Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:04 PM EDT

PDB ID	:	3AG1 / pdb_00003ag1
Title	:	Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 280 K
Authors	:	Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2010-03-19
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

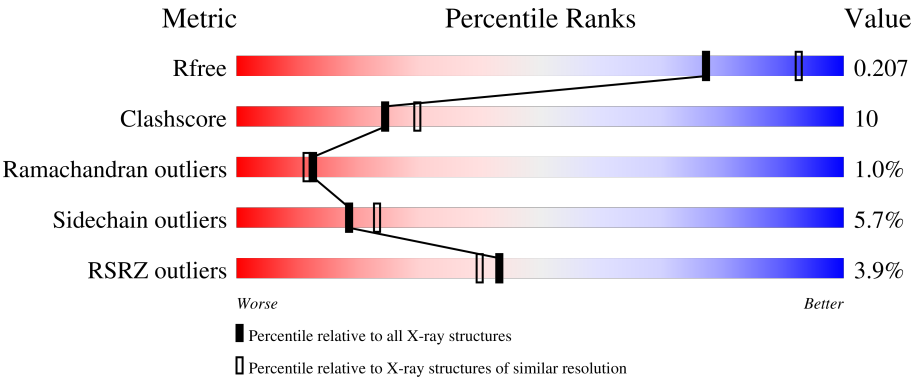
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



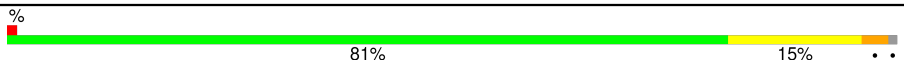
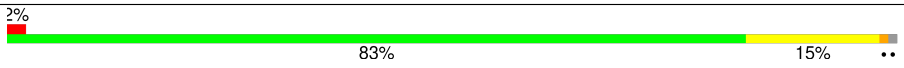
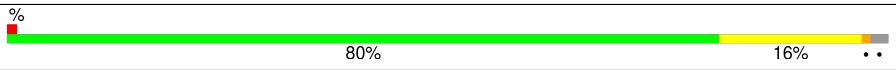
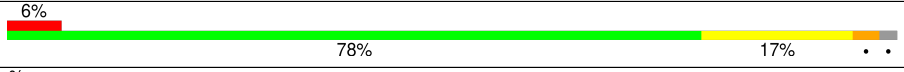
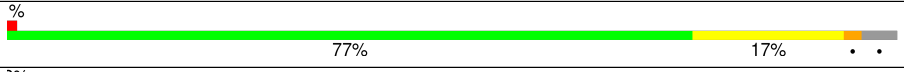
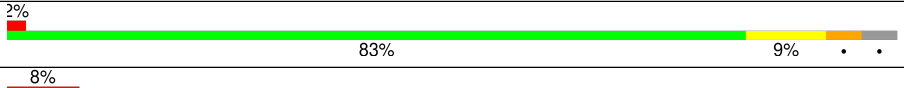
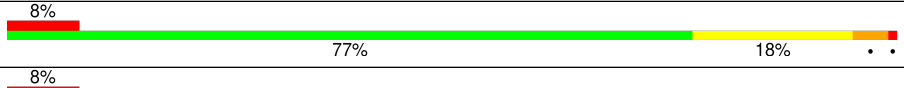
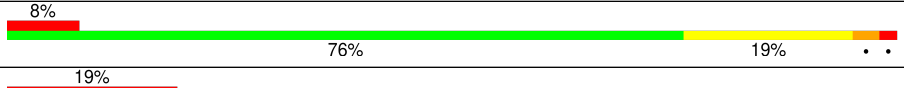
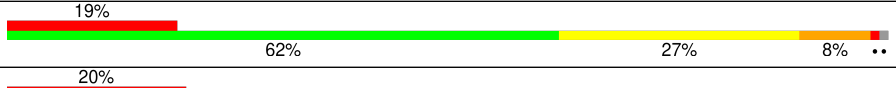
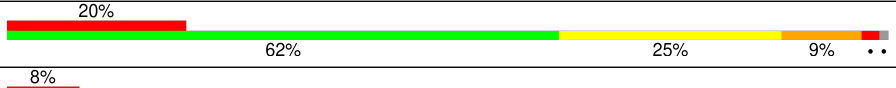
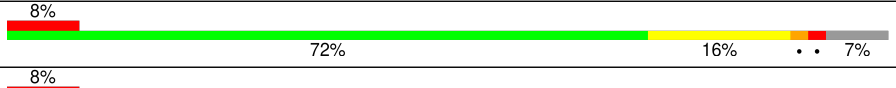
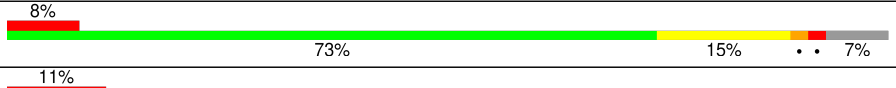
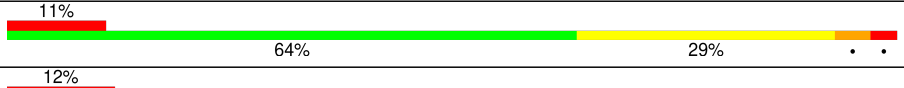
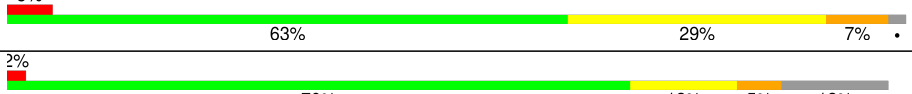
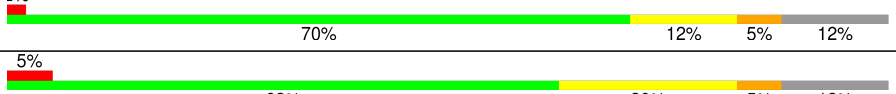
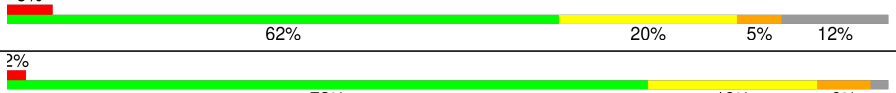
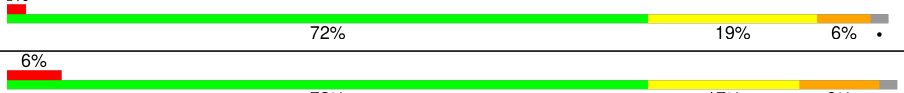
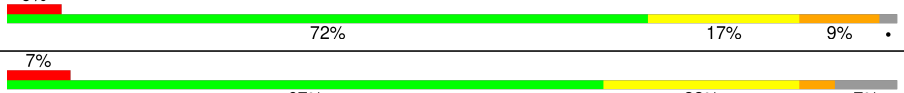
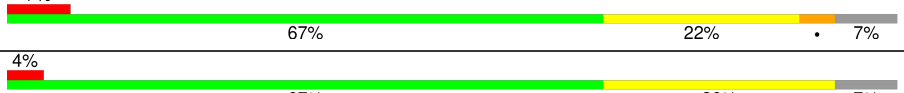
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	80% 18% .
1	N	514	% 80% 18% .
2	B	227	3% 64% 28% 7% .
2	O	227	4% 70% 25% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	B	1085	X	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	-
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	CDL	C	270	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	T	1269	-	-	X	-
26	DMU	C	272	X	-	-	-
26	DMU	M	526	X	-	-	-
26	DMU	T	1272	X	-	-	-
26	DMU	Z	1526	X	-	-	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32105 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

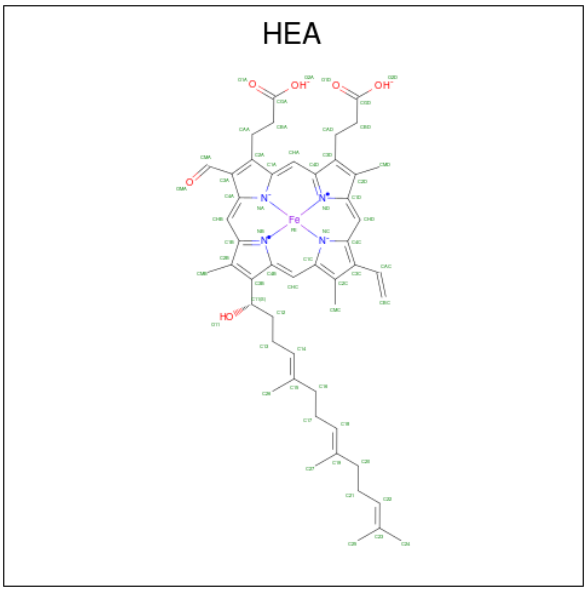
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

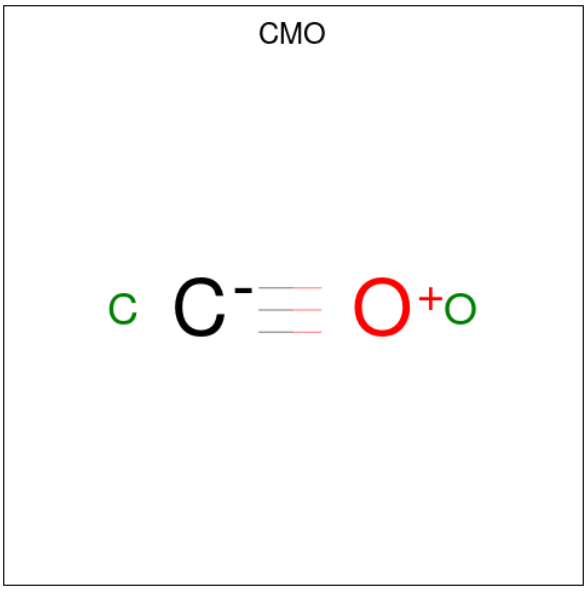
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O 2 1 1	0	0
15	N	1	Total C O 2 1 1	0	0

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Cu 1 1	0	0
16	N	1	Total Cu 1 1	0	0

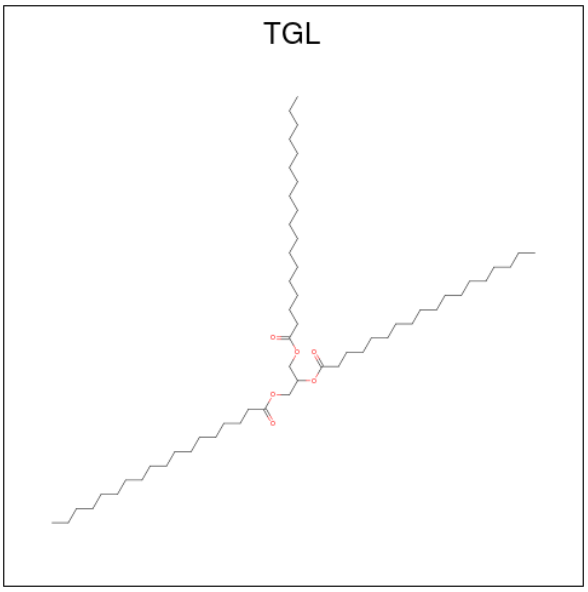
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

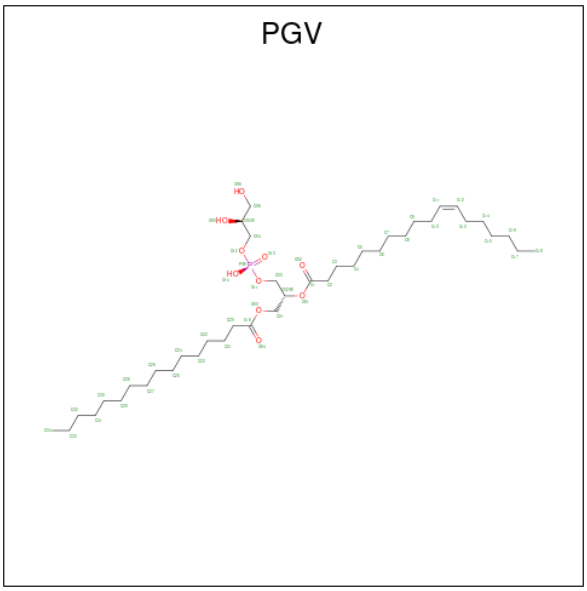
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



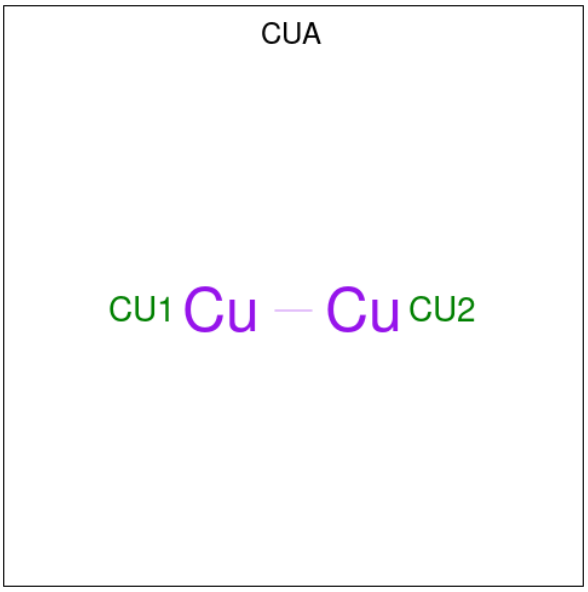
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	B	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



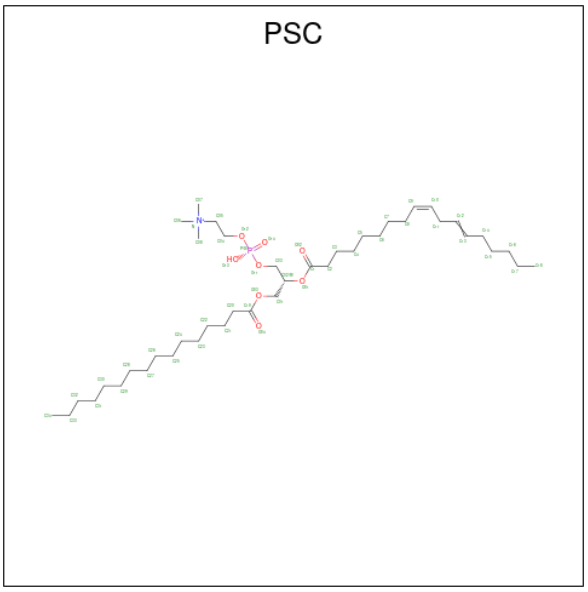
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



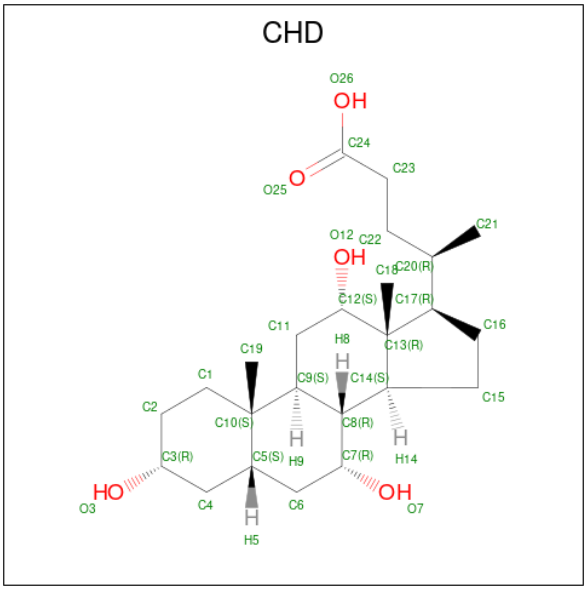
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C N O P 52 42 1 8 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

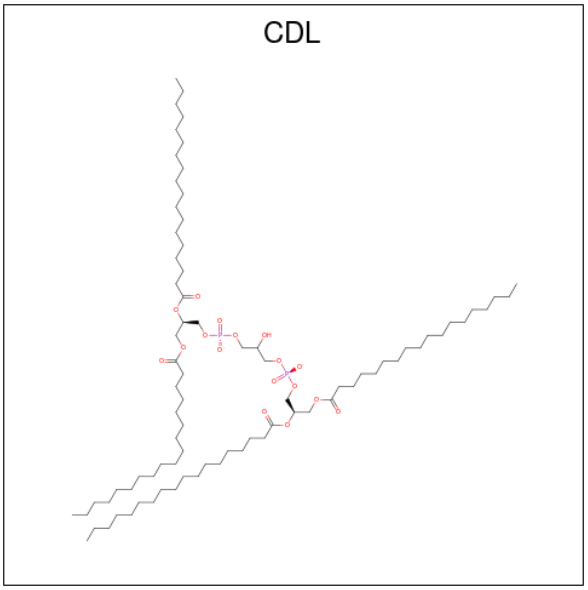


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	B	1	Total	C	O		0	0
			29	24	5			
23	C	1	Total	C	O		0	0
			29	24	5			
23	C	1	Total	C	O		0	0
			29	24	5			
23	J	1	Total	C	O		0	0
			29	24	5			
23	O	1	Total	C	O		0	0
			29	24	5			
23	P	1	Total	C	O		0	0
			29	24	5			
23	P	1	Total	C	O		0	0
			29	24	5			
23	W	1	Total	C	O		0	0
			29	24	5			

- Molecule 24 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

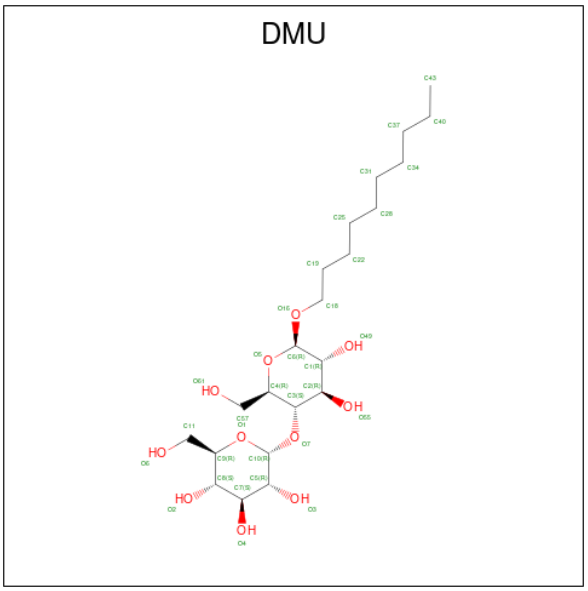
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total X 1 1	0	0
24	P	1	Total X 1 1	0	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O P 100 81 17 2	0	0
25	G	1	Total C O P 100 81 17 2	0	0
25	P	1	Total C O P 100 81 17 2	0	0
25	T	1	Total C O P 100 81 17 2	0	0

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

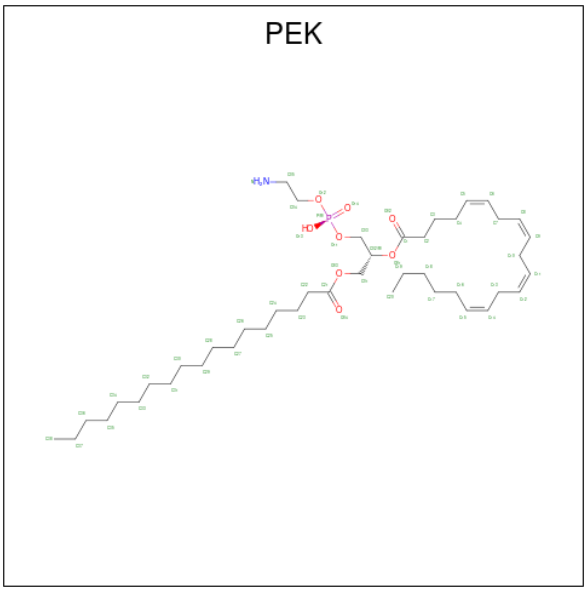


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 33 22 11	0	0
26	M	1	Total C O 33 22 11	0	0
26	T	1	Total C O 33 22 11	0	0
26	Z	1	Total C O 33 22 11	0	0

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	F	1	Total Zn 1 1	0	0
27	S	1	Total Zn 1 1	0	0

- Molecule 28 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	205	Total	O	0	0
			205	205		
29	B	121	Total	O	0	0
			121	121		
29	C	80	Total	O	0	0
			80	80		
29	D	75	Total	O	0	0
			75	75		
29	E	39	Total	O	0	0
			39	39		
29	F	70	Total	O	0	0
			70	70		

Continued on next page...

Continued from previous page...

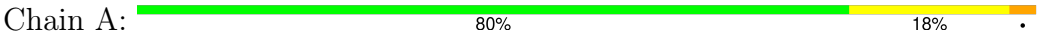
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	42	Total O 42 42	0	0
29	H	33	Total O 33 33	0	0
29	I	24	Total O 24 24	0	0
29	J	9	Total O 9 9	0	0
29	K	17	Total O 17 17	0	0
29	L	20	Total O 20 20	0	0
29	M	15	Total O 15 15	0	0
29	N	184	Total O 184 184	0	0
29	O	97	Total O 97 97	0	0
29	P	81	Total O 81 81	0	0
29	Q	47	Total O 47 47	0	0
29	R	27	Total O 27 27	0	0
29	S	52	Total O 52 52	0	0
29	T	37	Total O 37 37	0	0
29	U	28	Total O 28 28	0	0
29	V	17	Total O 17 17	0	0
29	W	12	Total O 12 12	0	0
29	X	12	Total O 12 12	0	0
29	Y	16	Total O 16 16	0	0
29	Z	9	Total O 9 9	0	0

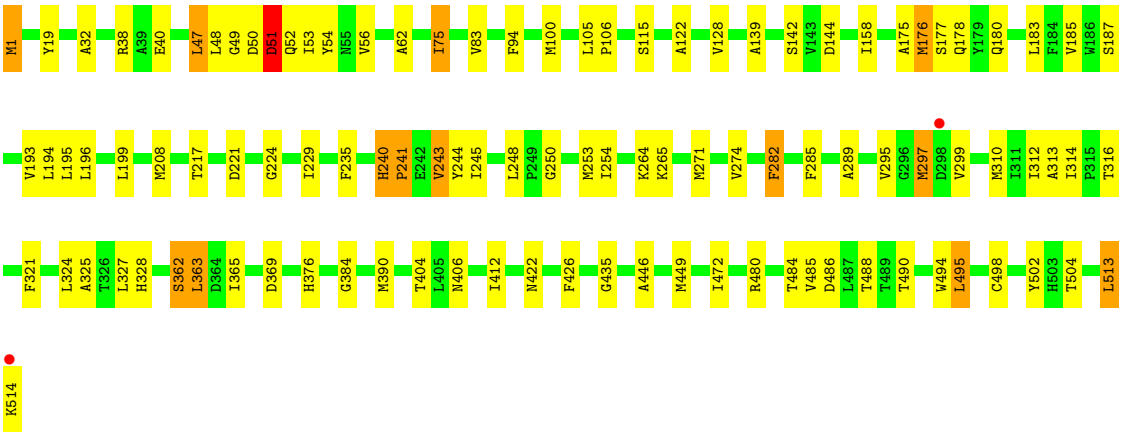
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c oxidase subunit 1

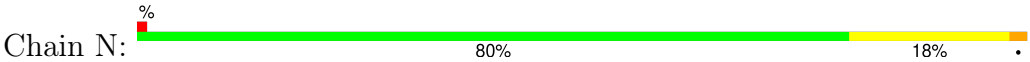
Chain A:

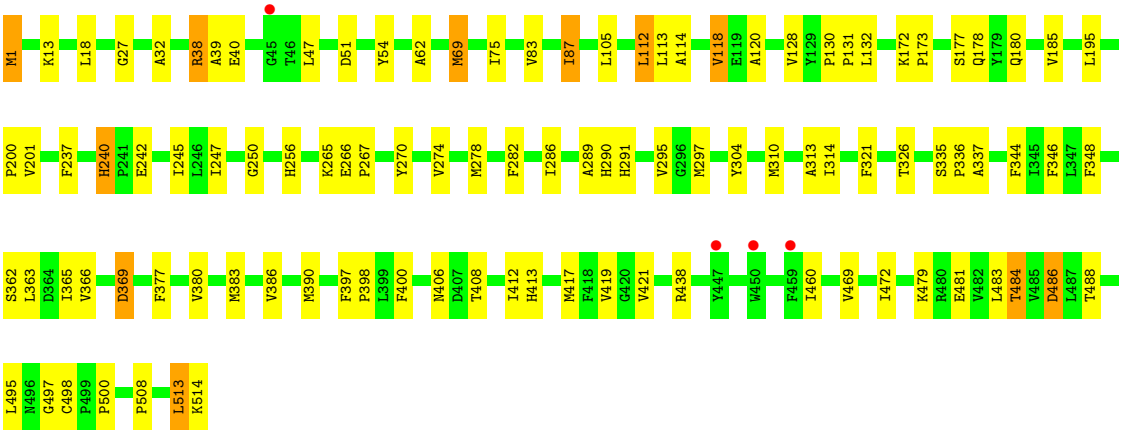




• Molecule 1: Cytochrome c oxidase subunit 1

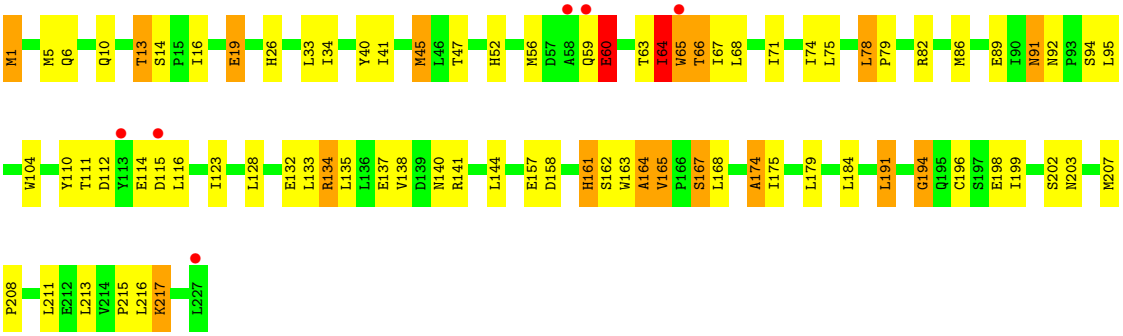
Chain N:



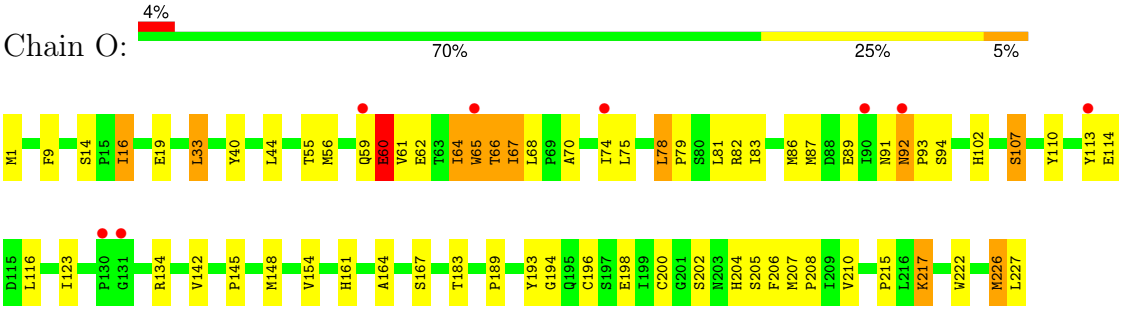


• Molecule 2: Cytochrome c oxidase subunit 2

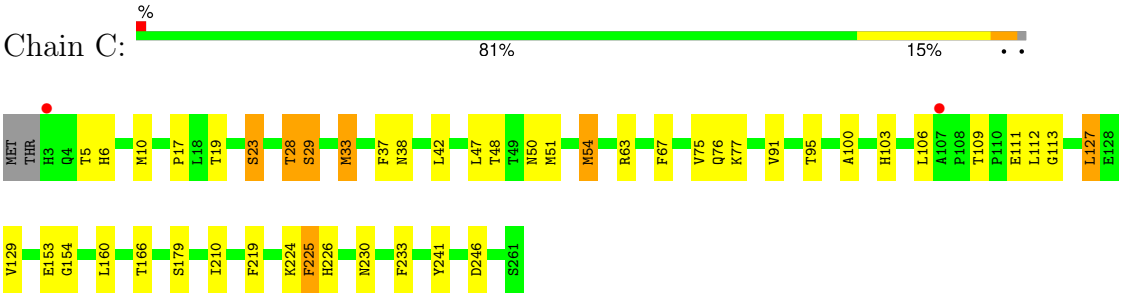
Chain B:



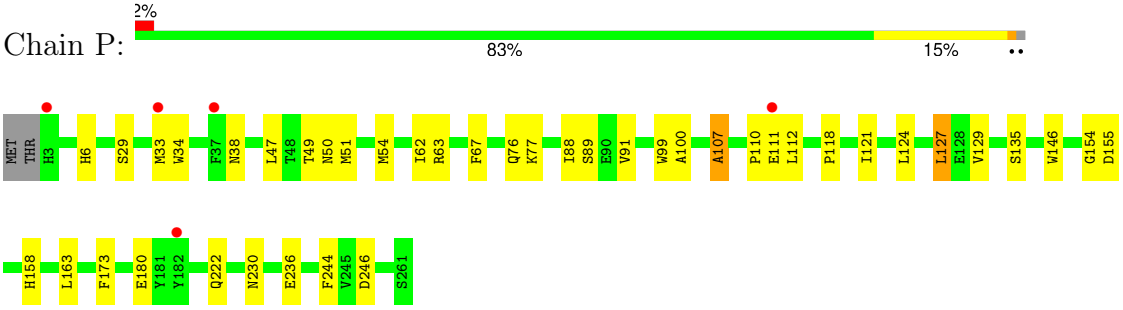
• Molecule 2: Cytochrome c oxidase subunit 2



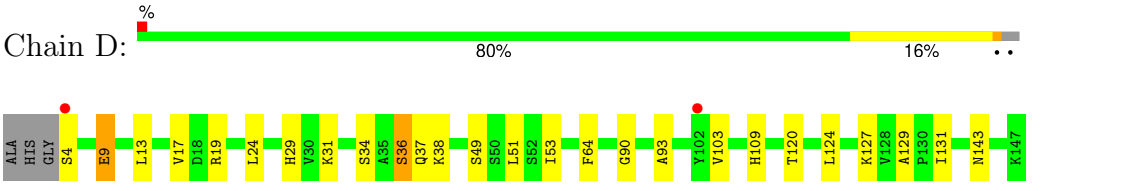
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 3: Cytochrome c oxidase subunit 3

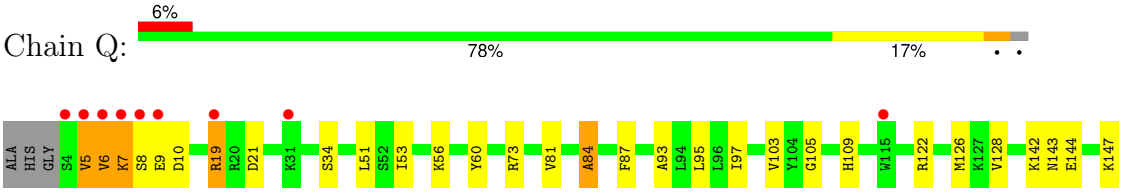


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



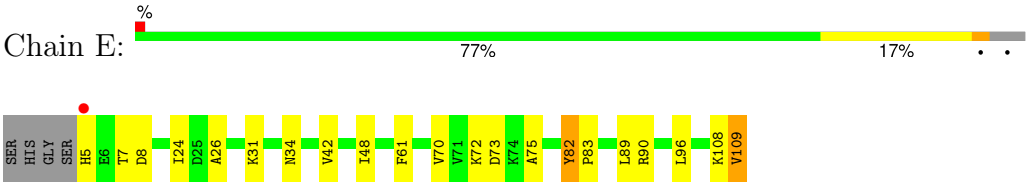
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



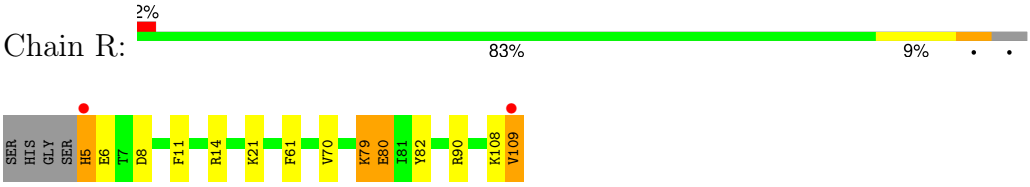
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:



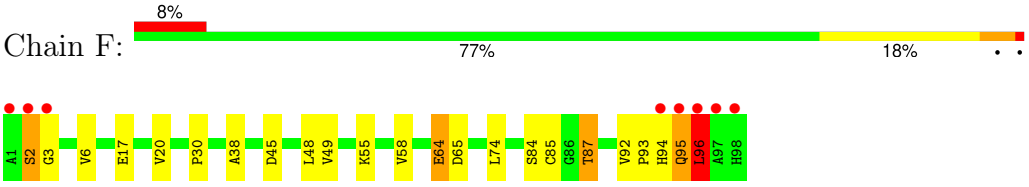
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



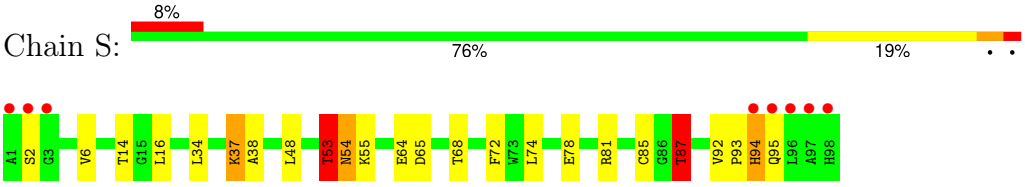
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



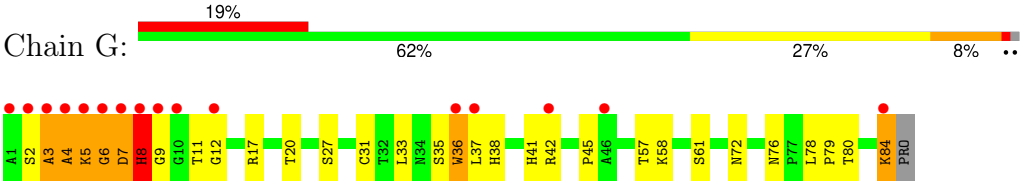
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:



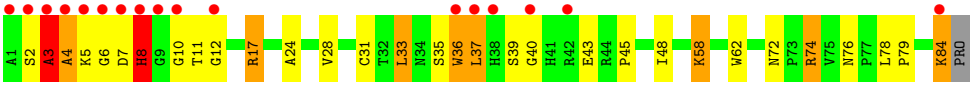
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G:



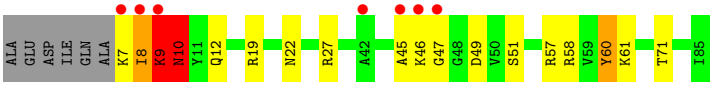
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T:



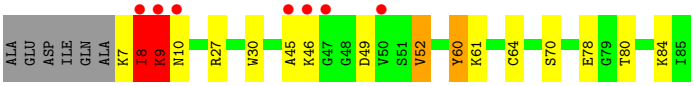
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



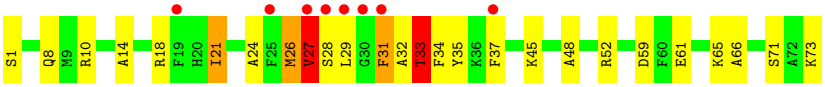
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



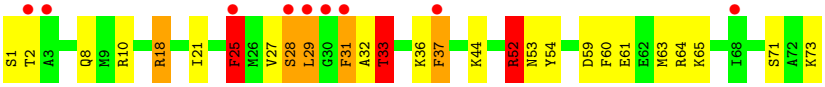
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



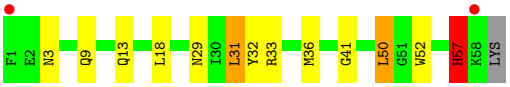
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



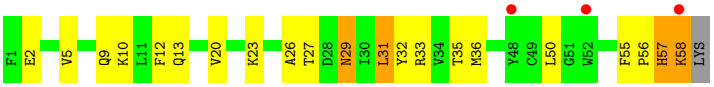
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain J:



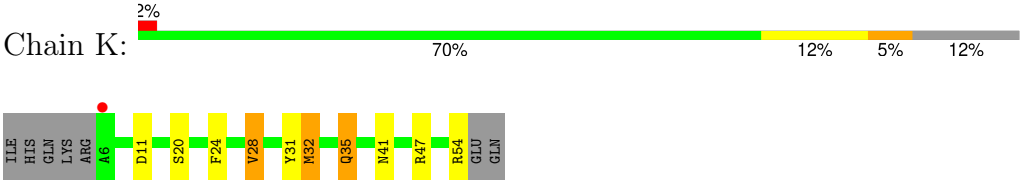
• Molecule 10: Cytochrome c oxidase polypeptide 7A1

Chain W:



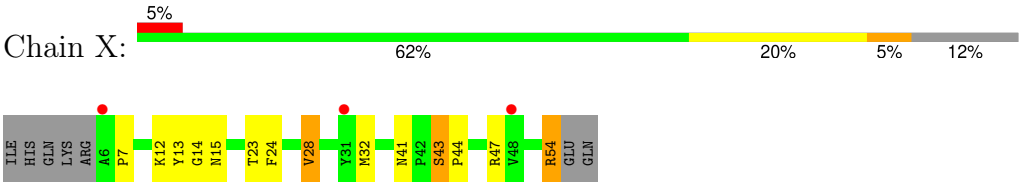
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



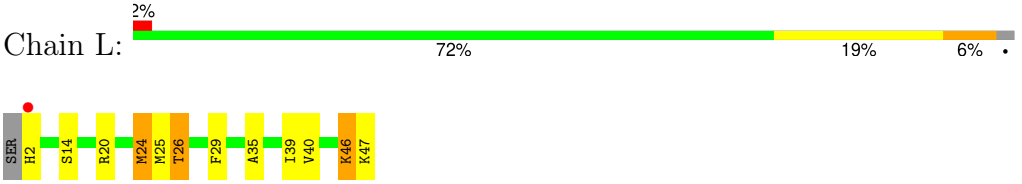
• Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



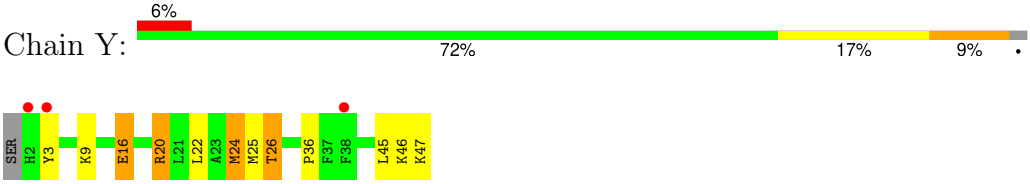
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:



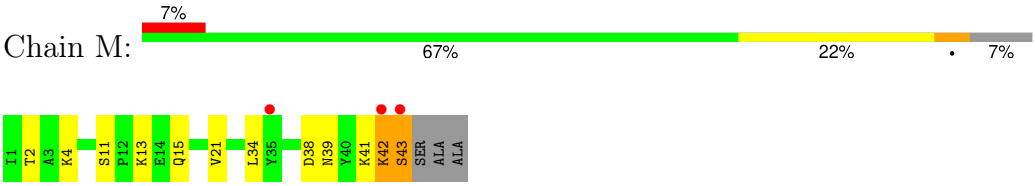
• Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:



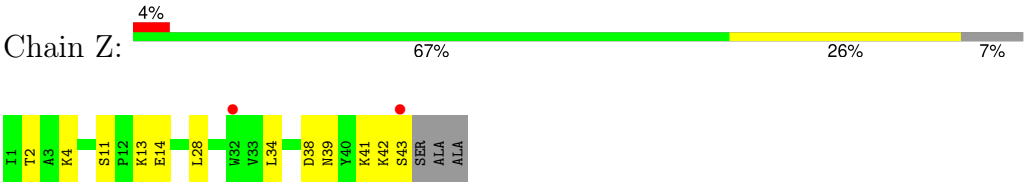
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.49Å 210.89Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.2 (40.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.162 , 0.192 0.180 , 0.207	Depositor DCC
R_{free} test set	17414 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, UNX, PEK, CDL, CUA, FME, CU, HEA, PGV, DMU, TGL, CMO, MG, ZN, NA, PSC, TPO, CHD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.84	45/4156 (1.1%)	1.44	27/5678 (0.5%)
1	N	1.54	24/4156 (0.6%)	1.31	20/5678 (0.4%)
2	B	1.83	28/1860 (1.5%)	1.50	19/2534 (0.7%)
2	O	1.46	9/1860 (0.5%)	1.35	14/2534 (0.6%)
3	C	1.68	14/2197 (0.6%)	1.30	14/3005 (0.5%)
3	P	1.47	9/2197 (0.4%)	1.26	10/3005 (0.3%)
4	D	1.65	8/1229 (0.7%)	1.39	5/1658 (0.3%)
4	Q	1.38	11/1229 (0.9%)	1.25	7/1658 (0.4%)
5	E	1.54	7/871 (0.8%)	1.33	4/1182 (0.3%)
5	R	1.25	1/871 (0.1%)	1.14	1/1182 (0.1%)
6	F	1.78	8/765 (1.0%)	1.50	7/1038 (0.7%)
6	S	1.53	5/765 (0.7%)	1.36	3/1038 (0.3%)
7	G	1.64	7/690 (1.0%)	1.43	10/937 (1.1%)
7	T	1.63	10/690 (1.4%)	1.37	5/937 (0.5%)
8	H	1.53	6/682 (0.9%)	1.28	2/921 (0.2%)
8	U	1.28	2/682 (0.3%)	1.23	3/921 (0.3%)
9	I	1.65	5/605 (0.8%)	1.38	4/802 (0.5%)
9	V	1.43	2/605 (0.3%)	1.35	5/802 (0.6%)
10	J	1.57	1/471 (0.2%)	1.37	5/636 (0.8%)
10	W	1.30	3/471 (0.6%)	1.22	3/636 (0.5%)
11	K	1.62	4/398 (1.0%)	1.37	2/546 (0.4%)
11	X	1.17	0/398	1.42	7/546 (1.3%)
12	L	1.70	4/393 (1.0%)	1.42	1/526 (0.2%)
12	Y	1.24	0/393	1.29	2/526 (0.4%)
13	M	1.54	0/345	1.49	3/470 (0.6%)
13	Z	1.19	0/345	1.19	0/470
All	All	1.59	213/29324 (0.7%)	1.35	183/39866 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	4

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	129	ALA	CA-CB	15.72	1.63	1.52
1	N	83	VAL	CA-CB	14.65	1.62	1.54
4	Q	5	VAL	CA-CB	12.07	1.66	1.53
2	B	198	GLU	C-O	11.90	1.38	1.23
2	O	198	GLU	C-O	11.90	1.38	1.23
1	A	498	CYS	C-O	-11.81	1.15	1.25
4	Q	6	VAL	CA-CB	9.98	1.64	1.54
8	H	8	ILE	CA-CB	9.91	1.68	1.54
11	K	41	ASN	C-O	-9.49	1.19	1.23
1	A	83	VAL	CA-CB	9.41	1.59	1.54
2	B	199	ILE	C-O	9.38	1.33	1.24
1	A	75	ILE	CA-CB	8.07	1.66	1.54
2	O	142	VAL	CA-CB	7.99	1.61	1.53
8	H	8	ILE	CA-C	7.95	1.62	1.52
1	A	295	VAL	CA-CB	7.95	1.64	1.54
6	F	45	ASP	CA-C	7.92	1.61	1.53
1	A	139	ALA	CA-CB	7.89	1.66	1.53
10	W	26	ALA	CA-CB	7.67	1.65	1.53
7	T	58	LYS	CE-NZ	7.67	1.72	1.49
3	P	129	VAL	CA-CB	-7.66	1.48	1.53
7	T	8	HIS	N-CA	7.64	1.56	1.46
1	N	240	HIS	CA-C	7.58	1.61	1.52
2	O	154	VAL	C-O	7.52	1.32	1.24
1	N	286	ILE	CA-CB	7.50	1.62	1.54
1	A	494	TRP	CA-C	7.47	1.62	1.52
6	S	2	SER	N-CA	7.15	1.54	1.46
3	C	109	THR	CA-C	7.15	1.61	1.52
1	A	106	PRO	CA-C	7.13	1.58	1.52
1	A	426	PHE	CA-C	7.12	1.61	1.52
7	T	36	TRP	CB-CG	7.04	1.72	1.50
4	Q	87	PHE	N-CA	-6.94	1.38	1.46
3	P	100	ALA	CA-CB	-6.93	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	3	ALA	CA-C	6.89	1.62	1.52
2	B	112	ASP	CA-C	6.79	1.61	1.52
1	A	52	GLN	N-CA	-6.78	1.38	1.46
1	N	386	VAL	CA-CB	6.77	1.63	1.54
4	Q	5	VAL	N-CA	6.75	1.55	1.46
2	B	163	TRP	N-CA	6.61	1.54	1.46
1	N	250	GLY	N-CA	6.61	1.54	1.45
1	A	485	VAL	C-O	-6.53	1.17	1.24
2	B	71	ILE	C-O	6.53	1.31	1.24
2	O	208	PRO	C-O	6.53	1.33	1.23
4	D	29	HIS	N-CA	-6.53	1.38	1.46
4	Q	5	VAL	CA-C	6.51	1.59	1.53
1	N	419	VAL	CA-CB	6.50	1.62	1.54
11	K	11	ASP	C-O	-6.46	1.16	1.24
11	K	20	SER	N-CA	-6.45	1.37	1.46
8	U	8	ILE	CA-CB	6.39	1.63	1.54
7	G	8	HIS	N-CA	6.36	1.54	1.46
1	A	56	VAL	CA-C	6.35	1.60	1.52
1	A	224	GLY	C-O	-6.34	1.18	1.24
1	A	217	THR	C-O	6.32	1.32	1.23
1	A	75	ILE	CG1-CD1	6.31	1.76	1.51
1	A	144	ASP	CA-C	6.28	1.60	1.52
1	A	175	ALA	CA-CB	6.26	1.64	1.53
7	T	7	ASP	N-CA	6.26	1.54	1.46
7	T	8	HIS	CA-C	6.24	1.61	1.52
1	N	337	ALA	CA-CB	6.22	1.62	1.53
6	F	20	VAL	CA-CB	6.20	1.61	1.54
1	A	185	VAL	CA-CB	6.20	1.61	1.54
1	N	295	VAL	CA-C	6.19	1.59	1.52
3	P	88	ILE	CA-CB	6.18	1.61	1.54
6	F	58	VAL	CA-CB	6.18	1.62	1.54
2	B	165	VAL	CA-CB	6.17	1.62	1.54
3	C	230	ASN	C-O	-6.17	1.16	1.23
4	Q	8	SER	CA-C	6.12	1.60	1.53
4	Q	84	ALA	N-CA	6.11	1.53	1.46
1	A	282	PHE	CA-C	6.10	1.60	1.52
8	H	10	ASN	CA-C	6.06	1.60	1.52
6	F	2	SER	N-CA	6.05	1.53	1.46
6	F	96	LEU	CA-C	6.01	1.60	1.52
5	E	61	PHE	CA-C	6.00	1.60	1.52
11	K	28	VAL	CA-C	5.99	1.61	1.52
5	E	96	LEU	C-O	-5.99	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	5.99	1.68	1.50
12	L	24	MET	CA-C	5.97	1.60	1.52
2	B	184	LEU	C-O	5.95	1.31	1.23
1	A	253	MET	SD-CE	-5.95	1.64	1.79
6	S	87	THR	CA-CB	5.93	1.63	1.53
9	I	14	ALA	C-O	-5.89	1.17	1.24
1	A	83	VAL	CA-C	5.87	1.58	1.52
1	N	397	PHE	CA-C	5.86	1.58	1.52
1	N	87	ILE	CA-CB	5.86	1.60	1.54
1	A	158	ILE	C-O	5.85	1.31	1.24
3	C	75	VAL	CA-C	5.85	1.60	1.52
7	G	8	HIS	CA-C	5.85	1.60	1.52
1	A	158	ILE	CA-C	5.85	1.60	1.52
2	B	47	THR	CA-CB	5.84	1.61	1.53
2	B	199	ILE	CA-CB	5.83	1.61	1.54
2	B	215	PRO	C-O	5.80	1.30	1.23
2	B	167	SER	N-CA	5.80	1.53	1.46
2	B	216	LEU	C-O	5.80	1.30	1.24
7	G	5	LYS	CB-CG	5.78	1.69	1.52
4	Q	8	SER	N-CA	5.78	1.53	1.46
1	A	480	ARG	CZ-NH2	5.77	1.41	1.33
3	C	112	LEU	CA-CB	5.77	1.63	1.53
3	C	100	ALA	CA-CB	5.76	1.62	1.53
1	A	122	ALA	CA-CB	5.76	1.60	1.53
3	P	222	GLN	CA-C	5.75	1.60	1.52
6	S	68	THR	CA-CB	5.75	1.61	1.53
5	R	82	TYR	CA-C	5.75	1.59	1.52
1	N	313	ALA	C-O	5.74	1.31	1.24
7	T	17	ARG	CG-CD	-5.72	1.35	1.52
1	A	94	PHE	CA-CB	5.70	1.60	1.53
9	I	33	THR	CA-C	5.70	1.60	1.52
2	B	134	ARG	CA-C	5.69	1.60	1.52
2	B	194	GLY	C-O	5.69	1.29	1.23
3	C	91	VAL	CA-CB	5.69	1.61	1.54
7	T	17	ARG	N-CA	-5.66	1.39	1.46
2	O	64	ILE	CA-CB	5.64	1.60	1.54
6	S	72	PHE	C-O	5.63	1.30	1.23
4	Q	103	VAL	CA-CB	5.59	1.61	1.55
6	F	2	SER	CA-C	5.58	1.60	1.52
10	J	41	GLY	C-O	5.58	1.30	1.23
8	H	22	ASN	N-CA	5.57	1.52	1.45
12	L	40	VAL	CA-C	5.57	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	SER	N-CA	5.54	1.53	1.46
1	A	243	VAL	CA-CB	5.54	1.61	1.54
2	B	116	LEU	CA-C	5.53	1.59	1.52
7	T	24	ALA	CA-CB	5.53	1.62	1.53
5	E	75	ALA	CA-CB	5.51	1.62	1.53
3	P	76	GLN	CA-C	5.51	1.59	1.52
1	N	326	THR	CA-CB	5.49	1.62	1.53
1	N	314	ILE	C-N	5.49	1.41	1.33
1	N	120	ALA	CA-C	5.48	1.60	1.52
3	C	28	THR	CA-CB	5.47	1.61	1.53
4	D	17	VAL	C-O	5.44	1.29	1.24
1	N	13	LYS	C-O	5.44	1.30	1.24
1	N	366	VAL	CA-CB	5.44	1.61	1.54
4	Q	9	GLU	N-CA	5.43	1.53	1.46
1	A	32	ALA	CA-C	5.42	1.59	1.52
1	A	412	ILE	CA-CB	5.41	1.61	1.54
10	W	20	VAL	CA-CB	5.40	1.61	1.54
3	C	103	HIS	CA-C	5.40	1.59	1.52
1	N	460	ILE	CA-CB	-5.39	1.48	1.54
1	A	19	TYR	CA-C	-5.38	1.45	1.52
6	S	2	SER	CA-C	5.37	1.58	1.52
9	I	71	SER	CA-C	5.37	1.60	1.52
2	O	67	ILE	CA-CB	5.36	1.61	1.54
9	V	33	THR	CA-CB	5.36	1.62	1.53
2	B	191	LEU	CA-C	5.36	1.58	1.52
2	B	174	ALA	CA-CB	5.34	1.60	1.53
7	G	80	THR	C-O	-5.34	1.16	1.24
2	B	10	GLN	C-O	5.34	1.30	1.23
9	I	59	ASP	C-O	-5.34	1.18	1.24
2	B	164	ALA	CA-CB	5.33	1.67	1.54
4	Q	7	LYS	CA-C	5.32	1.60	1.52
2	B	26	HIS	CA-C	5.32	1.59	1.52
1	N	130	PRO	CA-C	5.31	1.57	1.52
2	B	115	ASP	N-CA	-5.31	1.39	1.46
1	A	271	MET	CA-C	5.31	1.59	1.52
8	H	71	THR	CA-CB	5.30	1.61	1.53
1	A	193	VAL	CA-C	5.29	1.59	1.52
1	N	497	GLY	C-O	5.29	1.30	1.23
4	D	13	LEU	C-O	-5.29	1.18	1.24
2	O	40	TYR	N-CA	-5.29	1.40	1.46
1	N	270	TYR	CA-C	5.28	1.60	1.52
1	N	365	ILE	N-CA	5.28	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	64	PHE	CA-C	-5.28	1.46	1.52
9	I	48	ALA	CA-C	5.27	1.59	1.52
9	V	37	PHE	CB-CG	5.27	1.62	1.50
8	U	8	ILE	CA-C	5.26	1.59	1.52
5	E	42	VAL	N-CA	5.25	1.50	1.46
6	F	3	GLY	N-CA	5.25	1.51	1.45
10	W	5	VAL	CA-CB	5.24	1.60	1.54
3	P	121	ILE	CA-CB	5.24	1.60	1.54
1	A	310	MET	CG-SD	-5.24	1.67	1.80
1	A	328	HIS	N-CA	-5.23	1.39	1.46
3	C	166	THR	CA-CB	5.22	1.61	1.53
4	D	36	SER	C-O	-5.21	1.18	1.24
1	N	185	VAL	CA-C	5.21	1.59	1.52
2	B	158	ASP	CA-C	5.21	1.59	1.52
2	B	157	GLU	N-CA	-5.20	1.39	1.46
12	L	35	ALA	CA-C	5.19	1.58	1.52
3	P	49	THR	CA-C	5.19	1.59	1.52
1	A	404	THR	CA-C	5.18	1.59	1.52
7	T	28	VAL	N-CA	-5.17	1.40	1.46
1	A	196	LEU	C-O	-5.16	1.18	1.24
1	A	435	GLY	N-CA	5.16	1.52	1.45
4	D	124	LEU	N-CA	5.16	1.52	1.46
3	P	62	ILE	CA-C	5.15	1.59	1.52
6	F	96	LEU	N-CA	5.15	1.52	1.46
3	C	95	THR	CA-CB	5.15	1.61	1.53
12	L	39	ILE	CA-C	5.14	1.59	1.52
1	A	274	VAL	CA-C	5.14	1.59	1.52
1	A	316	THR	CA-CB	5.13	1.61	1.53
5	E	82	TYR	CA-C	5.13	1.58	1.52
5	E	73	ASP	C-O	-5.13	1.18	1.24
1	A	363	LEU	N-CA	-5.12	1.39	1.46
1	N	69	MET	N-CA	5.11	1.51	1.46
8	H	19	ARG	CA-C	5.10	1.59	1.52
1	N	247	ILE	CA-CB	5.10	1.60	1.54
3	C	54	MET	CG-SD	5.10	1.93	1.80
2	B	140	ASN	C-O	5.08	1.29	1.24
2	B	6	GLN	CA-C	5.08	1.59	1.52
3	P	107	ALA	CA-CB	5.08	1.58	1.53
1	A	495	LEU	CA-C	5.07	1.59	1.52
7	G	17	ARG	N-CA	-5.07	1.40	1.46
2	O	74	ILE	CA-CB	5.07	1.60	1.54
2	B	162	SER	C-O	5.06	1.29	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	134	ARG	CA-C	5.06	1.59	1.52
1	A	299	VAL	N-CA	-5.06	1.40	1.46
2	B	64	ILE	CA-CB	5.06	1.60	1.54
1	A	446	ALA	CA-CB	5.05	1.61	1.53
4	D	120	THR	CA-CB	-5.05	1.45	1.53
2	B	95	LEU	CA-C	5.04	1.58	1.52
3	C	10	MET	CB-CG	5.04	1.67	1.52
1	A	313	ALA	CA-CB	5.03	1.61	1.53
5	E	26	ALA	CA-CB	5.02	1.61	1.53
1	A	235	PHE	N-CA	-5.02	1.40	1.46
7	G	20	THR	CA-CB	5.02	1.61	1.53
3	C	76	GLN	CD-NE2	5.01	1.43	1.33
3	C	219	PHE	CA-C	5.01	1.59	1.52

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	TRP	N-CA-C	10.38	125.15	113.21
9	V	29	LEU	N-CA-C	9.65	123.01	111.33
7	T	8	HIS	N-CA-C	8.87	129.69	110.80
7	T	7	ASP	N-CA-C	8.71	129.35	110.80
2	B	64	ILE	N-CA-C	-8.58	102.18	110.42
1	N	105	LEU	CA-C-N	-8.29	111.84	120.38
1	N	105	LEU	C-N-CA	-8.29	111.84	120.38
11	X	43	SER	CA-C-N	8.27	128.37	119.28
11	X	43	SER	C-N-CA	8.27	128.37	119.28
4	D	103	VAL	N-CA-C	-8.25	105.19	112.12
9	I	52	ARG	CA-C-N	-8.12	110.44	122.86
9	I	52	ARG	C-N-CA	-8.12	110.44	122.86
1	A	240	HIS	CA-CB-CG	-8.04	105.75	113.80
4	Q	105	GLY	CA-C-N	-7.98	112.49	120.31
4	Q	105	GLY	C-N-CA	-7.98	112.49	120.31
6	F	49	VAL	CA-C-N	-7.95	112.16	120.03
6	F	49	VAL	C-N-CA	-7.95	112.16	120.03
6	S	2	SER	N-CA-C	7.83	121.16	108.32
7	G	7	ASP	N-CA-C	7.75	127.31	110.80
1	N	500	PRO	CA-C-N	-7.54	111.67	120.11
1	N	500	PRO	C-N-CA	-7.54	111.67	120.11
1	A	105	LEU	CA-C-N	-7.47	112.68	120.38
1	A	105	LEU	C-N-CA	-7.47	112.68	120.38
4	Q	8	SER	N-CA-C	7.44	122.94	111.56
1	A	240	HIS	N-CA-CB	7.29	117.31	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	141	ARG	N-CA-C	7.28	120.14	110.53
2	B	167	SER	CB-CA-C	-7.17	97.36	110.63
1	A	49	GLY	N-CA-C	-7.17	106.31	115.42
1	N	240	HIS	N-CA-CB	7.15	118.86	110.42
3	C	129	VAL	CA-C-N	-7.11	111.46	119.28
3	C	129	VAL	C-N-CA	-7.11	111.46	119.28
5	R	79	LYS	N-CA-C	7.00	119.76	111.71
3	C	37	PHE	N-CA-C	-6.91	102.45	111.71
7	T	6	GLY	N-CA-C	6.89	129.51	113.18
1	N	195	LEU	N-CA-C	-6.83	103.76	111.07
1	A	199	LEU	CA-C-N	-6.79	112.70	119.56
1	A	199	LEU	C-N-CA	-6.79	112.70	119.56
3	C	106	LEU	CA-C-N	-6.78	115.55	122.74
3	C	106	LEU	C-N-CA	-6.78	115.55	122.74
1	N	75	ILE	N-CA-C	6.76	117.38	110.82
3	C	113	GLY	N-CA-C	-6.73	105.61	115.63
11	X	23	THR	N-CA-C	-6.72	103.43	111.69
5	E	34	ASN	N-CA-C	-6.70	104.37	112.54
2	B	161	HIS	N-CA-C	-6.69	99.42	108.86
1	N	310	MET	CA-CB-CG	-6.66	100.77	114.10
4	Q	5	VAL	N-CA-C	6.57	116.70	107.37
7	G	8	HIS	N-CA-C	6.56	124.77	110.80
1	A	176	MET	CG-SD-CE	-6.47	86.66	100.90
1	N	47	LEU	N-CA-C	-6.46	105.41	113.55
2	O	68	LEU	CA-C-N	-6.46	112.17	119.28
2	O	68	LEU	C-N-CA	-6.46	112.17	119.28
1	N	240	HIS	CA-CB-CG	-6.41	107.39	113.80
3	P	246	ASP	N-CA-CB	-6.38	100.75	110.01
2	O	123	ILE	CB-CA-C	-6.38	105.01	110.94
2	O	14	SER	CA-C-N	6.38	126.13	119.05
2	O	14	SER	C-N-CA	6.38	126.13	119.05
1	N	39	ALA	N-CA-C	-6.37	104.26	111.14
1	N	256	HIS	N-CA-C	6.24	118.08	111.28
3	P	34	TRP	N-CA-C	6.20	117.84	111.14
1	A	244	TYR	CA-CB-CG	-6.16	102.81	113.90
1	A	314	ILE	CA-C-N	-6.15	112.51	119.28
1	A	314	ILE	C-N-CA	-6.15	112.51	119.28
3	C	6	HIS	N-CA-C	-6.13	101.14	110.14
11	K	32	MET	CG-SD-CE	6.12	114.36	100.90
10	J	57	HIS	CB-CA-C	6.11	121.07	111.72
7	G	57	THR	N-CA-C	-6.10	106.00	113.50
1	A	47	LEU	N-CA-C	-6.09	104.84	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	36	TRP	N-CA-C	-6.00	104.56	112.72
2	B	64	ILE	N-CA-CB	5.98	117.55	110.55
1	A	248	LEU	CA-C-N	-5.95	112.73	119.28
1	A	248	LEU	C-N-CA	-5.95	112.73	119.28
8	H	8	ILE	CB-CA-C	5.94	121.03	111.29
7	G	36	TRP	N-CA-C	-5.91	103.30	111.81
4	Q	6	VAL	N-CA-C	5.89	118.93	110.09
3	P	244	PHE	N-CA-C	-5.87	104.07	111.11
10	J	29	ASN	N-CA-C	5.87	117.67	111.28
3	C	225	PHE	N-CA-C	5.84	119.99	112.86
10	W	57	HIS	N-CA-C	5.84	118.82	108.24
2	B	68	LEU	CA-C-N	-5.84	112.85	119.28
2	B	68	LEU	C-N-CA	-5.84	112.85	119.28
9	I	66	ALA	N-CA-C	-5.83	106.16	113.28
2	B	92	ASN	N-CA-C	5.82	122.67	109.81
1	A	224	GLY	N-CA-C	-5.81	106.00	115.46
13	M	11	SER	CA-C-N	5.80	125.93	119.32
13	M	11	SER	C-N-CA	5.80	125.93	119.32
1	N	310	MET	CG-SD-CE	-5.78	88.17	100.90
13	M	21	VAL	N-CA-C	-5.78	104.88	110.72
6	F	17	GLU	N-CA-C	-5.76	105.01	111.28
2	O	65	TRP	N-CA-C	5.74	123.02	110.80
2	B	19	GLU	N-CA-CB	-5.73	101.69	110.12
1	A	376	HIS	N-CA-C	-5.72	104.73	110.97
2	B	217	LYS	CB-CA-C	-5.72	101.30	110.79
3	P	222	GLN	N-CA-C	-5.70	105.15	111.36
8	H	49	ASP	N-CA-C	5.69	117.93	108.20
1	A	362	SER	N-CA-CB	-5.68	100.89	110.49
12	Y	24	MET	CB-CA-C	-5.65	101.41	110.79
1	N	348	PHE	N-CA-C	-5.64	105.21	111.36
4	Q	60	TYR	N-CA-C	-5.63	105.22	111.36
1	A	365	ILE	CB-CA-C	-5.60	104.72	111.88
6	F	64	GLU	CA-C-N	-5.60	115.30	125.66
6	F	64	GLU	C-N-CA	-5.60	115.30	125.66
9	I	29	LEU	N-CA-C	5.59	122.71	110.80
3	P	230	ASN	CA-C-N	-5.59	114.90	122.95
3	P	230	ASN	C-N-CA	-5.59	114.90	122.95
12	Y	45	LEU	N-CA-C	5.57	120.06	113.16
2	O	92	ASN	CB-CA-C	5.54	121.08	110.17
3	P	29	SER	CB-CA-C	-5.54	101.59	110.79
6	S	53	THR	CB-CA-C	-5.54	100.59	114.11
11	K	35	GLN	CB-CA-C	-5.53	101.12	110.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	469	VAL	N-CA-C	-5.53	104.98	110.62
2	B	138	VAL	N-CA-C	5.52	117.07	109.46
2	O	161	HIS	N-CA-C	-5.47	101.42	109.18
11	X	7	PRO	N-CA-C	5.45	119.43	110.55
7	G	58	LYS	CA-C-N	-5.44	114.36	119.85
7	G	58	LYS	C-N-CA	-5.44	114.36	119.85
2	O	19	GLU	N-CA-CB	-5.42	102.15	110.12
1	A	221	ASP	CA-C-N	5.39	125.73	119.47
1	A	221	ASP	C-N-CA	5.39	125.73	119.47
9	V	25	PHE	CB-CA-C	5.39	119.30	110.95
3	P	99	TRP	N-CA-C	-5.38	105.31	111.07
7	T	36	TRP	CB-CA-C	5.38	117.83	111.22
3	C	29	SER	CA-CB-OG	-5.37	100.36	111.10
7	G	6	GLY	N-CA-C	5.36	125.88	113.18
3	P	89	SER	N-CA-C	-5.35	105.62	111.82
10	W	55	PHE	CB-CA-C	5.34	116.77	108.61
9	V	52	ARG	CA-C-N	-5.32	114.21	122.67
9	V	52	ARG	C-N-CA	-5.32	114.21	122.67
7	G	61	SER	CB-CA-C	-5.32	103.03	111.17
1	A	325	ALA	N-CA-C	-5.31	106.07	112.54
1	A	297	MET	CG-SD-CE	5.29	112.53	100.90
1	N	237	PHE	N-CA-C	-5.28	105.53	111.28
1	N	362	SER	CA-CB-OG	-5.27	100.56	111.10
9	V	53	ASN	N-CA-C	5.25	118.99	112.59
7	G	27	SER	CB-CA-C	-5.23	102.11	110.79
8	U	8	ILE	CB-CA-C	5.23	119.86	111.29
7	G	41	HIS	N-CA-C	5.23	117.89	110.10
2	O	92	ASN	N-CA-C	5.19	121.28	109.81
1	A	51	ASP	N-CA-C	-5.17	106.81	113.23
1	A	384	GLY	N-CA-C	-5.17	100.94	113.18
11	X	41	ASN	CA-C-N	-5.16	115.41	120.52
11	X	41	ASN	C-N-CA	-5.16	115.41	120.52
2	O	55	THR	N-CA-C	5.16	117.79	110.10
5	E	42	VAL	CA-C-N	-5.16	114.45	119.76
5	E	42	VAL	C-N-CA	-5.16	114.45	119.76
8	U	64	CYS	CA-C-N	-5.16	114.47	119.78
8	U	64	CYS	C-N-CA	-5.16	114.47	119.78
10	W	35	THR	N-CA-C	-5.15	105.56	111.07
4	D	24	LEU	CA-C-N	5.15	125.43	119.92
4	D	24	LEU	C-N-CA	5.15	125.43	119.92
1	N	346	PHE	N-CA-C	5.14	116.70	111.14
2	B	14	SER	N-CA-C	-5.14	102.23	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	9	PHE	CA-C-N	5.14	128.38	120.82
2	O	9	PHE	C-N-CA	5.14	128.38	120.82
1	A	19	TYR	CA-C-O	-5.13	115.11	120.55
10	J	18	LEU	CA-C-N	-5.13	114.95	120.03
10	J	18	LEU	C-N-CA	-5.13	114.95	120.03
5	E	72	LYS	N-CA-C	-5.13	105.77	111.36
3	C	153	GLU	N-CA-C	-5.12	106.87	113.02
3	C	48	THR	N-CA-C	5.12	116.55	111.07
1	A	208	MET	N-CA-C	-5.12	105.89	111.82
2	B	45	MET	CG-SD-CE	5.11	112.13	100.90
2	B	123	ILE	CA-C-N	-5.10	114.52	119.78
2	B	123	ILE	C-N-CA	-5.10	114.52	119.78
4	Q	7	LYS	N-CA-C	5.10	116.43	109.18
3	C	29	SER	CB-CA-C	-5.10	102.01	110.68
2	B	34	ILE	N-CA-C	5.09	115.81	110.62
2	O	44	LEU	N-CA-C	5.09	117.21	111.11
6	S	94	HIS	N-CA-C	5.09	121.64	110.80
1	A	32	ALA	N-CA-C	-5.08	105.82	111.36
3	P	163	LEU	N-CA-C	-5.08	105.92	111.82
6	F	92	VAL	CA-C-N	-5.08	114.57	119.90
6	F	92	VAL	C-N-CA	-5.08	114.57	119.90
1	N	201	VAL	N-CA-CB	5.06	117.05	110.57
12	L	26	THR	N-CA-CB	-5.05	102.68	110.01
2	B	13	THR	N-CA-C	-5.05	107.79	114.31
2	B	10	GLN	CA-CB-CG	-5.05	104.00	114.10
4	D	131	ILE	CB-CA-C	-5.03	105.50	112.24
3	C	241	TYR	N-CA-C	-5.03	105.98	111.82
3	C	233	PHE	N-CA-C	5.02	116.75	111.28
10	J	29	ASN	CB-CA-C	-5.02	102.46	110.79
4	D	90	GLY	N-CA-C	-5.01	106.35	112.77
11	X	12	LYS	N-CA-C	5.01	116.43	111.07
1	N	479	LYS	N-CA-C	5.01	118.04	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	44	0
1	N	4027	0	4001	55	0
2	B	1824	0	1833	39	0
2	O	1824	0	1833	44	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	24	0
4	D	1195	0	1183	9	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	11	0
5	R	852	0	845	10	0
6	F	748	0	728	10	0
6	S	748	0	728	14	0
7	G	675	0	644	26	0
7	T	675	0	644	42	0
8	H	662	0	623	8	0
8	U	662	0	623	12	0
9	I	601	0	613	23	0
9	V	601	0	613	26	0
10	J	460	0	459	7	0
10	W	460	0	459	12	0
11	K	384	0	366	3	0
11	X	384	0	366	7	0
12	L	380	0	380	14	0
12	Y	380	0	380	11	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	120	0	108	3	0
14	N	120	0	108	7	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	63	0	109	9	0
19	L	63	0	110	19	0
19	N	189	0	330	22	0
20	A	102	0	152	14	0
20	C	102	0	152	7	0
20	N	102	0	152	9	0
20	P	102	0	152	7	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	17	0
22	R	52	0	80	16	0
23	B	29	0	37	3	0
23	C	58	0	71	3	0
23	J	29	0	36	2	0
23	O	29	0	37	1	0
23	P	58	0	72	4	0
23	W	29	0	36	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	100	0	156	21	0
25	G	100	0	156	24	0
25	P	100	0	156	16	0
25	T	100	0	156	23	0
26	C	33	0	38	2	0
26	M	33	0	38	0	0
26	T	33	0	39	6	0
26	Z	33	0	39	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	22	0
28	S	53	0	77	6	0
28	T	106	0	154	19	0
29	A	205	0	0	3	0
29	B	121	0	0	3	0
29	C	80	0	0	2	0
29	D	75	0	0	1	0
29	E	39	0	0	1	0
29	F	70	0	0	2	0
29	G	42	0	0	5	0
29	H	33	0	0	5	0
29	I	24	0	0	1	0
29	J	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	17	0	0	0	0
29	L	20	0	0	2	0
29	M	15	0	0	0	0
29	N	184	0	0	6	0
29	O	97	0	0	2	0
29	P	81	0	0	7	0
29	Q	47	0	0	2	0
29	R	27	0	0	0	0
29	S	52	0	0	1	0
29	T	37	0	0	8	0
29	U	28	0	0	4	0
29	V	17	0	0	4	0
29	W	12	0	0	2	0
29	X	12	0	0	1	0
29	Y	16	0	0	0	0
29	Z	9	0	0	0	0
All	All	32105	0	31280	613	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (613) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:CD1	1:A:75:ILE:CG1	1.76	1.62
28:G:265:PEK:C7	28:G:265:PEK:C6	1.81	1.53
7:T:58:LYS:CE	7:T:58:LYS:NZ	1.72	1.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.40	1.36
7:T:45:PRO:CD	29:T:3099:HOH:O	1.75	1.35
7:T:5:LYS:CD	28:T:263:PEK:H382	1.73	1.19
7:T:5:LYS:HD2	28:T:263:PEK:C38	1.74	1.17
28:G:265:PEK:H383	25:G:269:CDL:C27	1.74	1.17
7:T:84:LYS:HD2	7:T:84:LYS:N	1.60	1.16
19:A:523:TGL:HG12	19:A:523:TGL:HC21	1.29	1.12
7:G:45:PRO:HD2	29:G:2099:HOH:O	1.49	1.11
7:T:5:LYS:HD2	28:T:263:PEK:H382	1.28	1.08
7:T:84:LYS:H	7:T:84:LYS:CD	1.67	1.07
7:T:45:PRO:HD2	29:T:3099:HOH:O	1.34	1.06
25:G:269:CDL:H112	25:G:269:CDL:HA21	1.32	1.05
29:P:4533:HOH:O	28:S:1265:PEK:H71	1.56	1.05
20:P:1267:PGV:H182	25:P:1270:CDL:H662	1.08	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:265:PEK:C38	25:G:269:CDL:H273	1.86	1.04
28:G:265:PEK:H383	25:G:269:CDL:H273	1.06	1.04
20:C:267:PGV:C12	20:C:267:PGV:H161	1.89	1.03
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.23	1.00
20:C:267:PGV:H161	20:C:267:PGV:H12	1.42	1.00
8:H:9:LYS:O	8:H:10:ASN:HB2	1.57	0.99
20:P:1267:PGV:C18	25:P:1270:CDL:H662	1.92	0.99
20:P:1267:PGV:H182	25:P:1270:CDL:C66	1.93	0.98
1:A:321:PHE:CD2	22:B:229:PSC:H341	1.99	0.98
3:C:111:GLU:HG3	29:H:4073:HOH:O	1.62	0.97
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.29	0.96
28:T:1264:PEK:H32	28:T:1264:PEK:H71	1.46	0.96
1:N:112:LEU:HD12	29:N:3701:HOH:O	1.64	0.95
8:U:8:ILE:HG21	29:U:4330:HOH:O	1.66	0.95
6:S:85:CYS:SG	6:S:87:THR:HG23	2.07	0.94
26:C:272:DMU:H29	26:C:272:DMU:O1	1.68	0.94
22:B:229:PSC:C07	9:I:10:ARG:HH21	1.80	0.93
5:R:8:ASP:OD1	22:R:1229:PSC:H081	1.69	0.93
25:G:269:CDL:H522	25:G:269:CDL:H231	1.51	0.92
7:T:45:PRO:HD3	29:T:3099:HOH:O	1.47	0.92
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.13	0.92
6:F:85:CYS:SG	6:F:87:THR:HG23	2.09	0.91
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.35	0.91
7:G:5:LYS:HD2	28:G:1263:PEK:H383	1.50	0.91
1:N:321:PHE:CD2	22:R:1229:PSC:H341	2.05	0.90
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.51	0.90
25:T:1269:CDL:HA21	25:T:1269:CDL:H111	1.53	0.90
19:B:521:TGL:H281	19:B:521:TGL:H102	1.52	0.89
7:T:5:LYS:CD	28:T:263:PEK:C38	2.41	0.89
22:R:1229:PSC:C07	9:V:10:ARG:HH21	1.85	0.89
7:T:62:TRP:HB3	26:T:1272:DMU:H30	1.52	0.89
7:T:84:LYS:HD2	7:T:84:LYS:H	0.77	0.88
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.34	0.88
12:L:20:ARG:HH21	19:L:522:TGL:HC32	1.36	0.86
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.39	0.86
25:G:269:CDL:H873	29:G:4364:HOH:O	1.75	0.86
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.17	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.22	0.85
8:H:9:LYS:O	8:H:10:ASN:CB	2.25	0.85
9:V:31:PHE:C	9:V:31:PHE:CD1	2.55	0.84
19:N:1521:TGL:C28	19:N:1521:TGL:H102	2.08	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:62:TRP:CB	26:T:1272:DMU:H30	2.07	0.83
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.43	0.83
9:V:36:LYS:HG3	29:V:4356:HOH:O	1.77	0.82
28:G:265:PEK:C7	28:G:265:PEK:C5	2.58	0.82
2:B:33:LEU:HD11	9:I:28:SER:HB3	1.59	0.82
20:C:267:PGV:H12	20:C:267:PGV:C16	2.07	0.82
25:T:1269:CDL:H511	25:T:1269:CDL:H181	1.61	0.81
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.64	0.81
7:G:45:PRO:CD	29:G:2099:HOH:O	2.16	0.80
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.46	0.80
7:T:72:ASN:H	7:T:76:ASN:HD22	1.26	0.80
7:T:76:ASN:HD21	28:T:1264:PEK:HN2	1.26	0.79
25:P:1270:CDL:HB32	25:P:1270:CDL:HB21	1.65	0.79
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.78
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.49	0.78
19:N:1521:TGL:H222	19:N:1521:TGL:HA81	1.65	0.78
19:A:523:TGL:HG12	19:A:523:TGL:CC2	2.13	0.77
25:P:1270:CDL:H611	25:P:1270:CDL:H652	1.67	0.77
19:B:521:TGL:H102	19:B:521:TGL:C28	2.14	0.77
9:I:31:PHE:CD1	9:I:31:PHE:C	2.63	0.77
25:C:270:CDL:H231	25:C:270:CDL:H642	1.68	0.76
5:R:80:GLU:H	5:R:80:GLU:CD	1.93	0.76
25:G:269:CDL:HA21	25:G:269:CDL:C11	2.14	0.76
7:T:62:TRP:HB3	26:T:1272:DMU:C57	2.15	0.75
28:S:1265:PEK:H383	25:T:1269:CDL:C27	2.17	0.75
19:L:522:TGL:HC51	19:L:522:TGL:OC1	1.86	0.74
22:R:1229:PSC:H072	9:V:10:ARG:HH21	1.51	0.74
22:B:229:PSC:H212	22:B:229:PSC:O01	1.87	0.74
19:N:1521:TGL:H102	19:N:1521:TGL:H281	1.69	0.73
8:H:27:ARG:NH1	29:H:2431:HOH:O	2.22	0.73
1:N:177:SER:H	1:N:180:GLN:HE21	1.36	0.73
28:G:265:PEK:C38	25:G:269:CDL:C27	2.57	0.72
28:G:265:PEK:C6	28:G:265:PEK:C8	2.67	0.72
1:A:50:ASP:HB3	1:A:53:ILE:HD12	1.71	0.72
20:A:524:PGV:H221	20:A:524:PGV:C01	2.19	0.72
9:I:26:MET:O	9:I:27:VAL:C	2.33	0.72
22:R:1229:PSC:H071	9:V:10:ARG:HH21	1.55	0.72
3:P:111:GLU:OE1	29:P:3467:HOH:O	2.08	0.71
7:G:5:LYS:CD	28:G:1263:PEK:H383	2.21	0.71
7:G:31:CYS:SG	25:G:269:CDL:H532	2.30	0.71
7:G:76:ASN:HD21	28:G:264:PEK:HN2	1.37	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:H	7:G:84:LYS:HD2	1.54	0.71
25:G:269:CDL:H792	25:G:269:CDL:H562	1.72	0.71
13:M:39:ASN:O	13:M:43:SER:HB2	1.91	0.70
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.72	0.70
19:A:523:TGL:H281	29:B:4178:HOH:O	1.91	0.70
25:T:1269:CDL:H181	25:T:1269:CDL:C51	2.22	0.69
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.58	0.69
6:F:64:GLU:O	6:F:65:ASP:HB2	1.92	0.69
25:G:269:CDL:H522	25:G:269:CDL:C23	2.21	0.69
3:P:107:ALA:HB2	20:P:1268:PGV:H031	1.73	0.69
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.25	0.68
1:N:484:THR:HB	13:Z:2:THR:OG1	1.93	0.68
25:C:270:CDL:HB32	25:C:270:CDL:HB21	1.74	0.68
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.09	0.68
3:C:246:ASP:HB2	29:C:4122:HOH:O	1.94	0.68
1:N:514:LYS:HA	6:S:38:ALA:CB	2.23	0.68
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.06	0.68
1:A:484:THR:HB	13:M:2:THR:OG1	1.94	0.68
19:B:521:TGL:HC72	29:B:4575:HOH:O	1.94	0.67
1:N:177:SER:H	1:N:180:GLN:NE2	1.92	0.67
22:R:1229:PSC:H071	9:V:10:ARG:NH2	2.09	0.67
25:P:1270:CDL:H122	25:P:1270:CDL:HA4	1.75	0.67
25:G:269:CDL:H231	25:G:269:CDL:C52	2.22	0.67
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.75	0.67
20:C:267:PGV:H182	25:C:270:CDL:H671	1.76	0.67
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.56	0.67
7:T:5:LYS:CG	28:T:263:PEK:H382	2.24	0.67
5:E:109:VAL:HG23	5:E:109:VAL:OXT	1.93	0.66
2:O:226:MET:HA	2:O:226:MET:HE3	1.75	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.76	0.66
3:P:33:MET:HG2	29:P:4161:HOH:O	1.95	0.66
28:S:1265:PEK:H383	25:T:1269:CDL:H272	1.77	0.66
25:T:1269:CDL:H181	25:T:1269:CDL:CB5	2.26	0.66
25:G:269:CDL:H792	25:G:269:CDL:C56	2.26	0.66
8:H:12:GLN:HG3	29:H:4563:HOH:O	1.95	0.66
20:A:524:PGV:H062	29:A:2126:HOH:O	1.95	0.65
1:A:75:ILE:CD1	1:A:75:ILE:CB	2.71	0.65
25:P:1270:CDL:HB21	25:P:1270:CDL:CB3	2.26	0.65
1:A:486:ASP:OD1	4:D:19:ARG:HD2	1.96	0.65
22:B:229:PSC:H342	22:B:229:PSC:H142	1.78	0.65
22:B:229:PSC:H142	22:B:229:PSC:C34	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	23:W:1059:CHD:C15	2.27	0.65
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.33	0.64
4:Q:19:ARG:HB3	4:Q:19:ARG:HH21	1.61	0.64
20:N:1524:PGV:C01	20:N:1524:PGV:H221	2.28	0.64
2:O:89:GLU:O	2:O:91:ASN:ND2	2.31	0.64
23:P:1271:CHD:H162	23:P:1271:CHD:H232	1.78	0.64
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.38	0.64
19:N:1521:TGL:HA71	19:N:1521:TGL:H101	1.79	0.64
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.09	0.64
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.80	0.63
1:N:488:THR:HB	1:N:495:LEU:HD13	1.81	0.63
2:B:33:LEU:HD11	9:I:28:SER:CB	2.26	0.63
10:W:33:ARG:HG2	23:W:1059:CHD:H152	1.81	0.63
7:G:5:LYS:HG3	28:G:1263:PEK:H382	1.81	0.63
23:P:1271:CHD:H232	23:P:1271:CHD:C16	2.29	0.63
2:B:59:GLN:O	2:B:60:GLU:HG3	1.99	0.63
7:G:8:HIS:ND1	28:G:1263:PEK:H332	2.13	0.63
7:G:72:ASN:H	7:G:76:ASN:ND2	1.97	0.62
8:H:57:ARG:HD2	29:H:4481:HOH:O	1.99	0.62
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.15	0.62
1:N:513:LEU:O	1:N:514:LYS:HB2	1.99	0.62
7:T:12:GLY:HA3	29:T:3372:HOH:O	1.99	0.62
20:A:524:PGV:C06	29:A:2126:HOH:O	2.46	0.62
2:O:61:VAL:HA	2:O:64:ILE:HD12	1.80	0.62
22:R:1229:PSC:C07	9:V:10:ARG:NH2	2.60	0.61
28:G:264:PEK:H71	28:G:264:PEK:H32	1.81	0.61
4:D:34:SER:H	4:D:37:GLN:NE2	1.98	0.61
7:T:36:TRP:HB3	29:T:4417:HOH:O	2.00	0.61
12:L:20:ARG:HH21	19:L:522:TGL:CC3	2.08	0.61
1:A:502:TYR:CD1	12:L:2:HIS:HE1	2.19	0.60
20:A:524:PGV:H221	20:A:524:PGV:H011	1.83	0.60
7:G:84:LYS:H	7:G:84:LYS:CD	2.13	0.60
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.01	0.60
9:V:18:ARG:HH11	9:V:18:ARG:CG	2.11	0.60
20:N:1524:PGV:H221	20:N:1524:PGV:H011	1.83	0.60
22:B:229:PSC:H081	5:E:8:ASP:OD1	2.01	0.59
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.31	0.59
7:T:3:ALA:O	7:T:4:ALA:HB2	2.03	0.59
9:I:31:PHE:CD1	9:I:32:ALA:N	2.71	0.59
28:S:1265:PEK:C38	25:T:1269:CDL:H273	2.32	0.59
7:G:3:ALA:O	7:G:4:ALA:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:127:LEU:HG	25:T:1269:CDL:OB3	2.03	0.58
4:Q:109:HIS:CD2	29:Q:3122:HOH:O	2.47	0.58
25:T:1269:CDL:H111	25:T:1269:CDL:CA2	2.31	0.58
19:N:1521:TGL:H281	19:N:1521:TGL:HB92	1.86	0.58
1:N:274:VAL:HG12	1:N:278:MET:HE2	1.85	0.58
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.69	0.58
5:E:31:LYS:HE3	29:F:4383:HOH:O	2.04	0.58
1:A:177:SER:H	1:A:180:GLN:NE2	2.02	0.58
19:N:1521:TGL:H102	19:N:1521:TGL:H283	1.86	0.58
7:G:4:ALA:CB	1:N:282:PHE:HA	2.34	0.57
8:U:49:ASP:O	8:U:52:VAL:HG22	2.04	0.57
1:A:47:LEU:O	13:M:41:LYS:HE3	2.04	0.57
6:F:85:CYS:SG	6:F:87:THR:CG2	2.89	0.57
7:G:5:LYS:HG3	28:G:1263:PEK:C38	2.33	0.57
5:R:8:ASP:HA	22:R:1229:PSC:H071	1.86	0.57
25:P:1270:CDL:H661	25:P:1270:CDL:H252	1.87	0.57
2:B:56:MET:HA	22:B:229:PSC:H202	1.85	0.57
7:T:5:LYS:HD3	28:T:263:PEK:H382	1.79	0.57
20:A:524:PGV:H222	13:M:15:GLN:HE22	1.70	0.56
26:C:272:DMU:H29	26:C:272:DMU:C10	2.35	0.56
9:I:31:PHE:O	9:I:34:PHE:N	2.32	0.56
4:Q:95:LEU:HD22	26:Z:1526:DMU:H13	1.86	0.56
3:C:19:THR:O	3:C:23:SER:HB3	2.06	0.56
20:A:524:PGV:H221	20:A:524:PGV:H012	1.86	0.56
25:C:270:CDL:HB32	25:C:270:CDL:CB2	2.35	0.56
25:P:1270:CDL:H431	29:W:4138:HOH:O	2.05	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.56
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.06	0.56
25:C:270:CDL:H672	25:C:270:CDL:H261	1.88	0.56
10:J:52:TRP:O	10:J:57:HIS:HE1	1.87	0.56
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.05	0.56
2:B:66:THR:HG22	2:B:67:ILE:N	2.20	0.56
25:C:270:CDL:HB21	25:C:270:CDL:CB3	2.36	0.56
23:B:1085:CHD:H12	23:B:1085:CHD:H212	1.87	0.56
1:A:513:LEU:O	1:A:514:LYS:HB2	2.06	0.56
4:Q:19:ARG:NH2	4:Q:21:ASP:OD1	2.39	0.55
28:G:264:PEK:H101	28:G:264:PEK:H161	1.88	0.55
25:C:270:CDL:H661	25:C:270:CDL:H242	1.88	0.55
10:J:50:LEU:HD22	10:J:50:LEU:O	2.06	0.55
25:T:1269:CDL:H522	25:T:1269:CDL:H202	1.87	0.55
1:N:508:PRO:HG3	3:P:6:HIS:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1523:TGL:CC2	19:N:1523:TGL:HG11	2.37	0.55
25:T:1269:CDL:OA7	25:T:1269:CDL:H311	2.05	0.55
25:G:269:CDL:H371	2:O:81:LEU:HD12	1.88	0.55
7:T:62:TRP:HB2	26:T:1272:DMU:H30	1.89	0.55
13:Z:39:ASN:O	13:Z:43:SER:HB2	2.07	0.55
7:G:2:SER:OG	28:G:1263:PEK:H301	2.07	0.55
3:P:33:MET:CG	29:P:4161:HOH:O	2.53	0.55
22:R:1229:PSC:H231	22:R:1229:PSC:H42	1.89	0.55
19:B:521:TGL:HA91	19:B:521:TGL:H252	1.88	0.55
7:G:3:ALA:O	7:G:4:ALA:CB	2.55	0.54
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.39	0.54
3:C:226:HIS:CE1	25:C:270:CDL:HB31	2.42	0.54
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.90	0.54
3:P:124:LEU:HD13	3:P:180:GLU:OE1	2.07	0.54
8:U:7:LYS:C	8:U:9:LYS:H	2.16	0.54
8:U:8:ILE:HG12	29:U:4330:HOH:O	2.08	0.54
19:L:522:TGL:H362	29:L:4269:HOH:O	2.08	0.54
7:T:5:LYS:HD3	28:T:263:PEK:C38	2.35	0.54
1:N:408:THR:O	1:N:412:ILE:HD12	2.08	0.54
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.40	0.54
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.23	0.53
11:X:24:PHE:O	11:X:28:VAL:HG12	2.08	0.53
10:J:9:GLN:O	10:J:13:GLN:HG3	2.09	0.53
4:Q:73:ARG:HB3	5:R:109:VAL:HG11	1.91	0.53
20:C:267:PGV:H182	25:C:270:CDL:C67	2.38	0.53
4:Q:19:ARG:NH2	4:Q:21:ASP:CG	2.66	0.53
19:B:521:TGL:H252	19:B:521:TGL:C20	2.39	0.53
8:U:60:TYR:CD1	8:U:60:TYR:C	2.87	0.53
3:C:226:HIS:HE1	25:C:270:CDL:HB31	1.74	0.53
10:W:29:ASN:HD22	10:W:29:ASN:H	1.54	0.53
2:B:13:THR:OG1	2:B:167:SER:HB3	2.09	0.53
12:L:25:MET:HG2	19:L:522:TGL:HA62	1.90	0.53
6:F:64:GLU:O	6:F:65:ASP:CB	2.57	0.53
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.24	0.52
1:N:1:FME:HE2	12:Y:3:TYR:CE1	2.43	0.52
25:C:270:CDL:HB22	25:C:270:CDL:OA5	2.08	0.52
1:N:112:LEU:CD1	29:N:3701:HOH:O	2.39	0.52
4:Q:122:ARG:HG2	4:Q:126:MET:HE2	1.90	0.52
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.91	0.52
2:B:33:LEU:CD1	9:I:28:SER:HB3	2.36	0.52
19:N:1523:TGL:HB52	4:Q:81:VAL:HG11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.90	0.52
6:S:64:GLU:O	6:S:65:ASP:HB2	2.09	0.52
25:T:1269:CDL:H172	29:T:4505:HOH:O	2.09	0.52
25:G:269:CDL:H231	25:G:269:CDL:C53	2.39	0.52
1:N:38:ARG:HD2	14:N:515:HEA:OMA	2.09	0.52
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.57	0.52
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.93	0.52
29:P:4415:HOH:O	26:T:1272:DMU:H24	2.10	0.52
2:O:62:GLU:HB2	29:O:4150:HOH:O	2.10	0.51
25:P:1270:CDL:PA1	25:P:1270:CDL:HB22	2.51	0.51
3:C:224:LYS:O	3:C:225:PHE:HB2	2.11	0.51
4:Q:56:LYS:HG2	5:R:61:PHE:CZ	2.46	0.51
10:W:29:ASN:H	10:W:29:ASN:ND2	2.09	0.51
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.40	0.51
2:O:33:LEU:CD1	9:V:28:SER:HB3	2.40	0.51
2:O:116:LEU:HD11	2:O:226:MET:CG	2.40	0.51
14:N:516:HEA:HBC1	14:N:516:HEA:HMC3	1.92	0.51
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.92	0.51
7:G:5:LYS:HB2	28:G:1263:PEK:H361	1.91	0.51
25:G:269:CDL:H542	25:G:269:CDL:H251	1.92	0.51
9:V:31:PHE:CD1	9:V:32:ALA:N	2.78	0.51
2:B:89:GLU:O	2:B:91:ASN:OD1	2.29	0.51
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.91	0.51
3:C:51:MET:HB2	25:C:270:CDL:H392	1.94	0.50
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.76	0.50
19:B:521:TGL:C28	19:B:521:TGL:C10	2.87	0.50
7:T:3:ALA:O	7:T:4:ALA:CB	2.59	0.50
2:O:78:LEU:CB	2:O:79:PRO:CD	2.89	0.50
9:V:59:ASP:OD2	9:V:63:MET:HE3	2.12	0.50
1:A:390:MET:HE3	1:A:390:MET:HA	1.93	0.50
20:A:524:PGV:H132	20:A:524:PGV:H302	1.93	0.50
25:G:269:CDL:H761	1:N:282:PHE:HZ	1.77	0.50
2:O:56:MET:HG2	22:R:1229:PSC:H211	1.94	0.50
1:A:422:ASN:HB3	19:B:521:TGL:H242	1.94	0.50
20:A:524:PGV:H322	20:A:524:PGV:H151	1.94	0.50
12:L:20:ARG:HH22	19:L:522:TGL:CC3	2.04	0.50
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.08	0.49
6:S:34:LEU:HD22	29:S:4590:HOH:O	2.12	0.49
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.94	0.49
19:N:1523:TGL:H352	29:V:4468:HOH:O	2.12	0.49
2:O:66:THR:HG22	2:O:67:ILE:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:15:ASN:HB2	29:X:3609:HOH:O	2.11	0.49
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.95	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.49
20:A:521:PGV:H182	3:C:28:THR:HG22	1.94	0.49
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.48	0.49
2:O:78:LEU:HB3	2:O:79:PRO:HD3	1.95	0.49
2:O:226:MET:HA	2:O:226:MET:CE	2.41	0.49
8:H:60:TYR:CD1	8:H:60:TYR:C	2.90	0.49
5:R:80:GLU:CD	5:R:80:GLU:N	2.68	0.49
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.94	0.48
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.95	0.48
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.78	0.48
4:D:93:ALA:HB3	11:K:28:VAL:HG22	1.95	0.48
12:L:20:ARG:NH2	19:L:522:TGL:HC62	2.08	0.48
19:N:1521:TGL:C28	19:N:1521:TGL:C10	2.88	0.48
10:W:9:GLN:O	10:W:13:GLN:HG3	2.12	0.48
4:D:34:SER:N	4:D:37:GLN:HE21	2.07	0.48
19:L:522:TGL:H351	29:L:4252:HOH:O	2.13	0.48
19:N:1521:TGL:H281	19:N:1521:TGL:C10	2.39	0.48
9:V:27:VAL:HG11	29:V:4562:HOH:O	2.13	0.48
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.25	0.48
1:N:417:MET:HE1	29:N:3166:HOH:O	2.13	0.48
19:N:1523:TGL:H242	19:N:1523:TGL:HA91	1.95	0.48
2:O:59:GLN:O	2:O:59:GLN:HG3	2.13	0.48
9:V:36:LYS:CG	29:V:4356:HOH:O	2.49	0.48
6:F:55:LYS:HA	6:F:74:LEU:O	2.13	0.48
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.11	0.48
2:O:102:HIS:HE2	2:O:107:SER:HG	1.62	0.48
1:N:400:PHE:HB3	19:N:1522:TGL:H282	1.94	0.48
3:P:236:GLU:HG2	29:P:4386:HOH:O	2.12	0.48
20:P:1267:PGV:H182	25:P:1270:CDL:C67	2.43	0.48
10:W:32:TYR:CE1	10:W:36:MET:HE3	2.47	0.48
1:N:87:ILE:O	1:N:173:PRO:HD3	2.14	0.48
7:T:2:SER:O	28:T:263:PEK:H331	2.14	0.48
7:T:5:LYS:CD	28:T:263:PEK:H383	2.40	0.48
29:W:4565:HOH:O	12:Y:47:LYS:HG3	2.13	0.48
22:B:229:PSC:H072	9:I:10:ARG:NH2	2.13	0.48
1:N:417:MET:CE	29:N:3166:HOH:O	2.62	0.48
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.96	0.48
25:T:1269:CDL:H762	25:T:1269:CDL:H561	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:31:PHE:O	9:I:32:ALA:C	2.56	0.47
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.95	0.47
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.72	0.47
1:A:177:SER:H	1:A:180:GLN:HE21	1.62	0.47
20:N:1524:PGV:H221	20:N:1524:PGV:H012	1.95	0.47
13:M:42:LYS:HA	13:M:42:LYS:CE	2.43	0.47
23:B:1085:CHD:H212	23:B:1085:CHD:C12	2.44	0.47
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.79	0.47
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.30	0.47
1:A:176:MET:HB2	1:A:176:MET:HE3	1.58	0.47
2:B:94:SER:HB2	29:B:4446:HOH:O	2.15	0.47
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.46	0.47
1:A:48:LEU:C	1:A:50:ASP:H	2.21	0.47
2:B:217:LYS:HD2	2:B:217:LYS:HA	1.60	0.47
1:A:51:ASP:HB3	2:B:202:SER:O	2.15	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.46
3:C:33:MET:CG	29:C:4096:HOH:O	2.63	0.46
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.96	0.46
1:N:472:ILE:HG21	19:N:1522:TGL:HA91	1.97	0.46
20:N:1524:PGV:H152	20:N:1524:PGV:H322	1.96	0.46
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.80	0.46
7:T:5:LYS:HD2	28:T:263:PEK:H383	1.83	0.46
13:M:39:ASN:O	13:M:43:SER:CB	2.61	0.46
2:O:78:LEU:CB	2:O:79:PRO:HD3	2.44	0.46
4:Q:19:ARG:HB3	4:Q:19:ARG:NH2	2.29	0.46
6:S:53:THR:HB	6:S:54:ASN:H	1.36	0.46
9:V:28:SER:O	9:V:32:ALA:N	2.41	0.46
19:L:522:TGL:H201	19:L:522:TGL:C24	2.46	0.46
3:P:146:TRP:CE2	7:T:17:ARG:HG3	2.50	0.46
6:S:92:VAL:O	6:S:92:VAL:HG23	2.14	0.46
28:S:1265:PEK:H381	25:T:1269:CDL:H273	1.97	0.46
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.80	0.46
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.95	0.46
20:P:1268:PGV:H21	20:P:1268:PGV:H51	1.36	0.46
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.98	0.46
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.97	0.46
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.46
2:O:33:LEU:HD11	9:V:28:SER:HB3	1.98	0.46
2:O:67:ILE:O	2:O:70:ALA:HB3	2.16	0.46
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.51	0.46
22:B:229:PSC:H142	22:B:229:PSC:H343	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:12:GLN:CG	29:H:4563:HOH:O	2.59	0.46
8:U:78:GLU:O	8:U:78:GLU:HG2	2.16	0.46
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.51	0.46
3:C:5:THR:HG22	6:F:96:LEU:HD22	1.97	0.46
25:C:270:CDL:H411	25:C:270:CDL:H382	1.83	0.46
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.46
2:B:52:HIS:CE1	22:B:229:PSC:H211	2.51	0.46
23:B:1085:CHD:H112	23:B:1085:CHD:H12A	1.69	0.46
25:G:269:CDL:H552	25:G:269:CDL:H582	1.60	0.46
12:L:46:LYS:O	12:L:47:LYS:CB	2.64	0.46
2:B:165:VAL:HG11	2:B:168:LEU:HD12	1.98	0.46
28:G:1263:PEK:H282	28:G:1263:PEK:H312	1.85	0.46
7:G:9:GLY:HA3	29:N:4361:HOH:O	2.16	0.45
1:N:398:PRO:O	1:N:498:CYS:HB3	2.16	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.45
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.51	0.45
7:T:8:HIS:CE1	28:T:263:PEK:H341	2.50	0.45
9:V:18:ARG:CG	9:V:18:ARG:NH1	2.77	0.45
2:O:200:CYS:SG	2:O:204:HIS:HA	2.57	0.45
2:O:226:MET:HE1	29:O:4398:HOH:O	2.17	0.45
28:T:1264:PEK:H32	28:T:1264:PEK:C7	2.31	0.45
1:A:50:ASP:CB	1:A:53:ILE:HD12	2.44	0.45
19:N:1521:TGL:H222	19:N:1521:TGL:CA8	2.42	0.45
5:R:8:ASP:HA	22:R:1229:PSC:C07	2.47	0.45
12:Y:9:LYS:HA	12:Y:9:LYS:HD3	1.61	0.45
1:A:514:LYS:HA	6:F:38:ALA:CB	2.47	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.16	0.45
22:R:1229:PSC:H251	22:R:1229:PSC:H221	1.39	0.45
8:U:7:LYS:O	8:U:8:ILE:HG22	2.16	0.45
12:Y:16:GLU:OE1	12:Y:16:GLU:HA	2.17	0.45
5:E:48:ILE:HG21	5:E:89:LEU:HD11	1.99	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.45
7:T:10:GLY:CA	29:T:4407:HOH:O	2.64	0.45
25:G:269:CDL:C87	29:G:4364:HOH:O	2.50	0.45
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB2	1.98	0.45
2:O:83:ILE:O	2:O:87:MET:HG3	2.17	0.45
4:D:9:GLU:CD	4:D:9:GLU:H	2.24	0.45
28:T:263:PEK:H231	28:T:263:PEK:H052	1.99	0.45
3:C:127:LEU:HG	25:G:269:CDL:OB3	2.16	0.45
2:O:59:GLN:C	2:O:60:GLU:HG3	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LYS:HD2	29:I:2618:HOH:O	2.18	0.44
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.29	0.44
5:E:31:LYS:CE	29:F:4383:HOH:O	2.63	0.44
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.82	0.44
8:H:58:ARG:HD2	8:H:58:ARG:HA	1.85	0.44
7:T:33:LEU:O	7:T:37:LEU:HB2	2.17	0.44
20:A:524:PGV:H011	20:A:524:PGV:H22	1.99	0.44
19:B:521:TGL:H281	19:B:521:TGL:C10	2.36	0.44
3:C:154:GLY:HA2	6:F:6:VAL:HB	1.99	0.44
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.00	0.44
25:T:1269:CDL:H541	25:T:1269:CDL:C23	2.34	0.44
10:W:12:PHE:O	10:W:23:LYS:HE2	2.17	0.44
1:N:369:ASP:HA	1:N:438:ARG:HD3	2.00	0.44
11:X:43:SER:HA	11:X:44:PRO:HD3	1.84	0.44
1:A:50:ASP:OD1	29:A:2067:HOH:O	2.21	0.44
22:B:229:PSC:H201	22:B:229:PSC:H232	1.33	0.44
7:G:5:LYS:CG	28:G:1263:PEK:H383	2.48	0.44
7:G:12:GLY:HA3	29:G:2372:HOH:O	2.18	0.44
2:O:66:THR:CG2	2:O:67:ILE:N	2.80	0.44
1:A:513:LEU:O	1:A:514:LYS:CB	2.66	0.44
2:B:86:MET:HE3	2:B:86:MET:HB2	1.82	0.44
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.99	0.44
6:F:30:PRO:O	6:F:96:LEU:HD21	2.18	0.44
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.41	0.44
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.99	0.44
2:O:207:MET:HE3	2:O:207:MET:HB2	1.83	0.44
1:A:321:PHE:CE2	22:B:229:PSC:H341	2.48	0.44
2:B:59:GLN:C	2:B:60:GLU:HG3	2.43	0.44
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.53	0.44
10:J:3:ASN:OD1	10:J:3:ASN:C	2.61	0.43
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.53	0.43
3:P:155:ASP:OD2	3:P:158:HIS:ND1	2.38	0.43
6:S:14:THR:HG1	10:W:13:GLN:HE22	1.64	0.43
2:B:111:THR:HA	2:B:114:GLU:O	2.19	0.43
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.99	0.43
28:G:265:PEK:H383	25:G:269:CDL:H272	1.84	0.43
1:N:114:ALA:O	1:N:118:VAL:HG13	2.18	0.43
1:N:321:PHE:HB3	2:O:65:TRP:CE3	2.53	0.43
20:N:1524:PGV:C01	20:N:1524:PGV:C22	2.96	0.43
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.99	0.43
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.52	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.01	0.43
1:N:18:LEU:HD22	19:N:1522:TGL:HB32	2.01	0.43
19:N:1521:TGL:H281	19:N:1521:TGL:CB9	2.48	0.43
9:V:31:PHE:HD1	9:V:32:ALA:N	2.16	0.43
2:B:78:LEU:CB	2:B:79:PRO:CD	2.97	0.43
20:N:1524:PGV:H242	20:N:1524:PGV:H41	1.99	0.43
11:X:13:TYR:O	11:X:14:GLY:C	2.61	0.43
1:A:250:GLY:O	1:A:254:ILE:HG12	2.19	0.43
2:O:33:LEU:HA	2:O:33:LEU:HD13	1.32	0.43
1:N:200:PRO:HB3	20:N:1266:PGV:H341	2.01	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.60	0.43
2:O:33:LEU:CD1	9:V:28:SER:CB	2.96	0.43
28:S:1265:PEK:C38	25:T:1269:CDL:C27	2.88	0.43
23:W:1059:CHD:H12A	23:W:1059:CHD:H112	1.40	0.43
22:B:229:PSC:H071	9:I:10:ARG:NH2	2.31	0.43
19:N:1522:TGL:H162	12:Y:24:MET:HE1	1.99	0.43
7:T:74:ARG:HB2	29:T:3608:HOH:O	2.19	0.43
12:Y:22:LEU:O	12:Y:26:THR:HB	2.19	0.43
2:B:1:FME:HE1	2:B:133:LEU:HD22	2.00	0.43
2:B:13:THR:O	2:B:13:THR:HG22	2.18	0.43
2:O:114:GLU:HB3	2:O:227:LEU:HD21	2.01	0.43
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.68	0.43
22:R:1229:PSC:H212	22:R:1229:PSC:O01	2.19	0.43
7:T:2:SER:O	28:T:263:PEK:H322	2.19	0.43
1:N:377:PHE:HA	1:N:380:VAL:HG22	2.01	0.42
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.79	0.42
2:O:114:GLU:HG3	2:O:227:LEU:HD11	2.00	0.42
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.85	0.42
2:O:33:LEU:HD11	9:V:28:SER:CB	2.49	0.42
3:P:47:LEU:O	3:P:51:MET:HG2	2.19	0.42
1:N:486:ASP:HB2	29:N:3142:HOH:O	2.18	0.42
22:R:1229:PSC:H212	22:R:1229:PSC:C02	2.49	0.42
1:A:240:HIS:CD2	1:A:240:HIS:C	2.98	0.42
20:C:267:PGV:H182	25:C:270:CDL:C66	2.49	0.42
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.54	0.42
6:S:16:LEU:HD12	6:S:16:LEU:HA	1.83	0.42
7:T:35:SER:C	7:T:37:LEU:H	2.27	0.42
28:T:1264:PEK:H71	28:T:1264:PEK:C3	2.34	0.42
23:C:271:CHD:H112	23:C:271:CHD:H12A	1.62	0.42
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:HE1	20:A:521:PGV:H81	2.02	0.42
1:A:472:ILE:HG21	19:L:522:TGL:HA92	2.02	0.42
9:I:26:MET:O	9:I:27:VAL:O	2.36	0.42
2:O:222:TRP:HB2	9:V:71:SER:HB2	2.01	0.42
6:S:37:LYS:HD3	6:S:37:LYS:HA	1.83	0.42
5:E:24:ILE:HG23	5:E:24:ILE:O	2.17	0.42
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.50	0.42
9:I:31:PHE:O	9:I:34:PHE:HB3	2.20	0.42
12:L:14:SER:H	19:L:522:TGL:HC31	1.85	0.42
1:N:412:ILE:HG12	4:Q:84:ALA:HB3	2.01	0.42
3:P:135:SER:HB3	25:T:1269:CDL:H572	2.02	0.42
1:A:48:LEU:C	1:A:50:ASP:N	2.77	0.42
1:A:115:SER:HB2	1:A:142:SER:O	2.19	0.42
9:I:31:PHE:HD1	9:I:32:ALA:N	2.15	0.42
19:L:522:TGL:H202	19:L:522:TGL:H231	1.72	0.42
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.01	0.42
28:T:263:PEK:O04	28:T:263:PEK:H242	2.19	0.42
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.75	0.42
14:N:515:HEA:HAC	14:N:515:HEA:HHD	1.91	0.42
20:P:1267:PGV:H331	29:P:4415:HOH:O	2.19	0.42
1:N:27:GLY:HA2	1:N:69:MET:HG3	2.02	0.42
2:B:63:THR:O	2:B:64:ILE:C	2.62	0.41
9:I:61:GLU:HG3	9:I:65:LYS:HE3	2.02	0.41
9:V:25:PHE:CZ	9:V:29:LEU:HD22	2.54	0.41
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.85	0.41
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.84	0.41
3:C:160:LEU:HD13	23:C:271:CHD:H181	2.02	0.41
19:N:1522:TGL:HC32	19:N:1522:TGL:HC62	1.90	0.41
4:Q:144:GLU:OE1	4:Q:147:LYS:HE3	2.19	0.41
6:S:81:ARG:HA	6:S:87:THR:O	2.19	0.41
1:A:488:THR:HB	1:A:495:LEU:HD13	2.02	0.41
5:E:82:TYR:N	5:E:83:PRO:CD	2.83	0.41
1:N:266:GLU:HB2	1:N:267:PRO:HD2	2.02	0.41
10:W:58:LYS:HA	10:W:58:LYS:HD3	1.81	0.41
10:J:33:ARG:HG2	23:J:60:CHD:H151	2.01	0.41
3:P:67:PHE:HA	10:W:9:GLN:HG2	2.02	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.02	0.41
14:A:516:HEA:HMC3	14:A:516:HEA:HBC1	2.03	0.41
19:B:521:TGL:C24	19:B:521:TGL:H201	2.50	0.41
28:G:264:PEK:H161	28:G:264:PEK:C10	2.49	0.41
28:G:1263:PEK:H161	3:P:91:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:522:TGL:C24	19:L:522:TGL:C20	2.95	0.41
1:N:344:PHE:CD1	1:N:344:PHE:C	2.98	0.41
20:N:1524:PGV:H011	20:N:1524:PGV:C22	2.49	0.41
5:R:5:HIS:HB3	5:R:6:GLU:H	1.41	0.41
12:L:29:PHE:CZ	19:L:522:TGL:HA82	2.56	0.41
1:N:289:ALA:HB1	1:N:297:MET:HE1	2.02	0.41
2:O:196:CYS:CB	2:O:207:MET:HG3	2.50	0.41
8:U:8:ILE:CG2	29:U:4330:HOH:O	2.44	0.41
25:C:270:CDL:HA4	25:C:270:CDL:H122	2.02	0.41
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.02	0.41
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.87	0.41
7:T:58:LYS:NZ	7:T:58:LYS:CD	2.72	0.41
1:A:324:LEU:O	1:A:327:LEU:HB2	2.21	0.41
1:A:1:FME:CE	1:A:1:FME:HA	2.49	0.41
2:B:82:ARG:CZ	2:B:86:MET:HE1	2.51	0.41
25:C:270:CDL:H852	25:C:270:CDL:H812	2.03	0.41
25:G:269:CDL:OA7	25:G:269:CDL:H342	2.21	0.41
9:I:27:VAL:HG12	9:I:28:SER:N	2.36	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.20	0.41
20:A:524:PGV:H242	13:M:15:GLN:NE2	2.35	0.41
2:B:33:LEU:HD11	9:I:28:SER:CA	2.51	0.41
2:B:41:ILE:O	2:B:45:MET:HG2	2.21	0.41
2:B:144:LEU:HB2	2:B:213:LEU:HD13	2.03	0.41
22:B:229:PSC:H212	22:B:229:PSC:C02	2.50	0.41
22:B:229:PSC:H071	5:E:8:ASP:HA	2.02	0.41
5:R:11:PHE:HB3	22:R:1229:PSC:H073	2.02	0.41
7:T:62:TRP:HB3	26:T:1272:DMU:H29	2.01	0.41
14:A:515:HEA:HHC	14:A:515:HEA:H11	1.83	0.40
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.55	0.40
2:B:191:LEU:HA	2:B:211:LEU:O	2.21	0.40
23:C:525:CHD:H12A	23:C:525:CHD:H112	1.52	0.40
5:E:90:ARG:NH2	29:E:4208:HOH:O	2.54	0.40
9:I:32:ALA:C	9:I:34:PHE:H	2.28	0.40
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.56	0.40
25:T:1269:CDL:H821	25:T:1269:CDL:H791	1.70	0.40
8:U:78:GLU:HG2	8:U:80:THR:HG23	2.04	0.40
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.98	0.40
20:A:524:PGV:H202	20:A:524:PGV:H231	1.95	0.40
5:E:108:LYS:O	5:E:108:LYS:HG2	2.20	0.40
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.96	0.40
10:J:32:TYR:CE1	10:J:36:MET:HE3	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:PRO:O	1:N:132:LEU:C	2.63	0.40
14:N:516:HEA:HHA	14:N:516:HEA:HAD2	1.83	0.40
3:P:173:PHE:CD2	3:P:173:PHE:C	2.99	0.40
23:P:1271:CHD:C16	23:P:1271:CHD:C23	2.96	0.40
22:R:1229:PSC:H063	22:R:1229:PSC:H042	1.84	0.40
2:B:135:LEU:O	2:B:208:PRO:HG3	2.22	0.40
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.40
11:K:31:TYR:CD2	11:K:35:GLN:HG3	2.56	0.40
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.03	0.40
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.40
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.20	0.40
8:U:9:LYS:O	8:U:10:ASN:CB	2.68	0.40
1:A:449:MET:SD	2:B:5:MET:HG2	2.61	0.40
2:B:74:ILE:HD11	25:T:1269:CDL:H461	2.04	0.40
4:D:109:HIS:HD2	29:D:2122:HOH:O	2.03	0.40
1:N:240:HIS:CD2	1:N:240:HIS:C	2.99	0.40
19:N:1523:TGL:HC22	19:N:1523:TGL:HC51	1.88	0.40
4:D:34:SER:O	4:D:38:LYS:HG3	2.21	0.40
19:N:1522:TGL:HA51	12:Y:25:MET:HG2	2.02	0.40
7:T:8:HIS:ND1	28:T:263:PEK:H321	2.37	0.40
25:T:1269:CDL:OA7	25:T:1269:CDL:H342	2.22	0.40
9:V:52:ARG:CZ	9:V:52:ARG:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	30	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	30	34
3	C	257/261 (98%)	253 (98%)	3 (1%)	1 (0%)	30	34
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	30	34
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	18	19
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	3	1
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	3
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	1	0
7	T	81/85 (95%)	65 (80%)	11 (14%)	5 (6%)	1	0
8	H	77/85 (91%)	66 (86%)	5 (6%)	6 (8%)	1	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	0
9	I	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	4	2
9	V	71/73 (97%)	64 (90%)	4 (6%)	3 (4%)	2	1
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	3
All	All	3504/3614 (97%)	3339 (95%)	129 (4%)	36 (1%)	12	11

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	8	HIS
8	U	8	ILE
8	U	45	ALA
2	B	60	GLU
3	C	38	ASN
8	H	47	GLY
9	I	27	VAL
9	I	33	THR
2	O	60	GLU
3	P	38	ASN
7	T	3	ALA
7	T	40	GLY
6	F	95	GLN
8	H	10	ASN
8	H	45	ALA
7	T	39	SER
8	U	46	LYS
6	F	96	LEU
8	H	9	LYS
8	U	9	LYS
9	V	28	SER
9	V	33	THR
9	V	37	PHE
4	Q	142	LYS
6	S	95	GLN
13	Z	41	LYS
7	G	6	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/426 (100%)	413 (97%)	13 (3%)	35 48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	426/426 (100%)	415 (97%)	11 (3%)	40 55
2	B	210/210 (100%)	201 (96%)	9 (4%)	26 35
2	O	210/210 (100%)	194 (92%)	16 (8%)	12 14
3	C	224/226 (99%)	218 (97%)	6 (3%)	39 53
3	P	224/226 (99%)	222 (99%)	2 (1%)	70 84
4	D	128/129 (99%)	120 (94%)	8 (6%)	16 19
4	Q	128/129 (99%)	121 (94%)	7 (6%)	19 24
5	E	92/95 (97%)	88 (96%)	4 (4%)	26 35
5	R	92/95 (97%)	84 (91%)	8 (9%)	9 10
6	F	81/81 (100%)	75 (93%)	6 (7%)	13 14
6	S	81/81 (100%)	75 (93%)	6 (7%)	13 14
7	G	67/68 (98%)	61 (91%)	6 (9%)	9 9
7	T	67/68 (98%)	61 (91%)	6 (9%)	9 9
8	H	71/75 (95%)	66 (93%)	5 (7%)	14 16
8	U	71/75 (95%)	64 (90%)	7 (10%)	7 8
9	I	57/57 (100%)	47 (82%)	10 (18%)	2 1
9	V	57/57 (100%)	46 (81%)	11 (19%)	1 1
10	J	49/50 (98%)	47 (96%)	2 (4%)	27 37
10	W	49/50 (98%)	42 (86%)	7 (14%)	3 3
11	K	39/46 (85%)	36 (92%)	3 (8%)	12 13
11	X	39/46 (85%)	35 (90%)	4 (10%)	7 7
12	L	39/40 (98%)	36 (92%)	3 (8%)	12 13
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12 13
13	M	37/38 (97%)	31 (84%)	6 (16%)	2 2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4 3
All	All	3040/3082 (99%)	2866 (94%)	174 (6%)	18 23

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	51	ASP
1	A	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	178	GLN
1	A	241	PRO
1	A	243	VAL
1	A	264	LYS
1	A	312	ILE
1	A	362	SER
1	A	363	LEU
1	A	369	ASP
1	A	504	THR
1	A	513	LEU
2	B	19	GLU
2	B	60	GLU
2	B	64	ILE
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	179	LEU
3	C	17	PRO
3	C	23	SER
3	C	33	MET
3	C	77	LYS
3	C	127	LEU
3	C	179	SER
4	D	4	SER
4	D	9	GLU
4	D	31	LYS
4	D	36	SER
4	D	49	SER
4	D	51	LEU
4	D	53	ILE
4	D	143	ASN
5	E	5	HIS
5	E	7	THR
5	E	70	VAL
5	E	109	VAL
6	F	2	SER
6	F	48	LEU
6	F	84	SER
6	F	87	THR
6	F	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	96	LEU
7	G	8	HIS
7	G	33	LEU
7	G	35	SER
7	G	36	TRP
7	G	42	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	18	ARG
9	I	21	ILE
9	I	26	MET
9	I	27	VAL
9	I	31	PHE
9	I	33	THR
9	I	37	PHE
9	I	45	LYS
9	I	73	LYS
10	J	31	LEU
10	J	50	LEU
11	K	32	MET
11	K	47	ARG
11	K	54	ARG
12	L	24	MET
12	L	26	THR
12	L	46	LYS
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	112	LEU
1	N	118	VAL
1	N	128	VAL
1	N	265	LYS
1	N	363	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	369	ASP
1	N	483	LEU
1	N	484	THR
1	N	486	ASP
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	107	SER
2	O	110	TYR
2	O	113	TYR
2	O	167	SER
2	O	183	THR
2	O	202	SER
2	O	205	SER
2	O	217	LYS
2	O	226	MET
3	P	77	LYS
3	P	127	LEU
4	Q	5	VAL
4	Q	6	VAL
4	Q	19	ARG
4	Q	34	SER
4	Q	51	LEU
4	Q	53	ILE
4	Q	143	ASN
5	R	5	HIS
5	R	21	LYS
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	108	LYS
5	R	109	VAL
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	S	78	GLU
6	S	87	THR
7	T	33	LEU
7	T	37	LEU
7	T	43	GLU
7	T	48	ILE
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
8	U	70	SER
8	U	84	LYS
9	V	2	THR
9	V	8	GLN
9	V	18	ARG
9	V	21	ILE
9	V	25	PHE
9	V	31	PHE
9	V	33	THR
9	V	44	LYS
9	V	52	ARG
9	V	65	LYS
9	V	73	LYS
10	W	2	GLU
10	W	10	LYS
10	W	27	THR
10	W	29	ASN
10	W	31	LEU
10	W	50	LEU
10	W	58	LYS
11	X	28	VAL
11	X	32	MET
11	X	47	ARG
11	X	54	ARG
12	Y	16	GLU
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
4	D	37	GLN
4	D	119	GLN
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	31	GLN
10	J	21	HIS
10	J	57	HIS
12	L	2	HIS
13	M	15	GLN
1	N	170	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	422	ASN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	161	GLN
4	Q	37	GLN
5	R	94	ASN
6	S	88	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	T	76	ASN
8	U	22	ASN
10	W	29	ASN
11	X	35	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	N	1	1	8,9,10	0.85	0	8,9,11	4.38	4 (50%)
1	FME	A	1	1	8,9,10	0.66	0	8,9,11	4.94	5 (62%)
2	FME	B	1	2	8,9,10	1.16	1 (12%)	8,9,11	6.17	4 (50%)
7	TPO	G	11	7	8,10,11	2.56	6 (75%)	10,14,16	2.21	3 (30%)
7	TPO	T	11	7	8,10,11	2.70	5 (62%)	10,14,16	2.30	4 (40%)
9	SAC	I	1	9	7,8,9	3.73	2 (28%)	7,9,11	3.64	2 (28%)
2	FME	O	1	2	8,9,10	0.90	0	8,9,11	3.72	4 (50%)
9	SAC	V	1	9	7,8,9	3.67	2 (28%)	7,9,11	2.71	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	4/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	3/9/11/13	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	3/7/8/10	-
2	FME	O	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	7.29	1.57	1.46
9	I	1	SAC	CA-N	6.68	1.56	1.46
9	I	1	SAC	OAC-C1A	6.52	1.37	1.23
9	V	1	SAC	OAC-C1A	5.55	1.35	1.23
7	T	11	TPO	P-OG1	4.47	1.67	1.59
7	G	11	TPO	P-O1P	4.03	1.63	1.50
7	T	11	TPO	P-O1P	3.80	1.62	1.50
7	G	11	TPO	P-OG1	3.56	1.65	1.59
7	T	11	TPO	P-O3P	2.51	1.64	1.54
7	G	11	TPO	CG2-CB	2.50	1.57	1.51
2	B	1	FME	O1-CN	-2.42	1.12	1.22
7	T	11	TPO	O-C	2.37	1.29	1.20
7	T	11	TPO	CG2-CB	2.35	1.57	1.51
7	G	11	TPO	O-C	2.30	1.28	1.20
7	G	11	TPO	P-O2P	2.22	1.63	1.54
7	G	11	TPO	P-O3P	2.04	1.62	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-16.81	96.98	122.82
1	A	1	FME	CA-N-CN	-12.33	103.86	122.82
1	N	1	FME	CA-N-CN	-10.28	107.00	122.82
2	O	1	FME	CA-N-CN	-9.32	108.49	122.82
9	I	1	SAC	C-CA-N	8.94	126.74	109.50
7	G	11	TPO	CG2-CB-CA	5.59	124.15	113.26
1	N	1	FME	CB-CA-N	5.28	120.14	110.52
7	T	11	TPO	CG2-CB-CA	4.87	122.75	113.26
9	V	1	SAC	C2A-C1A-N	4.28	123.22	116.12
1	A	1	FME	CB-CA-N	3.80	117.45	110.52
1	A	1	FME	CE-SD-CG	3.72	119.60	100.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CE-SD-CG	3.26	117.22	100.32
9	V	1	SAC	CB-CA-C	3.14	118.26	111.35
7	T	11	TPO	O3P-P-OG1	2.96	117.38	105.85
9	V	1	SAC	C-CA-N	2.93	115.16	109.50
7	G	11	TPO	O2P-P-OG1	2.91	117.21	105.85
7	T	11	TPO	O-C-CA	-2.88	117.37	124.77
9	V	1	SAC	OAC-C1A-C2A	-2.83	117.01	122.05
2	O	1	FME	O1-CN-N	-2.77	118.17	125.32
2	B	1	FME	O-C-CA	-2.63	118.00	124.77
1	A	1	FME	CG-CB-CA	-2.63	104.84	112.87
2	B	1	FME	CB-CA-N	2.62	115.30	110.52
2	O	1	FME	C-CA-N	2.48	114.28	109.50
9	I	1	SAC	OAC-C1A-N	2.32	126.08	121.98
2	O	1	FME	O-C-CA	-2.32	118.80	124.77
2	B	1	FME	O1-CN-N	-2.30	119.36	125.32
7	G	11	TPO	O-C-CA	-2.29	118.88	124.77
7	T	11	TPO	O2P-P-OG1	2.06	113.89	105.85
1	N	1	FME	O1-CN-N	2.06	130.63	125.32
1	A	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C-CA-N-C1A
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	N	1	FME	C-CA-CB-CG
9	V	1	SAC	C-CA-N-C1A
9	I	1	SAC	N-CA-CB-OG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	1	0
1	A	1	FME	1	0
2	B	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CDL	C	270	-	99,99,99	1.55	15 (15%)	105,111,111	1.48	15 (14%)
21	CUA	B	228	2	0,1,1	-	-	-		
14	HEA	A	515	1	67,67,67	2.06	22 (32%)	81,103,103	2.24	24 (29%)
19	TGL	N	1523	-	62,62,62	1.51	8 (12%)	65,65,65	1.44	11 (16%)
20	PGV	P	1267	-	50,50,50	1.03	2 (4%)	53,56,56	1.03	3 (5%)
14	HEA	N	515	1	67,67,67	2.06	21 (31%)	81,103,103	1.88	27 (33%)
19	TGL	A	523	-	62,62,62	1.48	6 (9%)	65,65,65	1.71	14 (21%)
26	DMU	M	526	-	34,34,34	1.28	2 (5%)	45,45,45	3.46	22 (48%)
21	CUA	O	228	2	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	PGV	A	524	-	50,50,50	1.34	3 (6%)	53,56,56	1.42	8 (15%)
28	PEK	T	1264	-	52,52,52	0.92	4 (7%)	55,57,57	1.42	11 (20%)
22	PSC	R	1229	-	51,51,51	1.38	3 (5%)	57,59,59	1.27	6 (10%)
25	CDL	T	1269	-	99,99,99	1.60	12 (12%)	105,111,111	1.51	14 (13%)
26	DMU	Z	1526	-	34,34,34	1.01	3 (8%)	45,45,45	3.15	21 (46%)
23	CHD	P	1271	-	32,32,32	0.91	1 (3%)	51,51,51	5.16	35 (68%)
22	PSC	B	229	-	51,51,51	1.42	3 (5%)	57,59,59	1.31	7 (12%)
26	DMU	T	1272	-	34,34,34	1.38	3 (8%)	45,45,45	3.16	22 (48%)
25	CDL	P	1270	-	99,99,99	1.55	13 (13%)	105,111,111	1.43	12 (11%)
23	CHD	W	1059	-	32,32,32	0.80	1 (3%)	51,51,51	5.03	34 (66%)
20	PGV	N	1524	-	50,50,50	1.28	2 (4%)	53,56,56	1.23	6 (11%)
15	CMO	N	520	14	0,1,1	-	-	-		
20	PGV	P	1268	-	50,50,50	1.44	2 (4%)	53,56,56	1.63	8 (15%)
23	CHD	B	1085	-	32,32,32	1.63	4 (12%)	51,51,51	5.54	37 (72%)
26	DMU	C	272	-	34,34,34	1.34	5 (14%)	45,45,45	3.38	21 (46%)
28	PEK	G	1263	-	52,52,52	1.42	5 (9%)	55,57,57	1.50	8 (14%)
19	TGL	N	1522	-	62,62,62	1.70	7 (11%)	65,65,65	1.81	16 (24%)
28	PEK	G	265	-	52,52,52	1.63	6 (11%)	55,57,57	1.54	11 (20%)
28	PEK	G	264	-	52,52,52	1.06	5 (9%)	55,57,57	1.58	10 (18%)
25	CDL	G	269	-	99,99,99	1.53	13 (13%)	105,111,111	1.45	17 (16%)
23	CHD	C	271	-	32,32,32	0.94	3 (9%)	51,51,51	4.96	34 (66%)
28	PEK	T	263	-	52,52,52	1.42	4 (7%)	55,57,57	1.22	5 (9%)
23	CHD	O	229	-	32,32,32	1.54	6 (18%)	51,51,51	5.49	37 (72%)
20	PGV	C	268	-	50,50,50	1.48	3 (6%)	53,56,56	1.72	7 (13%)
28	PEK	S	1265	-	52,52,52	1.30	3 (5%)	55,57,57	1.33	5 (9%)
19	TGL	L	522	-	62,62,62	1.77	9 (14%)	65,65,65	2.01	16 (24%)
23	CHD	J	60	-	32,32,32	1.11	2 (6%)	51,51,51	5.28	37 (72%)
14	HEA	A	516	1	67,67,67	2.08	23 (34%)	81,103,103	2.19	29 (35%)
20	PGV	C	267	-	50,50,50	0.91	2 (4%)	53,56,56	1.20	6 (11%)
23	CHD	C	525	-	32,32,32	1.46	4 (12%)	51,51,51	4.99	39 (76%)
15	CMO	A	520	-	0,1,1	-	-	-		
20	PGV	N	1266	-	50,50,50	0.87	3 (6%)	53,56,56	1.39	5 (9%)
20	PGV	A	521	-	50,50,50	0.83	2 (4%)	53,56,56	1.75	7 (13%)
19	TGL	B	521	-	62,62,62	1.55	8 (12%)	65,65,65	2.51	18 (27%)
19	TGL	N	1521	-	62,62,62	1.50	9 (14%)	65,65,65	2.24	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	N	516	15,1	67,67,67	1.95	25 (37%)	81,103,103	2.21	27 (33%)
23	CHD	P	1525	-	32,32,32	1.11	3 (9%)	51,51,51	5.41	38 (74%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	C	270	-	-	68/110/110/110	-
14	HEA	A	515	1	-	6/36/76/76	-
19	TGL	N	1523	-	-	32/65/65/65	-
20	PGV	P	1267	-	-	14/55/55/55	-
26	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
14	HEA	N	515	1	-	6/36/76/76	-
19	TGL	A	523	-	-	33/65/65/65	-
20	PGV	A	524	-	-	32/55/55/55	-
28	PEK	T	1264	-	-	21/56/56/56	-
22	PSC	R	1229	-	-	28/55/55/55	-
25	CDL	T	1269	-	-	59/110/110/110	-
26	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
23	CHD	P	1271	-	1/1/12/12	6/9/74/74	0/4/4/4
22	PSC	B	229	-	-	33/55/55/55	-
26	DMU	T	1272	-	6/6/10/10	12/19/59/59	0/2/2/2
25	CDL	P	1270	-	-	78/110/110/110	-
23	CHD	W	1059	-	2/2/12/12	6/9/74/74	0/4/4/4
20	PGV	N	1524	-	-	29/55/55/55	-
23	CHD	B	1085	-	1/1/12/12	2/9/74/74	0/4/4/4
20	PGV	P	1268	-	-	35/55/55/55	-
26	DMU	C	272	-	5/5/10/10	11/19/59/59	0/2/2/2
28	PEK	G	1263	-	-	32/56/56/56	-
19	TGL	N	1522	-	-	36/65/65/65	-
28	PEK	G	265	-	-	24/56/56/56	-
28	PEK	G	264	-	-	23/56/56/56	-
25	CDL	G	269	-	-	58/110/110/110	-
23	CHD	C	271	-	1/1/12/12	7/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEK	T	263	-	-	26/56/56/56	-
23	CHD	O	229	-	1/1/12/12	5/9/74/74	0/4/4/4
20	PGV	C	268	-	-	29/55/55/55	-
28	PEK	S	1265	-	-	27/56/56/56	-
19	TGL	L	522	-	-	42/65/65/65	-
23	CHD	J	60	-	1/1/12/12	7/9/74/74	0/4/4/4
14	HEA	A	516	1	-	6/36/76/76	-
20	PGV	C	267	-	-	13/55/55/55	-
23	CHD	C	525	-	-	1/9/74/74	0/4/4/4
20	PGV	N	1266	-	-	14/55/55/55	-
20	PGV	A	521	-	-	14/55/55/55	-
19	TGL	B	521	-	-	36/65/65/65	-
19	TGL	N	1521	-	-	36/65/65/65	-
14	HEA	N	516	15,1	-	9/36/76/76	-
23	CHD	P	1525	-	-	4/9/74/74	0/4/4/4

All (280) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	522	TGL	OG2-CB1	7.62	1.55	1.34
19	N	1522	TGL	OG2-CB1	7.47	1.55	1.34
20	C	268	PGV	O01-C1	7.20	1.54	1.34
20	P	1268	PGV	O01-C1	7.09	1.54	1.34
14	A	516	HEA	FE-NA	6.76	2.17	1.95
14	N	515	HEA	FE-ND	6.49	2.14	1.94
28	G	1263	PEK	O03-C21	6.44	1.52	1.33
28	T	263	PEK	O03-C21	6.37	1.51	1.33
19	A	523	TGL	OG2-CB1	5.97	1.51	1.34
19	N	1523	TGL	OG2-CB1	5.94	1.51	1.34
20	A	524	PGV	O03-C19	5.77	1.50	1.33
22	B	229	PSC	O01-C1	5.59	1.50	1.34
25	G	269	CDL	OB6-CB5	5.58	1.50	1.34
19	L	522	TGL	OG1-CA1	5.49	1.49	1.33
25	T	1269	CDL	OB8-CB7	5.45	1.49	1.33
26	T	1272	DMU	O16-C6	5.42	1.49	1.40
28	S	1265	PEK	O01-C1	5.37	1.49	1.34
28	T	263	PEK	O01-C1	5.37	1.49	1.34
28	G	265	PEK	O01-C1	5.35	1.49	1.34
19	L	522	TGL	OG3-CC1	5.34	1.48	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1269	CDL	OA6-CA5	5.33	1.49	1.34
25	T	1269	CDL	OB6-CB5	5.33	1.49	1.34
25	C	270	CDL	OA6-CA5	5.32	1.49	1.34
19	N	1522	TGL	OG3-CC1	5.32	1.48	1.33
25	P	1270	CDL	OA6-CA5	5.31	1.49	1.34
22	R	1229	PSC	O01-C1	5.26	1.49	1.34
25	G	269	CDL	OA6-CA5	5.25	1.49	1.34
19	N	1522	TGL	OG1-CA1	5.23	1.48	1.33
25	P	1270	CDL	OA8-CA7	5.21	1.48	1.33
20	N	1524	PGV	O03-C19	5.18	1.48	1.33
28	S	1265	PEK	O03-C21	5.16	1.48	1.33
23	C	525	CHD	C18-C13	5.12	1.62	1.54
19	N	1523	TGL	OG3-CC1	5.11	1.48	1.33
19	A	523	TGL	OG3-CC1	5.04	1.48	1.33
19	B	521	TGL	OG1-CA1	5.04	1.48	1.33
25	T	1269	CDL	OA8-CA7	5.04	1.48	1.33
19	N	1521	TGL	OG1-CA1	5.01	1.47	1.33
20	C	268	PGV	O03-C19	4.98	1.47	1.33
20	N	1524	PGV	O01-C1	4.97	1.48	1.34
28	G	1263	PEK	O01-C1	4.89	1.48	1.34
26	C	272	DMU	O16-C6	4.80	1.48	1.40
14	A	515	HEA	FE-NA	4.79	2.11	1.95
25	G	269	CDL	OB8-CB7	4.79	1.47	1.33
25	P	1270	CDL	OB6-CB5	4.76	1.47	1.34
25	P	1270	CDL	OB8-CB7	4.73	1.47	1.33
19	B	521	TGL	OG2-CB1	4.73	1.47	1.34
22	R	1229	PSC	O03-C19	4.73	1.47	1.33
14	N	516	HEA	FE-NA	4.68	2.10	1.95
22	B	229	PSC	O03-C19	4.61	1.46	1.33
19	B	521	TGL	OC1-CC1	-4.61	1.08	1.22
23	B	1085	CHD	C18-C13	4.61	1.61	1.54
14	A	515	HEA	FE-NC	4.56	2.10	1.95
28	G	265	PEK	C17-C16	4.54	1.71	1.52
20	P	1268	PGV	O03-C19	4.50	1.46	1.33
19	N	1521	TGL	OG2-CB1	4.49	1.47	1.34
14	A	516	HEA	FE-NC	4.45	2.09	1.95
25	G	269	CDL	OA8-CA7	4.42	1.46	1.33
14	A	515	HEA	CHD-C1D	4.42	1.47	1.38
25	C	270	CDL	OB8-CB7	4.41	1.46	1.33
20	A	524	PGV	O01-C1	4.39	1.46	1.34
25	C	270	CDL	OB6-CB5	4.32	1.46	1.34
14	N	515	HEA	CHA-C1A	4.30	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	229	PSC	C13-C12	4.29	1.56	1.31
19	A	523	TGL	OG1-CA1	4.28	1.45	1.33
22	R	1229	PSC	C13-C12	4.28	1.56	1.31
28	G	265	PEK	C7-C6	4.27	1.81	1.51
14	A	515	HEA	CHA-C1A	4.21	1.46	1.38
19	N	1521	TGL	OG3-CC1	4.21	1.45	1.33
25	T	1269	CDL	C59-C58	-4.15	1.31	1.51
19	N	1523	TGL	OG1-CA1	4.13	1.45	1.33
14	A	516	HEA	CHA-C1A	4.13	1.46	1.38
25	C	270	CDL	OA8-CA7	4.12	1.45	1.33
14	N	515	HEA	CHA-C4D	4.11	1.48	1.39
14	A	516	HEA	C4A-NA	-4.05	1.32	1.39
26	M	526	DMU	O16-C6	4.02	1.46	1.40
20	P	1267	PGV	O03-C19	3.96	1.44	1.33
25	P	1270	CDL	C59-C58	-3.96	1.32	1.51
19	B	521	TGL	C10-CB9	-3.90	1.32	1.51
26	M	526	DMU	C3-C4	-3.90	1.42	1.52
14	N	516	HEA	C4A-NA	-3.88	1.32	1.39
28	G	265	PEK	O03-C21	3.86	1.44	1.33
25	C	270	CDL	C40-C39	3.84	1.70	1.51
19	L	522	TGL	C20-CA9	-3.81	1.32	1.51
23	O	229	CHD	C13-C14	-3.80	1.49	1.55
25	C	270	CDL	C59-C58	-3.79	1.32	1.51
25	G	269	CDL	C59-C58	-3.78	1.33	1.51
14	A	516	HEA	CHC-C4B	3.78	1.46	1.38
19	N	1521	TGL	C10-CB9	-3.76	1.33	1.51
25	T	1269	CDL	C62-C61	-3.75	1.33	1.51
14	N	515	HEA	C3A-C4A	-3.72	1.39	1.46
28	G	264	PEK	O01-C1	3.72	1.44	1.34
14	N	516	HEA	C4D-ND	-3.72	1.31	1.38
14	A	515	HEA	C13-C14	3.68	1.61	1.50
25	G	269	CDL	C62-C61	-3.68	1.33	1.51
25	T	1269	CDL	C42-C41	-3.63	1.33	1.51
19	N	1522	TGL	C20-CA9	-3.63	1.33	1.51
20	N	1266	PGV	O01-C1	3.61	1.44	1.34
19	N	1522	TGL	C10-CB9	-3.61	1.33	1.51
19	N	1523	TGL	C10-CB9	-3.60	1.33	1.51
14	A	516	HEA	C1D-C2D	-3.57	1.37	1.44
14	N	516	HEA	C1D-ND	-3.54	1.34	1.40
25	P	1270	CDL	C62-C61	-3.54	1.34	1.51
14	N	515	HEA	C4C-NC	-3.52	1.33	1.39
25	T	1269	CDL	C19-C18	-3.51	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	265	PEK	C6-C5	3.50	1.51	1.31
14	N	516	HEA	CHB-C4A	3.48	1.45	1.38
25	P	1270	CDL	C79-C78	-3.47	1.34	1.51
14	A	516	HEA	C4B-C3B	-3.46	1.38	1.44
19	B	521	TGL	C20-CA9	-3.45	1.34	1.51
25	C	270	CDL	C62-C61	-3.45	1.34	1.51
26	Z	1526	DMU	O16-C6	3.45	1.45	1.40
14	N	515	HEA	CHD-C1D	3.43	1.45	1.38
20	A	521	PGV	O03-C19	3.42	1.43	1.33
14	A	515	HEA	C3A-C4A	-3.41	1.40	1.46
14	N	515	HEA	FE-NA	3.39	2.06	1.95
14	A	515	HEA	CMB-C2B	3.39	1.57	1.50
28	T	1264	PEK	O01-C1	3.39	1.43	1.34
14	A	515	HEA	C1A-NA	-3.36	1.33	1.39
25	P	1270	CDL	C39-C38	-3.36	1.35	1.51
14	A	515	HEA	CHC-C4B	3.35	1.45	1.38
25	C	270	CDL	C82-C81	-3.34	1.35	1.51
25	P	1270	CDL	C22-C21	-3.34	1.35	1.51
14	N	515	HEA	CHD-C4C	3.34	1.46	1.39
25	C	270	CDL	C37-C36	3.33	1.68	1.51
19	A	523	TGL	C10-CB9	-3.33	1.35	1.51
25	C	270	CDL	C22-C21	-3.32	1.35	1.51
19	A	523	TGL	C20-CA9	-3.30	1.35	1.51
25	P	1270	CDL	C82-C81	-3.29	1.35	1.51
14	N	516	HEA	C18-C19	3.28	1.40	1.33
19	N	1521	TGL	C20-CA9	-3.28	1.35	1.51
14	A	515	HEA	FE-ND	3.28	2.05	1.94
19	B	521	TGL	OG3-CC1	3.27	1.42	1.33
20	P	1267	PGV	O01-C1	3.27	1.43	1.34
19	L	522	TGL	C10-CB9	-3.25	1.35	1.51
25	C	270	CDL	C19-C18	-3.24	1.35	1.51
25	T	1269	CDL	C39-C38	-3.24	1.35	1.51
23	P	1271	CHD	C20-C17	3.23	1.59	1.54
25	P	1270	CDL	C19-C18	-3.21	1.35	1.51
25	T	1269	CDL	C79-C78	-3.19	1.35	1.51
14	N	515	HEA	C4B-C3B	-3.18	1.39	1.44
14	N	515	HEA	C4B-NB	-3.15	1.34	1.40
19	A	523	TGL	C15-CC9	-3.14	1.36	1.51
14	A	516	HEA	CHB-C1B	3.13	1.46	1.39
20	C	267	PGV	O01-C1	3.10	1.43	1.34
14	N	515	HEA	C4D-C3D	-3.07	1.39	1.45
25	G	269	CDL	C79-C78	-3.06	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1523	TGL	C20-CA9	-3.05	1.36	1.51
28	G	264	PEK	O03-C01	-3.05	1.38	1.45
25	T	1269	CDL	C22-C21	-3.05	1.36	1.51
14	A	516	HEA	C1B-NB	-3.04	1.32	1.38
25	G	269	CDL	C22-C21	-3.03	1.36	1.51
14	A	515	HEA	CHB-C1B	3.01	1.46	1.39
23	B	1085	CHD	C10-C5	-3.00	1.50	1.55
25	T	1269	CDL	C82-C81	-3.00	1.36	1.51
14	A	516	HEA	CHC-C1C	2.96	1.46	1.39
19	N	1523	TGL	C17-C16	2.96	1.66	1.51
25	P	1270	CDL	C42-C41	-2.95	1.37	1.51
23	B	1085	CHD	C13-C14	-2.94	1.50	1.55
19	N	1521	TGL	C17-C16	2.91	1.66	1.51
14	N	515	HEA	C1D-ND	-2.91	1.35	1.40
25	G	269	CDL	C19-C18	-2.90	1.37	1.51
14	N	515	HEA	FE-NB	2.90	2.03	1.94
26	C	272	DMU	O1-C10	2.88	1.49	1.41
25	G	269	CDL	C39-C38	-2.88	1.37	1.51
23	B	1085	CHD	C4-C3	2.88	1.57	1.52
14	A	515	HEA	C4B-NB	-2.88	1.35	1.40
14	N	516	HEA	C4C-NC	-2.87	1.34	1.39
14	A	515	HEA	C20-C19	2.87	1.57	1.51
14	A	515	HEA	C1D-ND	-2.87	1.35	1.40
19	L	522	TGL	C15-CC9	-2.85	1.37	1.51
19	N	1523	TGL	C15-CC9	-2.84	1.37	1.51
23	J	60	CHD	C23-C24	2.84	1.57	1.50
25	G	269	CDL	C82-C81	-2.84	1.37	1.51
14	N	516	HEA	C3A-C4A	-2.83	1.41	1.46
14	A	516	HEA	C1A-NA	-2.83	1.34	1.39
14	N	516	HEA	C1A-C2A	-2.82	1.40	1.45
14	A	515	HEA	C3A-C2A	2.81	1.43	1.37
14	A	516	HEA	C3A-C4A	-2.81	1.41	1.46
26	Z	1526	DMU	C3-C4	-2.81	1.45	1.52
14	N	516	HEA	CHA-C4D	2.80	1.45	1.39
14	N	516	HEA	C4B-NB	-2.77	1.35	1.40
28	T	1264	PEK	O01-C02	-2.76	1.40	1.46
23	O	229	CHD	C4-C3	2.74	1.56	1.52
25	G	269	CDL	C42-C41	-2.73	1.38	1.51
19	N	1522	TGL	C15-CC9	-2.73	1.38	1.51
14	A	516	HEA	CHB-C4A	2.71	1.43	1.38
20	C	267	PGV	O03-C19	2.70	1.41	1.33
14	N	516	HEA	CHA-C1A	2.70	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	522	TGL	CC2-CC1	2.70	1.58	1.50
14	A	516	HEA	C4C-NC	-2.68	1.34	1.39
28	G	264	PEK	O01-C02	-2.68	1.40	1.46
20	N	1266	PGV	O03-C19	2.65	1.41	1.33
26	C	272	DMU	C8-C7	2.61	1.59	1.52
14	N	516	HEA	CHC-C4B	2.60	1.43	1.38
14	N	516	HEA	C1A-NA	-2.59	1.34	1.39
14	A	516	HEA	C4D-C3D	-2.58	1.40	1.45
23	P	1525	CHD	C13-C14	-2.57	1.51	1.55
14	A	516	HEA	CHD-C1D	2.57	1.43	1.38
25	C	270	CDL	OB6-CB4	-2.57	1.40	1.46
28	T	1264	PEK	O03-C01	-2.56	1.39	1.45
14	N	516	HEA	CHD-C1D	2.56	1.43	1.38
28	G	1263	PEK	C01-C02	2.54	1.58	1.50
28	T	263	PEK	C01-C02	2.54	1.58	1.50
28	G	264	PEK	O03-C21	2.54	1.40	1.33
19	B	521	TGL	C15-CC9	-2.53	1.39	1.51
14	N	516	HEA	FE-NC	2.49	2.03	1.95
20	A	521	PGV	O03-C01	2.49	1.50	1.45
28	G	1263	PEK	P-O12	2.49	1.69	1.59
14	N	516	HEA	C1D-C2D	-2.48	1.39	1.44
19	N	1521	TGL	OG1-CG1	-2.48	1.39	1.45
14	N	515	HEA	C1C-NC	-2.47	1.35	1.39
25	C	270	CDL	CB2-C1	2.45	1.59	1.51
14	N	515	HEA	CMD-C2D	2.45	1.55	1.50
14	A	516	HEA	C3D-C2D	2.44	1.42	1.36
14	N	516	HEA	CHC-C1C	2.43	1.44	1.39
14	N	516	HEA	C4D-C3D	-2.42	1.40	1.45
14	N	516	HEA	CHB-C1B	2.41	1.44	1.39
14	N	516	HEA	O11-C11	2.41	1.48	1.42
23	C	525	CHD	O26-C24	-2.41	1.22	1.30
23	C	271	CHD	C10-C9	-2.40	1.51	1.56
14	N	515	HEA	C3B-C2B	2.39	1.40	1.34
23	O	229	CHD	C11-C9	2.39	1.57	1.53
19	N	1521	TGL	C18-C17	2.39	1.63	1.51
14	N	516	HEA	C4B-C3B	-2.38	1.40	1.44
19	L	522	TGL	CG3-CG2	2.37	1.58	1.50
23	C	525	CHD	C19-C10	2.36	1.58	1.54
14	N	515	HEA	CHC-C1C	2.36	1.44	1.39
14	A	516	HEA	C1A-C2A	-2.36	1.41	1.45
25	P	1270	CDL	CB2-C1	2.35	1.59	1.51
26	T	1272	DMU	O5-C6	2.34	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	516	HEA	FE-ND	2.33	2.02	1.94
20	A	524	PGV	P-O11	2.33	1.68	1.59
25	C	270	CDL	PB2-OB2	2.32	1.68	1.59
28	G	265	PEK	P-O12	2.32	1.68	1.59
14	A	515	HEA	C11-C3B	2.32	1.54	1.51
14	N	516	HEA	C1B-C2B	-2.31	1.39	1.44
19	N	1521	TGL	OC1-CC1	-2.30	1.15	1.22
23	P	1525	CHD	C11-C9	2.28	1.57	1.53
19	N	1522	TGL	CG3-CG2	2.27	1.57	1.50
19	B	521	TGL	OG1-CG1	-2.26	1.40	1.45
14	A	515	HEA	O11-C11	2.25	1.47	1.42
14	A	515	HEA	CHB-C4A	2.25	1.42	1.38
14	A	516	HEA	C14-C15	2.25	1.38	1.33
14	N	515	HEA	C1B-C2B	-2.24	1.40	1.44
14	A	515	HEA	CMC-C2C	2.23	1.55	1.50
25	C	270	CDL	C80-C79	2.22	1.62	1.51
26	T	1272	DMU	O1-C10	2.22	1.47	1.41
19	L	522	TGL	OG2-CG2	2.22	1.51	1.46
23	C	271	CHD	O26-C24	-2.21	1.23	1.30
23	J	60	CHD	C20-C17	2.19	1.58	1.54
14	A	515	HEA	C4D-C3D	-2.19	1.41	1.45
20	C	268	PGV	P-O11	2.18	1.67	1.59
28	T	263	PEK	C03-C02	2.18	1.57	1.50
14	A	516	HEA	O2D-CGD	-2.18	1.23	1.30
14	N	515	HEA	C4A-NA	-2.18	1.35	1.39
20	N	1266	PGV	O01-C02	-2.17	1.41	1.46
19	N	1523	TGL	C18-C17	2.17	1.62	1.51
28	T	1264	PEK	O03-C21	2.16	1.39	1.33
23	O	229	CHD	C13-C17	-2.13	1.51	1.55
28	S	1265	PEK	P-O12	2.13	1.67	1.59
14	A	515	HEA	C1A-C2A	-2.12	1.41	1.45
28	G	1263	PEK	P-O11	2.11	1.67	1.59
14	N	515	HEA	CMA-C3A	2.11	1.50	1.45
23	C	271	CHD	C20-C17	2.11	1.58	1.54
23	O	229	CHD	C8-C14	-2.09	1.49	1.53
14	A	516	HEA	C4D-ND	-2.09	1.34	1.38
23	C	525	CHD	C13-C14	-2.08	1.52	1.55
26	C	272	DMU	O5-C6	2.08	1.47	1.41
23	W	1059	CHD	C23-C24	2.07	1.55	1.50
14	A	516	HEA	C22-C23	2.06	1.38	1.32
14	N	516	HEA	C1B-NB	-2.06	1.34	1.38
28	G	264	PEK	C2-C1	2.05	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	272	DMU	C3-C4	-2.04	1.47	1.52
14	A	516	HEA	CMD-C2D	2.04	1.54	1.50
14	N	515	HEA	C3D-C2D	2.03	1.41	1.36
26	Z	1526	DMU	O1-C10	2.02	1.47	1.41
23	O	229	CHD	C21-C20	2.02	1.58	1.53
23	P	1525	CHD	C10-C5	-2.02	1.52	1.55
14	A	515	HEA	CBD-CGD	2.02	1.55	1.50
25	G	269	CDL	CB3-CB4	2.00	1.57	1.50

All (745) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1525	CHD	C6-C5-C10	14.73	128.34	112.66
23	J	60	CHD	C10-C9-C8	13.45	126.83	111.84
23	B	1085	CHD	C6-C5-C10	13.38	126.90	112.66
23	C	271	CHD	C10-C9-C8	13.15	126.50	111.84
23	P	1525	CHD	C1-C10-C5	12.99	126.39	107.75
23	P	1271	CHD	C10-C9-C8	12.43	125.70	111.84
23	W	1059	CHD	C10-C9-C8	12.41	125.67	111.84
23	O	229	CHD	C14-C13-C12	12.11	118.48	107.42
23	O	229	CHD	C1-C10-C5	12.02	125.00	107.75
23	O	229	CHD	C6-C5-C10	11.99	125.42	112.66
23	P	1525	CHD	C4-C3-C2	11.84	125.07	110.62
23	B	1085	CHD	C18-C13-C12	-11.73	97.32	109.06
23	O	229	CHD	C18-C13-C12	-11.73	97.32	109.06
23	B	1085	CHD	C1-C10-C5	11.09	123.67	107.75
23	O	229	CHD	C19-C10-C9	-10.81	96.65	111.18
23	B	1085	CHD	C14-C13-C12	10.68	117.17	107.42
23	C	525	CHD	C10-C9-C8	10.36	123.39	111.84
23	C	525	CHD	C6-C5-C10	10.34	123.66	112.66
23	C	525	CHD	C1-C10-C5	10.31	122.55	107.75
23	J	60	CHD	C18-C13-C12	-9.97	99.07	109.06
23	B	1085	CHD	C10-C9-C8	9.77	122.73	111.84
23	P	1525	CHD	C19-C10-C9	-9.70	98.13	111.18
23	P	1525	CHD	C17-C13-C12	9.44	126.16	117.67
23	O	229	CHD	C10-C9-C8	9.44	122.36	111.84
19	N	1521	TGL	CG2-OG2-CB1	9.21	139.85	117.80
23	J	60	CHD	C17-C13-C12	9.20	125.94	117.67
23	C	271	CHD	C1-C2-C3	9.15	122.61	110.48
23	B	1085	CHD	C5-C4-C3	9.12	126.46	112.71
19	B	521	TGL	CG2-OG2-CB1	9.06	139.47	117.80
23	P	1271	CHD	C6-C7-C8	9.05	121.39	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	229	CHD	C17-C13-C12	8.94	125.71	117.67
23	C	525	CHD	O12-C12-C13	-8.93	95.93	111.02
23	B	1085	CHD	C17-C13-C14	8.89	109.03	100.11
23	C	525	CHD	C14-C13-C12	8.81	115.47	107.42
23	P	1271	CHD	C16-C17-C20	8.81	125.50	112.18
23	J	60	CHD	C6-C7-C8	8.74	121.04	111.50
23	P	1525	CHD	C14-C13-C12	8.73	115.40	107.42
23	J	60	CHD	C6-C5-C10	8.61	121.83	112.66
23	P	1271	CHD	C18-C13-C12	-8.46	100.58	109.06
23	J	60	CHD	C13-C17-C20	8.46	129.73	119.48
23	C	525	CHD	C18-C13-C12	-8.44	100.61	109.06
23	C	271	CHD	C4-C5-C10	8.29	121.48	112.66
23	W	1059	CHD	C6-C7-C8	8.29	120.55	111.50
23	O	229	CHD	C15-C14-C13	8.27	111.56	103.54
23	C	271	CHD	C15-C14-C8	8.23	129.65	118.36
23	P	1271	CHD	C14-C13-C12	8.17	114.88	107.42
23	W	1059	CHD	C4-C3-C2	8.09	120.49	110.62
23	B	1085	CHD	C1-C2-C3	8.08	121.19	110.48
23	C	525	CHD	C4-C3-C2	8.07	120.46	110.62
26	M	526	DMU	O1-C9-C8	8.00	124.12	109.70
23	W	1059	CHD	C6-C5-C4	-7.98	102.11	111.23
26	C	272	DMU	O16-C6-C1	7.96	120.36	108.27
23	P	1525	CHD	C15-C14-C13	7.92	111.22	103.54
19	A	523	TGL	OG2-CB1-CB2	7.91	128.60	111.48
23	W	1059	CHD	C13-C17-C20	7.87	129.01	119.48
23	P	1271	CHD	C17-C13-C12	7.84	124.72	117.67
26	C	272	DMU	O1-C10-C5	7.83	126.45	110.37
23	B	1085	CHD	C17-C13-C12	7.82	124.70	117.67
23	J	60	CHD	C1-C10-C5	7.80	118.95	107.75
23	B	1085	CHD	C16-C17-C20	7.74	123.90	112.18
23	W	1059	CHD	C1-C10-C5	7.74	118.86	107.75
23	C	271	CHD	C6-C7-C8	7.74	119.95	111.50
14	N	515	HEA	C13-C12-C11	-7.67	102.14	114.39
23	P	1525	CHD	C10-C9-C8	7.59	120.30	111.84
23	C	271	CHD	C6-C5-C10	7.50	120.65	112.66
23	O	229	CHD	C4-C3-C2	7.45	119.71	110.62
23	C	271	CHD	C16-C17-C20	7.43	123.43	112.18
23	W	1059	CHD	C1-C10-C9	-7.43	99.81	111.34
23	W	1059	CHD	C16-C17-C13	7.41	110.73	103.54
23	C	525	CHD	C11-C12-C13	7.39	118.78	111.26
23	P	1525	CHD	C18-C13-C14	-7.39	99.63	111.20
23	J	60	CHD	C5-C4-C3	7.35	123.80	112.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	271	CHD	C16-C17-C13	7.35	110.67	103.54
23	J	60	CHD	C6-C5-C4	-7.32	102.86	111.23
19	N	1521	TGL	OG2-CB1-CB2	7.30	127.27	111.48
23	P	1271	CHD	C15-C14-C8	7.17	128.19	118.36
23	P	1525	CHD	C11-C12-C13	7.15	118.54	111.26
26	T	1272	DMU	O1-C10-C5	7.11	124.98	110.37
23	W	1059	CHD	C15-C14-C13	7.10	110.43	103.54
19	B	521	TGL	CG3-OG3-CC1	7.10	143.07	117.12
14	N	516	HEA	CHB-C1B-NB	7.09	132.06	124.42
23	C	525	CHD	C19-C10-C9	-7.07	101.68	111.18
23	C	271	CHD	C18-C13-C12	-7.07	101.98	109.06
23	B	1085	CHD	C6-C5-C4	-7.05	103.17	111.23
23	P	1271	CHD	C18-C13-C17	-7.02	100.20	111.20
23	B	1085	CHD	C19-C10-C9	-7.01	101.75	111.18
23	O	229	CHD	C6-C5-C4	-7.00	103.23	111.23
25	P	1270	CDL	OA6-CA5-C11	6.99	126.60	111.48
23	P	1271	CHD	C4-C5-C10	6.98	120.08	112.66
23	P	1271	CHD	C4-C3-C2	6.96	119.11	110.62
23	P	1271	CHD	C1-C2-C3	6.95	119.69	110.48
23	C	271	CHD	C19-C10-C9	-6.93	101.86	111.18
23	J	60	CHD	C11-C12-C13	6.92	118.30	111.26
23	C	525	CHD	C17-C13-C12	6.91	123.88	117.67
23	W	1059	CHD	C6-C5-C10	6.91	120.01	112.66
23	W	1059	CHD	C14-C13-C12	6.88	113.71	107.42
26	M	526	DMU	O1-C10-C5	6.88	124.51	110.37
23	C	271	CHD	C11-C12-C13	6.85	118.23	111.26
23	P	1271	CHD	C11-C9-C8	6.82	121.00	110.89
23	O	229	CHD	C16-C17-C20	6.82	122.50	112.18
23	O	229	CHD	O12-C12-C13	-6.72	99.67	111.02
26	M	526	DMU	O16-C6-C1	6.72	118.48	108.27
26	T	1272	DMU	O1-C9-C8	6.70	121.78	109.70
23	C	271	CHD	C15-C14-C13	6.70	110.04	103.54
26	Z	1526	DMU	O1-C9-C8	6.68	121.73	109.70
26	Z	1526	DMU	O1-C10-C5	6.65	124.03	110.37
23	O	229	CHD	C18-C13-C17	-6.65	100.79	111.20
20	A	521	PGV	O03-C19-O04	-6.61	107.10	123.63
20	C	268	PGV	O01-C1-C2	6.56	125.68	111.48
23	O	229	CHD	C5-C4-C3	6.54	122.58	112.71
26	Z	1526	DMU	O5-C4-C3	6.52	123.20	109.72
23	P	1271	CHD	C1-C10-C5	6.51	117.09	107.75
26	Z	1526	DMU	O16-C6-C1	6.50	118.15	108.27
23	B	1085	CHD	O12-C12-C13	-6.49	100.05	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	1085	CHD	C18-C13-C14	-6.46	101.08	111.20
26	M	526	DMU	O5-C4-C57	6.43	122.39	106.44
23	J	60	CHD	C4-C3-C2	6.43	118.47	110.62
25	C	270	CDL	OA6-CA5-C11	6.38	125.29	111.48
23	W	1059	CHD	C5-C4-C3	6.37	122.32	112.71
23	W	1059	CHD	C2-C1-C10	6.35	123.45	112.74
25	T	1269	CDL	OB6-CB5-C51	6.35	125.21	111.48
23	J	60	CHD	C14-C13-C12	6.32	113.20	107.42
23	C	271	CHD	C11-C9-C8	6.32	120.25	110.89
26	C	272	DMU	O5-C4-C57	6.31	122.08	106.44
23	P	1271	CHD	C19-C10-C9	-6.28	102.73	111.18
23	B	1085	CHD	C11-C9-C10	6.28	120.07	113.70
23	J	60	CHD	C2-C1-C10	6.27	123.32	112.74
20	P	1268	PGV	O03-C19-C20	6.27	130.94	111.83
23	P	1525	CHD	C6-C7-C8	6.26	118.33	111.50
23	W	1059	CHD	C15-C14-C8	6.25	126.93	118.36
23	W	1059	CHD	C14-C8-C7	6.24	120.13	111.85
20	A	521	PGV	O03-C19-C20	6.20	130.74	111.83
26	Z	1526	DMU	O5-C6-C1	6.16	123.02	110.37
26	T	1272	DMU	O16-C6-C1	6.14	117.60	108.27
23	J	60	CHD	O7-C7-C6	-6.12	94.64	109.86
23	C	271	CHD	C5-C6-C7	6.10	121.65	114.40
23	P	1271	CHD	O7-C7-C6	-6.06	94.80	109.86
23	P	1271	CHD	C5-C6-C7	6.04	121.59	114.40
23	C	525	CHD	C6-C7-C8	6.01	118.06	111.50
23	J	60	CHD	C15-C14-C8	5.98	126.56	118.36
14	A	515	HEA	CAA-CBA-CGA	-5.96	97.85	113.67
23	C	525	CHD	C15-C14-C8	5.92	126.48	118.36
23	C	271	CHD	C5-C4-C3	5.92	121.64	112.71
23	J	60	CHD	C9-C11-C12	5.92	122.03	114.29
23	B	1085	CHD	C14-C8-C9	5.92	118.01	109.75
25	T	1269	CDL	OA6-CA5-C11	5.90	124.24	111.48
26	M	526	DMU	O5-C4-C3	5.88	121.89	109.72
23	P	1271	CHD	C6-C5-C10	5.87	118.90	112.66
23	W	1059	CHD	C11-C9-C8	5.87	119.58	110.89
19	L	522	TGL	CG2-OG2-CB1	5.86	131.81	117.80
26	M	526	DMU	O1-C9-C11	5.81	120.83	106.44
23	B	1085	CHD	C18-C13-C17	-5.80	102.11	111.20
23	P	1271	CHD	C5-C4-C3	5.75	121.38	112.71
23	P	1271	CHD	C2-C1-C10	5.74	122.43	112.74
23	P	1525	CHD	C18-C13-C12	-5.74	103.31	109.06
26	C	272	DMU	O1-C9-C8	5.74	120.03	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1525	CHD	C6-C5-C4	-5.73	104.68	111.23
23	C	525	CHD	C17-C13-C14	5.72	105.85	100.11
26	C	272	DMU	O1-C9-C11	5.71	120.60	106.44
23	J	60	CHD	C1-C2-C3	5.70	118.03	110.48
23	P	1271	CHD	C17-C13-C14	5.70	105.83	100.11
23	C	271	CHD	C1-C10-C5	5.69	115.92	107.75
23	C	271	CHD	O7-C7-C6	-5.69	95.71	109.86
19	B	521	TGL	OG3-CG3-CG2	-5.68	92.01	108.40
23	W	1059	CHD	C5-C6-C7	5.68	121.15	114.40
23	B	1085	CHD	C6-C7-C8	5.66	117.68	111.50
20	C	268	PGV	O03-C19-C20	5.66	129.09	111.83
19	B	521	TGL	OG2-CG2-CG3	5.66	128.65	108.34
26	C	272	DMU	C8-C7-C5	5.63	120.72	110.83
23	C	525	CHD	C5-C4-C3	5.63	121.20	112.71
14	A	516	HEA	CHB-C1B-NB	5.60	130.45	124.42
26	T	1272	DMU	O5-C4-C3	5.59	121.28	109.72
14	A	516	HEA	CHA-C4D-ND	5.54	130.39	124.42
23	P	1525	CHD	C11-C9-C10	5.53	119.31	113.70
14	N	516	HEA	CHB-C1B-C2B	-5.50	116.34	125.03
28	S	1265	PEK	O03-C21-C22	5.49	128.59	111.83
20	P	1268	PGV	O01-C1-C2	5.45	123.28	111.48
19	B	521	TGL	OG1-CA1-CA2	5.43	128.39	111.83
23	J	60	CHD	C16-C17-C20	5.42	120.38	112.18
25	G	269	CDL	OB6-CB5-C51	5.42	123.20	111.48
23	P	1525	CHD	C9-C8-C7	5.38	118.63	111.86
26	T	1272	DMU	C8-C7-C5	5.35	120.23	110.83
23	W	1059	CHD	C11-C12-C13	5.34	116.70	111.26
26	C	272	DMU	O5-C6-C1	5.33	121.32	110.37
19	N	1522	TGL	CG2-OG2-CB1	5.33	130.55	117.80
26	M	526	DMU	O5-C6-C1	5.32	121.31	110.37
23	W	1059	CHD	C17-C13-C12	5.32	122.46	117.67
23	P	1525	CHD	C11-C9-C8	5.31	118.76	110.89
23	P	1525	CHD	O12-C12-C13	-5.30	102.06	111.02
14	A	515	HEA	C13-C12-C11	-5.28	105.96	114.39
23	C	271	CHD	C2-C1-C10	5.27	121.63	112.74
23	C	271	CHD	C14-C13-C12	5.25	112.21	107.42
23	O	229	CHD	C1-C2-C3	5.25	117.43	110.48
23	W	1059	CHD	O12-C12-C11	-5.24	98.46	109.12
23	J	60	CHD	C5-C6-C7	5.18	120.56	114.40
28	G	265	PEK	O03-C21-C22	5.18	127.63	111.83
23	J	60	CHD	C15-C14-C13	5.17	108.55	103.54
23	J	60	CHD	C14-C8-C7	5.16	118.70	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	272	DMU	C2-C3-C4	5.16	122.37	110.93
23	W	1059	CHD	C9-C11-C12	5.15	121.04	114.29
28	G	264	PEK	O03-C01-C02	-5.15	93.56	108.40
23	C	525	CHD	C11-C9-C8	5.14	118.50	110.89
26	M	526	DMU	C8-C7-C5	5.12	119.83	110.83
19	N	1521	TGL	CG3-OG3-CC1	5.11	135.78	117.12
23	C	525	CHD	C2-C1-C10	5.11	121.36	112.74
23	B	1085	CHD	C15-C14-C13	5.08	108.47	103.54
14	A	515	HEA	CHA-C4D-C3D	-5.05	117.41	124.77
28	G	1263	PEK	O01-C1-C2	5.04	122.39	111.48
26	Z	1526	DMU	O1-C9-C11	5.04	118.93	106.44
19	N	1521	TGL	OG1-CA1-CA2	5.04	127.19	111.83
26	M	526	DMU	C2-C3-C4	5.03	122.08	110.93
23	W	1059	CHD	C1-C2-C3	5.03	117.14	110.48
23	P	1271	CHD	C14-C8-C7	5.01	118.50	111.85
20	N	1266	PGV	O03-C19-O04	-4.98	111.17	123.63
23	P	1271	CHD	C16-C17-C13	4.97	108.36	103.54
14	N	516	HEA	C12-C11-C3B	4.97	119.89	112.12
19	L	522	TGL	OG2-CB1-CB2	4.95	122.19	111.48
23	P	1271	CHD	C21-C20-C17	4.93	120.29	112.88
19	L	522	TGL	OG3-CC1-OC1	-4.93	111.30	123.63
23	C	525	CHD	C6-C5-C4	-4.93	105.60	111.23
14	A	516	HEA	CMD-C2D-C1D	4.92	132.72	125.03
23	J	60	CHD	C1-C10-C9	-4.90	103.74	111.34
23	B	1085	CHD	C9-C11-C12	4.89	120.69	114.29
23	O	229	CHD	C11-C9-C8	4.88	118.11	110.89
23	O	229	CHD	C14-C8-C9	4.88	116.56	109.75
23	P	1525	CHD	C14-C8-C9	4.87	116.55	109.75
26	M	526	DMU	O7-C10-C5	-4.86	96.13	108.09
28	G	1263	PEK	O03-C01-C02	4.84	122.36	108.40
26	Z	1526	DMU	C8-C7-C5	4.82	119.30	110.83
26	C	272	DMU	C7-C8-C9	4.81	118.95	110.23
23	C	271	CHD	C17-C13-C12	4.80	121.99	117.67
19	B	521	TGL	OG1-CA1-OA1	-4.79	111.65	123.63
23	P	1271	CHD	C11-C12-C13	4.76	116.11	111.26
26	Z	1526	DMU	O5-C4-C57	4.76	118.23	106.44
23	C	525	CHD	C18-C13-C17	-4.75	103.75	111.20
28	G	1263	PEK	O03-C21-C22	4.71	126.21	111.83
28	T	1264	PEK	O03-C01-C02	-4.71	94.83	108.40
19	N	1523	TGL	OG2-CB1-CB2	4.71	121.66	111.48
23	O	229	CHD	C9-C8-C7	4.69	117.77	111.86
23	W	1059	CHD	C4-C5-C10	4.68	117.64	112.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C9-C10-C5	4.65	114.97	108.51
23	C	271	CHD	C4-C3-C2	4.63	116.26	110.62
20	N	1266	PGV	O03-C19-C20	4.62	125.92	111.83
23	W	1059	CHD	O7-C7-C6	-4.62	98.37	109.86
23	W	1059	CHD	C22-C20-C17	4.60	119.87	110.33
23	J	60	CHD	C16-C17-C13	4.60	108.00	103.54
26	Z	1526	DMU	C7-C8-C9	4.59	118.56	110.23
14	N	516	HEA	C1D-C2D-C3D	-4.59	102.15	106.98
23	C	525	CHD	C15-C14-C13	4.58	107.98	103.54
14	A	516	HEA	C3A-C2A-C1A	-4.58	102.72	107.05
23	W	1059	CHD	C18-C13-C12	-4.57	104.48	109.06
19	N	1522	TGL	OG2-CB1-CB2	4.57	121.37	111.48
23	J	60	CHD	C11-C9-C8	4.55	117.62	110.89
23	P	1525	CHD	C16-C17-C13	4.55	107.95	103.54
14	A	515	HEA	CHA-C4D-ND	4.54	129.31	124.42
23	O	229	CHD	C11-C9-C10	4.53	118.30	113.70
23	C	271	CHD	C6-C5-C4	-4.52	106.06	111.23
26	C	272	DMU	O5-C4-C3	4.52	119.06	109.72
23	W	1059	CHD	C18-C13-C14	-4.51	104.14	111.20
26	T	1272	DMU	O5-C6-C1	4.49	119.60	110.37
28	G	265	PEK	O01-C1-C2	4.49	121.19	111.48
23	W	1059	CHD	C9-C10-C5	4.47	114.73	108.51
23	C	271	CHD	C14-C8-C7	4.46	117.77	111.85
19	B	521	TGL	OG2-CB1-CB2	4.45	121.10	111.48
26	T	1272	DMU	O1-C9-C11	4.44	117.44	106.44
23	P	1271	CHD	C15-C14-C13	4.43	107.83	103.54
23	P	1525	CHD	O7-C7-C6	-4.42	98.86	109.86
23	O	229	CHD	C17-C13-C14	4.41	104.53	100.11
23	J	60	CHD	O12-C12-C11	-4.40	100.17	109.12
23	P	1525	CHD	C15-C14-C8	4.37	124.36	118.36
14	A	515	HEA	O1A-CGA-CBA	-4.36	109.25	123.09
23	J	60	CHD	C18-C13-C14	-4.36	104.37	111.20
14	A	516	HEA	O1A-CGA-CBA	-4.35	109.29	123.09
14	N	515	HEA	C26-C15-C16	4.35	122.78	115.23
23	W	1059	CHD	C16-C17-C20	4.33	118.73	112.18
14	A	516	HEA	CAD-CBD-CGD	-4.32	102.20	113.67
26	T	1272	DMU	C6-C1-C2	4.32	119.09	110.01
23	C	525	CHD	O7-C7-C6	-4.31	99.13	109.86
14	A	515	HEA	O2A-CGA-CBA	4.31	127.62	114.00
26	T	1272	DMU	O7-C10-C5	4.31	118.69	108.09
23	P	1271	CHD	C9-C11-C12	4.31	119.93	114.29
26	T	1272	DMU	O5-C4-C57	4.30	117.09	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C6-C5-C4	-4.30	106.31	111.23
26	M	526	DMU	O16-C18-C19	4.29	123.91	109.37
14	A	515	HEA	C16-C15-C14	4.27	130.75	121.17
19	N	1522	TGL	OG3-CC1-OC1	-4.26	112.97	123.63
14	N	516	HEA	C1C-CHC-C4B	-4.26	116.23	126.25
23	O	229	CHD	C5-C6-C7	4.25	119.45	114.40
19	N	1521	TGL	OG2-CG2-CG3	4.25	123.58	108.34
23	C	525	CHD	C13-C17-C20	4.24	124.62	119.48
23	J	60	CHD	C17-C13-C14	4.23	104.36	100.11
14	A	516	HEA	CAA-CBA-CGA	-4.22	102.46	113.67
23	O	229	CHD	C1-C10-C9	-4.22	104.78	111.34
14	N	516	HEA	CHC-C4B-NB	4.22	129.59	124.37
26	T	1272	DMU	C7-C8-C9	4.19	117.83	110.23
23	P	1525	CHD	O12-C12-C11	-4.18	100.61	109.12
23	C	525	CHD	C14-C8-C9	4.18	115.58	109.75
23	C	525	CHD	C5-C6-C7	4.15	119.33	114.40
22	R	1229	PSC	O01-C1-C2	4.14	120.44	111.48
20	A	524	PGV	O03-C19-C20	4.14	124.44	111.83
23	J	60	CHD	C4-C5-C10	4.13	117.06	112.66
26	M	526	DMU	O7-C3-C2	4.12	117.71	107.23
23	J	60	CHD	C22-C20-C17	4.10	118.84	110.33
25	G	269	CDL	OA6-CA5-C11	4.09	120.34	111.48
23	C	525	CHD	C18-C13-C14	-4.08	104.82	111.20
19	L	522	TGL	OG3-CC1-CC2	4.07	124.25	111.83
26	M	526	DMU	O5-C6-O16	4.05	119.61	110.04
23	C	525	CHD	C22-C20-C17	-4.02	102.00	110.33
26	T	1272	DMU	C1-C2-C3	4.02	118.80	109.68
23	P	1525	CHD	C18-C13-C17	-4.02	104.91	111.20
14	A	515	HEA	CHB-C1B-NB	-3.98	120.14	124.42
22	B	229	PSC	O01-C1-C2	3.97	120.06	111.48
14	N	516	HEA	C2A-C1A-NA	3.96	114.15	110.32
26	C	272	DMU	C6-O5-C4	3.96	121.46	113.72
19	L	522	TGL	CC3-CC2-CC1	3.96	128.20	113.69
23	B	1085	CHD	C19-C10-C5	-3.94	103.84	110.44
23	C	525	CHD	C1-C2-C3	3.94	115.70	110.48
28	G	264	PEK	O01-C1-O02	-3.94	114.49	123.70
26	T	1272	DMU	C2-C3-C4	3.94	119.66	110.93
26	T	1272	DMU	C6-O5-C4	3.93	121.39	113.72
26	M	526	DMU	C22-C19-C18	-3.91	96.47	113.47
28	T	263	PEK	O03-C21-C22	3.91	123.75	111.83
19	B	521	TGL	OG1-CG1-CG2	3.91	119.66	108.40
23	O	229	CHD	O7-C7-C6	-3.91	100.14	109.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C19-C10-C5	-3.91	103.91	110.44
23	P	1271	CHD	O12-C12-C11	-3.90	101.18	109.12
26	T	1272	DMU	C18-O16-C6	3.90	120.34	113.68
14	N	516	HEA	C3A-C2A-C1A	-3.89	103.36	107.05
26	Z	1526	DMU	C2-C3-C4	3.88	119.53	110.93
20	A	524	PGV	C4-C3-C2	-3.88	98.87	113.13
14	A	515	HEA	C3C-C4C-NC	3.85	113.04	109.80
22	R	1229	PSC	O03-C19-C20	3.85	123.57	111.83
23	C	271	CHD	C9-C11-C12	3.85	119.33	114.29
28	S	1265	PEK	O01-C1-C2	3.84	119.79	111.48
19	N	1522	TGL	OG3-CC1-CC2	3.83	123.53	111.83
14	A	515	HEA	C13-C14-C15	-3.83	118.85	127.62
19	B	521	TGL	OG2-CG2-CG1	3.83	122.08	108.34
14	N	515	HEA	C1C-CHC-C4B	-3.82	117.26	126.25
19	A	523	TGL	OG3-CC1-CC2	3.80	123.42	111.83
26	C	272	DMU	C6-C1-C2	3.79	117.99	110.01
23	C	271	CHD	C18-C13-C17	-3.78	105.28	111.20
19	B	521	TGL	OG3-CC1-CC2	3.77	123.34	111.83
23	O	229	CHD	C9-C11-C12	3.77	119.22	114.29
19	B	521	TGL	CG3-CG2-CG1	-3.76	103.03	111.78
28	T	263	PEK	O03-C01-C02	3.75	119.21	108.40
14	A	516	HEA	CHC-C4B-NB	3.74	129.00	124.37
26	M	526	DMU	C6-C1-C2	3.73	117.86	110.01
25	T	1269	CDL	OA8-CA7-C31	3.73	123.20	111.83
23	P	1525	CHD	C5-C4-C3	3.72	118.31	112.71
26	Z	1526	DMU	O5-C6-O16	3.71	118.80	110.04
25	C	270	CDL	OA8-CA7-C31	3.70	123.11	111.83
23	J	60	CHD	C13-C14-C8	3.69	119.40	114.72
25	P	1270	CDL	OB8-CB7-C71	3.69	123.09	111.83
23	B	1085	CHD	C23-C22-C20	-3.68	107.59	114.46
14	A	515	HEA	C1A-CHA-C4D	-3.67	118.21	126.02
23	O	229	CHD	C22-C20-C17	-3.67	102.72	110.33
26	Z	1526	DMU	C6-C1-C2	3.67	117.74	110.01
23	P	1525	CHD	C17-C13-C14	3.67	103.79	100.11
14	A	515	HEA	C1B-C2B-C3B	-3.66	102.56	106.80
23	O	229	CHD	C16-C17-C13	3.65	107.08	103.54
23	C	271	CHD	O12-C12-C13	-3.62	104.91	111.02
14	A	515	HEA	O11-C11-C3B	-3.62	104.62	111.26
14	N	516	HEA	OMA-CMA-C3A	-3.62	117.45	125.62
23	B	1085	CHD	C9-C8-C7	3.61	116.40	111.86
23	P	1525	CHD	C13-C17-C20	3.61	123.85	119.48
25	C	270	CDL	C52-C51-CB5	-3.60	100.49	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	516	HEA	C20-C19-C18	-3.60	113.08	121.17
23	C	525	CHD	C23-C22-C20	-3.59	107.75	114.46
23	P	1525	CHD	C16-C17-C20	3.59	117.61	112.18
14	A	515	HEA	CHD-C1D-ND	3.58	128.80	124.37
23	C	525	CHD	O3-C3-C4	3.57	116.95	109.84
23	B	1085	CHD	C1-C10-C9	-3.57	105.80	111.34
14	N	516	HEA	CHA-C4D-ND	3.57	128.26	124.42
20	C	267	PGV	C22-C21-C20	-3.56	100.06	113.13
26	M	526	DMU	C7-C8-C9	3.54	116.66	110.23
23	B	1085	CHD	C11-C12-C13	3.54	114.86	111.26
23	P	1525	CHD	C1-C10-C9	-3.52	105.88	111.34
14	A	516	HEA	O2A-CGA-CBA	3.51	125.10	114.00
20	N	1524	PGV	C02-O01-C1	3.49	126.14	117.80
26	C	272	DMU	C1-C2-C3	3.48	117.59	109.68
25	C	270	CDL	OB8-CB7-OB9	-3.48	114.92	123.63
23	C	525	CHD	C21-C20-C22	-3.47	104.97	110.34
28	T	1264	PEK	O01-C1-O02	-3.47	115.60	123.70
19	B	521	TGL	OG3-CC1-OC1	-3.46	114.97	123.63
26	M	526	DMU	C6-O5-C4	3.45	120.45	113.72
26	M	526	DMU	C10-C5-C7	3.44	117.25	110.01
23	B	1085	CHD	C11-C9-C8	3.43	115.97	110.89
23	C	271	CHD	C17-C13-C14	3.42	103.54	100.11
23	C	525	CHD	C1-C10-C9	-3.42	106.03	111.34
19	N	1521	TGL	OG1-CA1-OA1	-3.42	115.08	123.63
23	C	271	CHD	C21-C20-C17	3.41	118.00	112.88
28	G	265	PEK	O03-C21-O04	-3.41	115.11	123.63
23	P	1271	CHD	C23-C22-C20	-3.40	108.10	114.46
19	L	522	TGL	CG3-OG3-CC1	3.39	129.50	117.12
25	C	270	CDL	CB4-OB6-CB5	-3.38	109.72	117.80
26	C	272	DMU	O7-C3-C4	3.37	118.33	109.48
19	N	1523	TGL	OG1-CA1-CA2	3.37	122.12	111.83
26	C	272	DMU	O5-C6-O16	3.37	118.00	110.04
23	C	271	CHD	C19-C10-C1	-3.36	102.96	108.31
25	C	270	CDL	OA8-CA7-OA9	-3.36	115.22	123.63
23	B	1085	CHD	C2-C1-C10	3.35	118.40	112.74
20	P	1267	PGV	O03-C19-O04	-3.33	115.29	123.63
26	Z	1526	DMU	C1-C2-C3	3.32	117.21	109.68
25	C	270	CDL	OB8-CB7-C71	3.31	121.93	111.83
19	L	522	TGL	OG2-CG2-CG3	3.30	120.17	108.34
26	C	272	DMU	O61-C57-C4	3.29	122.55	111.33
25	P	1270	CDL	OA6-CA5-OA7	-3.29	116.02	123.70
19	L	522	TGL	OB1-CB1-CB2	-3.28	110.96	123.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	229	CHD	C11-C12-C13	3.27	114.59	111.26
20	C	268	PGV	O03-C01-C02	3.26	117.78	108.40
23	B	1085	CHD	C15-C16-C17	3.26	111.52	105.14
20	A	524	PGV	C02-O01-C1	3.25	125.58	117.80
19	N	1521	TGL	OG2-CB1-OB1	-3.25	116.10	123.70
26	C	272	DMU	C10-O1-C9	3.24	120.05	113.72
19	N	1523	TGL	OG1-CA1-OA1	-3.24	115.53	123.63
20	P	1268	PGV	O04-C19-C20	-3.23	111.14	123.78
14	N	516	HEA	O1A-CGA-CBA	-3.23	112.85	123.09
20	C	268	PGV	O04-C19-C20	-3.23	111.17	123.78
14	A	515	HEA	C27-C19-C18	-3.22	115.34	123.63
26	T	1272	DMU	C10-O1-C9	3.22	120.02	113.72
20	A	521	PGV	C02-O01-C1	-3.21	110.11	117.80
20	N	1524	PGV	O03-C19-C20	3.21	121.62	111.83
14	N	515	HEA	O2A-CGA-CBA	3.20	124.11	114.00
23	O	229	CHD	C2-C1-C10	3.19	118.13	112.74
19	N	1521	TGL	CG1-OG1-CA1	-3.19	105.44	117.12
19	N	1521	TGL	OG3-CC1-CC2	3.19	121.57	111.83
23	C	525	CHD	C19-C10-C5	-3.19	105.10	110.44
23	B	1085	CHD	C21-C20-C17	-3.19	108.10	112.88
20	C	267	PGV	C27-C26-C25	-3.18	98.29	114.37
28	T	1264	PEK	C32-C31-C30	-3.18	98.29	114.37
19	N	1523	TGL	OG3-CC1-CC2	3.17	121.51	111.83
23	P	1271	CHD	C13-C17-C20	3.17	123.33	119.48
23	B	1085	CHD	O26-C24-C23	3.17	124.02	114.00
19	N	1522	TGL	OB1-CB1-CB2	-3.17	111.40	123.78
25	T	1269	CDL	CB2-C1-CA2	-3.16	103.55	112.65
14	N	516	HEA	O2A-CGA-CBA	3.16	123.97	114.00
23	O	229	CHD	C21-C20-C17	3.14	117.60	112.88
14	A	516	HEA	CHA-C4D-C3D	-3.14	120.19	124.77
26	T	1272	DMU	C11-C9-C8	3.14	120.73	113.02
14	A	516	HEA	C20-C21-C22	3.13	127.51	112.02
28	G	264	PEK	C24-C23-C22	-3.13	101.62	113.13
14	N	515	HEA	C2B-C1B-NB	3.13	113.52	109.90
23	B	1085	CHD	C22-C20-C17	3.13	116.82	110.33
19	B	521	TGL	C15-CC9-CC8	3.13	130.19	114.37
23	W	1059	CHD	C19-C10-C9	-3.13	106.97	111.18
23	C	271	CHD	C23-C22-C20	-3.13	108.62	114.46
26	Z	1526	DMU	C10-C5-C7	3.11	116.56	110.01
28	S	1265	PEK	O03-C21-O04	-3.10	115.87	123.63
23	P	1525	CHD	C1-C2-C3	3.09	114.58	110.48
14	A	515	HEA	C26-C15-C16	-3.09	109.86	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	272	DMU	C18-O16-C6	3.09	118.95	113.68
26	Z	1526	DMU	O16-C18-C19	3.07	119.80	109.37
26	Z	1526	DMU	C10-O1-C9	3.07	119.72	113.72
14	A	516	HEA	C1D-C2D-C3D	-3.07	103.75	106.98
20	N	1266	PGV	O03-C01-C02	3.06	117.22	108.40
19	N	1522	TGL	CC3-CC2-CC1	3.06	124.91	113.69
23	O	229	CHD	C18-C13-C14	-3.06	106.41	111.20
26	C	272	DMU	O7-C3-C2	3.06	115.01	107.23
19	L	522	TGL	CA5-CA4-CA3	-3.05	98.93	114.37
14	N	516	HEA	C20-C21-C22	3.05	127.12	112.02
28	G	1263	PEK	C01-O03-C21	3.05	128.28	117.12
20	A	524	PGV	O03-C01-C02	3.05	117.19	108.40
20	C	268	PGV	O02-C1-C2	-3.05	111.86	123.78
14	A	515	HEA	C12-C11-C3B	3.05	116.89	112.12
25	P	1270	CDL	OA8-CA7-C31	3.05	121.12	111.83
23	C	271	CHD	C9-C10-C5	3.04	112.74	108.51
23	C	525	CHD	C14-C8-C7	3.04	115.88	111.85
26	C	272	DMU	O16-C18-C19	3.03	119.64	109.37
23	C	525	CHD	C9-C8-C7	3.03	115.67	111.86
28	T	263	PEK	O01-C1-C2	3.02	118.03	111.48
20	N	1266	PGV	O01-C1-O02	-3.02	116.64	123.70
23	B	1085	CHD	O7-C7-C8	-3.02	102.60	109.52
28	G	264	PEK	O01-C02-C03	-3.02	97.52	108.34
25	T	1269	CDL	CB6-OB8-CB7	3.01	128.13	117.12
19	L	522	TGL	OG1-CA1-CA2	3.01	121.02	111.83
23	J	60	CHD	C22-C23-C24	2.99	120.48	112.49
23	C	525	CHD	C9-C11-C12	2.98	118.20	114.29
23	C	525	CHD	C16-C17-C13	2.98	106.43	103.54
23	C	271	CHD	O12-C12-C11	-2.98	103.07	109.12
23	J	60	CHD	C14-C8-C9	2.97	113.90	109.75
14	A	515	HEA	C2B-C1B-NB	2.96	113.33	109.90
26	T	1272	DMU	C57-C4-C3	2.93	121.62	113.38
26	M	526	DMU	C1-C2-C3	2.93	116.33	109.68
23	P	1525	CHD	C19-C10-C5	-2.92	105.55	110.44
19	A	523	TGL	OG1-CA1-CA2	2.91	120.72	111.83
14	N	515	HEA	CAA-C2A-C1A	2.91	130.76	124.85
28	G	264	PEK	C27-C26-C25	-2.90	99.70	114.37
20	A	521	PGV	O01-C1-O02	-2.89	116.94	123.70
23	C	271	CHD	C13-C17-C20	2.88	122.98	119.48
28	G	265	PEK	O01-C1-O02	-2.88	116.97	123.70
19	B	521	TGL	CG1-OG1-CA1	-2.88	106.60	117.12
14	N	516	HEA	CAD-C3D-C4D	-2.87	119.69	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	1271	CHD	C1-C10-C9	-2.87	106.88	111.34
14	N	516	HEA	C2D-C1D-ND	2.87	113.14	109.84
25	G	269	CDL	C22-C21-C20	2.86	128.83	114.37
25	P	1270	CDL	CA4-OA6-CA5	2.86	124.64	117.80
14	N	515	HEA	C1D-C2D-C3D	-2.86	103.97	106.98
14	A	516	HEA	C12-C11-C3B	2.86	116.59	112.12
14	N	515	HEA	O1A-CGA-CBA	-2.86	114.03	123.09
28	G	264	PEK	O01-C02-C01	-2.86	98.10	108.34
23	C	525	CHD	O12-C12-C11	-2.85	103.31	109.12
19	N	1523	TGL	CG3-OG3-CC1	2.85	127.53	117.12
20	N	1524	PGV	O01-C1-C2	2.85	117.64	111.48
25	G	269	CDL	C42-C41-C40	2.84	128.73	114.37
25	G	269	CDL	C80-C79-C78	2.84	128.72	114.37
14	N	515	HEA	CHD-C4C-NC	2.84	129.00	123.86
20	P	1268	PGV	C03-C02-C01	-2.83	105.18	111.78
22	R	1229	PSC	C32-C31-C30	-2.83	100.08	114.37
20	C	267	PGV	O03-C19-O04	-2.82	116.56	123.63
19	N	1522	TGL	CA4-CA3-CA2	-2.82	102.76	113.13
14	A	516	HEA	C4A-C3A-C2A	2.82	109.26	106.81
19	N	1522	TGL	C16-C15-CC9	2.82	128.60	114.37
19	A	523	TGL	CG3-OG3-CC1	2.81	127.39	117.12
23	B	1085	CHD	C15-C14-C8	2.80	122.20	118.36
25	G	269	CDL	C83-C82-C81	2.79	128.49	114.37
20	A	524	PGV	C01-O03-C19	2.79	127.31	117.12
22	B	229	PSC	C02-O01-C1	2.79	124.46	117.80
26	T	1272	DMU	O5-C6-O16	2.77	116.60	110.04
20	A	524	PGV	O03-C19-O04	-2.77	116.70	123.63
26	Z	1526	DMU	C6-O5-C4	2.76	119.12	113.72
19	N	1523	TGL	CG3-CG2-CG1	-2.76	105.35	111.78
19	A	523	TGL	OB1-CB1-CB2	-2.76	113.00	123.78
22	B	229	PSC	C32-C31-C30	-2.75	100.44	114.37
14	N	515	HEA	C26-C15-C14	-2.75	116.56	123.63
28	G	264	PEK	C3-C2-C1	-2.75	103.62	113.69
14	A	516	HEA	CHD-C1D-ND	2.75	127.77	124.37
14	A	516	HEA	O2D-CGD-CBD	2.75	122.69	114.00
19	L	522	TGL	CA8-CA7-CA6	-2.75	100.49	114.37
23	P	1271	CHD	O12-C12-C13	-2.74	106.39	111.02
25	T	1269	CDL	C83-C82-C81	2.74	128.23	114.37
25	P	1270	CDL	C58-C57-C56	-2.73	100.57	114.37
19	A	523	TGL	CG3-CG2-CG1	-2.73	105.42	111.78
23	B	1085	CHD	C19-C10-C1	2.72	112.63	108.31
28	S	1265	PEK	C03-C02-C01	-2.71	105.46	111.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	1269	CDL	OA6-CA5-OA7	-2.71	117.37	123.70
19	L	522	TGL	C16-C15-CC9	2.71	128.06	114.37
14	A	516	HEA	C2D-C1D-ND	2.70	112.94	109.84
14	A	516	HEA	CHD-C1D-C2D	-2.70	119.28	126.95
23	O	229	CHD	C6-C7-C8	2.70	114.44	111.50
26	M	526	DMU	O2-C8-C7	-2.70	104.02	110.38
19	N	1521	TGL	OG1-CG1-CG2	2.69	116.15	108.40
19	A	523	TGL	CG1-OG1-CA1	2.69	126.94	117.12
25	C	270	CDL	C42-C41-C40	2.69	127.95	114.37
23	B	1085	CHD	O7-C7-C6	-2.69	103.18	109.86
25	T	1269	CDL	OA6-CA4-CA6	2.68	117.97	108.34
20	P	1268	PGV	C02-O01-C1	2.68	124.21	117.80
14	N	516	HEA	C20-C19-C18	-2.66	115.19	121.17
25	P	1270	CDL	C54-C53-C52	-2.66	100.92	114.37
22	B	229	PSC	O03-C01-C02	2.66	116.06	108.40
25	G	269	CDL	C43-C42-C41	2.66	127.80	114.37
26	T	1272	DMU	O7-C3-C4	2.66	116.45	109.48
14	A	515	HEA	C27-C19-C20	2.65	119.83	115.23
14	N	515	HEA	C3B-C4B-NB	2.65	112.89	109.84
28	G	265	PEK	C7-C6-C5	-2.64	101.25	123.57
28	G	264	PEK	C25-C24-C23	-2.62	101.11	114.37
28	G	264	PEK	O01-C1-C2	2.62	117.15	111.48
20	N	1524	PGV	O03-C01-C02	2.62	115.94	108.40
14	A	515	HEA	CHD-C1D-C2D	-2.61	119.54	126.95
20	N	1524	PGV	O01-C02-C03	2.60	117.67	108.34
23	P	1525	CHD	O3-C3-C4	2.60	115.01	109.84
14	N	516	HEA	CHC-C4B-C3B	-2.59	119.26	125.80
23	P	1525	CHD	C2-C1-C10	2.59	117.11	112.74
23	B	1085	CHD	C4-C3-C2	2.59	113.78	110.62
26	C	272	DMU	C11-C9-C8	2.58	119.36	113.02
20	A	524	PGV	O01-C02-C03	2.58	117.60	108.34
26	T	1272	DMU	O61-C57-C4	2.58	120.12	111.33
26	Z	1526	DMU	C11-C9-C8	2.57	119.33	113.02
25	C	270	CDL	OA6-CA5-OA7	-2.56	117.71	123.70
14	N	515	HEA	CHB-C4A-NA	2.55	127.23	124.45
22	B	229	PSC	C03-C02-C01	-2.55	105.84	111.78
28	T	1264	PEK	C2-C3-C4	2.55	118.91	113.35
19	N	1522	TGL	OG1-CG1-CG2	2.54	115.72	108.40
19	N	1522	TGL	C15-CC9-CC8	2.53	127.16	114.37
14	A	516	HEA	C4B-NB-C1B	2.53	108.20	105.21
23	W	1059	CHD	O3-C3-C2	-2.52	103.58	110.17
19	N	1522	TGL	C26-C25-C24	-2.51	101.66	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	J	60	CHD	C9-C10-C5	2.51	112.00	108.51
25	P	1270	CDL	OB8-CB7-OB9	-2.51	117.34	123.63
14	A	516	HEA	O11-C11-C12	2.51	115.80	109.14
25	G	269	CDL	CB6-OB8-CB7	2.51	126.28	117.12
28	G	1263	PEK	O04-C21-C22	-2.50	114.01	123.78
14	N	516	HEA	C4A-CHB-C1B	-2.49	120.72	126.02
25	T	1269	CDL	C80-C79-C78	2.49	126.95	114.37
14	N	515	HEA	C3C-C2C-C1C	-2.48	104.24	107.17
25	G	269	CDL	C40-C39-C38	2.48	126.90	114.37
23	O	229	CHD	O26-C24-C23	2.48	121.83	114.00
25	G	269	CDL	C19-C18-C17	2.48	126.90	114.37
23	O	229	CHD	C21-C20-C22	2.47	114.17	110.34
19	N	1522	TGL	OG1-CA1-CA2	2.47	119.37	111.83
25	G	269	CDL	C23-C22-C21	2.47	126.86	114.37
19	A	523	TGL	OG1-CA1-OA1	-2.47	117.45	123.63
19	B	521	TGL	OB1-CB1-CB2	-2.46	114.14	123.78
20	A	521	PGV	C4-C3-C2	-2.46	104.08	113.13
23	P	1525	CHD	O26-C24-C23	2.46	121.78	114.00
25	C	270	CDL	C38-C37-C36	-2.46	101.94	114.37
20	P	1267	PGV	C27-C26-C25	-2.46	101.94	114.37
19	N	1523	TGL	C20-CA9-CA8	2.45	126.78	114.37
26	M	526	DMU	O3-C5-C7	2.45	116.16	110.38
23	J	60	CHD	C19-C10-C9	-2.45	107.89	111.18
20	C	268	PGV	C03-C02-C01	-2.44	106.10	111.78
19	N	1521	TGL	OG2-CG2-CG1	2.43	117.07	108.34
20	P	1268	PGV	O02-C1-C2	-2.43	114.28	123.78
26	M	526	DMU	C31-C28-C25	-2.43	102.09	114.37
20	A	521	PGV	O03-C01-C02	2.43	115.39	108.40
14	N	516	HEA	O11-C11-C3B	-2.42	106.82	111.26
28	G	265	PEK	C03-C02-C01	-2.40	106.18	111.78
14	N	515	HEA	C20-C19-C18	2.40	126.56	121.17
19	N	1522	TGL	OG3-CG3-CG2	2.40	115.32	108.40
14	A	516	HEA	C13-C14-C15	-2.40	122.12	127.62
25	C	270	CDL	O1-C1-CB2	2.40	117.99	109.70
25	P	1270	CDL	C56-C55-C54	-2.40	102.24	114.37
23	P	1271	CHD	C22-C23-C24	-2.39	106.12	112.49
14	N	515	HEA	C1B-C2B-C3B	-2.39	104.03	106.80
25	P	1270	CDL	OA8-CA7-OA9	-2.39	117.65	123.63
23	C	271	CHD	C22-C23-C24	-2.39	106.13	112.49
20	N	1524	PGV	C3-C2-C1	-2.38	104.97	113.69
23	W	1059	CHD	O7-C7-C8	-2.38	104.07	109.52
23	O	229	CHD	C15-C14-C8	2.38	121.61	118.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	516	HEA	C4A-CHB-C1B	-2.37	120.99	126.02
14	N	515	HEA	CHB-C1B-C2B	-2.37	121.29	125.03
28	G	265	PEK	C23-C22-C21	-2.36	105.04	113.69
19	A	523	TGL	CB4-CB3-CB2	2.35	121.77	113.13
23	B	1085	CHD	C5-C6-C7	2.35	117.19	114.40
28	G	1263	PEK	O01-C1-O02	-2.35	118.22	123.70
14	N	516	HEA	C27-C19-C18	2.34	129.64	123.63
25	C	270	CDL	C53-C52-C51	-2.33	104.55	113.13
23	C	525	CHD	C11-C9-C10	2.33	116.07	113.70
14	N	515	HEA	CAD-CBD-CGD	-2.33	107.49	113.67
19	L	522	TGL	C15-CC9-CC8	2.33	126.14	114.37
19	N	1522	TGL	OG2-CG2-CG3	2.33	116.69	108.34
14	A	516	HEA	CHB-C1B-C2B	-2.33	121.36	125.03
25	G	269	CDL	OA6-CA4-CA6	2.32	116.68	108.34
14	A	515	HEA	CMD-C2D-C1D	2.32	128.66	125.03
26	T	1272	DMU	C10-C5-C7	2.32	114.90	110.01
28	T	1264	PEK	C30-C29-C28	-2.31	102.67	114.37
25	C	270	CDL	OA4-PA1-OA3	2.31	123.19	112.44
28	T	263	PEK	O04-C21-C22	-2.31	114.75	123.78
19	L	522	TGL	CA4-CA3-CA2	-2.30	104.66	113.13
14	N	516	HEA	C26-C15-C14	-2.30	117.71	123.63
25	T	1269	CDL	OB6-CB5-OB7	-2.30	118.33	123.70
22	B	229	PSC	C29-C28-C27	-2.30	102.74	114.37
14	N	515	HEA	C13-C14-C15	-2.30	122.37	127.62
19	B	521	TGL	C16-C15-CC9	2.29	125.94	114.37
14	N	516	HEA	CMC-C2C-C3C	2.29	131.93	126.55
19	A	523	TGL	OG2-CB1-OB1	-2.29	118.36	123.70
25	P	1270	CDL	CA6-OA8-CA7	2.29	125.48	117.12
20	P	1268	PGV	O03-C19-O04	-2.28	117.91	123.63
14	N	515	HEA	C2A-C1A-NA	-2.28	108.12	110.32
28	T	263	PEK	C01-O03-C21	2.28	125.44	117.12
20	A	521	PGV	C25-C24-C23	-2.27	102.89	114.37
23	W	1059	CHD	C13-C14-C8	2.27	117.59	114.72
23	P	1525	CHD	O7-C7-C8	-2.27	104.33	109.52
14	N	515	HEA	CHC-C4B-C3B	-2.26	120.09	125.80
14	N	515	HEA	CMD-C2D-C3D	2.26	132.27	126.15
19	L	522	TGL	OG1-CG1-CG2	2.26	114.91	108.40
23	W	1059	CHD	O3-C3-C4	-2.25	105.36	109.84
25	G	269	CDL	C82-C81-C80	2.25	125.75	114.37
19	N	1522	TGL	CA8-CA7-CA6	-2.25	102.99	114.37
25	C	270	CDL	C39-C38-C37	2.25	125.74	114.37
25	P	1270	CDL	C42-C41-C40	2.24	125.70	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	1268	PGV	O14-P-O13	2.24	122.87	112.44
14	A	515	HEA	C4A-NA-C1A	2.24	109.47	105.82
25	G	269	CDL	OA6-CA5-OA7	-2.24	118.47	123.70
14	N	515	HEA	CBA-CAA-C2A	2.24	118.72	112.53
23	J	60	CHD	O26-C24-O25	-2.24	117.58	123.33
19	L	522	TGL	CA3-CA2-CA1	-2.23	105.51	113.69
28	G	264	PEK	C29-C28-C27	-2.22	103.15	114.37
28	T	1264	PEK	C24-C23-C22	-2.22	104.97	113.13
28	G	265	PEK	P-O12-C04	2.21	131.79	121.26
20	C	268	PGV	C01-O03-C19	2.21	125.20	117.12
14	A	516	HEA	C3C-C2C-C1C	-2.21	104.57	107.17
14	A	516	HEA	CMC-C2C-C3C	2.21	131.74	126.55
23	P	1525	CHD	C23-C22-C20	-2.20	110.35	114.46
26	Z	1526	DMU	O49-C1-C6	-2.20	104.83	110.08
20	P	1267	PGV	O03-C19-C20	2.20	118.54	111.83
14	N	516	HEA	CAD-C3D-C2D	2.20	131.98	127.87
28	G	265	PEK	C8-C7-C6	-2.20	101.21	112.02
19	A	523	TGL	OG3-CC1-OC1	-2.19	118.14	123.63
25	T	1269	CDL	C82-C81-C80	2.19	125.44	114.37
19	N	1522	TGL	CG3-OG3-CC1	2.19	125.11	117.12
26	Z	1526	DMU	O3-C5-C7	2.18	115.52	110.38
25	G	269	CDL	C79-C78-C77	2.17	125.36	114.37
14	A	516	HEA	C2A-C1A-NA	2.17	112.42	110.32
14	N	515	HEA	C21-C20-C19	-2.16	106.04	113.19
23	J	60	CHD	C18-C13-C17	-2.15	107.84	111.20
25	G	269	CDL	C39-C38-C37	2.14	125.18	114.37
23	P	1525	CHD	C9-C11-C12	2.13	117.08	114.29
28	T	1264	PEK	O01-C02-C01	-2.13	100.71	108.34
14	A	516	HEA	O11-C11-C3B	-2.13	107.36	111.26
19	N	1521	TGL	CC3-CC2-CC1	2.12	121.48	113.69
19	N	1521	TGL	C21-C20-CA9	2.12	125.10	114.37
23	O	229	CHD	C22-C23-C24	2.12	118.15	112.49
23	P	1525	CHD	C4-C5-C10	-2.12	110.40	112.66
14	N	516	HEA	C3C-C2C-C1C	-2.12	104.67	107.17
25	C	270	CDL	C20-C19-C18	2.11	125.06	114.37
14	N	516	HEA	CHA-C1A-C2A	-2.11	121.53	124.86
28	G	265	PEK	O12-C04-C05	2.11	116.89	109.17
28	S	1265	PEK	O04-C21-C22	-2.11	115.54	123.78
23	C	525	CHD	C16-C17-C20	2.10	115.36	112.18
23	P	1271	CHD	O7-C7-C8	-2.10	104.70	109.52
20	C	267	PGV	C8-C9-C10	-2.10	103.76	113.86
25	T	1269	CDL	OB5-PB2-OB3	-2.10	100.62	108.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	1523	TGL	C21-C20-CA9	2.10	124.97	114.37
25	T	1269	CDL	OB8-CB6-CB4	2.10	114.44	108.40
23	C	525	CHD	O26-C24-O25	-2.09	117.95	123.33
19	N	1523	TGL	OG2-CG2-CG3	2.09	115.84	108.34
19	N	1521	TGL	C16-C15-CC9	2.09	124.93	114.37
28	T	1264	PEK	O01-C1-C2	2.09	116.00	111.48
22	B	229	PSC	O03-C19-C20	2.09	118.20	111.83
19	N	1523	TGL	CB3-CB2-CB1	-2.09	106.05	113.69
20	C	267	PGV	O01-C1-C2	2.09	115.99	111.48
23	P	1525	CHD	C22-C23-C24	-2.08	106.93	112.49
23	O	229	CHD	C4-C5-C10	-2.08	110.45	112.66
14	A	515	HEA	C21-C22-C23	2.08	134.57	127.64
19	A	523	TGL	OG2-CG2-CG3	2.08	115.80	108.34
22	R	1229	PSC	C29-C28-C27	-2.07	103.88	114.37
26	Z	1526	DMU	O2-C8-C7	-2.07	105.49	110.38
28	G	265	PEK	C2-C3-C4	-2.07	108.83	113.35
28	G	1263	PEK	O01-C02-C01	2.07	115.76	108.34
14	N	515	HEA	CHC-C4B-NB	2.07	126.92	124.37
14	A	516	HEA	C27-C19-C18	2.06	128.92	123.63
23	O	229	CHD	O7-C7-C8	-2.05	104.82	109.52
28	T	1264	PEK	C28-C27-C26	-2.05	104.00	114.37
28	G	1263	PEK	C02-O01-C1	2.05	122.70	117.80
19	N	1521	TGL	OB1-CB1-CB2	-2.05	115.77	123.78
22	R	1229	PSC	O03-C19-O04	-2.04	118.53	123.63
20	C	267	PGV	O03-C19-C20	2.04	118.04	111.83
19	B	521	TGL	C21-C20-CA9	2.03	124.64	114.37
14	N	516	HEA	CMD-C2D-C1D	2.03	128.20	125.03
14	N	515	HEA	C2D-C1D-ND	2.03	112.17	109.84
20	N	1266	PGV	C15-C14-C13	-2.03	104.12	113.86
28	T	1264	PEK	C01-O03-C21	2.03	124.53	117.12
14	N	515	HEA	CHC-C1C-NC	2.03	127.53	123.86
20	A	524	PGV	C3-C2-C1	-2.02	106.28	113.69
14	N	516	HEA	C12-C13-C14	-2.02	106.86	112.16
22	R	1229	PSC	O01-C1-O02	-2.02	118.99	123.70
25	G	269	CDL	OB5-PB2-OB3	-2.01	100.95	108.94
19	A	523	TGL	C11-C10-CB9	2.01	124.54	114.37
19	B	521	TGL	CA5-CA4-CA3	-2.01	104.20	114.37
19	A	523	TGL	C16-C15-CC9	2.01	124.53	114.37
19	N	1523	TGL	C16-C15-CC9	2.01	124.52	114.37
28	T	1264	PEK	C02-O01-C1	2.01	122.60	117.80
14	N	515	HEA	C1A-CHA-C4D	-2.01	121.75	126.02
14	A	515	HEA	O2D-CGD-CBD	2.01	120.34	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	1269	CDL	C23-C22-C21	2.01	124.50	114.37

All (28) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	1085	CHD	C9
23	C	271	CHD	C9
23	J	60	CHD	C9
23	O	229	CHD	C9
23	P	1271	CHD	C9
23	W	1059	CHD	C9
23	W	1059	CHD	C17
26	C	272	DMU	C5
26	C	272	DMU	C6
26	C	272	DMU	C4
26	C	272	DMU	C9
26	C	272	DMU	C2
26	M	526	DMU	C5
26	M	526	DMU	C6
26	M	526	DMU	C4
26	M	526	DMU	C9
26	M	526	DMU	C2
26	T	1272	DMU	C6
26	T	1272	DMU	C5
26	T	1272	DMU	C10
26	T	1272	DMU	C4
26	T	1272	DMU	C9
26	T	1272	DMU	C2
26	Z	1526	DMU	C5
26	Z	1526	DMU	C6
26	Z	1526	DMU	C4
26	Z	1526	DMU	C9
26	Z	1526	DMU	C2

All (978) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	516	HEA	C2A-C3A-CMA-OMA
14	A	516	HEA	C4A-C3A-CMA-OMA
14	N	515	HEA	C2A-C3A-CMA-OMA
14	N	515	HEA	C4A-C3A-CMA-OMA
14	N	516	HEA	C2A-C3A-CMA-OMA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	523	TGL	CC2-CC1-OG3-CG3
19	A	523	TGL	OC1-CC1-OG3-CG3
19	N	1521	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C03-O11-P-O13
20	A	524	PGV	C04-O12-P-O11
20	A	524	PGV	C04-O12-P-O14
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	C05-C04-O12-P
20	A	524	PGV	C04-C05-C06-O06
20	A	524	PGV	O02-C1-O01-C02
20	C	267	PGV	C04-O12-P-O14
20	C	268	PGV	O01-C02-C03-O11
20	C	268	PGV	C2-C1-O01-C02
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C04-O12-P-O13
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O12-C04-C05-C06
20	N	1524	PGV	O02-C1-O01-C02
20	P	1268	PGV	C03-O11-P-O13
20	P	1268	PGV	C04-O12-P-O13
20	P	1268	PGV	C2-C1-O01-C02
22	B	229	PSC	C04-O12-P-O11
22	B	229	PSC	C04-O12-P-O13
22	B	229	PSC	C04-O12-P-O14
22	R	1229	PSC	O12-C04-C05-N
22	R	1229	PSC	C05-C04-O12-P
23	J	60	CHD	C16-C17-C20-C22
23	W	1059	CHD	C16-C17-C20-C21
25	C	270	CDL	CA2-C1-CB2-OB2
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	OA7-CA5-OA6-CA4
25	C	270	CDL	CB2-OB2-PB2-OB3
25	C	270	CDL	CB2-OB2-PB2-OB4
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB3-OB5-PB2-OB2
25	G	269	CDL	CB3-OB5-PB2-OB3
25	G	269	CDL	CB3-OB5-PB2-OB4
25	G	269	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	CA2-OA2-PA1-OA3
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA2-OA2-PA1-OA5
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	CB2-OB2-PB2-OB4
25	P	1270	CDL	CB2-OB2-PB2-OB5
25	T	1269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB2-OB2-PB2-OB5
25	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	1269	CDL	CB3-OB5-PB2-OB3
26	C	272	DMU	C1-C6-O16-C18
26	C	272	DMU	O5-C6-O16-C18
26	M	526	DMU	O5-C6-O16-C18
26	Z	1526	DMU	O5-C6-O16-C18
28	G	264	PEK	C11-C12-C13-C14
28	G	264	PEK	C12-C13-C14-C15
28	G	265	PEK	C03-O11-P-O12
28	G	265	PEK	C03-O11-P-O13
28	G	265	PEK	C04-O12-P-O11
28	G	265	PEK	C04-O12-P-O13
28	G	265	PEK	C04-O12-P-O14
28	G	1263	PEK	C03-O11-P-O12
28	G	1263	PEK	C03-O11-P-O13
28	G	1263	PEK	C03-O11-P-O14
28	G	1263	PEK	O12-C04-C05-N
28	G	1263	PEK	C11-C10-C9-C8
28	S	1265	PEK	C04-O12-P-O11
28	S	1265	PEK	C04-O12-P-O13
28	S	1265	PEK	C04-O12-P-O14
28	T	263	PEK	C03-O11-P-O12
28	T	263	PEK	C03-O11-P-O14
28	T	263	PEK	O03-C01-C02-O01
28	T	263	PEK	O12-C04-C05-N
28	T	263	PEK	C6-C7-C8-C9
28	T	1264	PEK	C12-C13-C14-C15
20	N	1524	PGV	O04-C19-O03-C01
25	T	1269	CDL	OA9-CA7-OA8-CA6
20	N	1524	PGV	C20-C19-O03-C01
25	T	1269	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	O	229	CHD	C21-C20-C22-C23
19	N	1523	TGL	OC1-CC1-OG3-CG3
20	A	524	PGV	O04-C19-O03-C01
23	W	1059	CHD	C16-C17-C20-C22
19	B	521	TGL	OB1-CB1-OG2-CG2
20	A	524	PGV	C20-C19-O03-C01
22	R	1229	PSC	C20-C19-O03-C01
19	B	521	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
25	C	270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	C11-CA5-OA6-CA4
19	N	1521	TGL	OA1-CA1-OG1-CG1
19	N	1522	TGL	OA1-CA1-OG1-CG1
26	Z	1526	DMU	O5-C4-C57-O61
19	N	1521	TGL	CA2-CA1-OG1-CG1
19	N	1522	TGL	CA2-CA1-OG1-CG1
19	N	1523	TGL	CC2-CC1-OG3-CG3
19	L	522	TGL	CC1-CC2-CC3-CC4
20	N	1524	PGV	C10-C11-C12-C13
20	P	1267	PGV	C10-C11-C12-C13
20	P	1268	PGV	C10-C11-C12-C13
22	B	229	PSC	C11-C10-C9-C8
28	G	265	PEK	C7-C8-C9-C10
28	G	265	PEK	C10-C11-C12-C13
28	T	1264	PEK	C7-C8-C9-C10
28	T	1264	PEK	C10-C11-C12-C13
26	M	526	DMU	O6-C11-C9-O1
19	L	522	TGL	OA1-CA1-OG1-CG1
19	N	1521	TGL	OB1-CB1-OG2-CG2
20	C	268	PGV	O02-C1-O01-C02
20	P	1268	PGV	O02-C1-O01-C02
19	B	521	TGL	C22-C23-C24-C25
20	C	267	PGV	C28-C29-C30-C31
19	N	1521	TGL	C11-C10-CB9-CB8
19	N	1521	TGL	CC5-CC6-CC7-CC8
20	N	1524	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CB2-OB2
19	B	521	TGL	CA2-CA1-OG1-CG1
19	B	521	TGL	CC2-CC1-OG3-CG3
22	B	229	PSC	C20-C19-O03-C01
26	C	272	DMU	O6-C11-C9-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	521	TGL	OC1-CC1-OG3-CG3
22	R	1229	PSC	O04-C19-O03-C01
19	L	522	TGL	CA2-CA1-OG1-CG1
26	T	1272	DMU	O6-C11-C9-O1
25	C	270	CDL	C38-C39-C40-C41
23	W	1059	CHD	C21-C20-C22-C23
19	B	521	TGL	C20-C21-C22-C23
22	R	1229	PSC	C20-C21-C22-C23
19	N	1522	TGL	CC1-CC2-CC3-CC4
23	C	271	CHD	C17-C20-C22-C23
23	W	1059	CHD	C17-C20-C22-C23
20	A	521	PGV	C10-C11-C12-C13
20	C	267	PGV	C10-C11-C12-C13
22	R	1229	PSC	C11-C10-C9-C8
22	R	1229	PSC	C11-C12-C13-C14
28	G	264	PEK	C13-C14-C15-C16
28	G	1263	PEK	C4-C5-C6-C7
28	G	1263	PEK	C10-C11-C12-C13
28	S	1265	PEK	C7-C8-C9-C10
28	S	1265	PEK	C13-C14-C15-C16
28	T	263	PEK	C13-C14-C15-C16
22	B	229	PSC	O04-C19-O03-C01
25	T	1269	CDL	C31-C32-C33-C34
26	M	526	DMU	C3-C4-C57-O61
25	T	1269	CDL	C79-C80-C81-C82
26	Z	1526	DMU	O6-C11-C9-O1
25	T	1269	CDL	C22-C23-C24-C25
25	C	270	CDL	CB2-C1-CA2-OA2
25	G	269	CDL	CA2-C1-CB2-OB2
25	P	1270	CDL	CB2-C1-CA2-OA2
25	T	1269	CDL	C71-CB7-OB8-CB6
19	B	521	TGL	CB6-CB7-CB8-CB9
19	B	521	TGL	C11-C10-CB9-CB8
25	G	269	CDL	C80-C81-C82-C83
20	P	1268	PGV	C2-C3-C4-C5
22	B	229	PSC	C20-C21-C22-C23
25	G	269	CDL	C73-C74-C75-C76
26	C	272	DMU	C28-C31-C34-C37
20	N	1524	PGV	C20-C21-C22-C23
28	T	263	PEK	C29-C30-C31-C32
23	O	229	CHD	C17-C20-C22-C23
19	A	523	TGL	C11-C10-CB9-CB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	C38-C39-C40-C41
26	T	1272	DMU	C1-C6-O16-C18
19	B	521	TGL	OA1-CA1-OG1-CG1
23	J	60	CHD	C16-C17-C20-C21
19	N	1523	TGL	CB1-CB2-CB3-CB4
25	G	269	CDL	CA7-C31-C32-C33
19	N	1521	TGL	CB1-CB2-CB3-CB4
25	T	1269	CDL	CB5-C51-C52-C53
28	G	1263	PEK	C13-C14-C15-C16
28	T	263	PEK	C7-C8-C9-C10
23	J	60	CHD	C13-C17-C20-C21
25	P	1270	CDL	CB7-C71-C72-C73
23	C	271	CHD	C21-C20-C22-C23
25	T	1269	CDL	CB7-C71-C72-C73
19	N	1522	TGL	CC3-CC4-CC5-CC6
19	L	522	TGL	CB1-CB2-CB3-CB4
20	P	1268	PGV	C1-C2-C3-C4
25	C	270	CDL	CB7-C71-C72-C73
25	G	269	CDL	CB7-C71-C72-C73
25	T	1269	CDL	OB9-CB7-OB8-CB6
22	B	229	PSC	C19-C20-C21-C22
22	R	1229	PSC	C1-C2-C3-C4
25	C	270	CDL	CA5-C11-C12-C13
28	G	264	PEK	C1-C2-C3-C4
25	C	270	CDL	C19-C20-C21-C22
20	C	268	PGV	O12-C04-C05-O05
25	G	269	CDL	O1-C1-CB2-OB2
25	P	1270	CDL	O1-C1-CB2-OB2
20	C	267	PGV	C12-C13-C14-C15
20	P	1267	PGV	C12-C13-C14-C15
28	G	264	PEK	C10-C11-C12-C13
28	S	1265	PEK	C4-C5-C6-C7
26	C	272	DMU	O16-C18-C19-C22
22	B	229	PSC	C1-C2-C3-C4
25	T	1269	CDL	C11-CA5-OA6-CA4
19	B	521	TGL	CB1-CB2-CB3-CB4
28	T	263	PEK	C34-C35-C36-C37
26	T	1272	DMU	O5-C4-C57-O61
25	G	269	CDL	OA7-CA5-OA6-CA4
25	T	1269	CDL	OA7-CA5-OA6-CA4
25	P	1270	CDL	CA2-C1-CB2-OB2
19	L	522	TGL	CC3-CC4-CC5-CC6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	271	CHD	C16-C17-C20-C21
26	T	1272	DMU	C5-C10-O7-C3
22	R	1229	PSC	C04-C05-N-C06
22	R	1229	PSC	C04-C05-N-C08
25	P	1270	CDL	CB5-C51-C52-C53
25	G	269	CDL	C11-CA5-OA6-CA4
19	N	1521	TGL	C21-C20-CA9-CA8
20	A	524	PGV	C10-C11-C12-C13
20	C	268	PGV	C10-C11-C12-C13
22	B	229	PSC	C11-C12-C13-C14
25	C	270	CDL	O1-C1-CA2-OA2
25	P	1270	CDL	O1-C1-CA2-OA2
20	C	268	PGV	C20-C19-O03-C01
25	G	269	CDL	C15-C16-C17-C18
26	C	272	DMU	C3-C4-C57-O61
26	C	272	DMU	O5-C4-C57-O61
14	N	516	HEA	C2D-C3D-CAD-CBD
20	N	1524	PGV	C04-C05-C06-O06
19	N	1521	TGL	C16-C15-CC9-CC8
14	N	516	HEA	C4D-C3D-CAD-CBD
25	G	269	CDL	CA5-C11-C12-C13
19	L	522	TGL	C20-C21-C22-C23
28	G	1263	PEK	O03-C01-C02-O01
25	C	270	CDL	C31-CA7-OA8-CA6
25	G	269	CDL	C71-CB7-OB8-CB6
25	P	1270	CDL	C31-CA7-OA8-CA6
22	R	1229	PSC	C04-C05-N-C07
28	T	1264	PEK	C1-C2-C3-C4
23	C	271	CHD	C16-C17-C20-C22
23	W	1059	CHD	C13-C17-C20-C22
22	B	229	PSC	C02-C01-O03-C19
19	L	522	TGL	C16-C17-C18-C19
19	L	522	TGL	C22-C23-C24-C25
20	P	1268	PGV	C24-C25-C26-C27
25	C	270	CDL	C13-C14-C15-C16
25	C	270	CDL	C41-C42-C43-C44
19	A	523	TGL	CB3-CB4-CB5-CB6
19	L	522	TGL	C10-C11-C12-C13
20	A	524	PGV	C14-C15-C16-C17
20	C	268	PGV	C6-C7-C8-C9
22	R	1229	PSC	C26-C27-C28-C29
25	G	269	CDL	C43-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	S	1265	PEK	C27-C28-C29-C30
28	S	1265	PEK	C28-C29-C30-C31
19	L	522	TGL	CB5-CB6-CB7-CB8
19	L	522	TGL	C17-C18-C19-C33
19	N	1522	TGL	C16-C17-C18-C19
19	N	1523	TGL	C21-C20-CA9-CA8
25	P	1270	CDL	C72-C73-C74-C75
25	P	1270	CDL	C74-C75-C76-C77
26	Z	1526	DMU	C25-C28-C31-C34
28	G	1263	PEK	C22-C21-O03-C01
19	N	1522	TGL	CA2-CA3-CA4-CA5
22	B	229	PSC	C4-C5-C6-C7
25	G	269	CDL	C79-C80-C81-C82
25	P	1270	CDL	C19-C20-C21-C22
25	P	1270	CDL	C73-C74-C75-C76
20	A	524	PGV	O05-C05-C06-O06
20	N	1524	PGV	O05-C05-C06-O06
19	N	1523	TGL	CA6-CA7-CA8-CA9
25	C	270	CDL	C11-C12-C13-C14
25	G	269	CDL	CB5-C51-C52-C53
25	P	1270	CDL	CA5-C11-C12-C13
25	C	270	CDL	C22-C23-C24-C25
19	N	1523	TGL	CB2-CB3-CB4-CB5
19	L	522	TGL	CB2-CB1-OG2-CG2
19	L	522	TGL	C19-C33-C34-C35
20	C	268	PGV	C23-C24-C25-C26
19	N	1522	TGL	CB3-CB4-CB5-CB6
19	N	1522	TGL	C12-C13-C14-C29
19	N	1521	TGL	CB6-CB7-CB8-CB9
19	N	1521	TGL	CC6-CC7-CC8-CC9
25	G	269	CDL	C62-C63-C64-C65
25	T	1269	CDL	C34-C35-C36-C37
20	C	268	PGV	O04-C19-O03-C01
19	N	1522	TGL	C10-C11-C12-C13
20	P	1268	PGV	C29-C30-C31-C32
25	C	270	CDL	C16-C17-C18-C19
25	G	269	CDL	C59-C60-C61-C62
20	A	521	PGV	C4-C5-C6-C7
20	P	1267	PGV	C7-C8-C9-C10
25	T	1269	CDL	C33-C34-C35-C36
19	N	1523	TGL	CG2-CG3-OG3-CC1
25	G	269	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	521	TGL	CC5-CC6-CC7-CC8
19	L	522	TGL	C24-C25-C26-C27
19	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1523	TGL	C16-C15-CC9-CC8
23	J	60	CHD	C13-C17-C20-C22
25	C	270	CDL	C42-C43-C44-C45
19	N	1522	TGL	CA9-C20-C21-C22
19	N	1523	TGL	CC5-CC6-CC7-CC8
20	C	267	PGV	C30-C31-C32-C33
20	C	268	PGV	C22-C23-C24-C25
22	R	1229	PSC	C24-C25-C26-C27
28	G	264	PEK	C25-C26-C27-C28
28	T	263	PEK	C24-C25-C26-C27
28	T	1264	PEK	C23-C24-C25-C26
19	B	521	TGL	CA4-CA5-CA6-CA7
19	N	1521	TGL	C17-C18-C19-C33
19	N	1523	TGL	C20-C21-C22-C23
20	A	524	PGV	C21-C22-C23-C24
25	C	270	CDL	C73-C74-C75-C76
25	C	270	CDL	C83-C84-C85-C86
25	T	1269	CDL	C52-C53-C54-C55
19	N	1522	TGL	C21-C22-C23-C24
20	A	524	PGV	C4-C5-C6-C7
25	P	1270	CDL	C11-C12-C13-C14
25	P	1270	CDL	C40-C41-C42-C43
20	P	1268	PGV	C23-C24-C25-C26
19	L	522	TGL	CA5-CA6-CA7-CA8
19	N	1522	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	C23-C24-C25-C26
25	P	1270	CDL	C79-C80-C81-C82
28	G	1263	PEK	O04-C21-O03-C01
19	A	523	TGL	CB9-C10-C11-C12
25	C	270	CDL	C57-C58-C59-C60
28	T	263	PEK	C10-C11-C12-C13
28	T	1264	PEK	C13-C14-C15-C16
20	C	268	PGV	C24-C25-C26-C27
25	G	269	CDL	C52-C53-C54-C55
25	T	1269	CDL	C41-C42-C43-C44
25	T	1269	CDL	C62-C63-C64-C65
25	T	1269	CDL	C80-C81-C82-C83
28	T	1264	PEK	C26-C27-C28-C29
22	R	1229	PSC	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	M	526	DMU	C19-C22-C25-C28
20	A	521	PGV	C5-C6-C7-C8
22	R	1229	PSC	C22-C23-C24-C25
19	L	522	TGL	C21-C22-C23-C24
20	C	268	PGV	C25-C26-C27-C28
20	C	268	PGV	C28-C29-C30-C31
20	N	1266	PGV	C7-C8-C9-C10
20	P	1268	PGV	C22-C23-C24-C25
19	L	522	TGL	OB1-CB1-OG2-CG2
25	T	1269	CDL	C37-C38-C39-C40
19	L	522	TGL	C23-C24-C25-C26
19	N	1522	TGL	C22-C23-C24-C25
20	A	521	PGV	C27-C28-C29-C30
20	N	1266	PGV	C5-C6-C7-C8
25	P	1270	CDL	C54-C55-C56-C57
25	G	269	CDL	C13-C14-C15-C16
28	G	264	PEK	C31-C32-C33-C34
19	N	1521	TGL	CA5-CA6-CA7-CA8
19	A	523	TGL	C15-C16-C17-C18
22	R	1229	PSC	C3-C4-C5-C6
25	G	269	CDL	C31-C32-C33-C34
19	N	1523	TGL	CA2-CA3-CA4-CA5
28	G	264	PEK	C27-C28-C29-C30
25	C	270	CDL	CA7-C31-C32-C33
19	N	1523	TGL	CC4-CC5-CC6-CC7
25	P	1270	CDL	C14-C15-C16-C17
25	P	1270	CDL	C22-C23-C24-C25
25	T	1269	CDL	C20-C21-C22-C23
19	A	523	TGL	CB7-CB8-CB9-C10
19	N	1523	TGL	C24-C25-C26-C27
22	R	1229	PSC	C27-C28-C29-C30
20	P	1268	PGV	C20-C19-O03-C01
23	W	1059	CHD	C13-C17-C20-C21
25	P	1270	CDL	C51-CB5-OB6-CB4
19	B	521	TGL	CA5-CA6-CA7-CA8
19	N	1522	TGL	C16-C15-CC9-CC8
22	B	229	PSC	C24-C25-C26-C27
22	B	229	PSC	C13-C14-C15-C16
28	G	1263	PEK	C15-C16-C17-C18
25	P	1270	CDL	C59-C60-C61-C62
25	P	1270	CDL	OA9-CA7-OA8-CA6
19	A	523	TGL	CB5-CB6-CB7-CB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	523	TGL	C13-C14-C29-C30
19	L	522	TGL	CC6-CC7-CC8-CC9
19	N	1521	TGL	CC4-CC5-CC6-CC7
25	C	270	CDL	C43-C44-C45-C46
28	G	265	PEK	C24-C25-C26-C27
19	A	523	TGL	CB6-CB7-CB8-CB9
25	G	269	CDL	C58-C59-C60-C61
26	T	1272	DMU	C3-C4-C57-O61
19	B	521	TGL	CC4-CC5-CC6-CC7
25	G	269	CDL	C57-C58-C59-C60
28	G	1263	PEK	C33-C34-C35-C36
19	N	1521	TGL	C22-C23-C24-C25
25	C	270	CDL	OA9-CA7-OA8-CA6
25	P	1270	CDL	C13-C14-C15-C16
26	Z	1526	DMU	C28-C31-C34-C37
28	G	1263	PEK	C25-C26-C27-C28
28	G	1263	PEK	C32-C33-C34-C35
26	T	1272	DMU	C18-C19-C22-C25
19	N	1522	TGL	CA1-CA2-CA3-CA4
25	C	270	CDL	C14-C15-C16-C17
23	P	1271	CHD	C21-C20-C22-C23
19	A	523	TGL	C21-C20-CA9-CA8
19	N	1523	TGL	C17-C18-C19-C33
20	N	1266	PGV	C23-C24-C25-C26
20	P	1267	PGV	C13-C14-C15-C16
25	G	269	CDL	C37-C38-C39-C40
25	G	269	CDL	C76-C77-C78-C79
28	G	265	PEK	C2-C1-O01-C02
19	N	1522	TGL	CA3-CA4-CA5-CA6
20	C	268	PGV	C27-C28-C29-C30
20	P	1267	PGV	C14-C15-C16-C17
25	P	1270	CDL	C41-C42-C43-C44
25	C	270	CDL	CB5-C51-C52-C53
25	T	1269	CDL	CA7-C31-C32-C33
20	C	268	PGV	C13-C14-C15-C16
22	B	229	PSC	C26-C27-C28-C29
19	A	523	TGL	OG1-CG1-CG2-OG2
20	P	1268	PGV	C12-C13-C14-C15
25	T	1269	CDL	OB6-CB4-CB6-OB8
28	S	1265	PEK	C15-C16-C17-C18
25	C	270	CDL	C81-C82-C83-C84
20	A	524	PGV	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	C3-C4-C5-C6
25	T	1269	CDL	C56-C57-C58-C59
19	A	523	TGL	C22-C23-C24-C25
28	T	1264	PEK	C3-C4-C5-C6
25	P	1270	CDL	C71-C72-C73-C74
20	A	521	PGV	C7-C8-C9-C10
20	C	267	PGV	C25-C26-C27-C28
20	P	1268	PGV	C14-C15-C16-C17
25	P	1270	CDL	C42-C43-C44-C45
28	S	1265	PEK	C24-C25-C26-C27
25	G	269	CDL	C74-C75-C76-C77
28	G	265	PEK	C21-C22-C23-C24
20	C	268	PGV	O12-C04-C05-C06
25	T	1269	CDL	CB2-C1-CA2-OA2
19	N	1521	TGL	C10-C11-C12-C13
19	N	1523	TGL	CB9-C10-C11-C12
19	N	1523	TGL	C12-C13-C14-C29
19	A	523	TGL	CA6-CA7-CA8-CA9
20	N	1524	PGV	C29-C30-C31-C32
20	N	1266	PGV	C26-C27-C28-C29
20	P	1267	PGV	C25-C26-C27-C28
25	C	270	CDL	C79-C80-C81-C82
25	G	269	CDL	C78-C79-C80-C81
20	A	521	PGV	C24-C25-C26-C27
20	C	267	PGV	C7-C8-C9-C10
26	M	526	DMU	O16-C18-C19-C22
28	G	264	PEK	C24-C25-C26-C27
20	C	268	PGV	C01-C02-C03-O11
25	P	1270	CDL	OB5-CB3-CB4-CB6
28	G	265	PEK	O02-C1-O01-C02
19	L	522	TGL	C12-C13-C14-C29
20	N	1524	PGV	C23-C24-C25-C26
19	N	1522	TGL	CC4-CC5-CC6-CC7
25	P	1270	CDL	C63-C64-C65-C66
19	N	1522	TGL	C24-C25-C26-C27
25	C	270	CDL	C59-C60-C61-C62
28	G	1263	PEK	C2-C1-O01-C02
19	A	523	TGL	CC6-CC7-CC8-CC9
25	P	1270	CDL	C31-C32-C33-C34
20	A	524	PGV	C26-C27-C28-C29
25	G	269	CDL	C41-C42-C43-C44
25	P	1270	CDL	C81-C82-C83-C84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C15-C16-C17-C18
19	N	1522	TGL	OB1-CB1-OG2-CG2
26	Z	1526	DMU	C22-C25-C28-C31
28	S	1265	PEK	C22-C23-C24-C25
19	A	523	TGL	OG1-CG1-CG2-CG3
19	B	521	TGL	OG1-CG1-CG2-CG3
20	A	524	PGV	O03-C01-C02-C03
25	C	270	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CB3-CB4-CB6-OB8
28	G	1263	PEK	O03-C01-C02-C03
22	B	229	PSC	C6-C7-C8-C9
19	N	1521	TGL	C13-C14-C29-C30
25	C	270	CDL	C72-C73-C74-C75
28	G	1263	PEK	C29-C30-C31-C32
25	P	1270	CDL	C52-C53-C54-C55
25	P	1270	CDL	C83-C84-C85-C86
28	T	263	PEK	C32-C33-C34-C35
26	M	526	DMU	C25-C28-C31-C34
25	G	269	CDL	C23-C24-C25-C26
19	N	1521	TGL	CB3-CB4-CB5-CB6
20	P	1267	PGV	C28-C29-C30-C31
20	P	1268	PGV	O04-C19-O03-C01
19	N	1522	TGL	C17-C18-C19-C33
20	N	1524	PGV	C2-C3-C4-C5
25	T	1269	CDL	C61-C62-C63-C64
20	A	524	PGV	C2-C3-C4-C5
25	C	270	CDL	C71-C72-C73-C74
20	A	521	PGV	C19-C20-C21-C22
19	B	521	TGL	CA9-C20-C21-C22
19	N	1521	TGL	C14-C29-C30-C31
20	P	1268	PGV	C30-C31-C32-C33
28	G	265	PEK	C29-C30-C31-C32
20	N	1524	PGV	C03-C02-O01-C1
19	B	521	TGL	C15-C16-C17-C18
22	B	229	PSC	C29-C30-C31-C32
20	A	524	PGV	C11-C10-C9-C8
19	N	1521	TGL	CB4-CB5-CB6-CB7
19	N	1521	TGL	C15-C16-C17-C18
22	B	229	PSC	C27-C28-C29-C30
25	C	270	CDL	C53-C54-C55-C56
25	P	1270	CDL	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	515	HEA	C2A-C3A-CMA-OMA
25	P	1270	CDL	C55-C56-C57-C58
28	T	263	PEK	C16-C17-C18-C19
19	N	1521	TGL	CA1-CA2-CA3-CA4
22	R	1229	PSC	C19-C20-C21-C22
28	G	264	PEK	C4-C5-C6-C7
28	T	1264	PEK	C4-C5-C6-C7
25	P	1270	CDL	C82-C83-C84-C85
28	T	263	PEK	C14-C15-C16-C17
25	P	1270	CDL	OA5-CA3-CA4-OA6
25	G	269	CDL	C40-C41-C42-C43
19	B	521	TGL	C16-C17-C18-C19
25	G	269	CDL	C32-C33-C34-C35
28	G	1263	PEK	C26-C27-C28-C29
19	B	521	TGL	C25-C26-C27-C28
25	T	1269	CDL	C44-C45-C46-C47
26	Z	1526	DMU	C34-C37-C40-C43
19	B	521	TGL	CC7-CC8-CC9-C15
25	P	1270	CDL	C62-C63-C64-C65
26	T	1272	DMU	C31-C34-C37-C40
20	C	268	PGV	C14-C15-C16-C17
19	A	523	TGL	C29-C30-C31-C32
25	G	269	CDL	C24-C25-C26-C27
25	G	269	CDL	C64-C65-C66-C67
26	M	526	DMU	C34-C37-C40-C43
28	G	1263	PEK	C16-C17-C18-C19
25	P	1270	CDL	OA6-CA4-CA6-OA8
19	N	1522	TGL	CC5-CC6-CC7-CC8
25	C	270	CDL	C37-C38-C39-C40
19	N	1523	TGL	C29-C30-C31-C32
20	N	1266	PGV	C31-C32-C33-C34
25	G	269	CDL	C21-C22-C23-C24
25	P	1270	CDL	C76-C77-C78-C79
25	T	1269	CDL	C18-C19-C20-C21
19	N	1522	TGL	CC6-CC7-CC8-CC9
20	P	1268	PGV	C31-C32-C33-C34
19	N	1522	TGL	C25-C26-C27-C28
19	N	1522	TGL	C29-C30-C31-C32
19	N	1523	TGL	C33-C34-C35-C36
25	G	269	CDL	C44-C45-C46-C47
25	P	1270	CDL	C44-C45-C46-C47
28	G	264	PEK	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	522	TGL	C16-C15-CC9-CC8
20	C	268	PGV	C5-C6-C7-C8
25	C	270	CDL	C15-C16-C17-C18
26	T	1272	DMU	C34-C37-C40-C43
19	L	522	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	CB2-CB1-OG2-CG2
19	N	1521	TGL	C21-C22-C23-C24
28	T	1264	PEK	C33-C34-C35-C36
19	L	522	TGL	C33-C34-C35-C36
28	G	264	PEK	C7-C8-C9-C10
28	G	265	PEK	C4-C5-C6-C7
26	C	272	DMU	C18-C19-C22-C25
25	P	1270	CDL	C35-C36-C37-C38
28	S	1265	PEK	C22-C21-O03-C01
25	C	270	CDL	C32-C33-C34-C35
25	P	1270	CDL	OB7-CB5-OB6-CB4
20	A	521	PGV	C6-C7-C8-C9
25	T	1269	CDL	CB4-CB3-OB5-PB2
25	T	1269	CDL	C84-C85-C86-C87
19	N	1523	TGL	C13-C14-C29-C30
20	P	1268	PGV	C15-C16-C17-C18
19	N	1521	TGL	C16-C17-C18-C19
20	P	1268	PGV	C4-C5-C6-C7
25	T	1269	CDL	C16-C17-C18-C19
25	T	1269	CDL	C53-C54-C55-C56
25	T	1269	CDL	C81-C82-C83-C84
28	G	265	PEK	C27-C28-C29-C30
20	N	1524	PGV	C01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-CA6
25	P	1270	CDL	OA5-CA3-CA4-CA6
25	T	1269	CDL	C63-C64-C65-C66
20	C	268	PGV	C31-C32-C33-C34
20	N	1266	PGV	C6-C7-C8-C9
25	P	1270	CDL	C61-C62-C63-C64
20	P	1268	PGV	C9-C10-C11-C12
20	P	1268	PGV	C11-C12-C13-C14
19	N	1521	TGL	CB7-CB8-CB9-C10
25	P	1270	CDL	C18-C19-C20-C21
25	T	1269	CDL	C36-C37-C38-C39
25	T	1269	CDL	C57-C58-C59-C60
28	T	263	PEK	C28-C29-C30-C31
19	L	522	TGL	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	N	1521	TGL	C24-C25-C26-C27
19	A	523	TGL	CA2-CA3-CA4-CA5
28	G	264	PEK	C33-C34-C35-C36
25	C	270	CDL	CB3-CB4-CB6-OB8
25	T	1269	CDL	CA3-CA4-CA6-OA8
23	J	60	CHD	C17-C20-C22-C23
19	N	1521	TGL	C25-C26-C27-C28
28	G	264	PEK	C35-C36-C37-C38
25	G	269	CDL	C36-C37-C38-C39
28	T	263	PEK	C25-C26-C27-C28
19	N	1522	TGL	C19-C33-C34-C35
20	P	1268	PGV	C26-C27-C28-C29
25	G	269	CDL	C19-C20-C21-C22
20	P	1268	PGV	O01-C02-C03-O11
28	G	1263	PEK	O01-C02-C03-O11
28	T	263	PEK	O01-C02-C03-O11
19	L	522	TGL	CC5-CC6-CC7-CC8
25	P	1270	CDL	CA4-CA3-OA5-PA1
20	P	1268	PGV	C13-C14-C15-C16
28	G	1263	PEK	C30-C31-C32-C33
28	S	1265	PEK	C23-C24-C25-C26
19	A	523	TGL	CB2-CB3-CB4-CB5
20	A	521	PGV	C26-C27-C28-C29
20	N	1524	PGV	C14-C15-C16-C17
28	S	1265	PEK	C16-C17-C18-C19
19	A	523	TGL	C16-C15-CC9-CC8
22	B	229	PSC	C9-C10-C11-C12
22	B	229	PSC	C10-C11-C12-C13
22	R	1229	PSC	C9-C10-C11-C12
28	G	265	PEK	C11-C10-C9-C8
28	G	265	PEK	C9-C10-C11-C12
28	G	265	PEK	C12-C13-C14-C15
28	G	1263	PEK	C6-C7-C8-C9
28	G	1263	PEK	C9-C10-C11-C12
28	S	1265	PEK	C5-C6-C7-C8
28	S	1265	PEK	C9-C10-C11-C12
28	S	1265	PEK	C11-C12-C13-C14
28	T	263	PEK	C5-C6-C7-C8
28	T	263	PEK	C9-C10-C11-C12
28	T	1264	PEK	C9-C10-C11-C12
19	A	523	TGL	C10-C11-C12-C13
28	G	264	PEK	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CC4-CC5-CC6-CC7
28	T	1264	PEK	C28-C29-C30-C31
20	A	524	PGV	C22-C23-C24-C25
28	S	1265	PEK	C34-C35-C36-C37
25	T	1269	CDL	C39-C40-C41-C42
25	C	270	CDL	C36-C37-C38-C39
20	A	524	PGV	O03-C19-C20-C21
25	C	270	CDL	C31-C32-C33-C34
25	P	1270	CDL	C43-C44-C45-C46
20	P	1268	PGV	C25-C26-C27-C28
22	R	1229	PSC	C5-C6-C7-C8
28	G	264	PEK	C23-C24-C25-C26
28	T	1264	PEK	C25-C26-C27-C28
19	B	521	TGL	C13-C14-C29-C30
25	P	1270	CDL	C80-C81-C82-C83
22	B	229	PSC	C28-C29-C30-C31
28	T	1264	PEK	C17-C18-C19-C20
20	A	524	PGV	C25-C26-C27-C28
26	T	1272	DMU	C25-C28-C31-C34
19	B	521	TGL	C24-C25-C26-C27
28	T	1264	PEK	C34-C35-C36-C37
20	C	268	PGV	C05-C04-O12-P
25	G	269	CDL	C61-C62-C63-C64
26	M	526	DMU	C22-C25-C28-C31
20	N	1266	PGV	C15-C16-C17-C18
19	N	1522	TGL	C11-C10-CB9-CB8
20	N	1266	PGV	C24-C25-C26-C27
28	S	1265	PEK	O04-C21-O03-C01
19	L	522	TGL	CA7-CA8-CA9-C20
20	A	524	PGV	C03-C02-O01-C1
22	B	229	PSC	C03-C02-O01-C1
20	N	1266	PGV	C19-C20-C21-C22
26	C	272	DMU	C4-C3-O7-C10
20	A	521	PGV	C23-C24-C25-C26
25	C	270	CDL	C21-C22-C23-C24
25	G	269	CDL	O1-C1-CA2-OA2
20	P	1267	PGV	C31-C32-C33-C34
28	G	1263	PEK	C28-C29-C30-C31
22	B	229	PSC	O01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-OA6
25	C	270	CDL	OB5-CB3-CB4-OB6
20	P	1267	PGV	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	G	265	PEK	C16-C17-C18-C19
20	N	1524	PGV	O03-C01-C02-C03
25	P	1270	CDL	CB3-CB4-CB6-OB8
28	T	263	PEK	O03-C01-C02-C03
25	G	269	CDL	C22-C23-C24-C25
25	G	269	CDL	C53-C54-C55-C56
19	N	1523	TGL	CC1-CC2-CC3-CC4
20	N	1266	PGV	C10-C11-C12-C13
25	G	269	CDL	C34-C35-C36-C37
19	B	521	TGL	OG1-CG1-CG2-OG2
19	B	521	TGL	OG2-CG2-CG3-OG3
20	A	524	PGV	O03-C01-C02-O01
20	C	268	PGV	C12-C13-C14-C15
25	C	270	CDL	OA6-CA4-CA6-OA8
25	C	270	CDL	OB6-CB4-CB6-OB8
19	A	523	TGL	C19-C33-C34-C35
25	P	1270	CDL	C56-C57-C58-C59
19	N	1521	TGL	CA3-CA4-CA5-CA6
28	S	1265	PEK	C26-C27-C28-C29
22	B	229	PSC	C04-C05-N-C08
25	C	270	CDL	C34-C35-C36-C37
20	C	267	PGV	C29-C30-C31-C32
25	C	270	CDL	C20-C21-C22-C23
20	N	1524	PGV	C05-C04-O12-P
23	C	271	CHD	C20-C22-C23-C24
22	B	229	PSC	C23-C24-C25-C26
19	L	522	TGL	C11-C10-CB9-CB8
19	N	1523	TGL	CB6-CB7-CB8-CB9
28	G	265	PEK	C26-C27-C28-C29
19	B	521	TGL	CA3-CA4-CA5-CA6
20	P	1268	PGV	C21-C22-C23-C24
28	G	1263	PEK	C24-C25-C26-C27
19	N	1523	TGL	CB3-CB4-CB5-CB6
20	P	1267	PGV	C15-C16-C17-C18
26	C	272	DMU	C31-C34-C37-C40
25	C	270	CDL	C58-C59-C60-C61
22	B	229	PSC	C01-C02-C03-O11
25	T	1269	CDL	OB5-CB3-CB4-CB6
28	T	263	PEK	C01-C02-C03-O11
19	N	1523	TGL	C16-C17-C18-C19
28	G	1263	PEK	O02-C1-O01-C02
20	A	524	PGV	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C43-C44-C45-C46
19	L	522	TGL	CA3-CA4-CA5-CA6
19	N	1522	TGL	C11-C12-C13-C14
25	P	1270	CDL	C24-C25-C26-C27
19	N	1522	TGL	CB6-CB7-CB8-CB9
19	N	1523	TGL	CA5-CA6-CA7-CA8
25	C	270	CDL	C1-CA2-OA2-PA1
25	G	269	CDL	CB4-CB3-OB5-PB2
25	T	1269	CDL	C1-CA2-OA2-PA1
28	T	263	PEK	C02-C03-O11-P
23	P	1271	CHD	C16-C17-C20-C22
22	R	1229	PSC	O01-C02-C03-O11
25	P	1270	CDL	OB5-CB3-CB4-OB6
19	L	522	TGL	C25-C26-C27-C28
25	T	1269	CDL	C73-C74-C75-C76
14	A	515	HEA	C4A-C3A-CMA-OMA
14	N	516	HEA	C4A-C3A-CMA-OMA
26	C	272	DMU	C19-C22-C25-C28
28	T	1264	PEK	C24-C25-C26-C27
26	T	1272	DMU	O16-C18-C19-C22
28	G	264	PEK	C34-C35-C36-C37
20	N	1524	PGV	O03-C01-C02-O01
25	P	1270	CDL	OB6-CB4-CB6-OB8
25	P	1270	CDL	C37-C38-C39-C40
25	T	1269	CDL	C71-C72-C73-C74
19	L	522	TGL	CG1-CG2-CG3-OG3
19	N	1521	TGL	OG1-CG1-CG2-CG3
25	P	1270	CDL	CA3-CA4-CA6-OA8
25	C	270	CDL	C80-C81-C82-C83
20	C	268	PGV	C21-C22-C23-C24
19	N	1523	TGL	C18-C19-C33-C34
20	A	524	PGV	C04-O12-P-O13
20	P	1268	PGV	C03-O11-P-O12
20	P	1268	PGV	C03-O11-P-O14
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB5
25	C	270	CDL	CB3-OB5-PB2-OB3
25	P	1270	CDL	CA3-OA5-PA1-OA3
25	T	1269	CDL	CB3-OB5-PB2-OB4
28	G	265	PEK	C03-O11-P-O14
28	T	263	PEK	C03-O11-P-O13
25	P	1270	CDL	C57-C58-C59-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	521	TGL	CB9-C10-C11-C12
20	P	1268	PGV	C20-C21-C22-C23
19	N	1523	TGL	C22-C23-C24-C25
20	N	1266	PGV	C4-C5-C6-C7
25	G	269	CDL	C55-C56-C57-C58
20	C	267	PGV	C02-C03-O11-P
20	P	1268	PGV	C02-C03-O11-P
25	C	270	CDL	CA4-CA3-OA5-PA1
25	P	1270	CDL	C1-CA2-OA2-PA1
20	P	1267	PGV	C1-C2-C3-C4
19	N	1521	TGL	CA7-CA8-CA9-C20
20	P	1267	PGV	C30-C31-C32-C33
19	N	1523	TGL	CG1-CG2-OG2-CB1
19	N	1522	TGL	CB2-CB3-CB4-CB5
26	T	1272	DMU	C22-C25-C28-C31
20	A	524	PGV	C31-C32-C33-C34
22	R	1229	PSC	C01-C02-C03-O11
28	G	1263	PEK	C01-C02-C03-O11
20	N	1524	PGV	O01-C02-C03-O11
25	T	1269	CDL	OB5-CB3-CB4-OB6
25	C	270	CDL	C60-C61-C62-C63
19	B	521	TGL	CA1-CA2-CA3-CA4
22	B	229	PSC	O01-C1-C2-C3
19	A	523	TGL	CA9-C20-C21-C22
19	L	522	TGL	C13-C14-C29-C30
28	G	264	PEK	C16-C17-C18-C19
20	P	1267	PGV	C02-C03-O11-P
25	T	1269	CDL	OA6-CA4-CA6-OA8
19	A	523	TGL	C17-C18-C19-C33
22	R	1229	PSC	O03-C19-C20-C21
20	N	1524	PGV	C22-C23-C24-C25
25	P	1270	CDL	C33-C34-C35-C36
19	A	523	TGL	C16-C17-C18-C19
20	A	524	PGV	C24-C25-C26-C27
20	N	1524	PGV	C7-C8-C9-C10
25	C	270	CDL	C40-C41-C42-C43
19	A	523	TGL	CA4-CA5-CA6-CA7
19	A	523	TGL	C33-C34-C35-C36
20	A	521	PGV	O03-C19-C20-C21
23	P	1525	CHD	C13-C17-C20-C21
23	P	1271	CHD	C20-C22-C23-C24
20	A	521	PGV	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	C	267	PGV	C11-C10-C9-C8
25	P	1270	CDL	C12-C11-CA5-OA6
20	C	267	PGV	C05-C04-O12-P
22	R	1229	PSC	C31-C32-C33-C34
20	N	1524	PGV	C30-C31-C32-C33
23	P	1525	CHD	C13-C17-C20-C22
28	G	1263	PEK	C14-C15-C16-C17
20	P	1268	PGV	C01-C02-C03-O11
20	P	1268	PGV	C7-C8-C9-C10
25	C	270	CDL	C63-C64-C65-C66
19	N	1523	TGL	CB4-CB5-CB6-CB7
20	A	524	PGV	C11-C12-C13-C14
25	T	1269	CDL	C40-C41-C42-C43
19	N	1523	TGL	OG1-CG1-CG2-OG2
19	L	522	TGL	OG2-CB1-CB2-CB3
28	S	1265	PEK	C32-C33-C34-C35
25	P	1270	CDL	C21-C22-C23-C24
20	N	1524	PGV	C31-C32-C33-C34
23	O	229	CHD	C16-C17-C20-C22
20	P	1268	PGV	C11-C10-C9-C8
14	A	515	HEA	CAD-CBD-CGD-O1D
26	Z	1526	DMU	O6-C11-C9-C8
28	G	264	PEK	C26-C27-C28-C29
19	L	522	TGL	CB6-CB7-CB8-CB9
19	B	521	TGL	C11-C12-C13-C14
19	L	522	TGL	C11-C12-C13-C14
19	N	1523	TGL	OG1-CA1-CA2-CA3
20	N	1266	PGV	O03-C19-C20-C21
19	A	523	TGL	CG3-CG2-OG2-CB1
19	N	1521	TGL	CG1-CG2-OG2-CB1
22	R	1229	PSC	C01-C02-O01-C1
22	R	1229	PSC	C03-C02-O01-C1
28	T	263	PEK	C31-C32-C33-C34
20	C	268	PGV	C11-C10-C9-C8
25	T	1269	CDL	O1-C1-CB2-OB2
28	G	264	PEK	C3-C4-C5-C6
20	P	1267	PGV	C05-C04-O12-P
25	G	269	CDL	CA4-CA3-OA5-PA1
14	A	516	HEA	CAD-CBD-CGD-O1D
25	G	269	CDL	OB5-CB3-CB4-CB6
25	C	270	CDL	C52-C53-C54-C55
19	A	523	TGL	OG2-CG2-CG3-OG3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	G	264	PEK	O03-C01-C02-O01
28	G	1263	PEK	C17-C18-C19-C20
28	G	265	PEK	C5-C6-C7-C8
28	G	265	PEK	C6-C7-C8-C9
28	G	1263	PEK	C12-C13-C14-C15
28	S	1265	PEK	C6-C7-C8-C9
28	S	1265	PEK	C11-C10-C9-C8
28	T	1264	PEK	C11-C10-C9-C8
28	T	1264	PEK	C11-C12-C13-C14
20	C	267	PGV	C24-C25-C26-C27
22	B	229	PSC	C04-C05-N-C07
14	N	516	HEA	CAD-CBD-CGD-O2D
23	P	1271	CHD	C16-C17-C20-C21
19	N	1523	TGL	CC9-C15-C16-C17
22	B	229	PSC	C2-C3-C4-C5
14	N	516	HEA	CAA-CBA-CGA-O1A
28	T	263	PEK	C02-C01-O03-C21
23	C	271	CHD	C22-C23-C24-O26
23	O	229	CHD	C22-C23-C24-O25
19	N	1521	TGL	CC1-CC2-CC3-CC4
14	N	516	HEA	CAD-CBD-CGD-O1D
19	L	522	TGL	CB3-CB4-CB5-CB6
26	Z	1526	DMU	C19-C22-C25-C28
26	Z	1526	DMU	C19-C18-O16-C6
20	A	524	PGV	O04-C19-C20-C21
14	A	516	HEA	CAD-CBD-CGD-O2D
23	O	229	CHD	C22-C23-C24-O26
25	P	1270	CDL	C75-C76-C77-C78
25	C	270	CDL	C12-C13-C14-C15
25	T	1269	CDL	C13-C14-C15-C16
25	C	270	CDL	OB5-CB3-CB4-CB6
19	L	522	TGL	OG2-CG2-CG3-OG3
14	A	515	HEA	CAD-CBD-CGD-O2D
28	S	1265	PEK	C25-C26-C27-C28
28	S	1265	PEK	C29-C30-C31-C32
20	C	267	PGV	C15-C16-C17-C18
14	N	515	HEA	CAD-CBD-CGD-O1D
22	B	229	PSC	C12-C13-C14-C15
20	N	1266	PGV	C14-C15-C16-C17
22	B	229	PSC	C04-C05-N-C06
25	G	269	CDL	C38-C39-C40-C41
23	P	1271	CHD	C22-C23-C24-O26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C75-C76-C77-C78
23	P	1525	CHD	C22-C23-C24-O25
25	G	269	CDL	C33-C34-C35-C36
23	P	1525	CHD	C22-C23-C24-O26
20	A	521	PGV	C9-C10-C11-C12
22	R	1229	PSC	C12-C13-C14-C15
23	C	271	CHD	C22-C23-C24-O25
25	P	1270	CDL	C20-C21-C22-C23
23	P	1271	CHD	C22-C23-C24-O25
19	N	1523	TGL	CB5-CB6-CB7-CB8
19	B	521	TGL	C14-C29-C30-C31
20	N	1524	PGV	O03-C19-C20-C21
25	P	1270	CDL	C39-C40-C41-C42
28	T	1264	PEK	O03-C01-C02-O01
19	N	1521	TGL	OG3-CC1-CC2-CC3
19	N	1521	TGL	CC2-CC3-CC4-CC5
25	G	269	CDL	C52-C51-CB5-OB6
22	B	229	PSC	O02-C1-O01-C02
28	T	263	PEK	C4-C5-C6-C7
19	L	522	TGL	CA4-CA5-CA6-CA7
26	T	1272	DMU	C19-C22-C25-C28
20	A	521	PGV	C11-C12-C13-C14
20	N	1266	PGV	C9-C10-C11-C12
25	P	1270	CDL	C32-C31-CA7-OA8
25	G	269	CDL	C11-C12-C13-C14
19	A	523	TGL	OG1-CA1-CA2-CA3
19	B	521	TGL	OG3-CC1-CC2-CC3
28	G	264	PEK	O01-C1-C2-C3
28	S	1265	PEK	O01-C1-C2-C3
25	G	269	CDL	C71-C72-C73-C74
20	A	524	PGV	C23-C24-C25-C26
25	P	1270	CDL	C60-C61-C62-C63
19	L	522	TGL	CA2-CA3-CA4-CA5
23	B	1085	CHD	C22-C23-C24-O25
25	T	1269	CDL	C11-C12-C13-C14
23	J	60	CHD	C22-C23-C24-O26
20	C	268	PGV	C02-C03-O11-P
25	C	270	CDL	C32-C31-CA7-OA8
28	G	265	PEK	O01-C1-C2-C3
14	N	515	HEA	CAA-CBA-CGA-O1A
20	C	268	PGV	C1-C2-C3-C4
14	A	516	HEA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	515	HEA	CAA-CBA-CGA-O2A
14	N	516	HEA	CAA-CBA-CGA-O2A
23	J	60	CHD	C22-C23-C24-O25
14	N	515	HEA	CAD-CBD-CGD-O2D
20	C	268	PGV	O01-C1-C2-C3
28	G	265	PEK	C33-C34-C35-C36
23	B	1085	CHD	C22-C23-C24-O26
19	B	521	TGL	CB3-CB4-CB5-CB6
19	A	523	TGL	CA3-CA4-CA5-CA6
20	C	268	PGV	C30-C31-C32-C33
19	L	522	TGL	CB2-CB3-CB4-CB5
19	B	521	TGL	CG1-CG2-OG2-CB1
19	A	523	TGL	OG2-CB1-CB2-CB3
19	L	522	TGL	OG1-CA1-CA2-CA3
20	P	1268	PGV	C6-C7-C8-C9
28	T	1264	PEK	C30-C31-C32-C33
25	P	1270	CDL	C17-C18-C19-C20
28	G	1263	PEK	O01-C1-C2-C3
19	A	523	TGL	OA1-CA1-CA2-CA3
14	A	516	HEA	C26-C15-C16-C17
28	T	1264	PEK	O01-C1-C2-C3
19	N	1522	TGL	CC7-CC8-CC9-C15
19	N	1521	TGL	C18-C19-C33-C34
28	S	1265	PEK	O02-C1-C2-C3
25	C	270	CDL	C32-C31-CA7-OA9
25	P	1270	CDL	C32-C31-CA7-OA9
28	G	264	PEK	O02-C1-C2-C3
19	B	521	TGL	CA7-CA8-CA9-C20
19	N	1521	TGL	CA4-CA5-CA6-CA7
19	B	521	TGL	OC1-CC1-CC2-CC3
19	L	522	TGL	C21-C20-CA9-CA8
25	P	1270	CDL	C52-C51-CB5-OB6
23	C	525	CHD	C21-C20-C22-C23
25	G	269	CDL	OB7-CB5-OB6-CB4
14	N	516	HEA	C26-C15-C16-C17
19	B	521	TGL	C21-C20-CA9-CA8
14	A	515	HEA	CAA-CBA-CGA-O2A
25	T	1269	CDL	C54-C55-C56-C57
20	C	268	PGV	O02-C1-C2-C3
14	A	515	HEA	CAA-CBA-CGA-O1A
22	R	1229	PSC	O01-C1-C2-C3
25	C	270	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	229	PSC	C2-C1-O01-C02
19	N	1522	TGL	OG1-CA1-CA2-CA3
25	T	1269	CDL	C59-C60-C61-C62
19	N	1522	TGL	CB1-CB2-CB3-CB4
19	N	1522	TGL	C21-C20-CA9-CA8
25	G	269	CDL	C16-C17-C18-C19
25	T	1269	CDL	C78-C79-C80-C81

There are no ring outliers.

40 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	270	CDL	21	0
14	A	515	HEA	2	0
19	N	1523	TGL	5	0
20	P	1267	PGV	5	0
14	N	515	HEA	5	0
19	A	523	TGL	3	0
20	A	524	PGV	12	0
28	T	1264	PEK	4	0
22	R	1229	PSC	16	0
25	T	1269	CDL	23	0
26	Z	1526	DMU	1	0
23	P	1271	CHD	3	0
22	B	229	PSC	17	0
26	T	1272	DMU	6	0
25	P	1270	CDL	16	0
23	W	1059	CHD	3	0
20	N	1524	PGV	8	0
20	P	1268	PGV	2	0
23	B	1085	CHD	3	0
26	C	272	DMU	2	0
28	G	1263	PEK	10	0
19	N	1522	TGL	7	0
28	G	265	PEK	8	0
28	G	264	PEK	4	0
25	G	269	CDL	24	0
23	C	271	CHD	2	0
28	T	263	PEK	15	0
23	O	229	CHD	1	0
28	S	1265	PEK	6	0
19	L	522	TGL	19	0

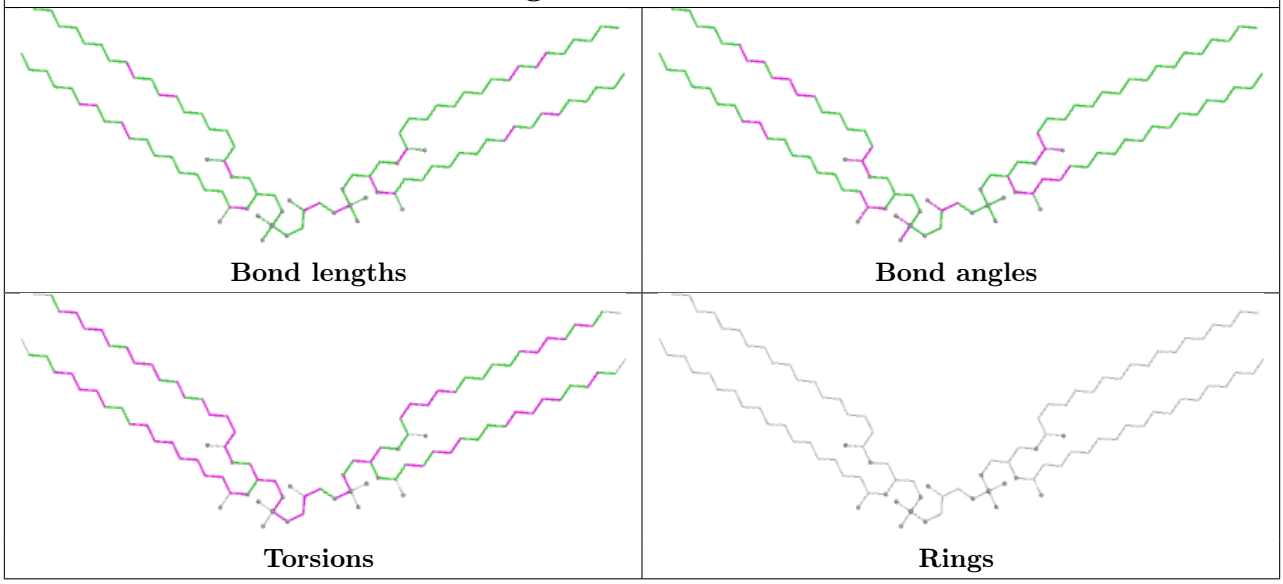
Continued on next page...

Continued from previous page...

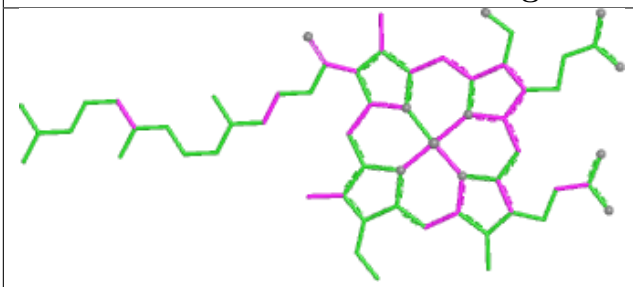
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	60	CHD	2	0
14	A	516	HEA	1	0
20	C	267	PGV	7	0
23	C	525	CHD	1	0
20	N	1266	PGV	1	0
20	A	521	PGV	2	0
19	B	521	TGL	9	0
19	N	1521	TGL	10	0
14	N	516	HEA	2	0
23	P	1525	CHD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

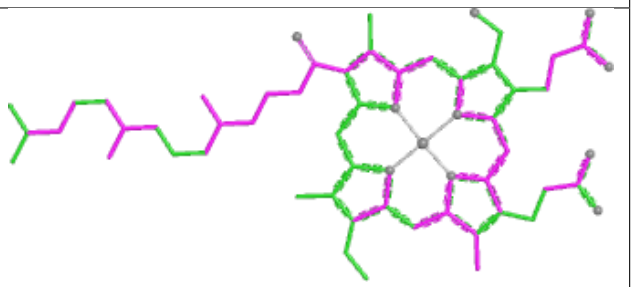
Ligand CDL C 270



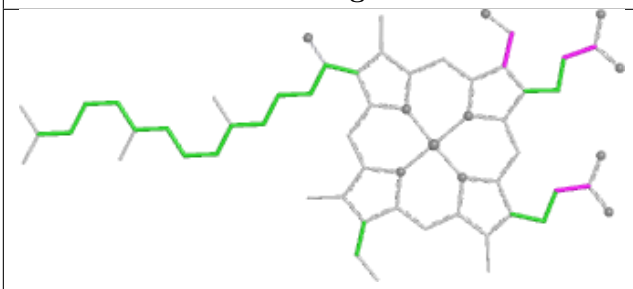
Ligand HEA A 515



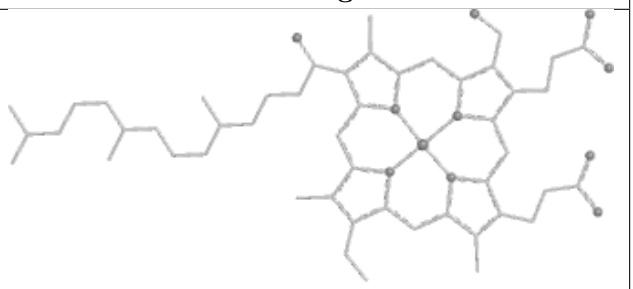
Bond lengths



Bond angles



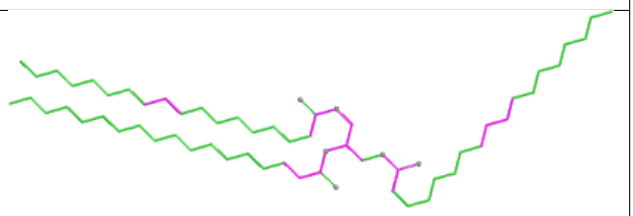
Torsions



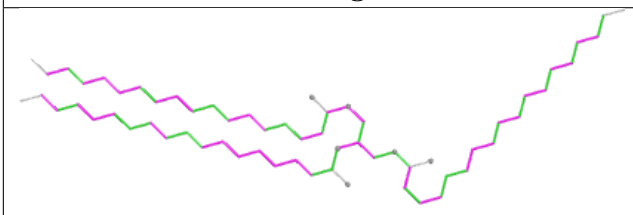
Rings

Ligand TGL N 1523

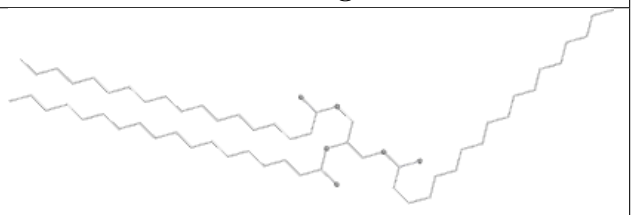
Bond lengths



Bond angles

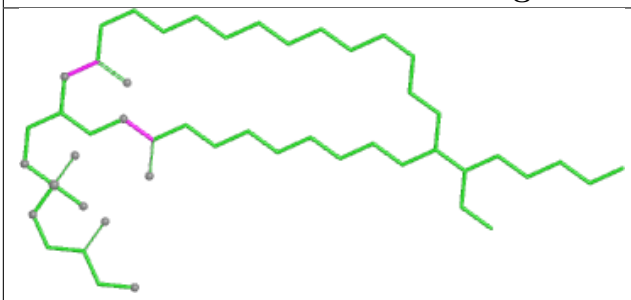


Torsions

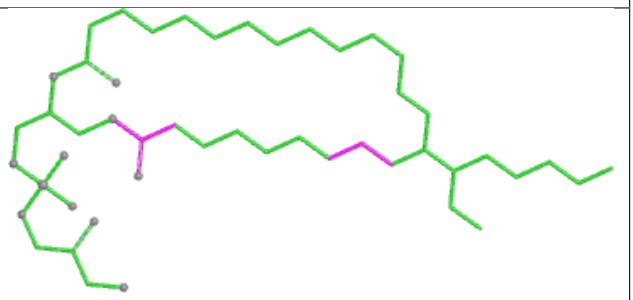


Rings

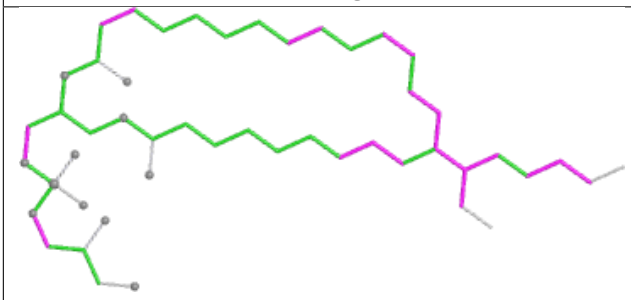
Ligand PGV P 1267



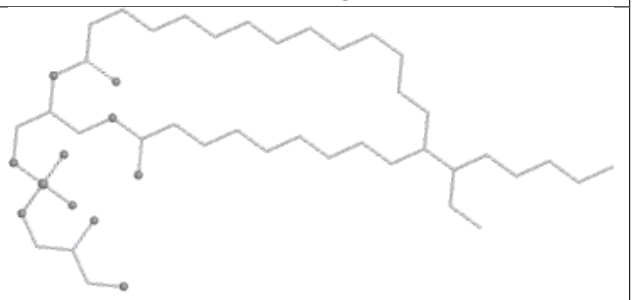
Bond lengths



Bond angles

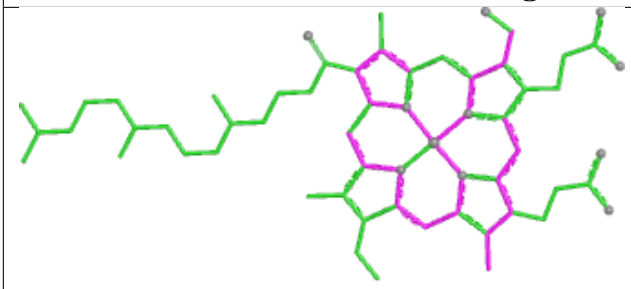


Torsions

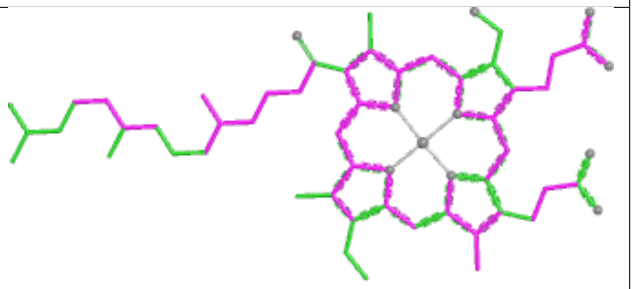


Rings

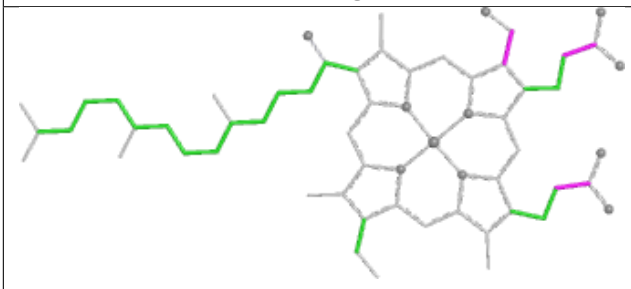
Ligand HEA N 515



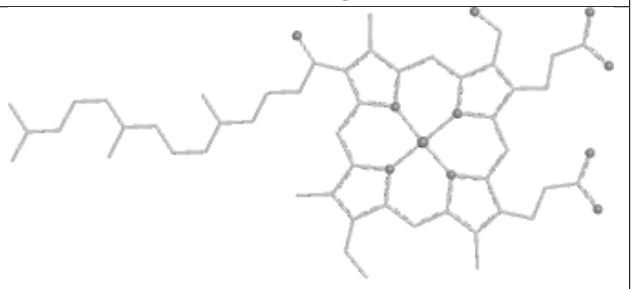
Bond lengths



Bond angles

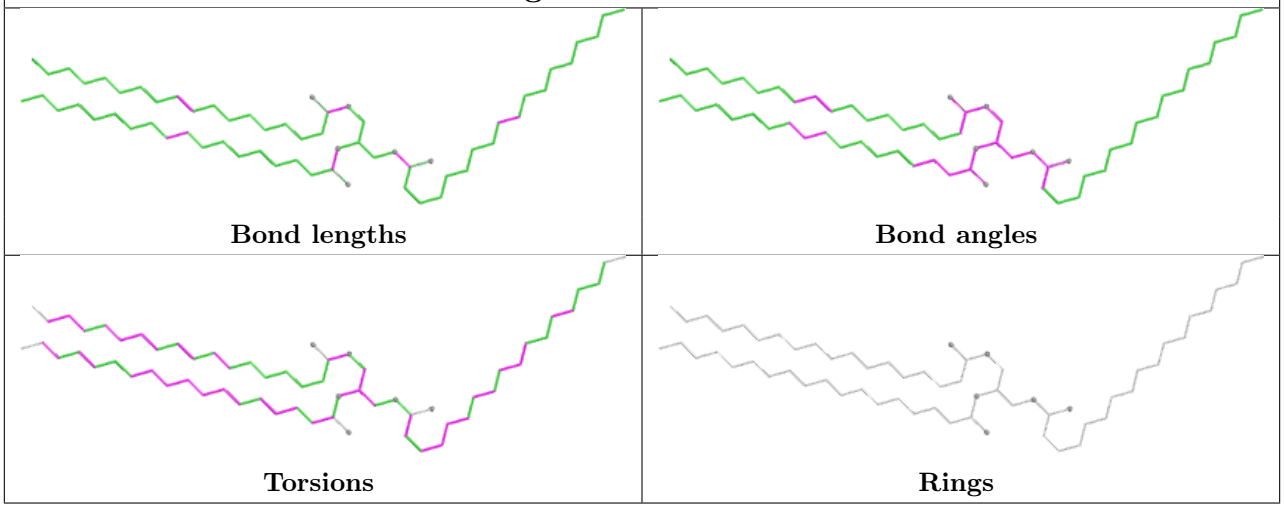


Torsions

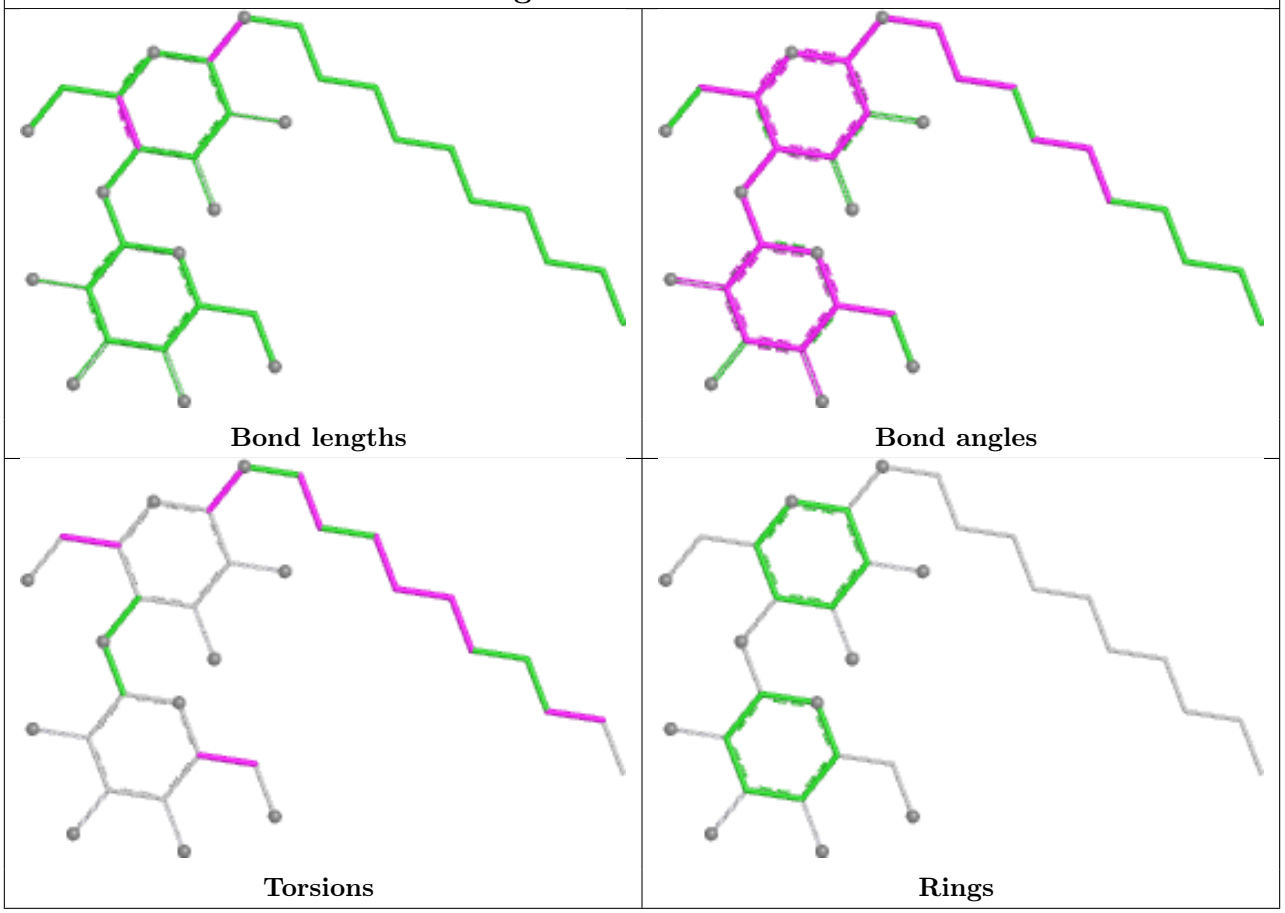


Rings

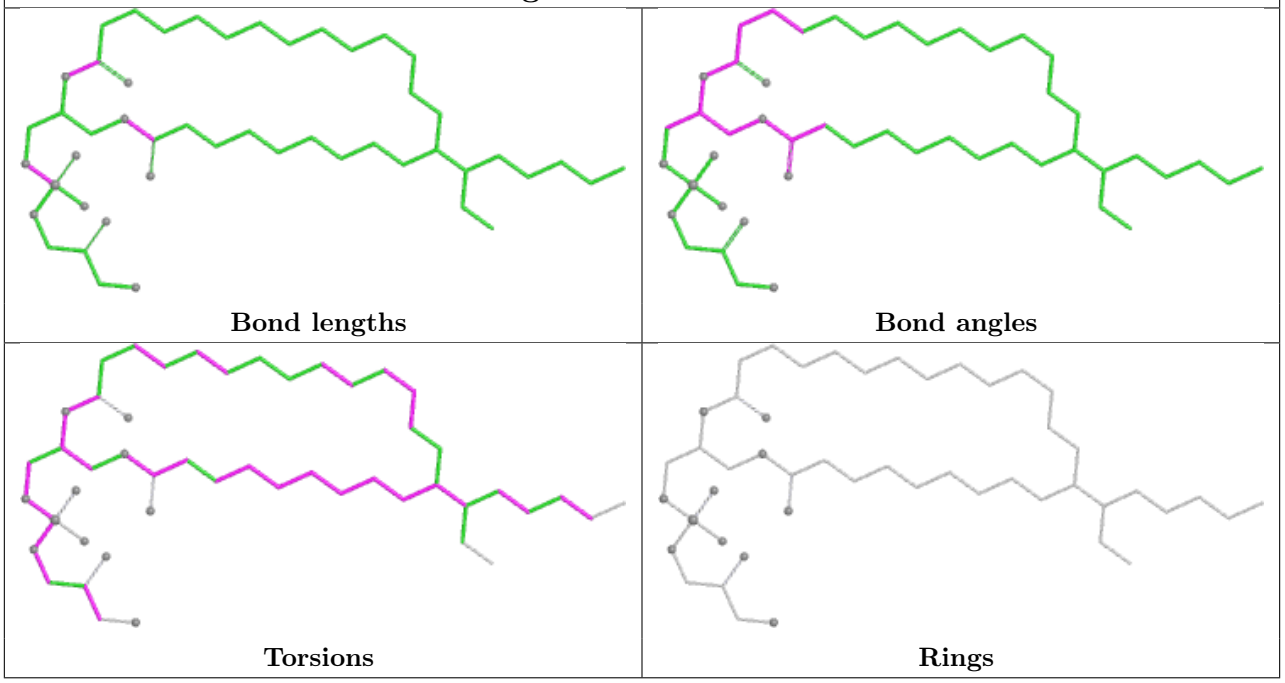
Ligand TGL A 523



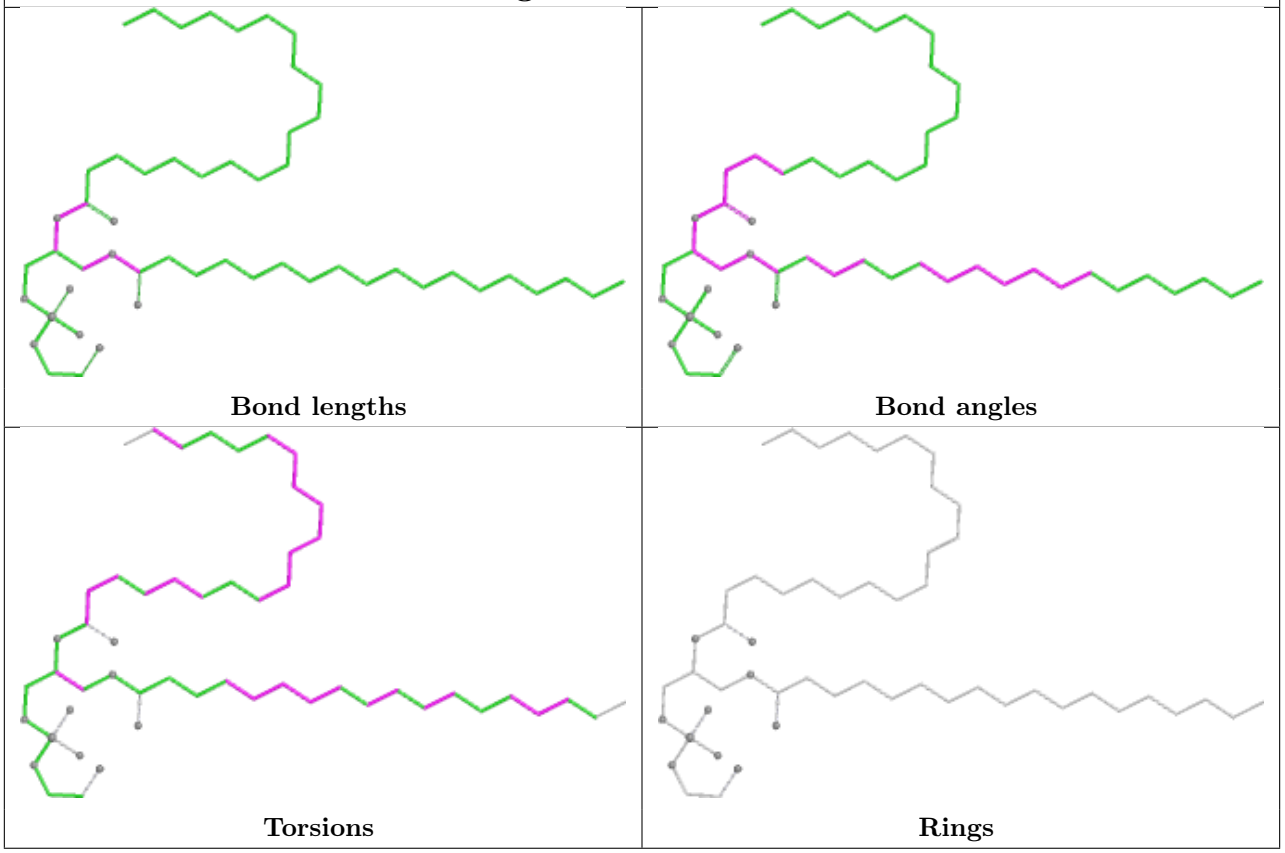
Ligand DMU M 526



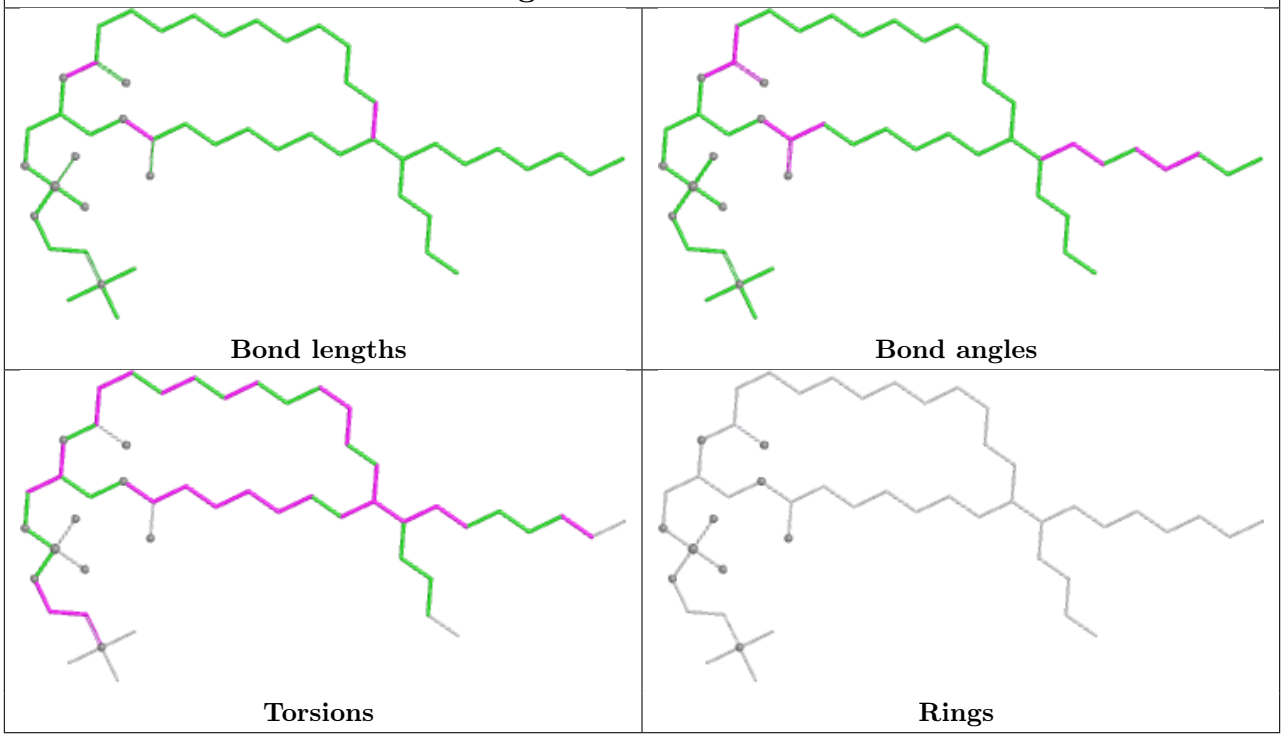
Ligand PGV A 524



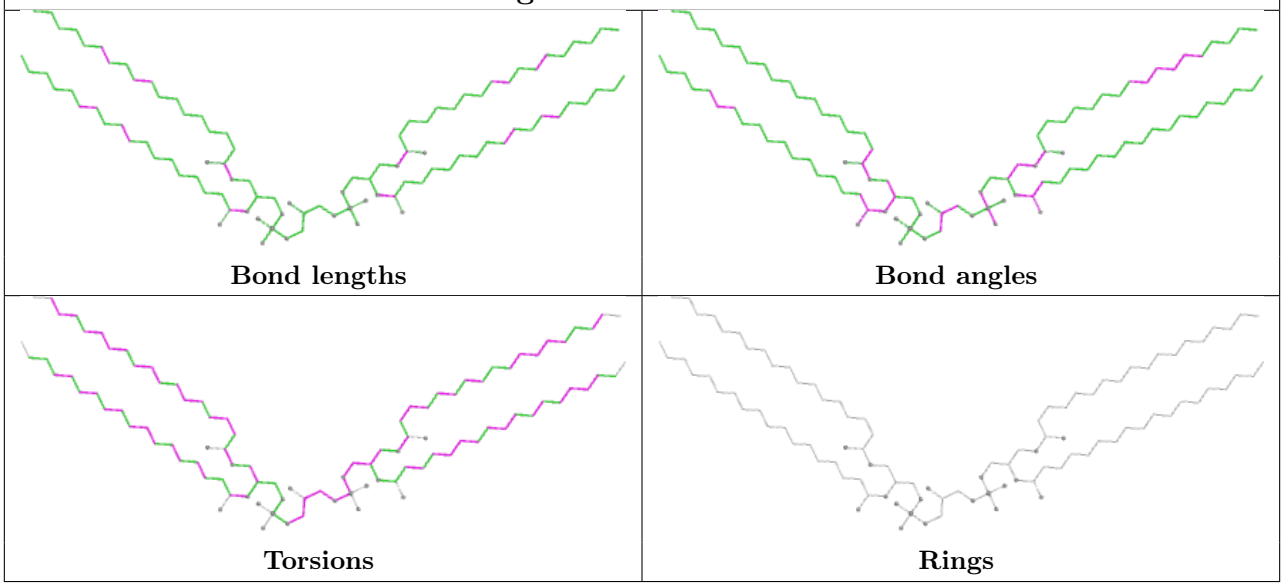
Ligand PEK T 1264



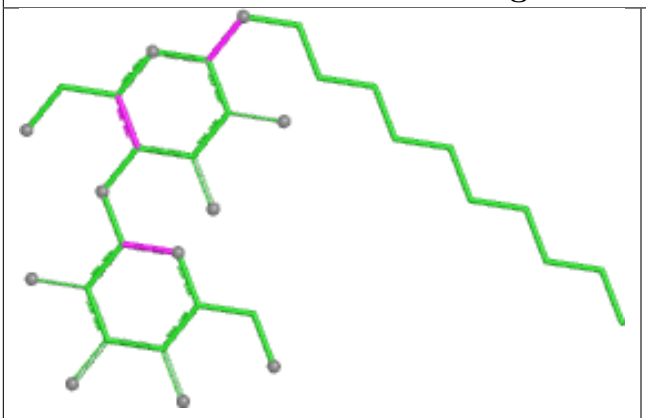
Ligand PSC R 1229



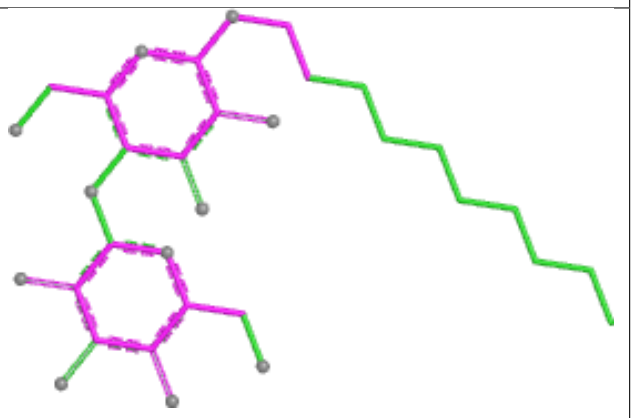
Ligand CDL T 1269



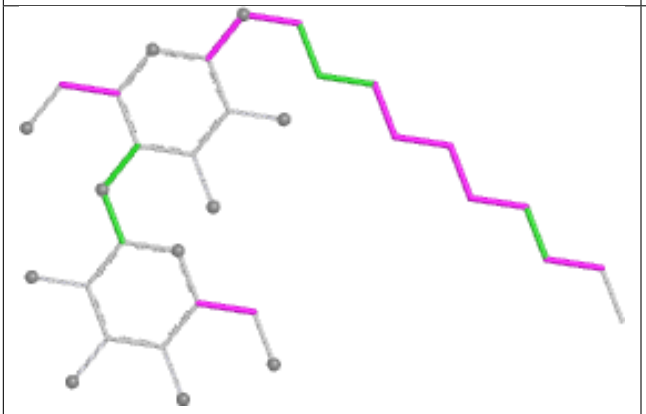
Ligand DMU Z 1526



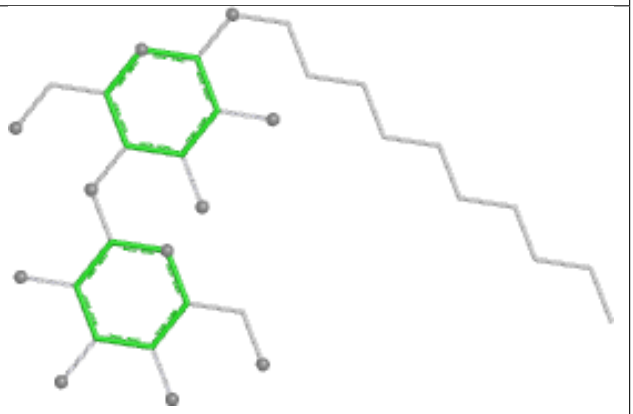
Bond lengths



Bond angles

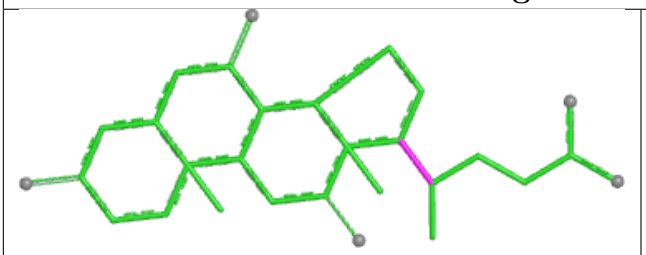


Torsions

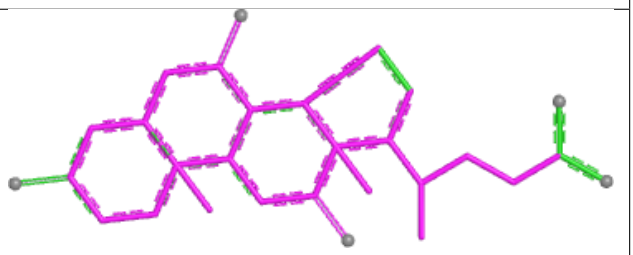


Rings

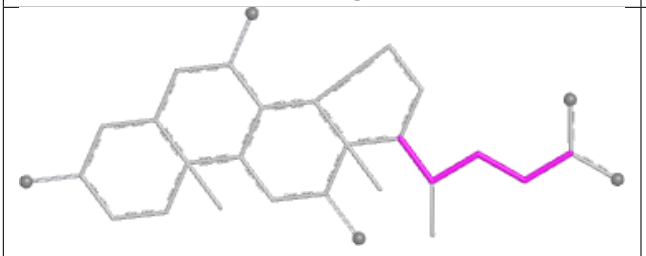
Ligand CHD P 1271



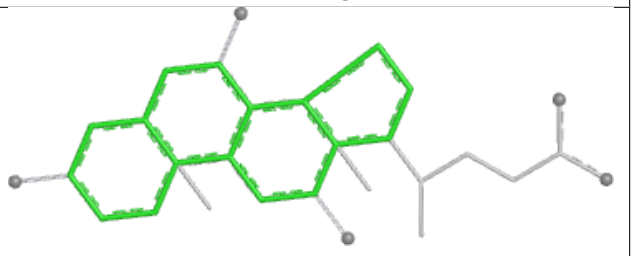
Bond lengths



Bond angles

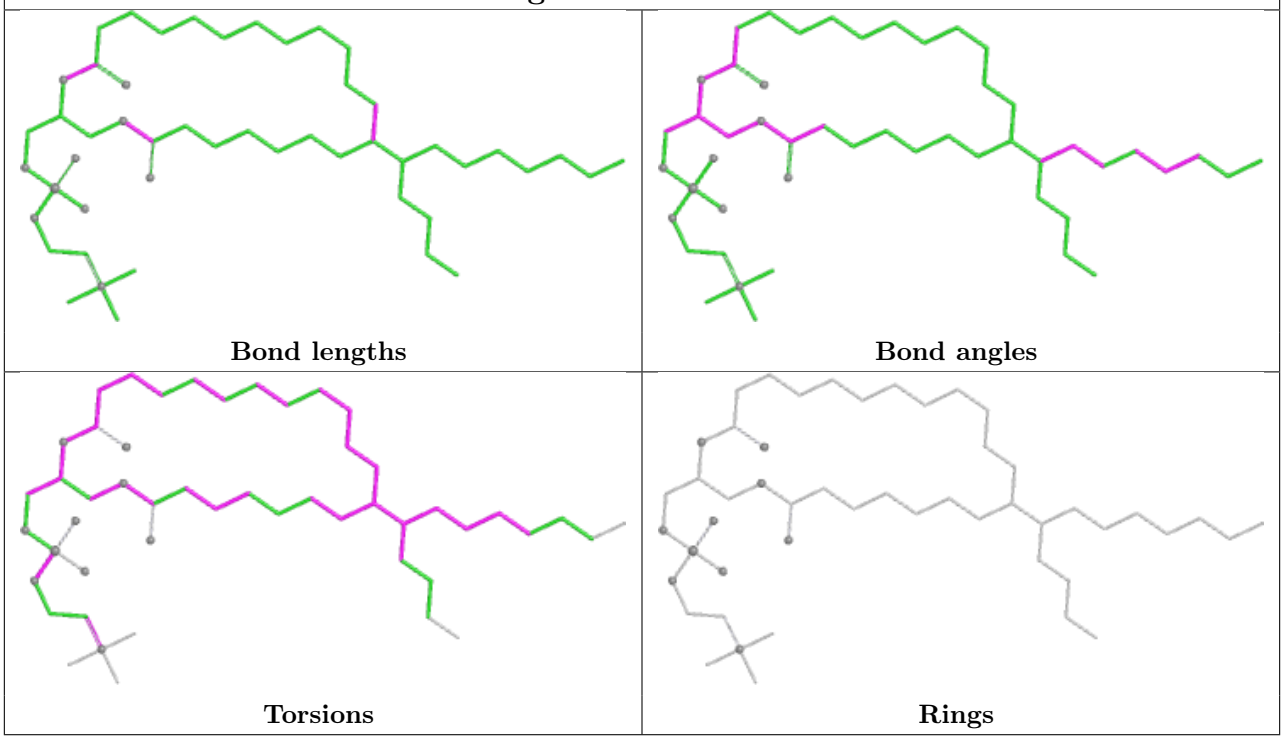


Torsions

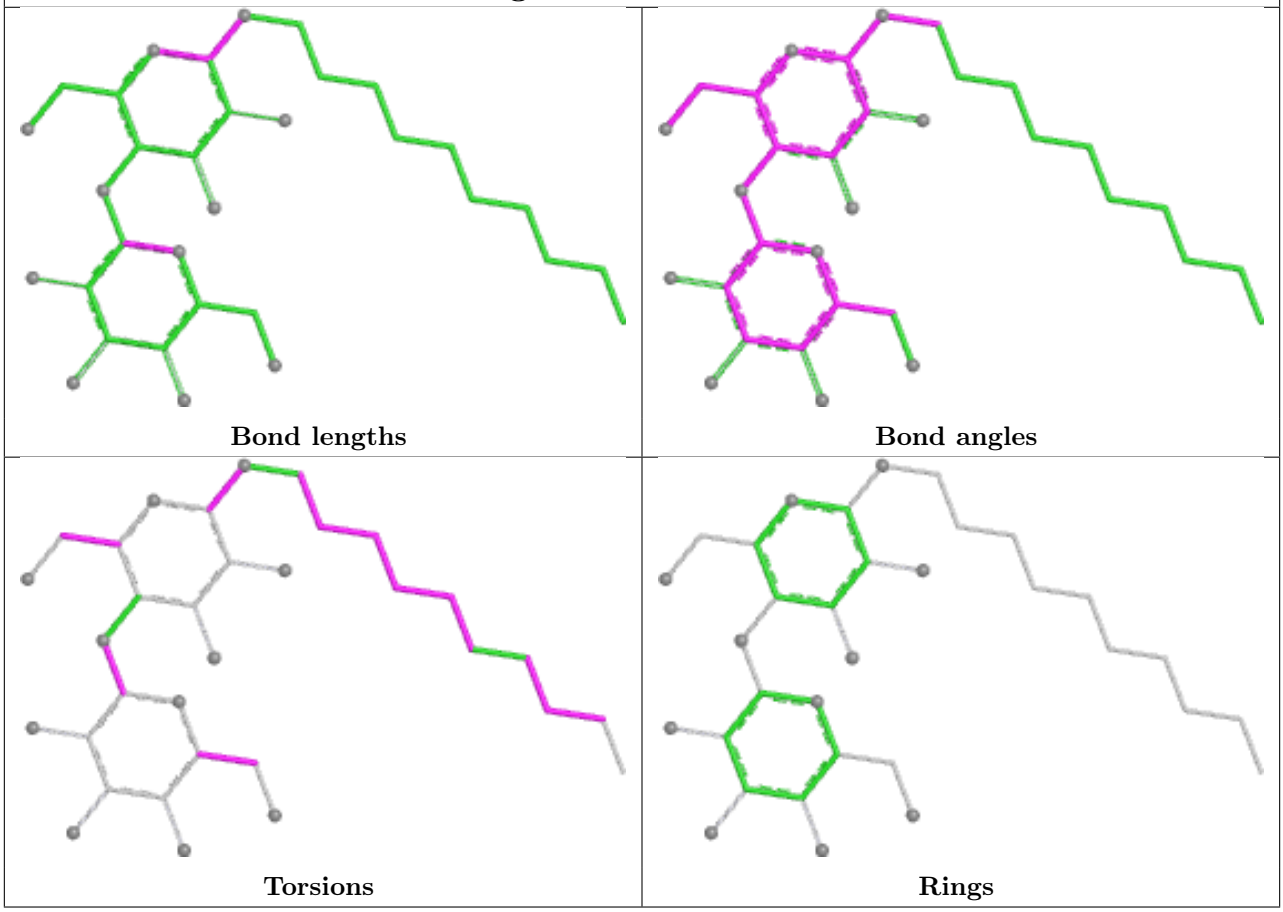


Rings

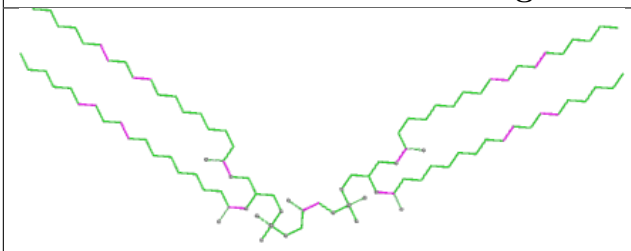
Ligand PSC B 229



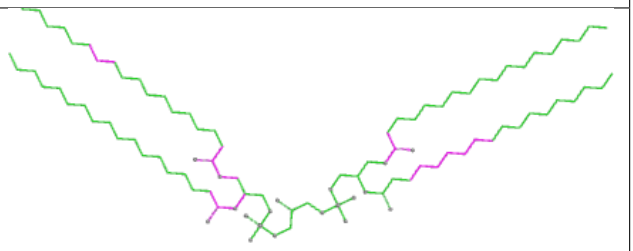
Ligand DMU T 1272



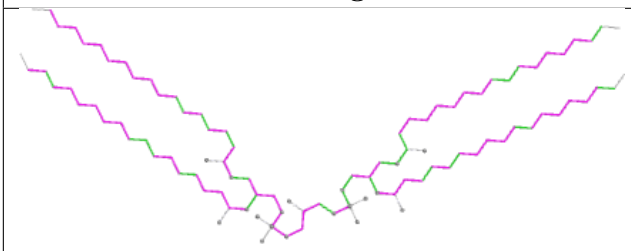
Ligand CDL P 1270



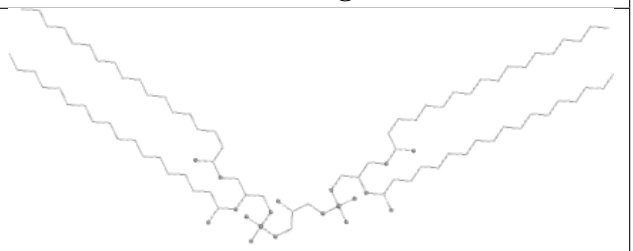
Bond lengths



Bond angles

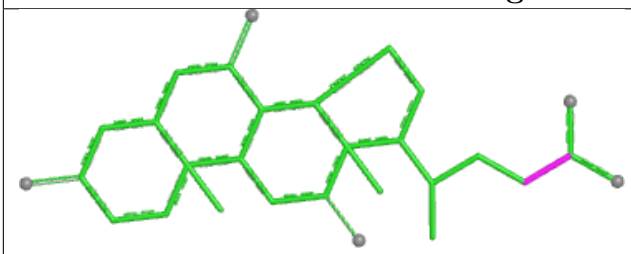


Torsions

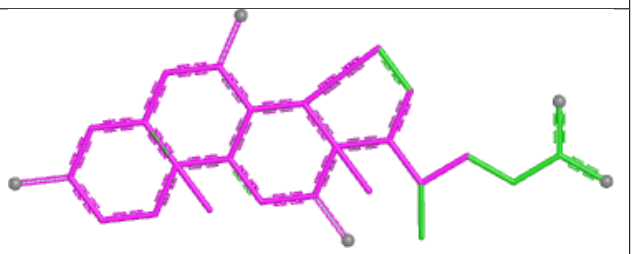


Rings

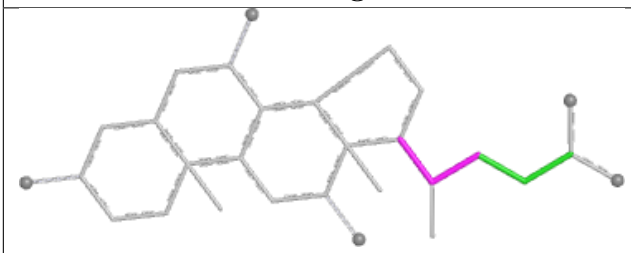
Ligand CHD W 1059



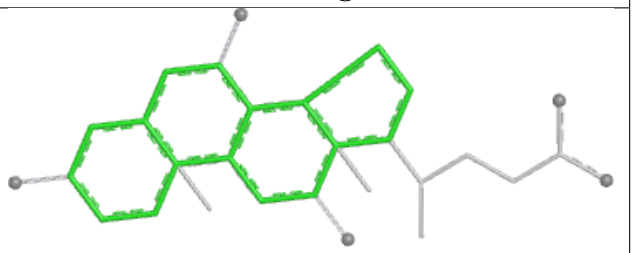
Bond lengths



Bond angles

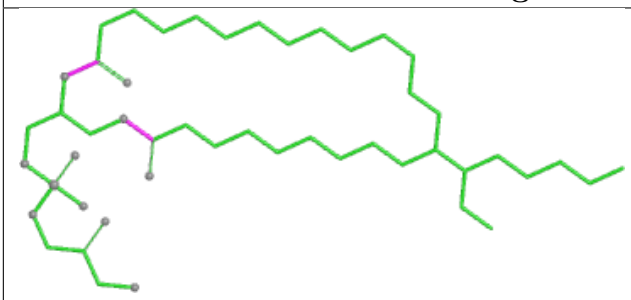


Torsions

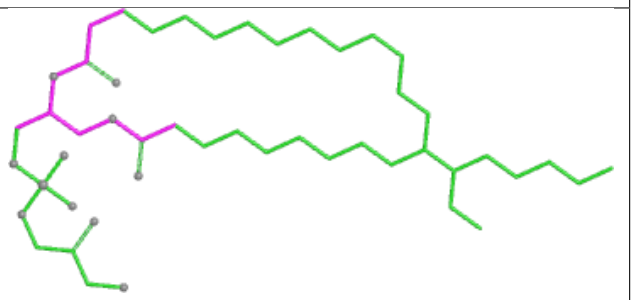


Rings

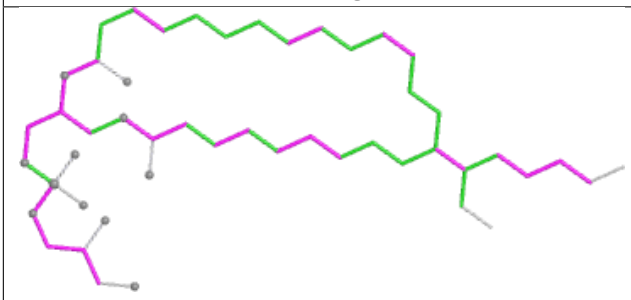
Ligand PGV N 1524



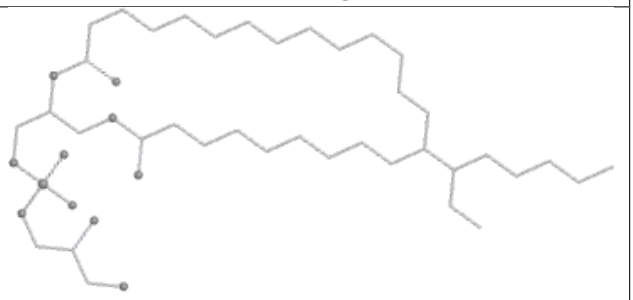
Bond lengths



Bond angles

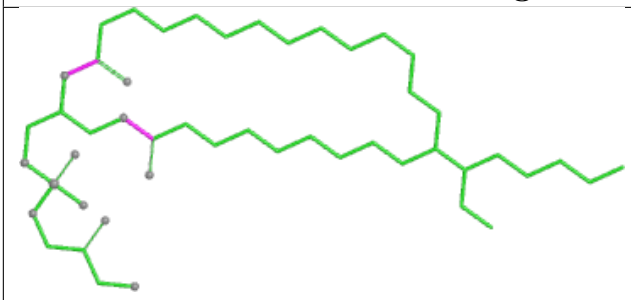


Torsions

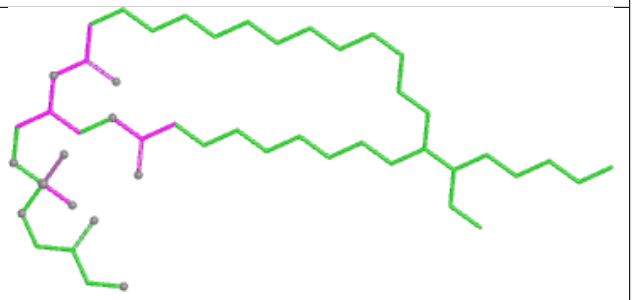


Rings

Ligand PGV P 1268

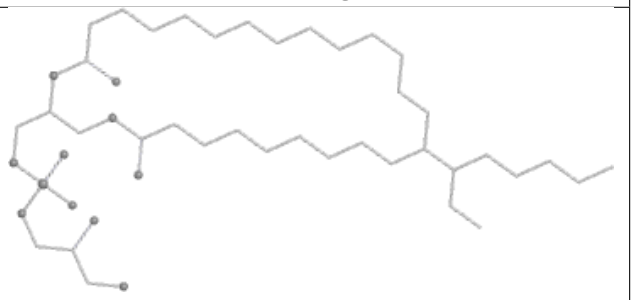


Bond lengths



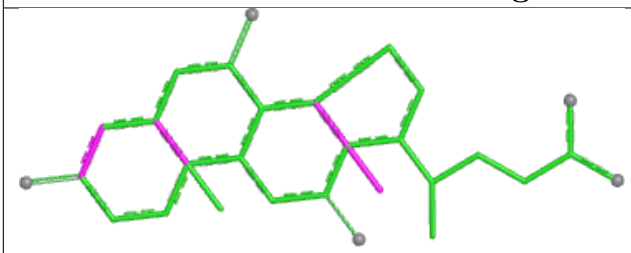
Bond angles

Torsions

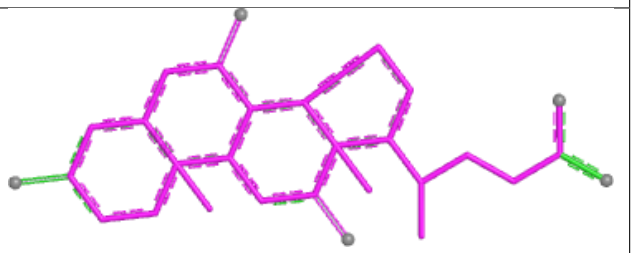


Rings

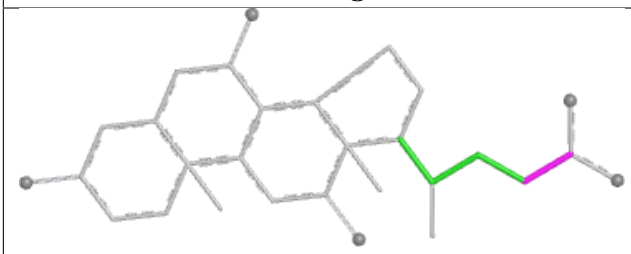
Ligand CHD B 1085



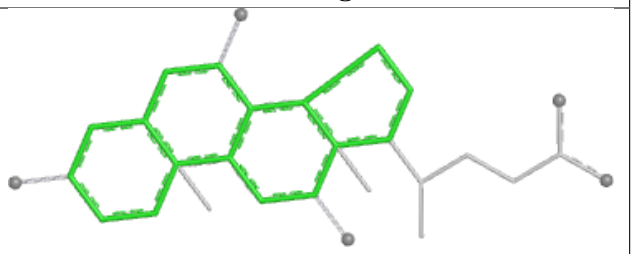
Bond lengths



Bond angles

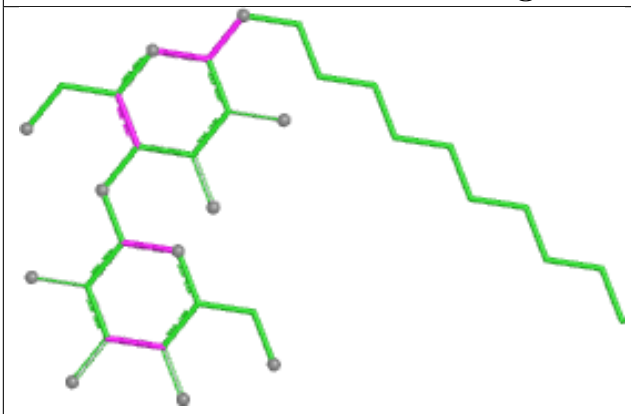


Torsions

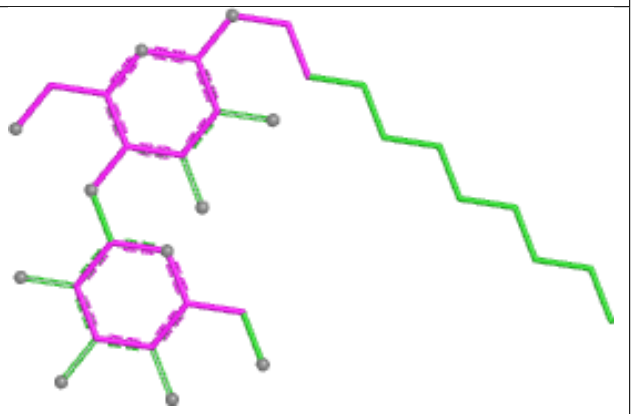


Rings

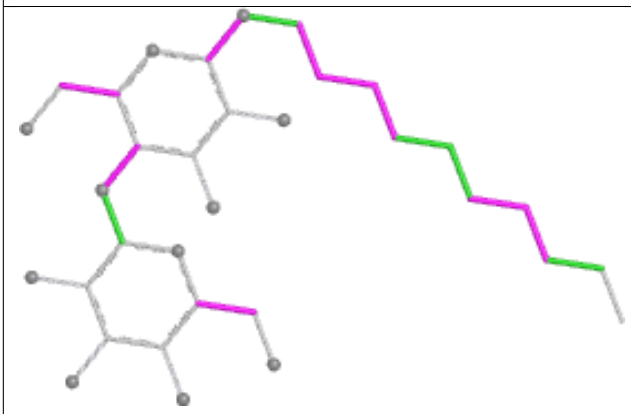
Ligand DMU C 272



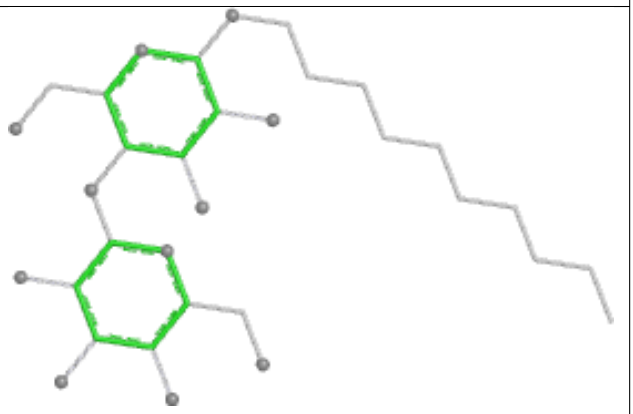
Bond lengths



Bond angles

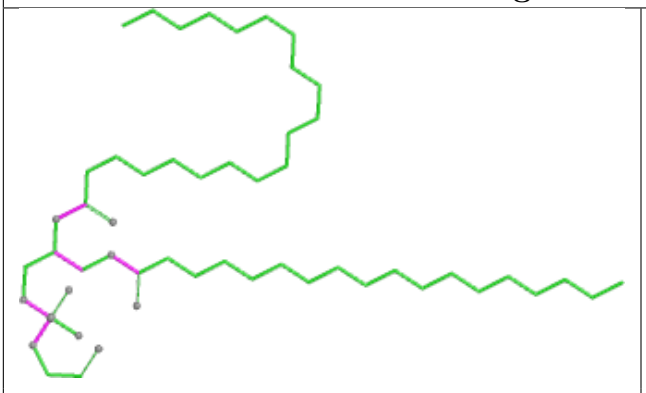


Torsions

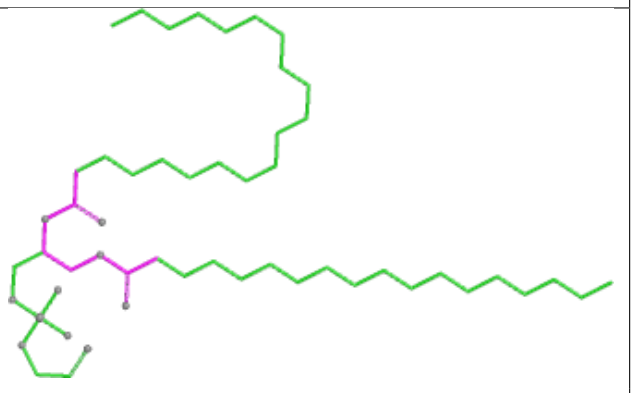


Rings

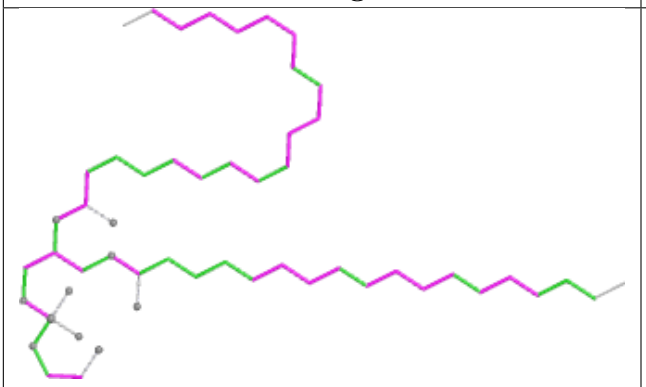
Ligand PEK G 1263



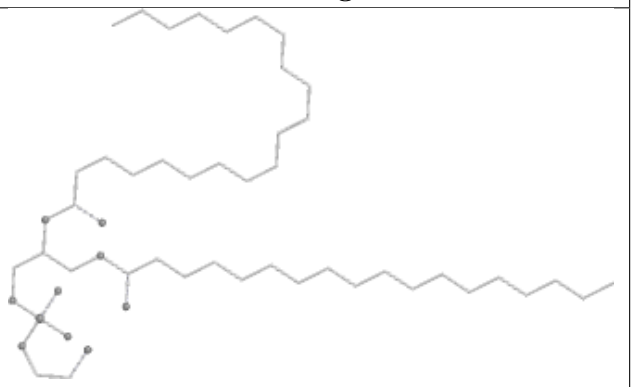
Bond lengths



Bond angles

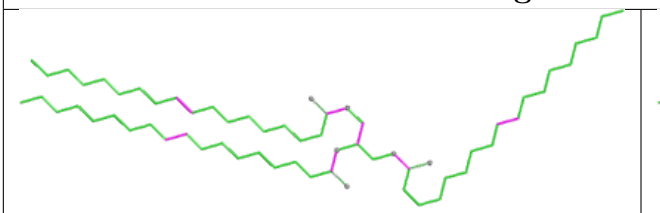


Torsions

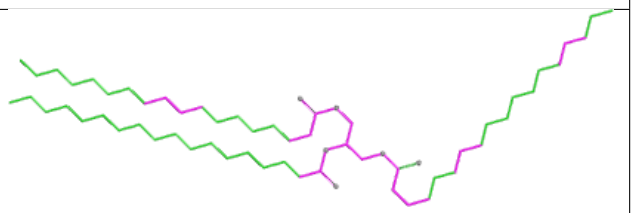


Rings

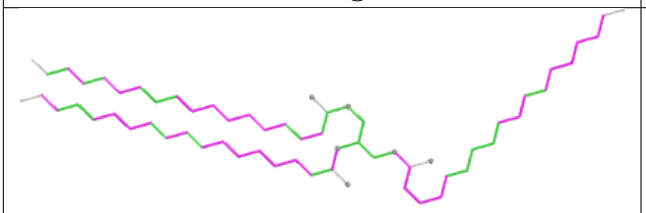
Ligand TGL N 1522



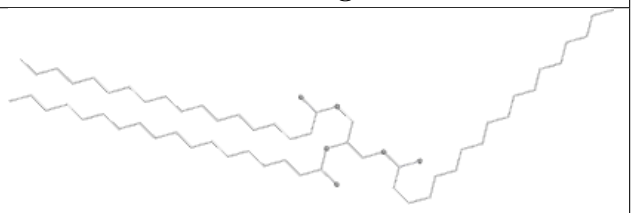
Bond lengths



Bond angles

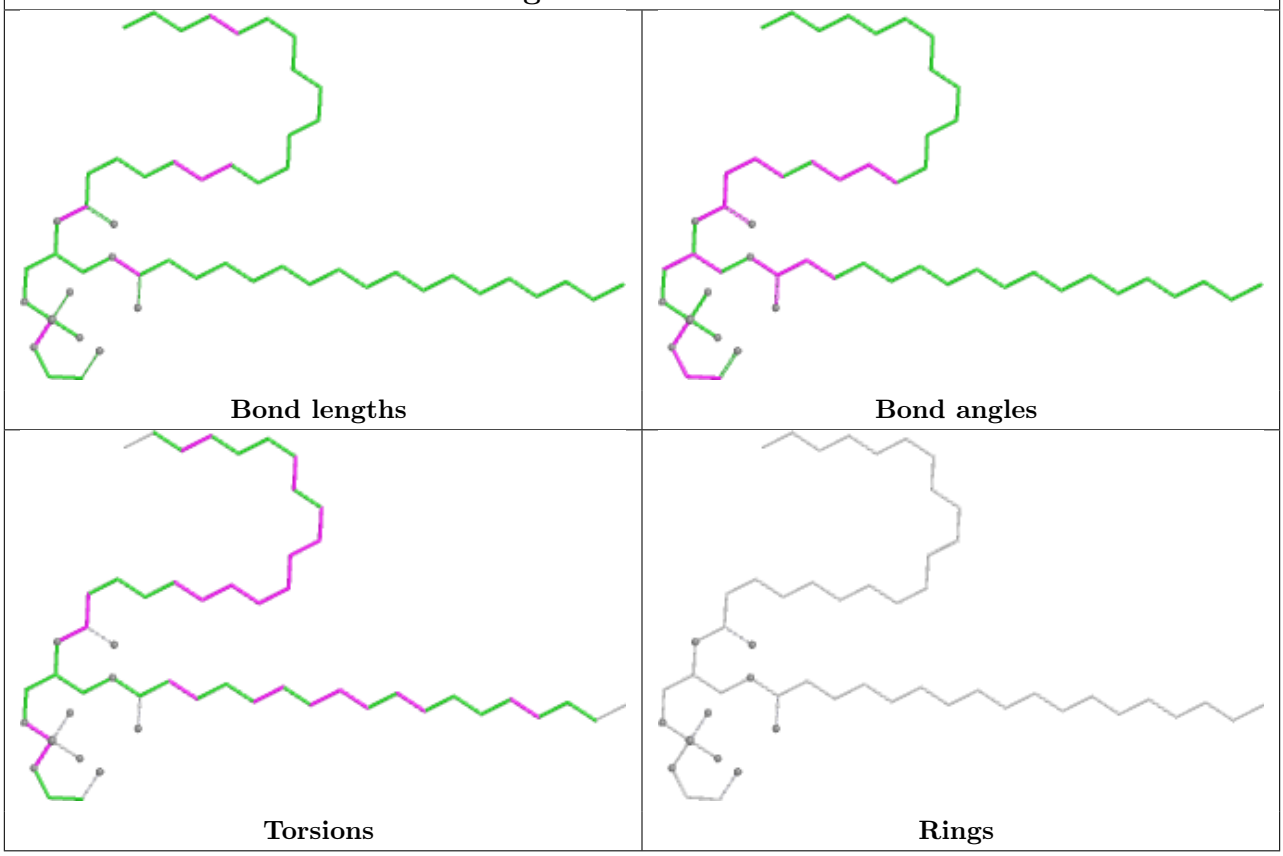


Torsions

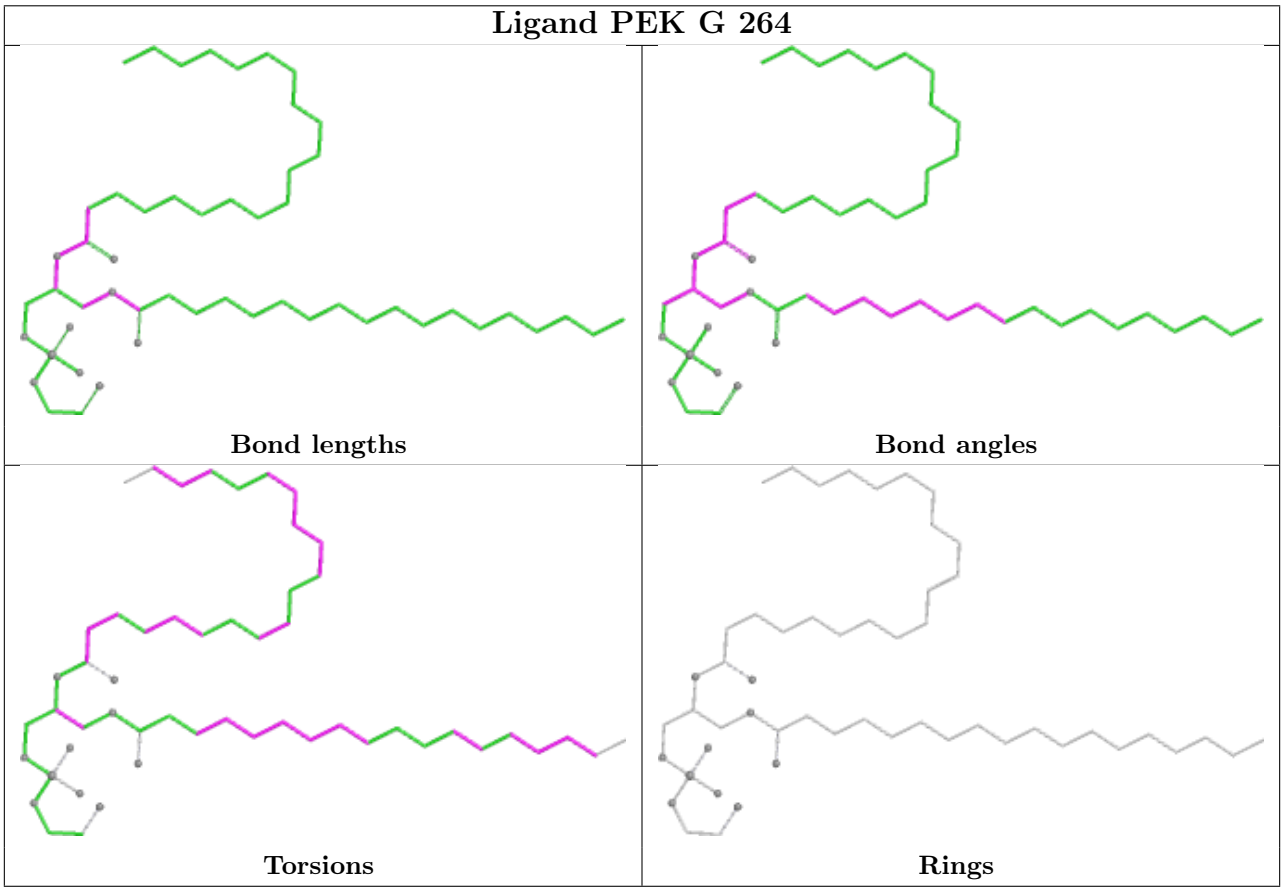


Rings

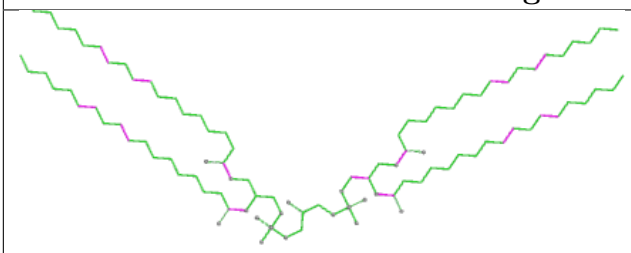
Ligand PEK G 265



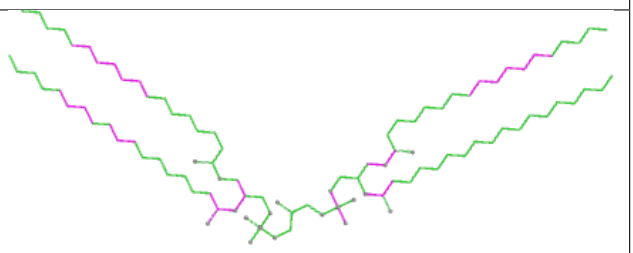
Ligand PEK G 264



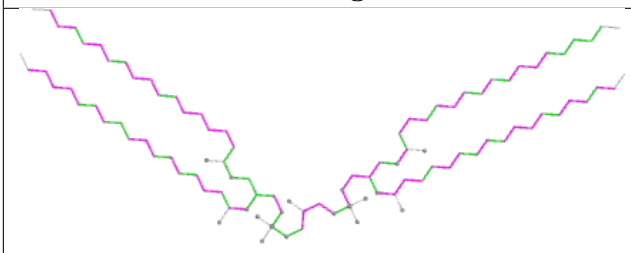
Ligand CDL G 269



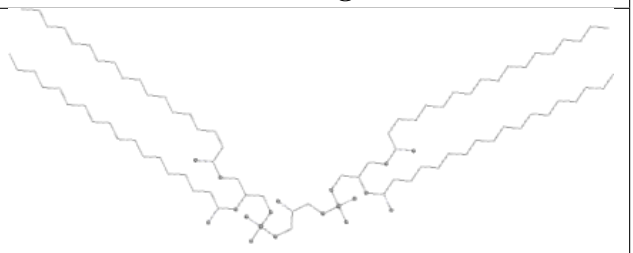
Bond lengths



Bond angles

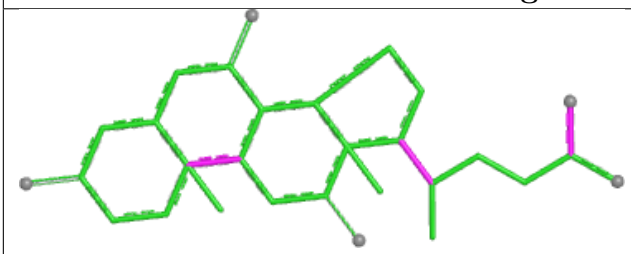


Torsions

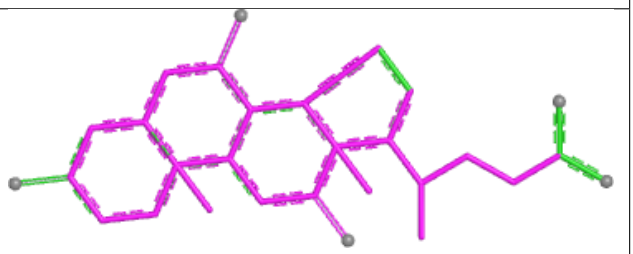


Rings

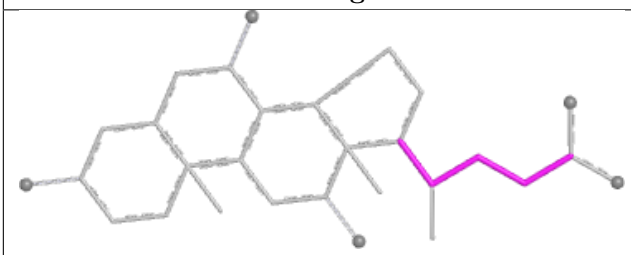
Ligand CHD C 271



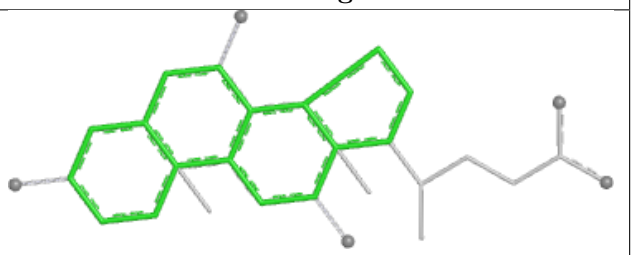
Bond lengths



Bond angles

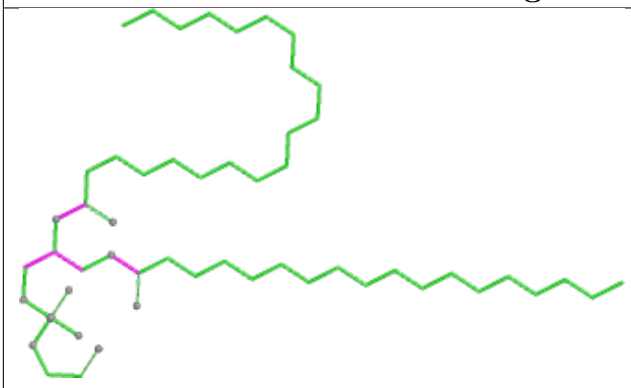


Torsions

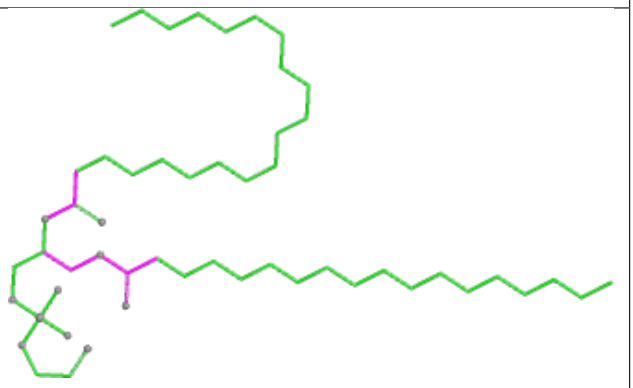


Rings

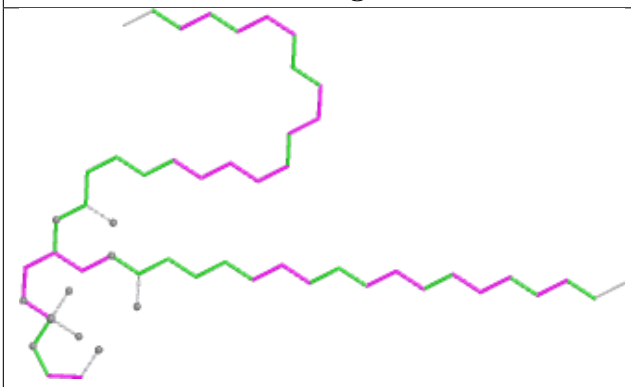
Ligand PEK T 263



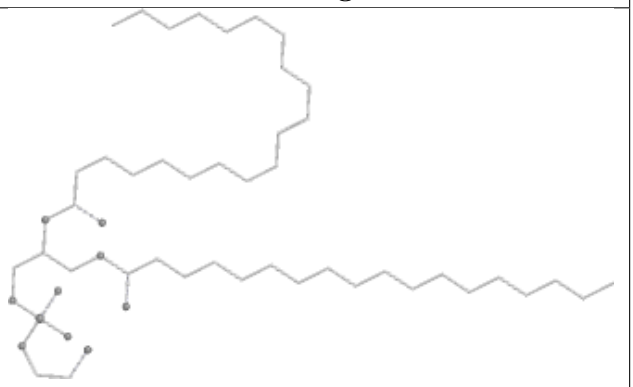
Bond lengths



Bond angles

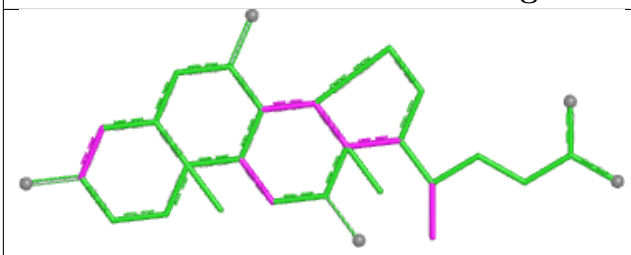


Torsions

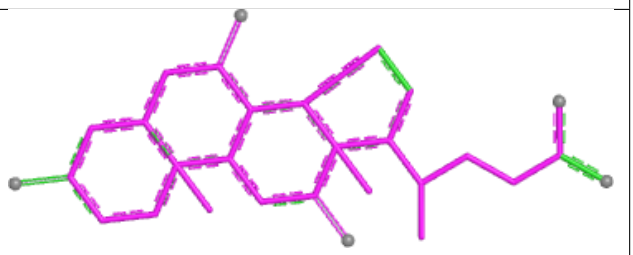


Rings

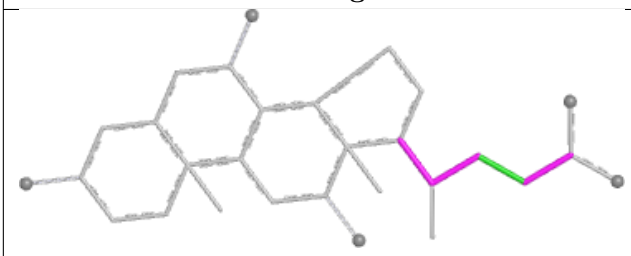
Ligand CHD O 229



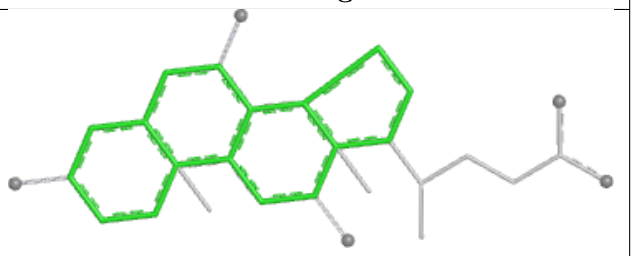
Bond lengths



Bond angles

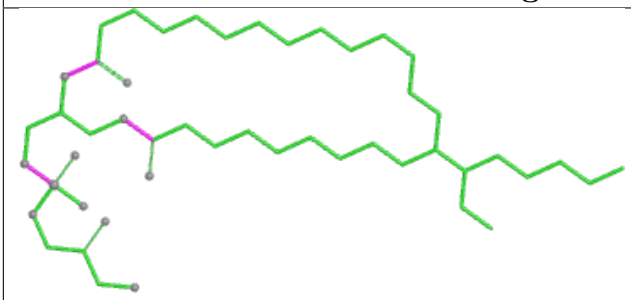


Torsions

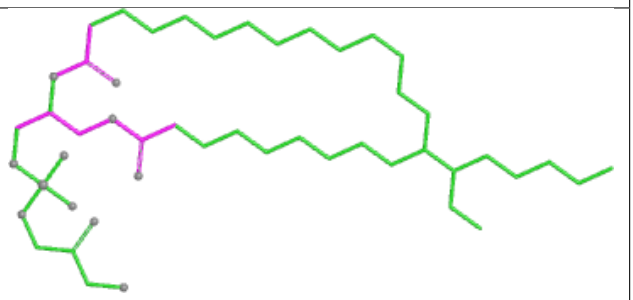


Rings

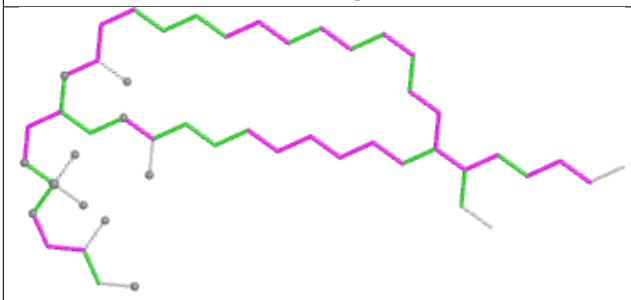
Ligand PGV C 268



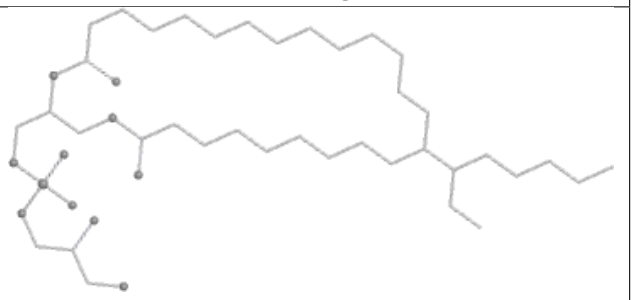
Bond lengths



Bond angles

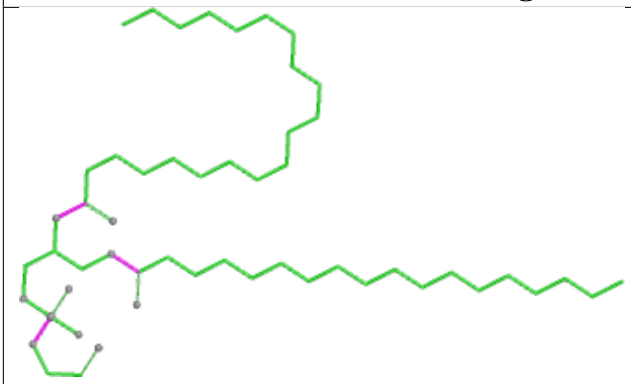


Torsions

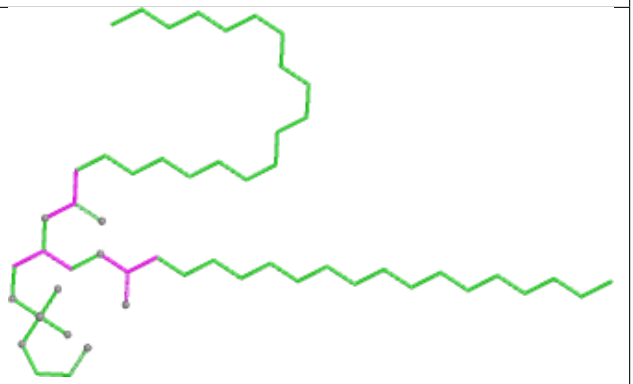


Rings

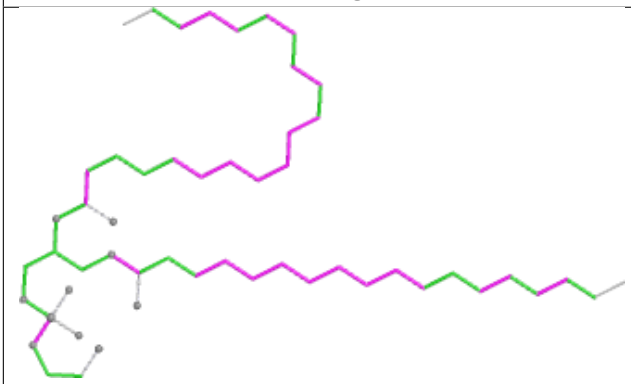
Ligand PEK S 1265



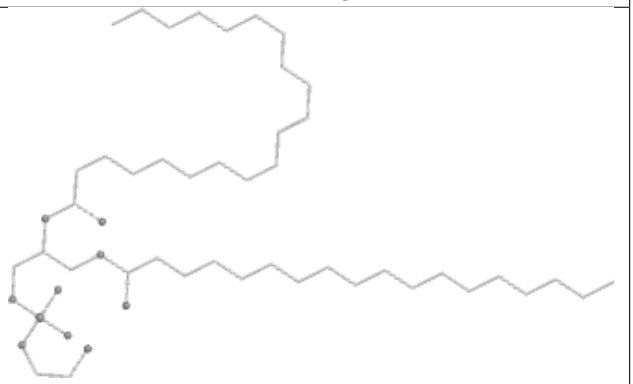
Bond lengths



Bond angles

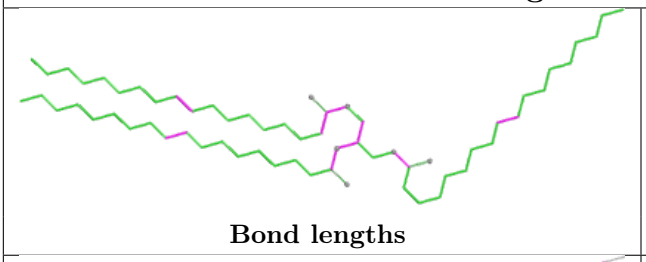


Torsions

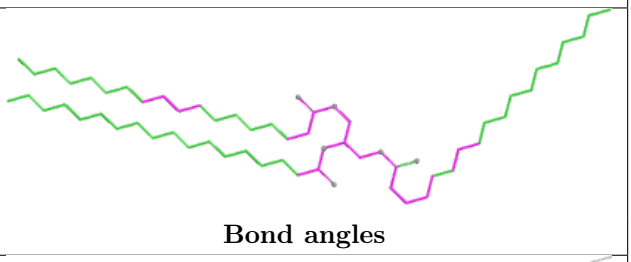


Rings

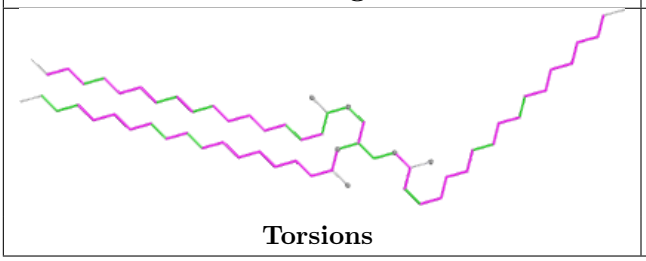
Ligand TGL L 522



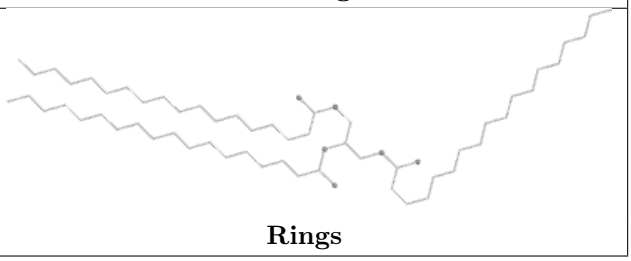
Bond lengths



Bond angles

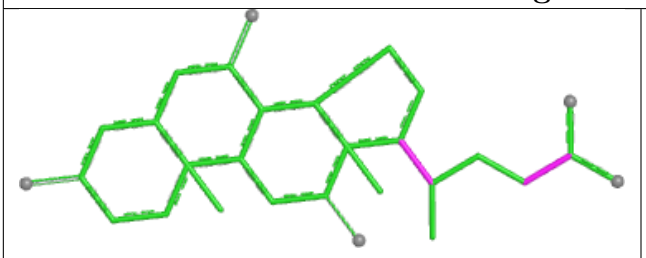


Torsions

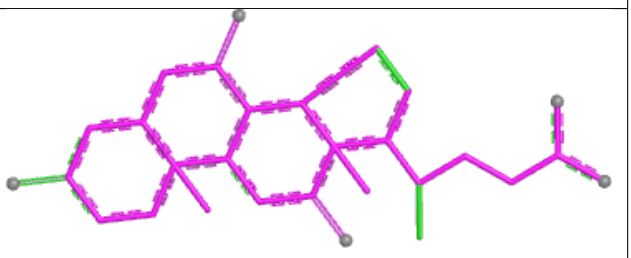


Rings

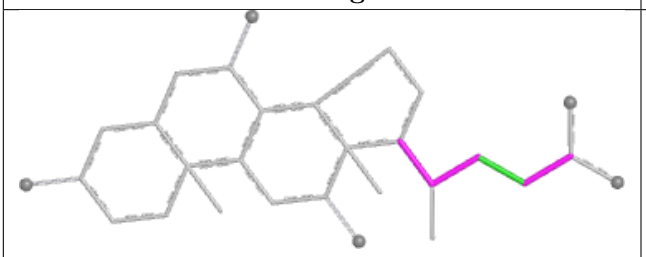
Ligand CHD J 60



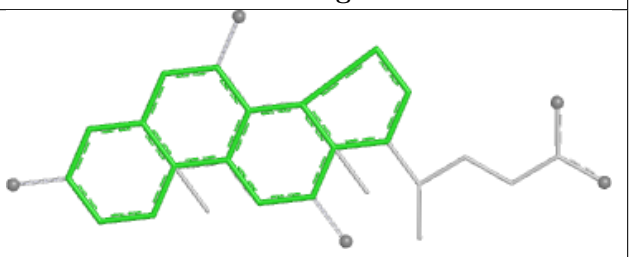
Bond lengths



Bond angles

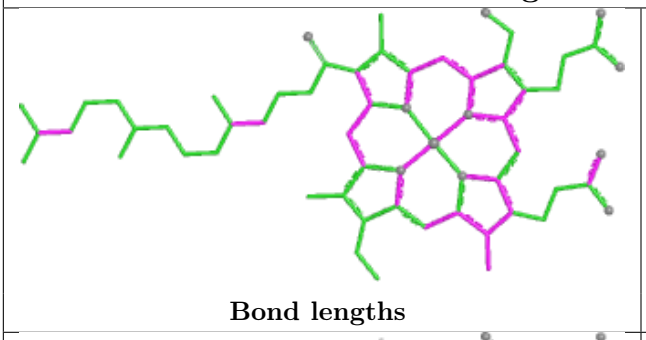


Torsions

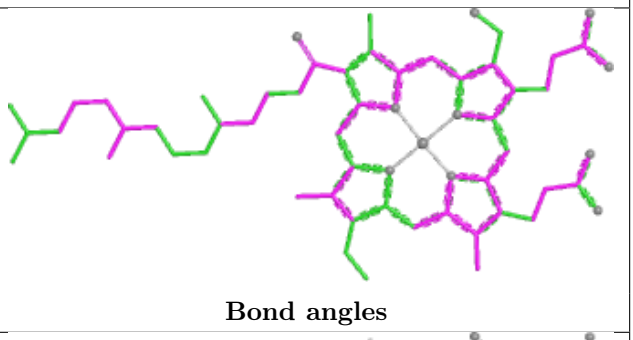


Rings

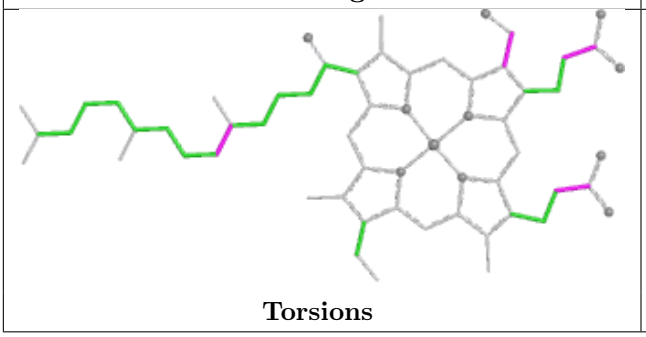
Ligand HEA A 516



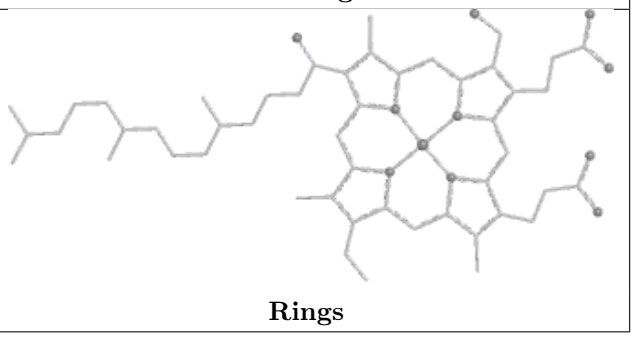
Bond lengths



Bond angles

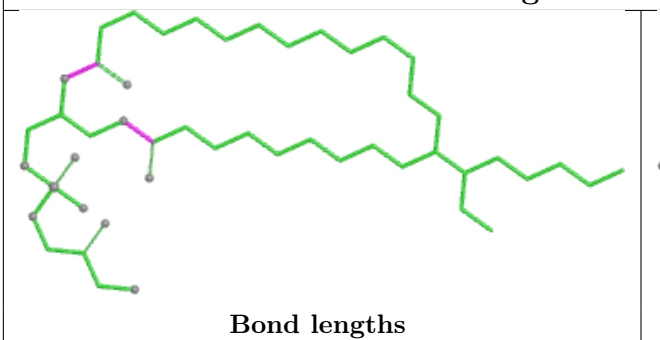


Torsions

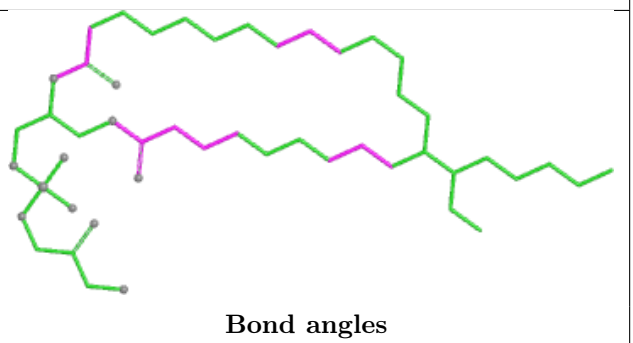


Rings

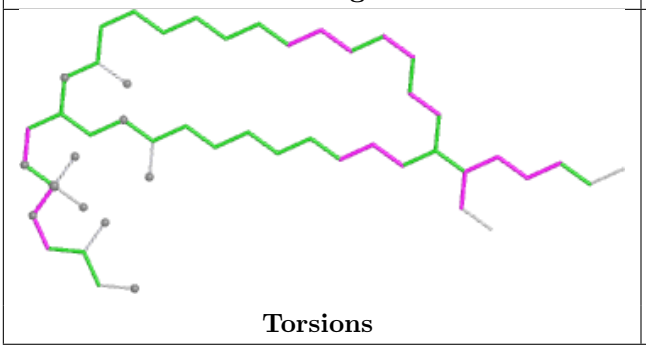
Ligand PGV C 267



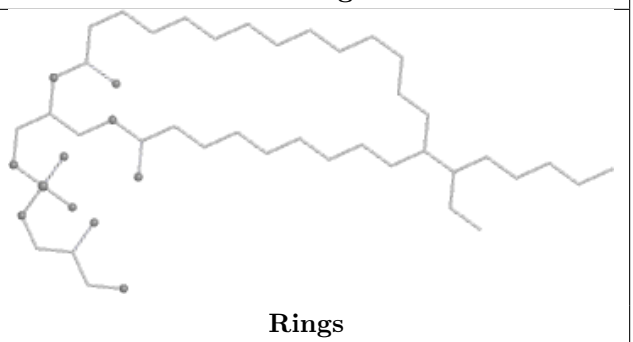
Bond lengths



Bond angles

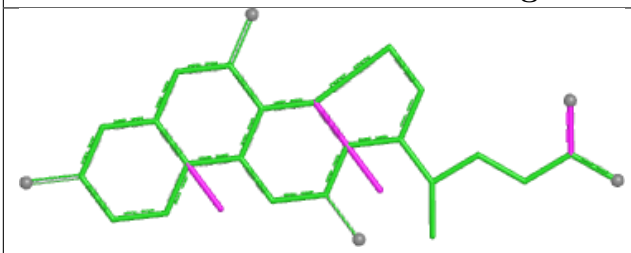


Torsions

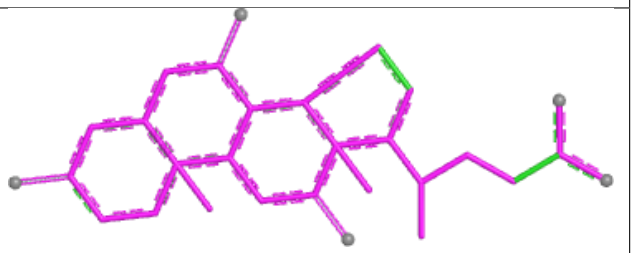


Rings

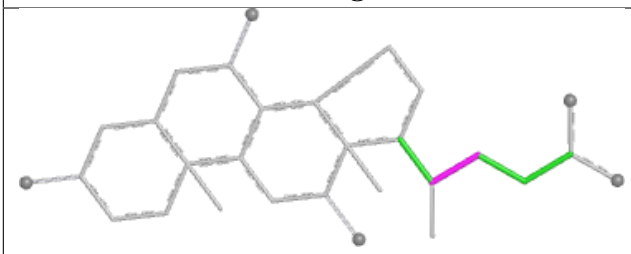
Ligand CHD C 525



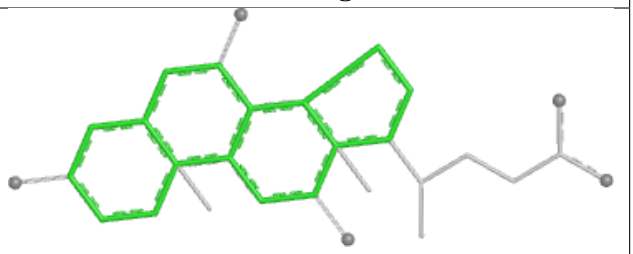
Bond lengths



Bond angles

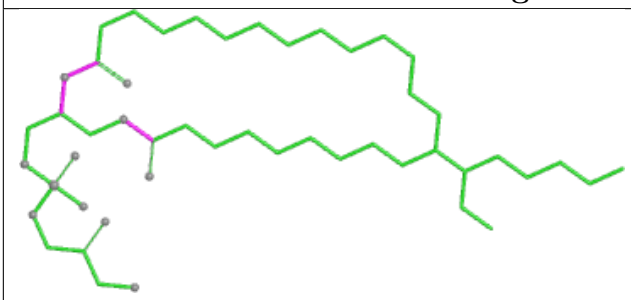


Torsions

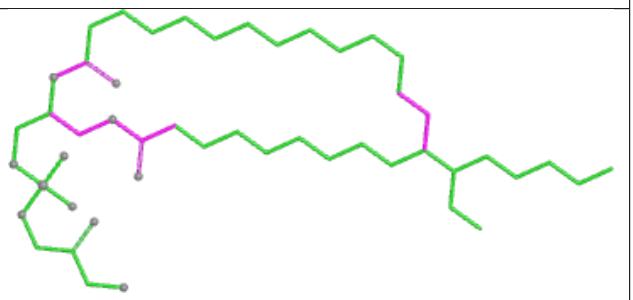


Rings

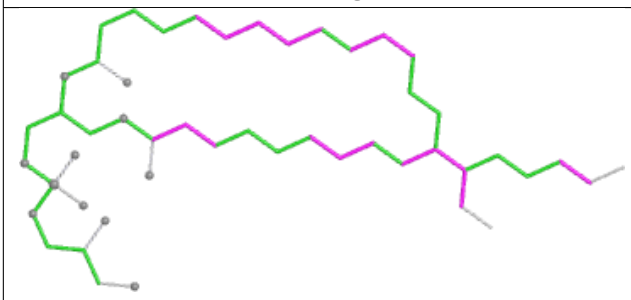
Ligand PGV N 1266



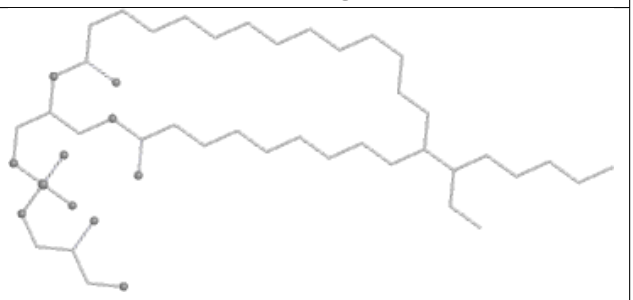
Bond lengths



Bond angles

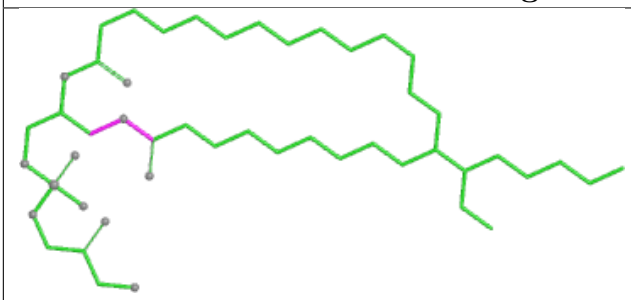


Torsions

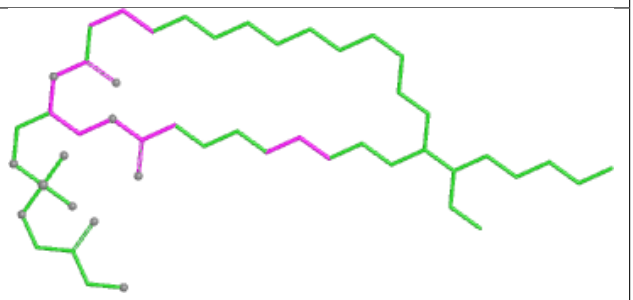


Rings

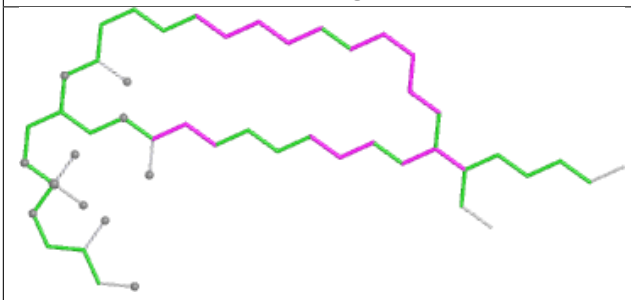
Ligand PGV A 521



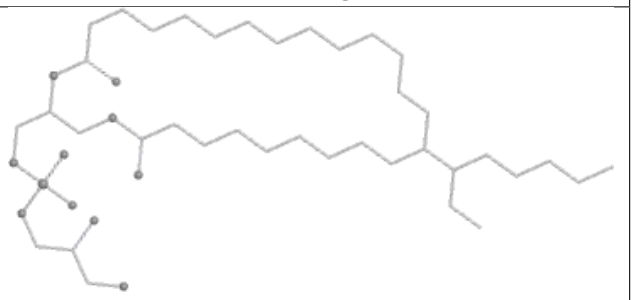
Bond lengths



Bond angles

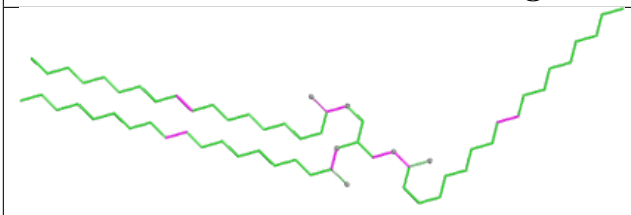


Torsions

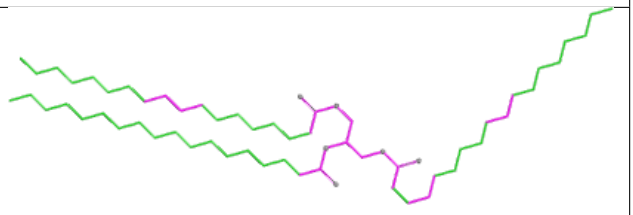


Rings

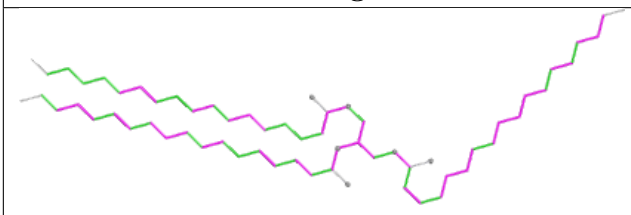
Ligand TGL B 521



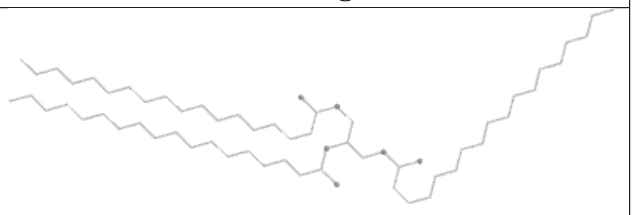
Bond lengths



Bond angles

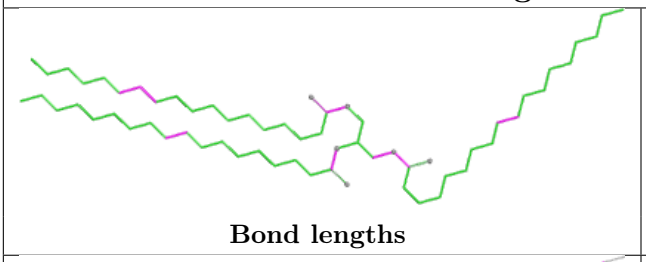


Torsions

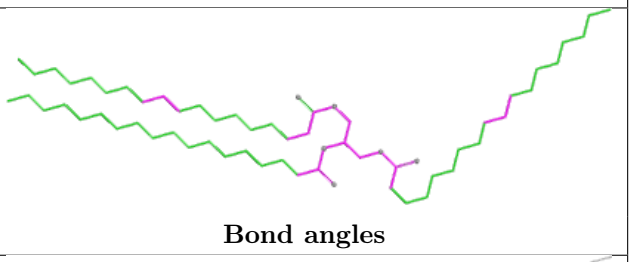


Rings

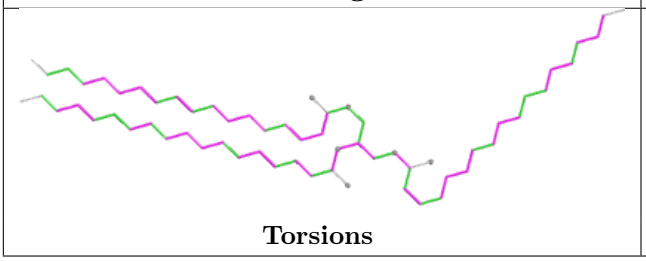
Ligand TGL N 1521



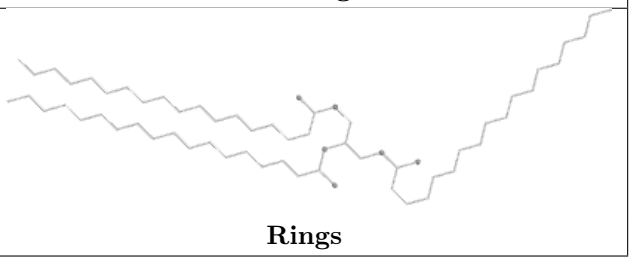
Bond lengths



Bond angles

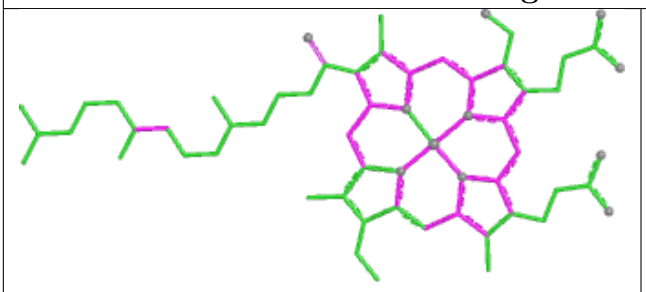


Torsions

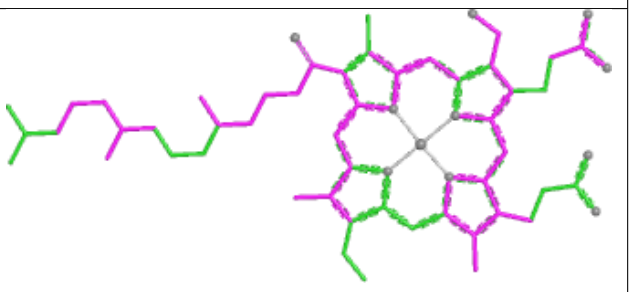


Rings

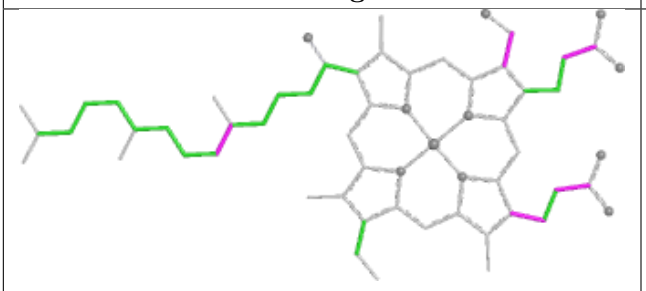
Ligand HEA N 516



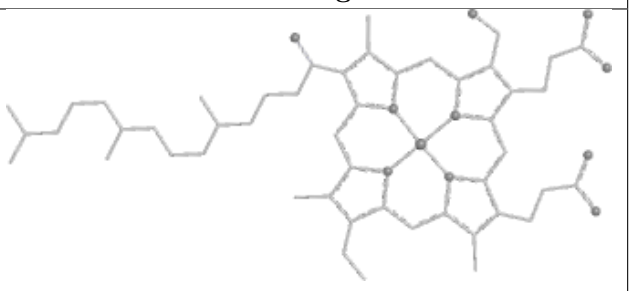
Bond lengths



Bond angles

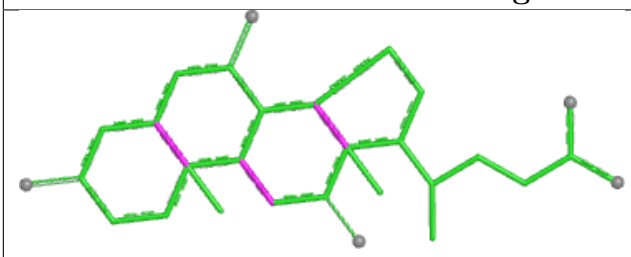


Torsions

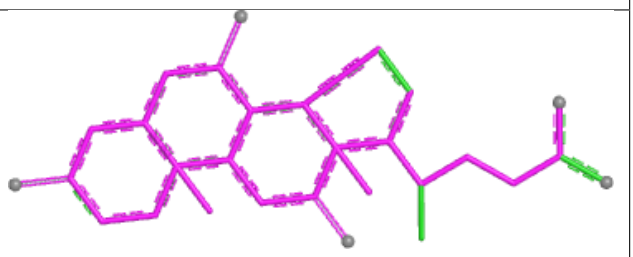


Rings

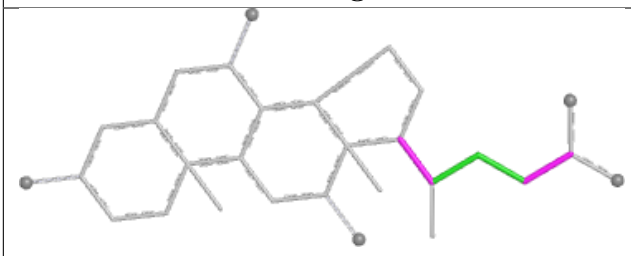
Ligand CHD P 1525



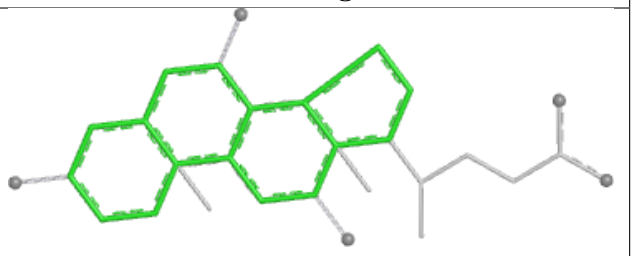
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.41	2 (0%) 88 87	36, 42, 52, 84	0
1	N	513/514 (99%)	0.08	4 (0%) 82 80	43, 51, 63, 92	0
2	B	226/227 (99%)	-0.07	6 (2%) 56 53	36, 48, 78, 111	0
2	O	226/227 (99%)	0.51	8 (3%) 47 44	49, 61, 93, 120	0
3	C	259/261 (99%)	-0.43	2 (0%) 82 80	38, 45, 59, 86	0
3	P	259/261 (99%)	-0.02	5 (1%) 66 63	44, 51, 68, 88	0
4	D	144/147 (97%)	-0.19	2 (1%) 73 71	43, 51, 75, 91	0
4	Q	144/147 (97%)	0.70	9 (6%) 26 23	55, 69, 96, 132	0
5	E	105/109 (96%)	-0.26	1 (0%) 79 77	43, 51, 83, 118	0
5	R	105/109 (96%)	0.05	2 (1%) 66 63	51, 63, 92, 123	0
6	F	98/98 (100%)	0.09	8 (8%) 17 15	40, 53, 112, 143	0
6	S	98/98 (100%)	0.24	8 (8%) 17 15	49, 61, 113, 144	0
7	G	83/85 (97%)	0.69	16 (19%) 3 2	42, 55, 123, 129	0
7	T	83/85 (97%)	0.79	17 (20%) 2 2	46, 62, 121, 133	0
8	H	79/85 (92%)	0.21	7 (8%) 15 13	46, 58, 119, 129	0
8	U	79/85 (92%)	0.45	7 (8%) 15 13	54, 69, 120, 127	0
9	I	72/73 (98%)	0.30	8 (11%) 10 8	48, 60, 105, 112	0
9	V	72/73 (98%)	0.74	9 (12%) 8 6	52, 74, 109, 112	0
10	J	58/59 (98%)	0.21	2 (3%) 48 45	45, 58, 86, 119	0
10	W	58/59 (98%)	0.68	3 (5%) 33 29	54, 66, 88, 120	0
11	K	49/56 (87%)	0.07	1 (2%) 65 62	45, 57, 75, 83	0
11	X	49/56 (87%)	0.66	3 (6%) 27 24	62, 69, 85, 99	0
12	L	46/47 (97%)	-0.09	1 (2%) 62 59	43, 48, 70, 100	0
12	Y	46/47 (97%)	0.72	3 (6%) 25 22	53, 61, 82, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.04	3 (6%) 22 19	44, 51, 88, 120	0
13	Z	43/46 (93%)	0.76	2 (4%) 36 33	57, 65, 96, 121	0
All	All	3550/3614 (98%)	0.08	139 (3%) 43 40	36, 53, 92, 144	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	8.2
6	F	1	ALA	8.1
8	H	8	ILE	7.8
6	S	1	ALA	7.2
7	G	3	ALA	7.2
7	G	5	LYS	7.0
4	Q	5	VAL	7.0
7	G	4	ALA	6.2
6	F	96	LEU	6.0
6	F	97	ALA	6.0
10	W	48	TYR	5.8
7	G	2	SER	5.8
7	T	5	LYS	5.7
8	U	8	ILE	5.6
7	T	36	TRP	5.6
7	T	3	ALA	5.1
7	G	10	GLY	5.1
7	G	7	ASP	5.0
6	S	96	LEU	5.0
6	S	97	ALA	5.0
7	G	8	HIS	4.8
7	G	36	TRP	4.7
7	T	1	ALA	4.7
7	T	4	ALA	4.4
4	Q	8	SER	4.4
9	I	29	LEU	4.3
4	Q	7	LYS	4.3
11	X	6	ALA	4.2
4	Q	4	SER	4.1
7	G	1	ALA	4.1
2	B	59	GLN	4.0
12	L	2	HIS	3.9
9	I	30	GLY	3.9
7	G	9	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	37	PHE	3.9
7	T	2	SER	3.8
4	D	4	SER	3.7
7	G	6	GLY	3.6
8	H	9	LYS	3.6
8	H	46	LYS	3.6
10	J	58	LYS	3.6
2	O	74	ILE	3.5
10	W	52	TRP	3.4
7	T	9	GLY	3.4
9	V	29	LEU	3.4
7	T	8	HIS	3.4
2	O	131	GLY	3.4
2	B	58	ALA	3.3
6	S	94	HIS	3.3
12	Y	2	HIS	3.3
9	V	2	THR	3.3
7	G	12	GLY	3.2
7	T	42	ARG	3.2
7	T	7	ASP	3.2
6	S	98	HIS	3.2
5	E	5	HIS	3.1
7	T	6	GLY	3.1
6	F	94	HIS	3.1
9	V	25	PHE	3.1
7	T	12	GLY	3.1
2	O	90	ILE	3.0
3	P	3	HIS	3.0
6	F	3	GLY	2.9
9	I	37	PHE	2.9
6	F	95	GLN	2.9
4	D	102	TYR	2.9
8	U	47	GLY	2.9
7	G	84	LYS	2.9
13	Z	43	SER	2.9
7	T	84	LYS	2.9
2	O	130	PRO	2.8
2	B	227	LEU	2.8
2	B	115	ASP	2.8
8	H	45	ALA	2.8
6	S	2	SER	2.7
10	W	58	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	447	TYR	2.7
12	Y	3	TYR	2.7
9	I	25	PHE	2.7
5	R	5	HIS	2.7
9	V	31	PHE	2.7
3	P	111	GLU	2.7
10	J	1	PHE	2.7
8	U	10	ASN	2.7
8	U	50	VAL	2.7
9	V	3	ALA	2.6
2	B	113	TYR	2.6
6	S	95	GLN	2.6
2	O	65	TRP	2.6
11	K	6	ALA	2.6
4	Q	31	LYS	2.6
13	Z	32	TRP	2.6
8	H	47	GLY	2.6
9	I	19	PHE	2.6
2	O	113	TYR	2.6
6	S	3	GLY	2.5
13	M	43	SER	2.5
7	T	10	GLY	2.5
9	I	31	PHE	2.5
13	M	35	TYR	2.5
8	U	46	LYS	2.5
4	Q	19	ARG	2.5
5	R	109	VAL	2.5
1	A	298	ASP	2.5
2	O	59	GLN	2.5
9	V	30	GLY	2.5
3	P	33	MET	2.4
11	X	31	TYR	2.4
1	A	514	LYS	2.4
1	N	459	PHE	2.4
8	U	9	LYS	2.4
6	F	98	HIS	2.4
7	T	40	GLY	2.3
6	F	2	SER	2.3
9	I	28	SER	2.3
9	V	28	SER	2.3
7	G	46	ALA	2.3
3	C	3	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	7	LYS	2.3
12	Y	38	PHE	2.2
13	M	42	LYS	2.2
7	T	37	LEU	2.2
4	Q	9	GLU	2.2
3	C	107	ALA	2.2
3	P	182	TYR	2.2
2	B	65	TRP	2.2
4	Q	115	TRP	2.2
8	U	45	ALA	2.1
7	G	37	LEU	2.1
9	I	27	VAL	2.1
11	X	48	VAL	2.1
3	P	37	PHE	2.1
1	N	45	GLY	2.1
1	N	450	TRP	2.1
2	O	92	ASN	2.0
8	H	42	ALA	2.0
7	T	38	HIS	2.0
7	G	42	ARG	2.0
9	V	68	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.34	0.21	110,112,114,115	0
7	TPO	T	11	11/12	0.39	0.28	97,105,129,130	0
9	SAC	I	1	9/10	0.45	0.22	99,103,106,106	0
7	TPO	G	11	11/12	0.48	0.34	93,102,125,127	0
1	FME	N	1	10/11	0.77	0.28	77,82,105,107	0
1	FME	A	1	10/11	0.83	0.20	63,70,93,102	0
2	FME	O	1	10/11	0.93	0.15	59,59,64,64	0
2	FME	B	1	10/11	0.98	0.07	46,48,51,61	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	UNX	C	262	1/1	0.56	0.52	75,75,75,75	0
24	UNX	P	262	1/1	0.70	0.45	75,75,75,75	0
28	PEK	G	1263	53/53	0.75	0.29	83,126,150,150	0
28	PEK	T	263	53/53	0.76	0.27	78,123,145,149	0
23	CHD	W	1059	29/29	0.77	0.20	110,117,120,122	0
22	PSC	B	229	52/52	0.78	0.24	70,117,150,150	0
23	CHD	J	60	29/29	0.80	0.18	103,112,119,120	0
26	DMU	C	272	33/33	0.80	0.20	96,129,132,134	0
20	PGV	C	268	51/51	0.81	0.26	78,103,119,120	0
26	DMU	T	1272	33/33	0.81	0.21	111,140,141,141	0
22	PSC	R	1229	52/52	0.81	0.26	73,120,150,150	0
20	PGV	P	1268	51/51	0.81	0.26	78,108,125,126	0
19	TGL	A	523	63/63	0.82	0.31	78,102,131,132	0
19	TGL	N	1523	63/63	0.82	0.29	84,111,131,133	0
19	TGL	N	1522	63/63	0.83	0.27	72,95,111,112	0
28	PEK	G	265	53/53	0.83	0.23	70,109,135,138	0
25	CDL	G	269	100/100	0.83	0.28	89,118,138,141	0
20	PGV	N	1524	51/51	0.83	0.24	67,106,139,140	0
25	CDL	T	1269	100/100	0.85	0.26	92,117,138,143	0
28	PEK	S	1265	53/53	0.85	0.25	75,112,133,136	0
19	TGL	B	521	63/63	0.85	0.25	54,96,118,120	0
20	PGV	A	524	51/51	0.86	0.22	62,101,132,135	0
19	TGL	N	1521	63/63	0.86	0.24	69,101,120,123	0
25	CDL	C	270	100/100	0.87	0.22	56,112,137,139	0
19	TGL	L	522	63/63	0.87	0.25	57,89,109,113	0
25	CDL	P	1270	100/100	0.87	0.23	69,119,136,137	0
26	DMU	Z	1526	33/33	0.87	0.15	73,80,94,96	0
18	NA	N	519	1/1	0.91	0.22	58,58,58,58	0
23	CHD	C	271	29/29	0.92	0.15	86,97,99,99	0
26	DMU	M	526	33/33	0.92	0.10	52,63,87,91	0
23	CHD	P	1271	29/29	0.94	0.12	98,101,103,104	0
23	CHD	P	1525	29/29	0.95	0.09	48,54,57,59	0

Continued on next page...

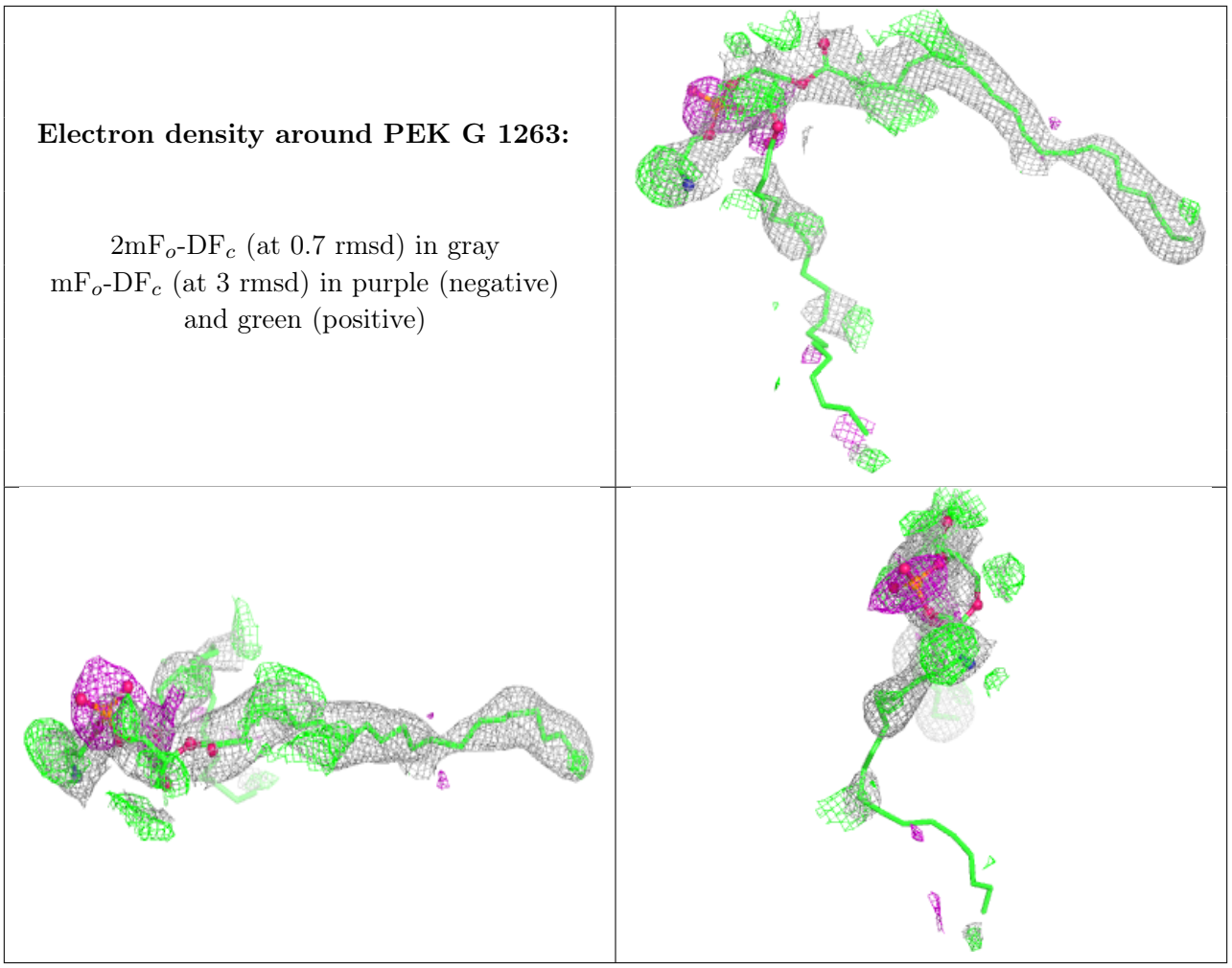
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	PEK	G	264	53/53	0.95	0.14	44,65,107,109	0
23	CHD	B	1085	29/29	0.96	0.07	46,50,53,59	0
23	CHD	O	229	29/29	0.96	0.07	45,49,56,62	0
28	PEK	T	1264	53/53	0.96	0.14	49,70,109,111	0
20	PGV	N	1266	51/51	0.97	0.11	45,60,81,84	0
23	CHD	C	525	29/29	0.97	0.07	38,50,57,65	0
20	PGV	P	1267	51/51	0.97	0.12	45,56,102,106	0
20	PGV	A	521	51/51	0.97	0.10	36,53,77,79	0
15	CMO	N	520	2/2	0.97	0.06	47,47,47,48	0
17	MG	N	518	1/1	0.97	0.04	50,50,50,50	0
17	MG	A	518	1/1	0.98	0.07	40,40,40,40	0
21	CUA	O	228	2/2	0.98	0.04	52,52,52,54	0
20	PGV	C	267	51/51	0.98	0.10	38,52,95,97	0
14	HEA	N	515	60/60	0.98	0.09	47,52,65,66	0
14	HEA	N	516	60/60	0.98	0.07	42,48,69,74	0
15	CMO	A	520	2/2	0.98	0.05	39,39,39,41	0
14	HEA	A	516	60/60	0.98	0.06	32,40,56,64	0
21	CUA	B	228	2/2	0.99	0.03	41,41,41,42	0
27	ZN	F	99	1/1	0.99	0.02	48,48,48,48	0
18	NA	A	519	1/1	0.99	0.06	47,47,47,47	0
14	HEA	A	515	60/60	0.99	0.06	33,40,54,68	0
16	CU	N	517	1/1	1.00	0.02	49,49,49,49	0
16	CU	A	517	1/1	1.00	0.04	40,40,40,40	0
27	ZN	S	99	1/1	1.00	0.01	56,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

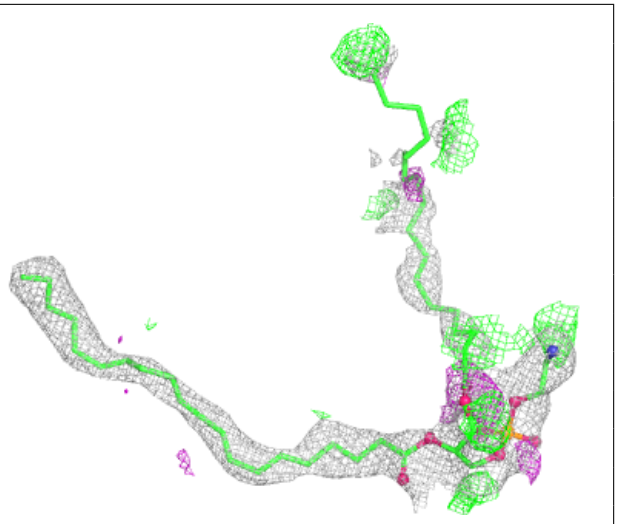
Electron density around PEK G 1263:

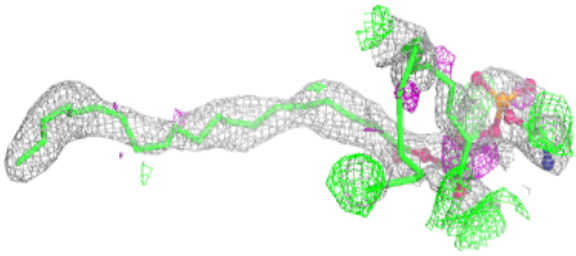
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

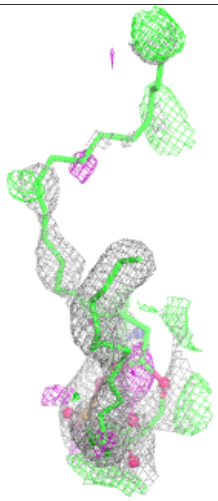


Electron density around PEK T 263:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

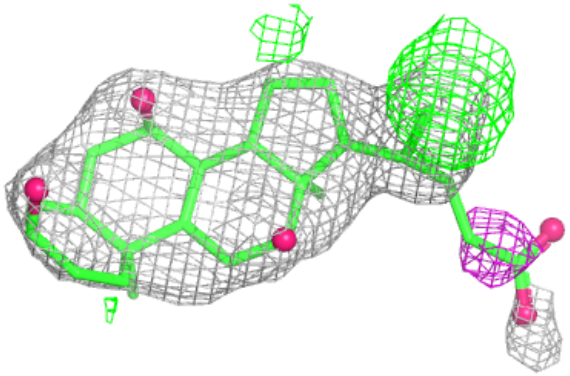


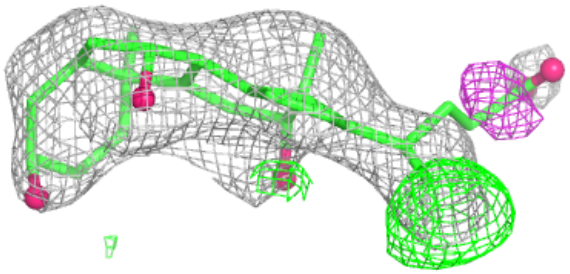


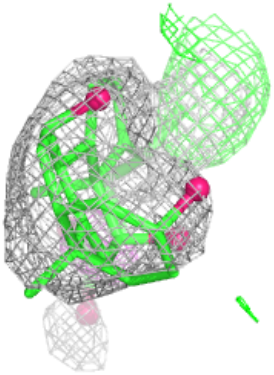


Electron density around CHD W 1059:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

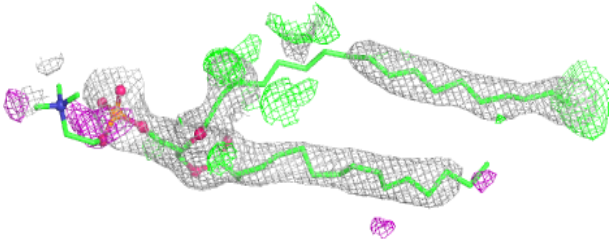


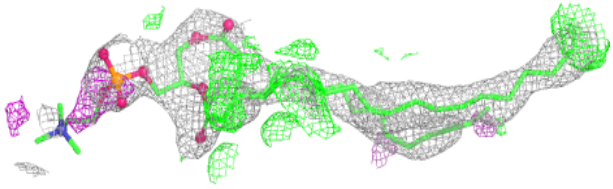


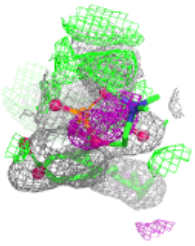


Electron density around PSC B 229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

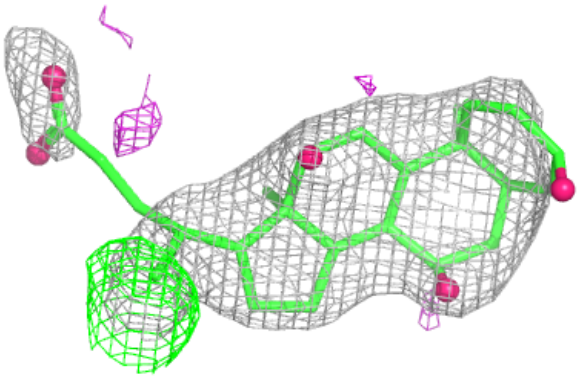


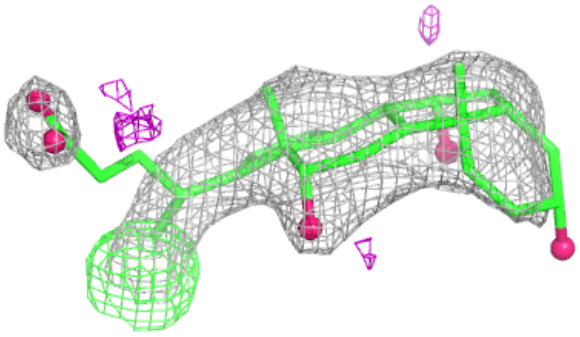


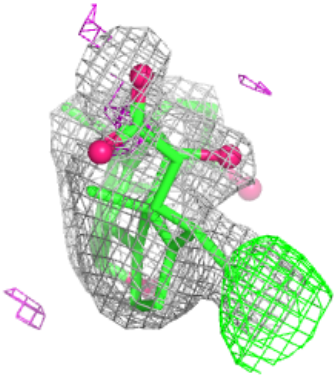


Electron density around CHD J 60:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

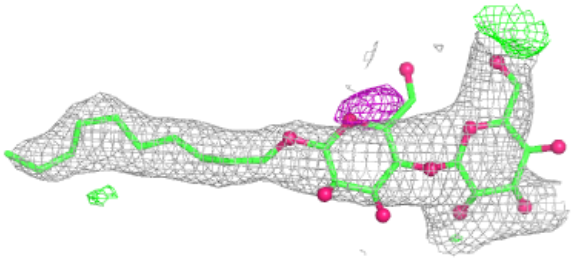


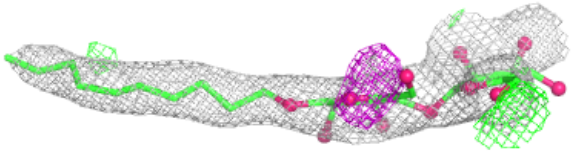


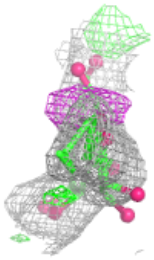


Electron density around DMU C 272:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

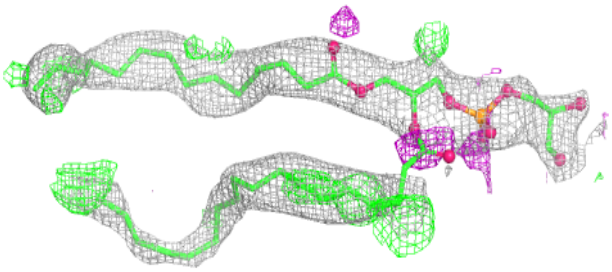


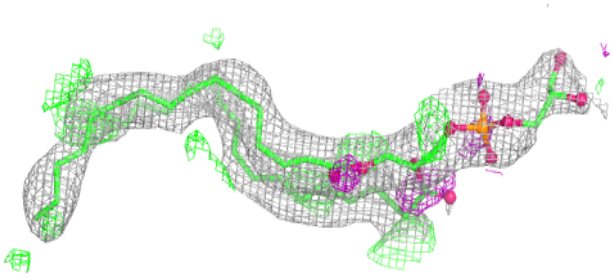


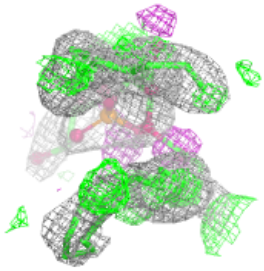


Electron density around PGV C 268:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

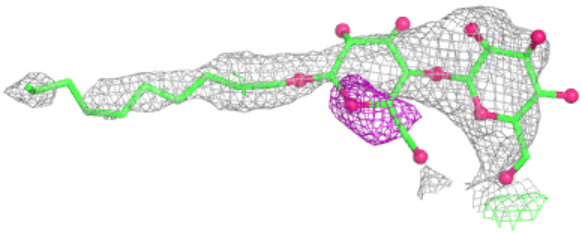


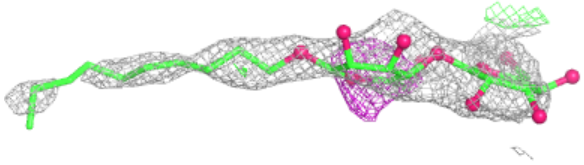


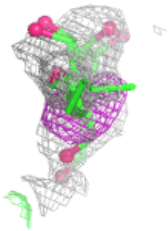


Electron density around DMU T 1272:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

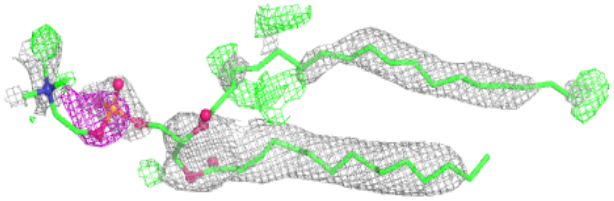


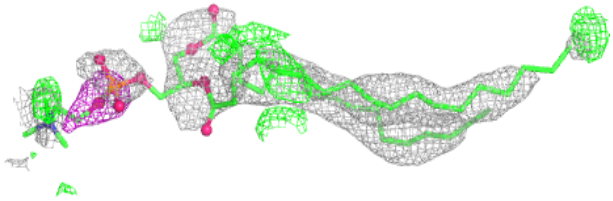


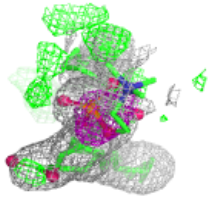


Electron density around PSC R 1229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

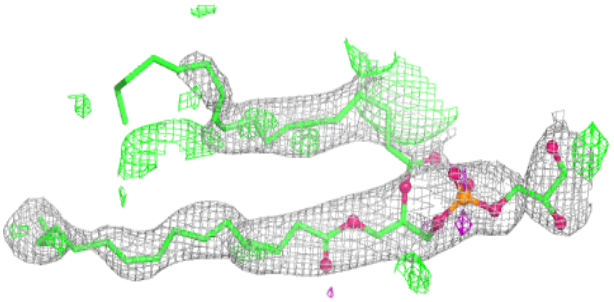


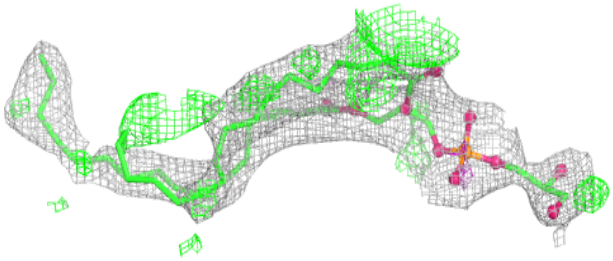


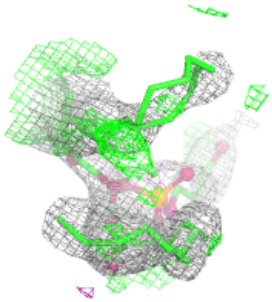


Electron density around PGV P 1268:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

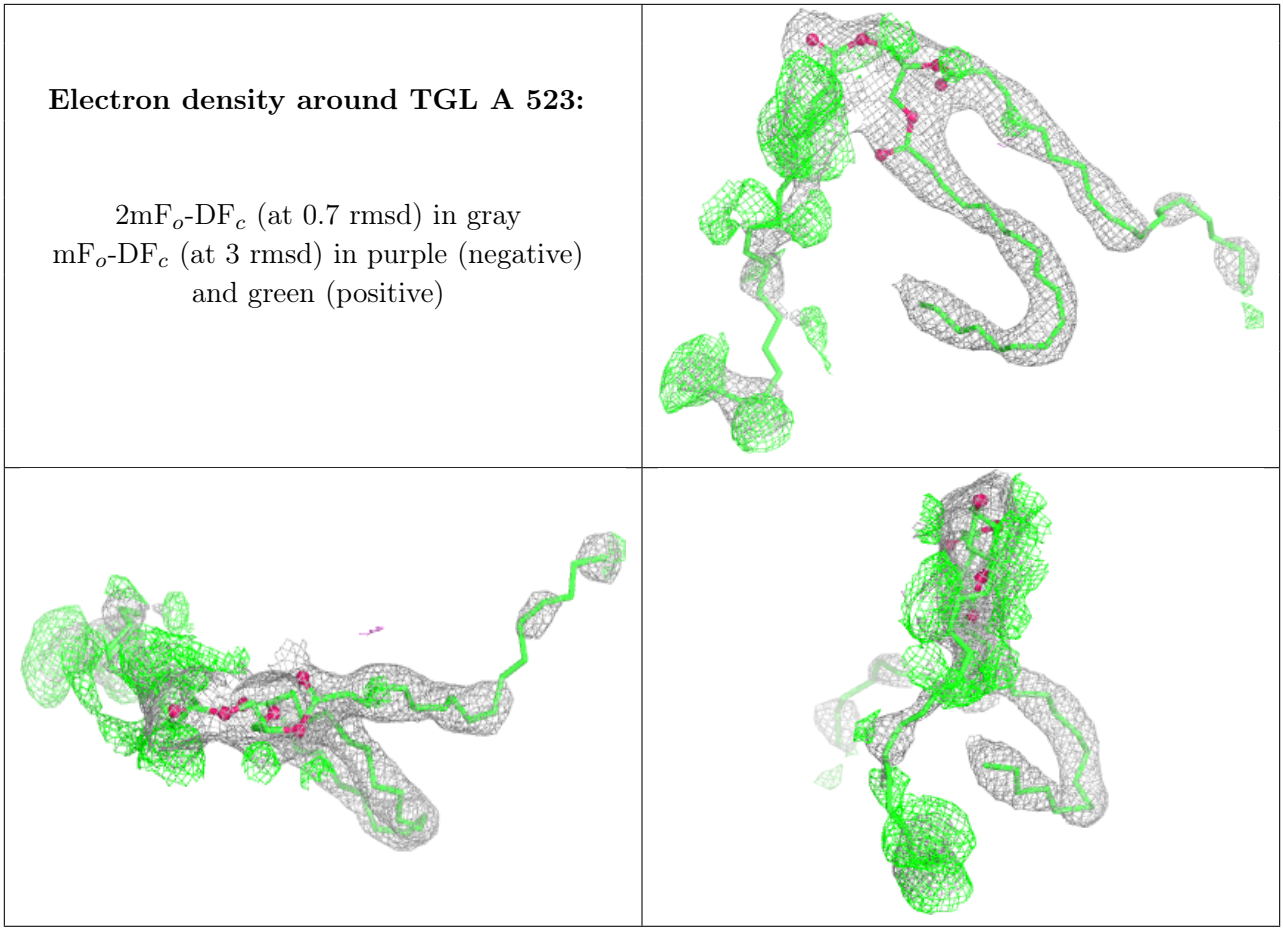






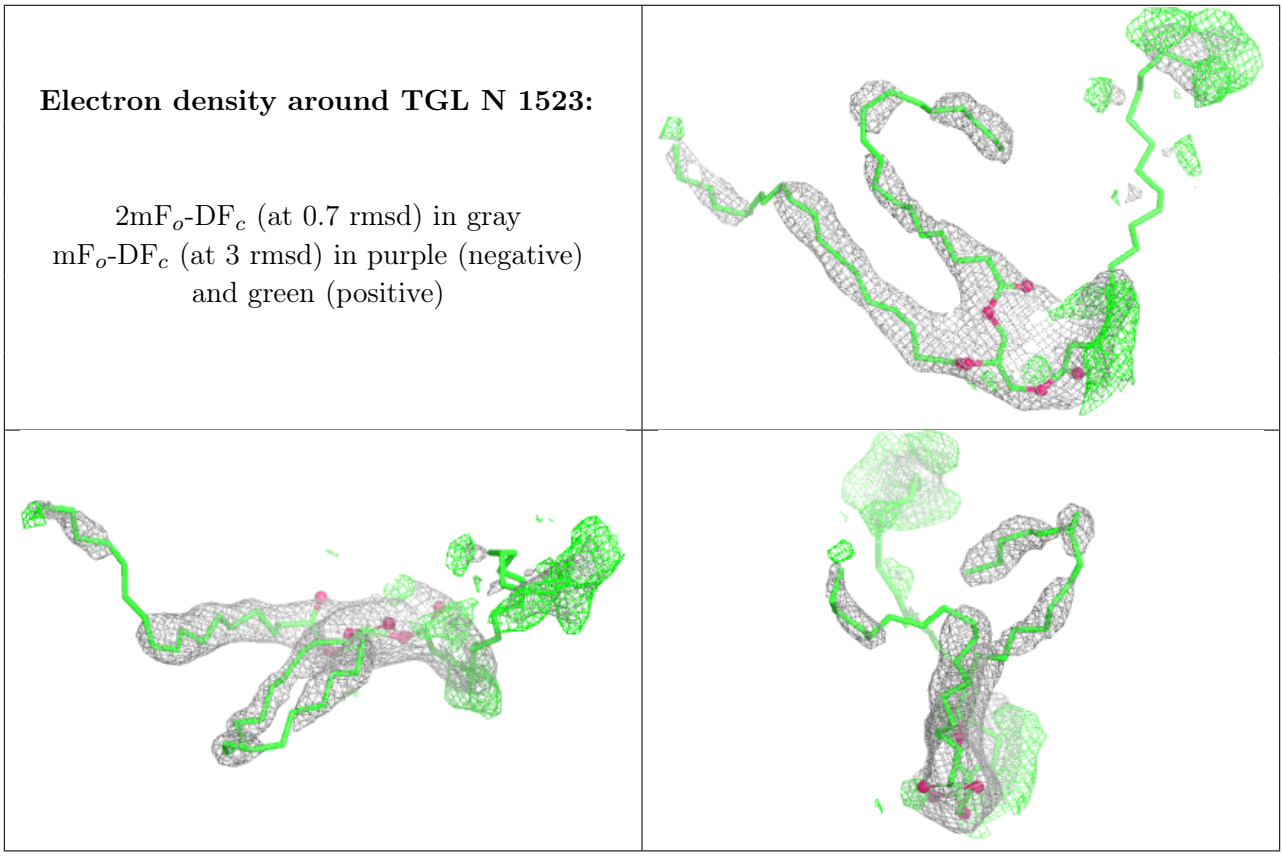
Electron density around TGL A 523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



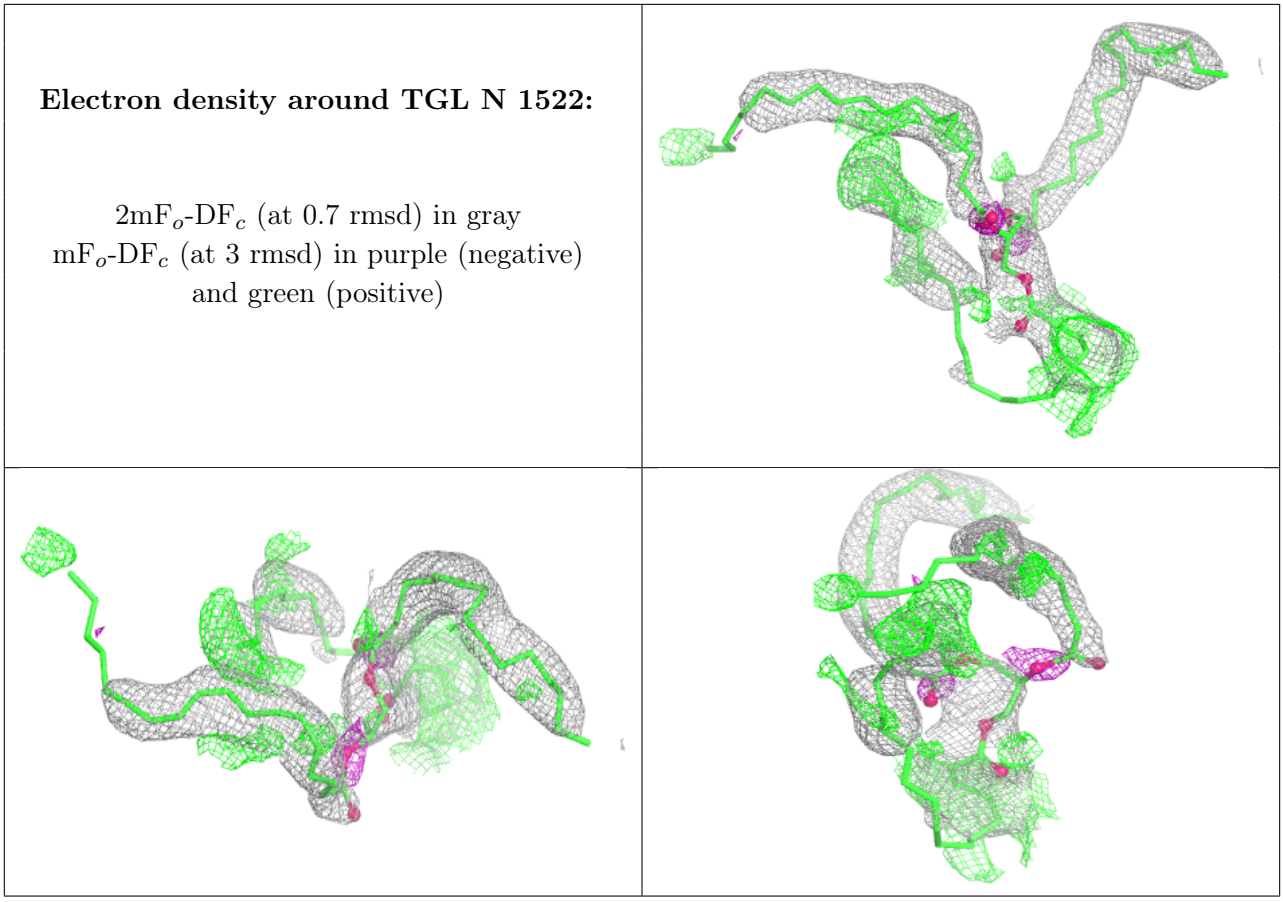
Electron density around TGL N 1523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



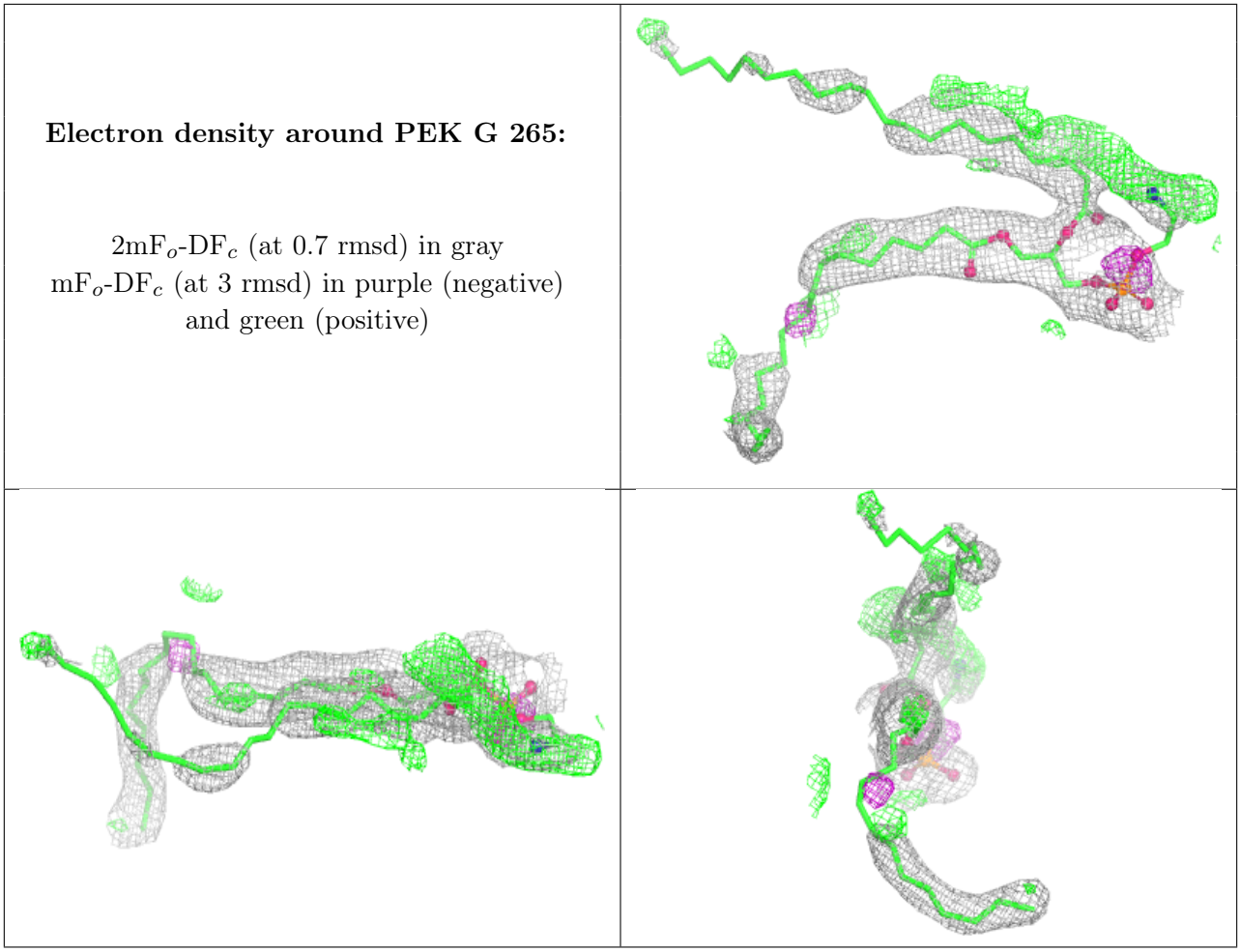
Electron density around TGL N 1522:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



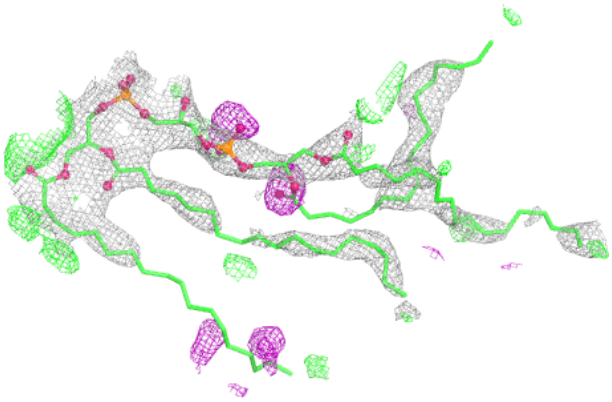
Electron density around PEK G 265:

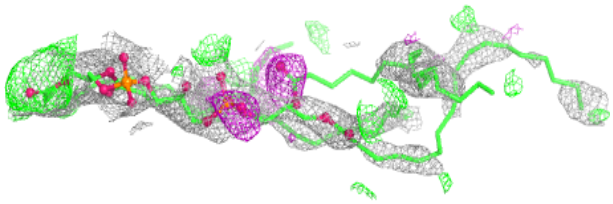
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

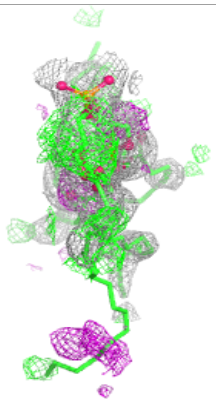


Electron density around CDL G 269:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

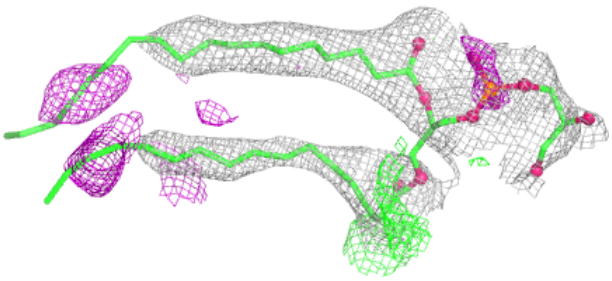


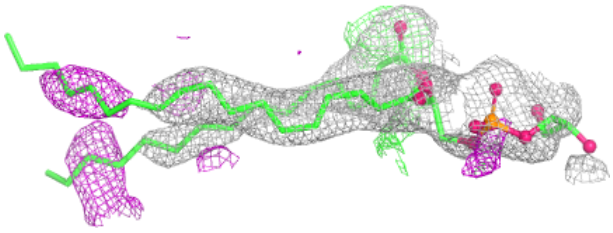


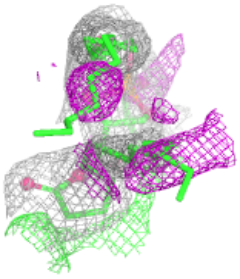


Electron density around PGV N 1524:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

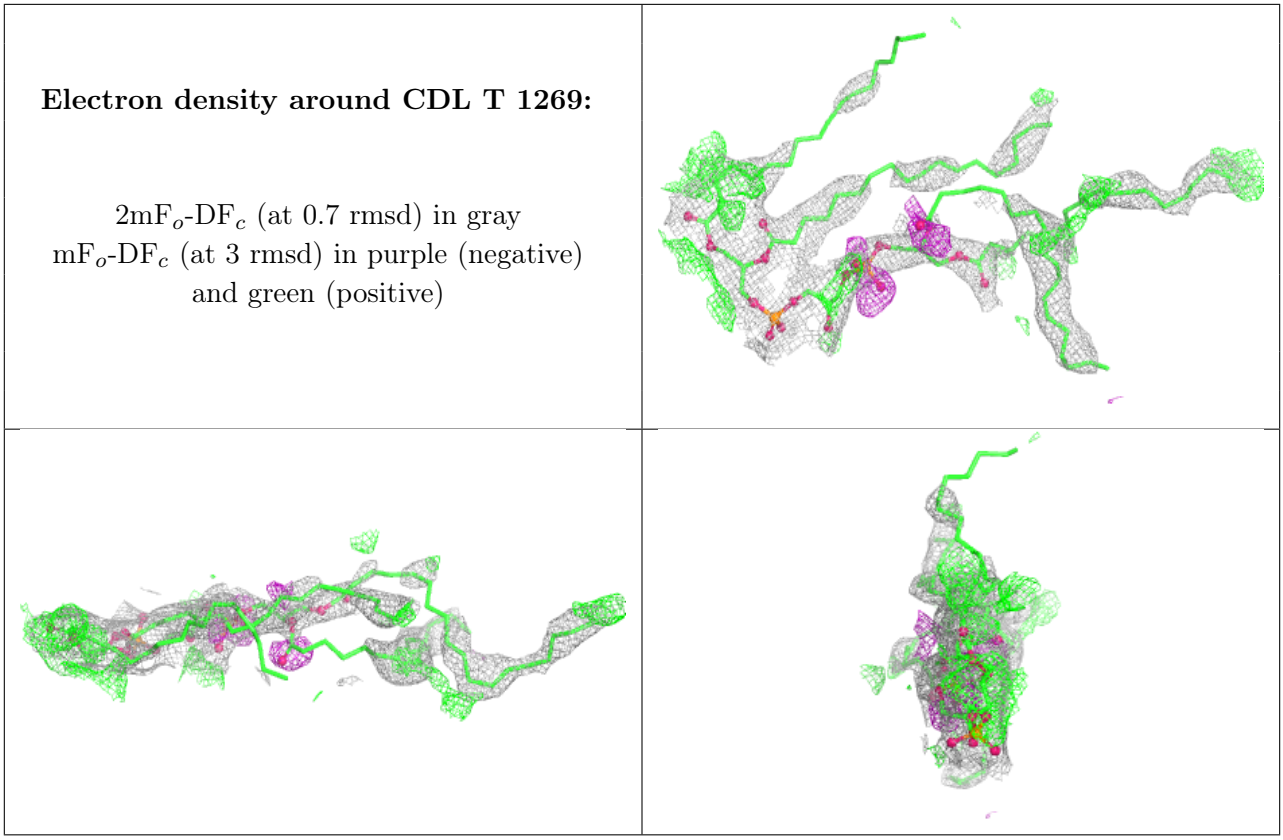






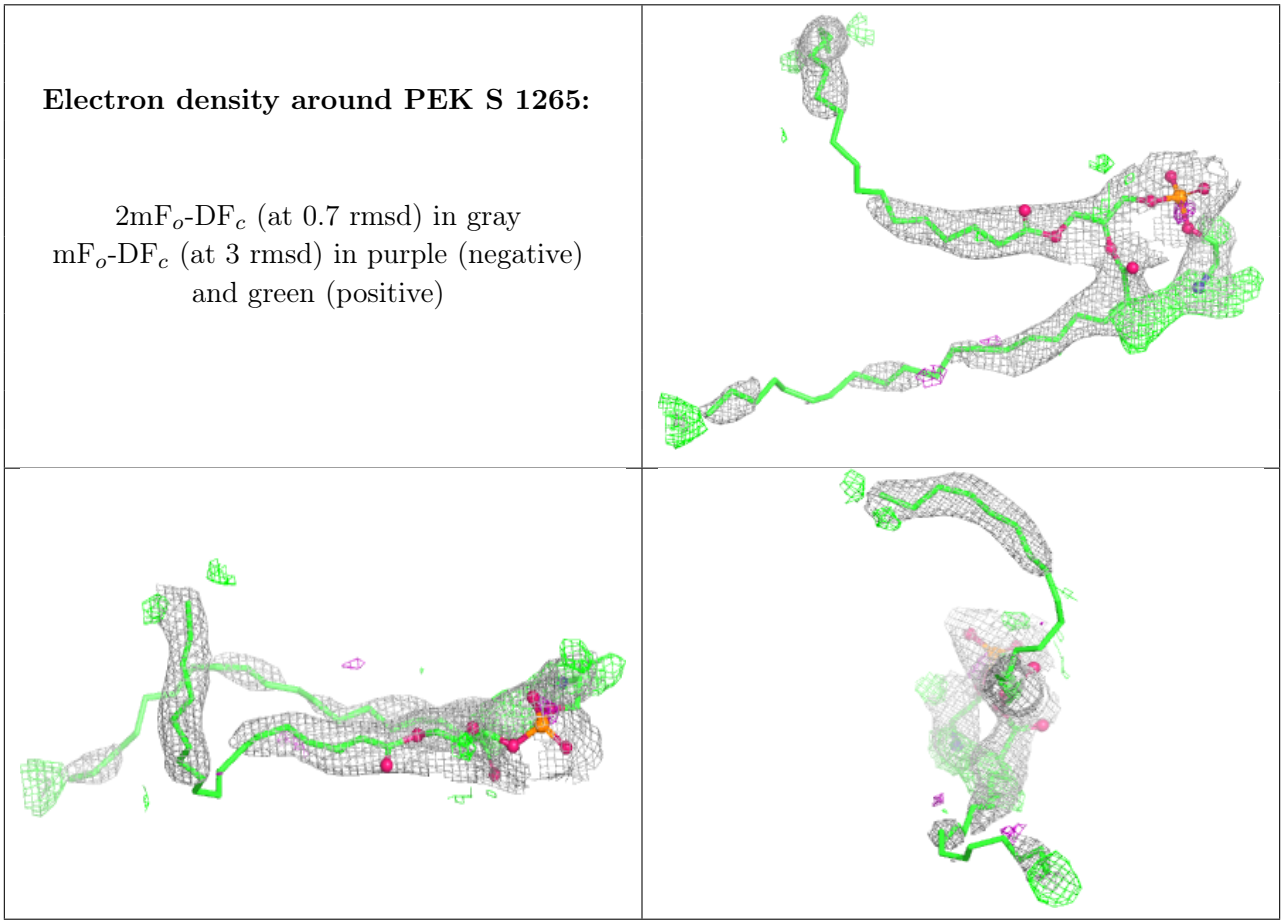
Electron density around CDL T 1269:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



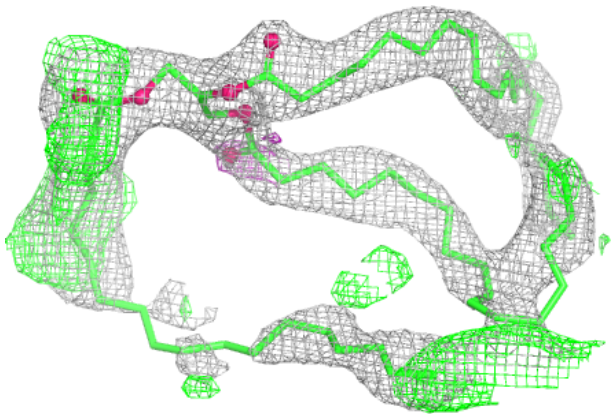
Electron density around PEK S 1265:

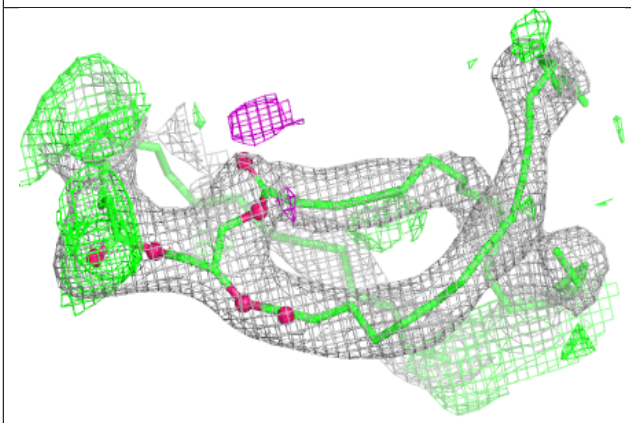
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

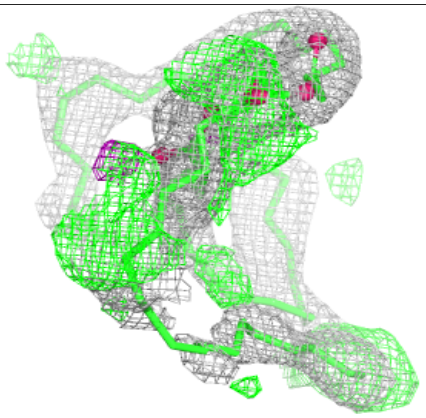


Electron density around TGL B 521:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

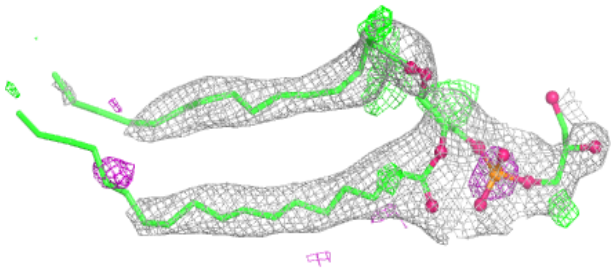


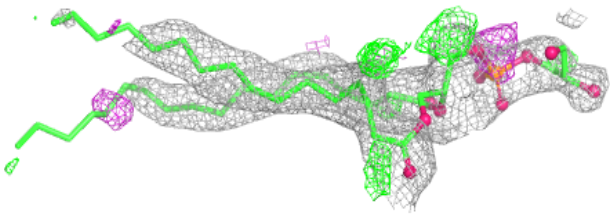


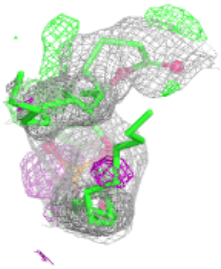


Electron density around PGV A 524:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

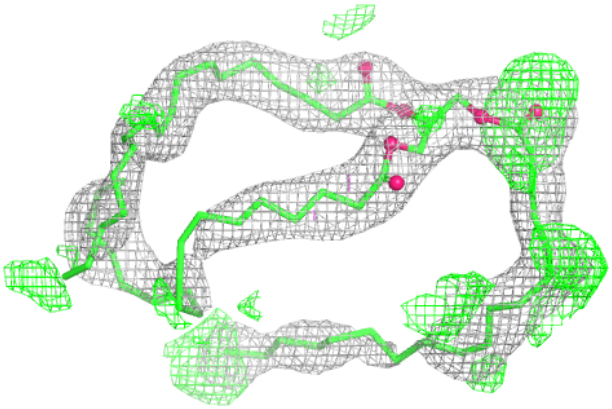


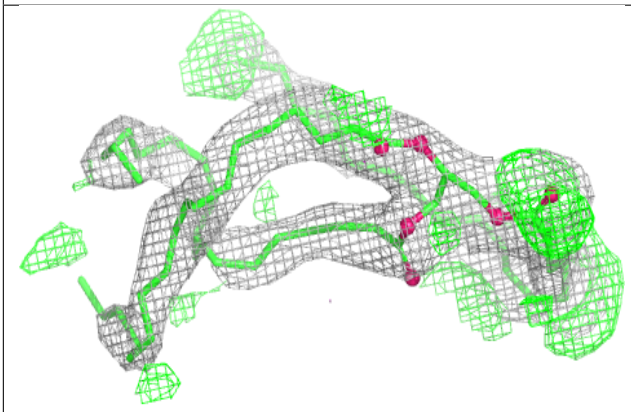


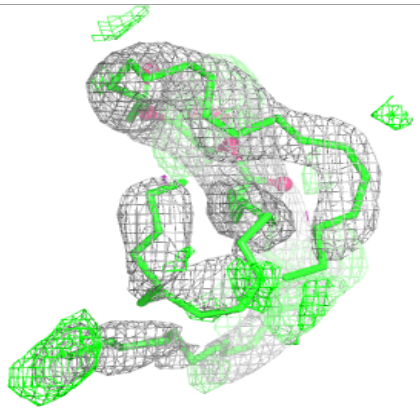


Electron density around TGL N 1521:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

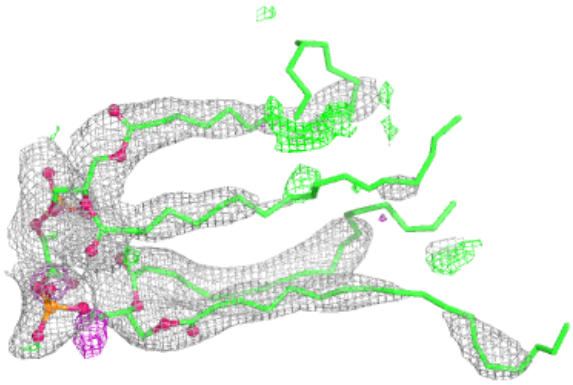


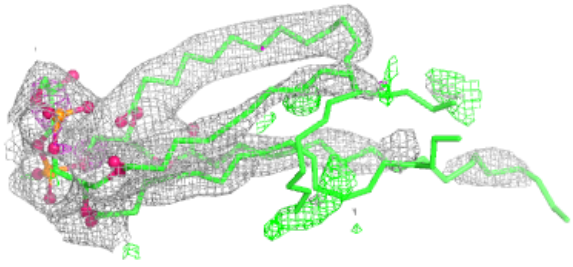


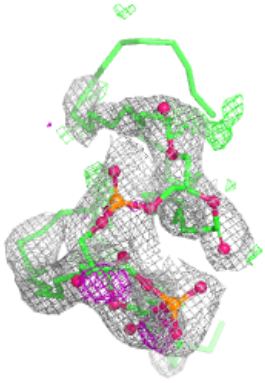


Electron density around CDL C 270:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

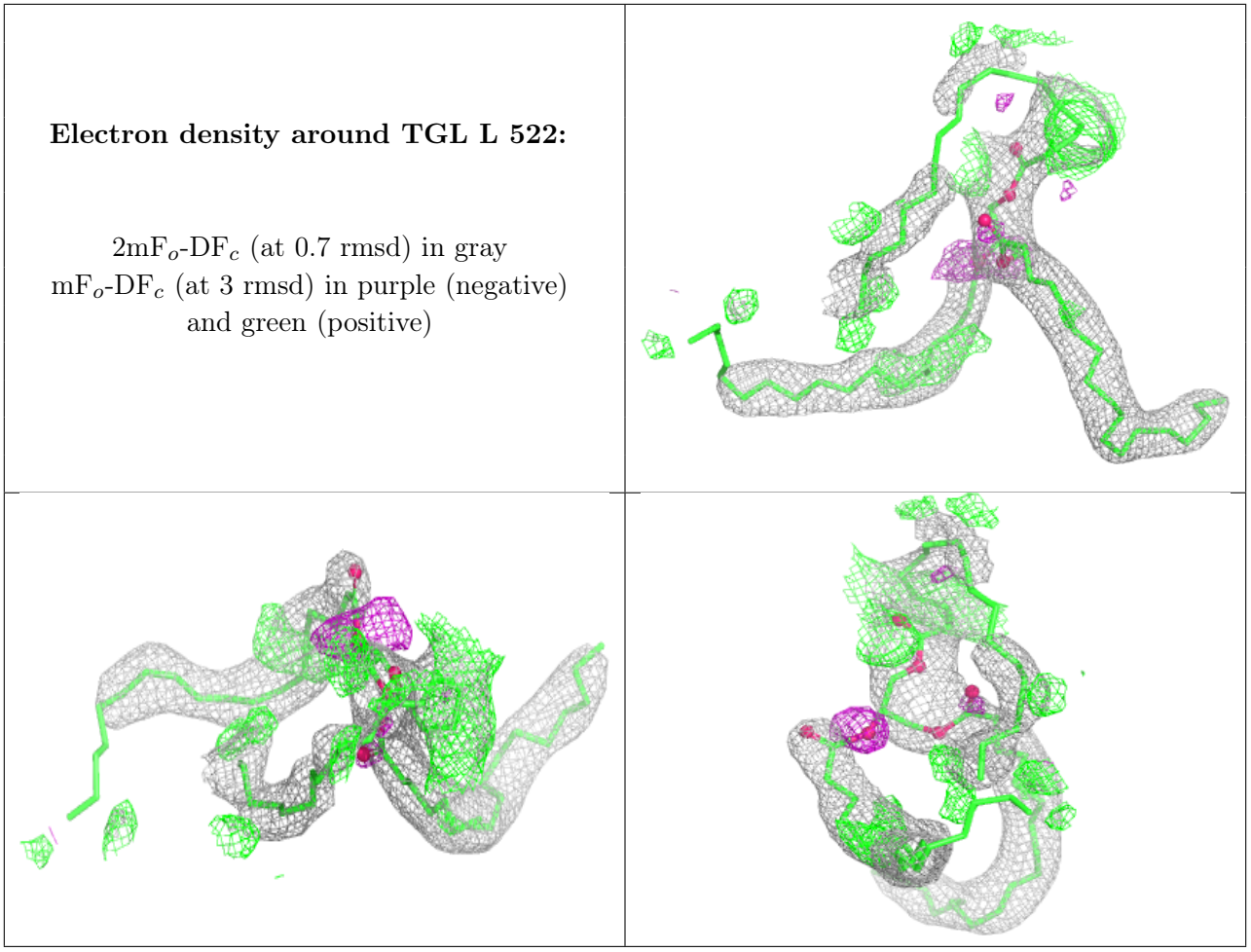






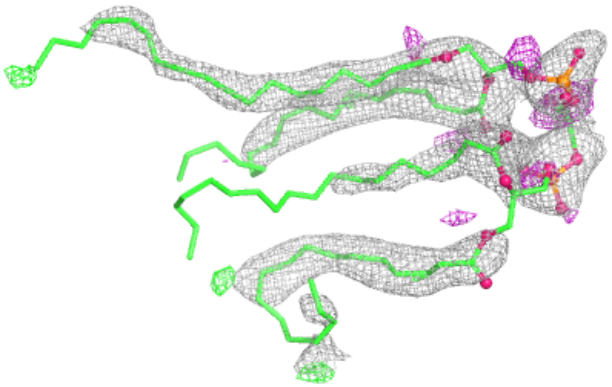
Electron density around TGL L 522:

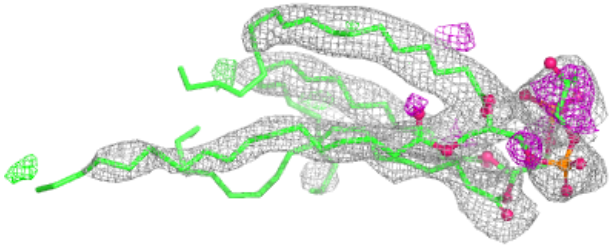
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

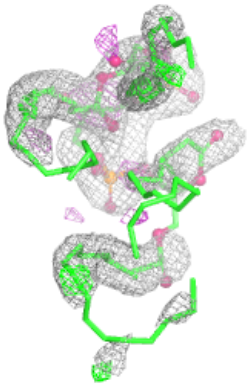


Electron density around CDL P 1270:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

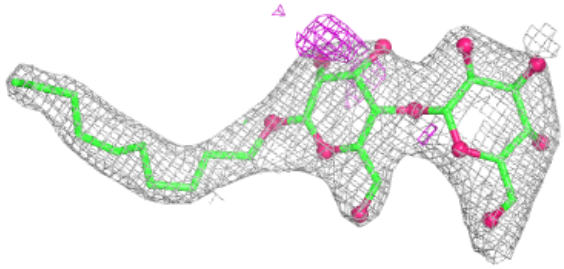


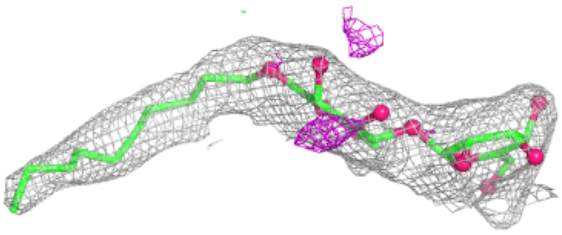


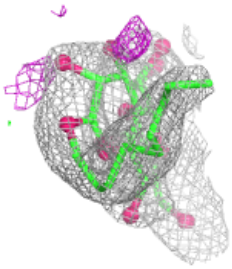


Electron density around DMU Z 1526:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

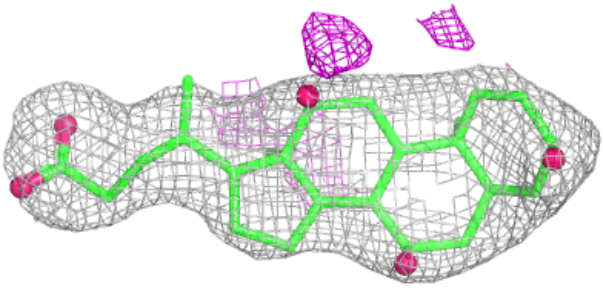


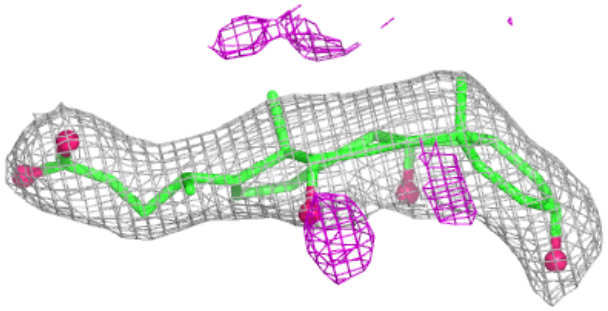


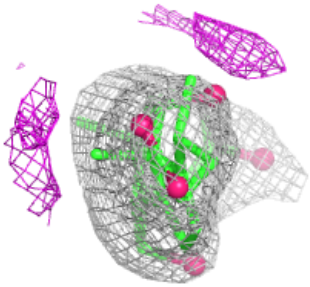


Electron density around CHD C 271:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

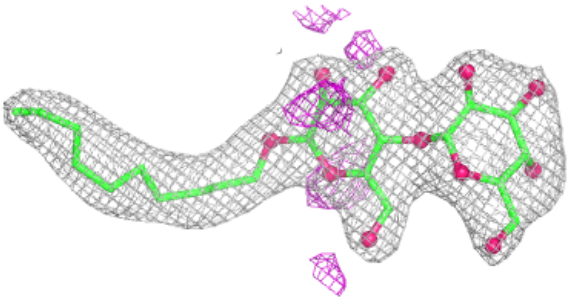


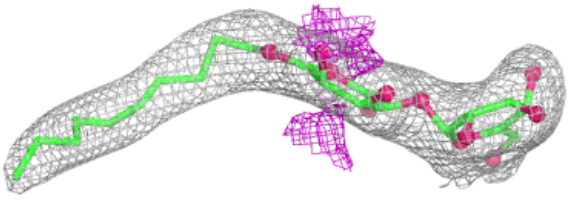


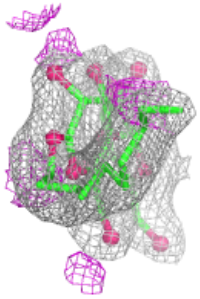


Electron density around DMU M 526:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

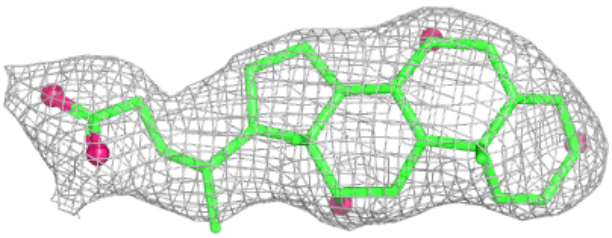


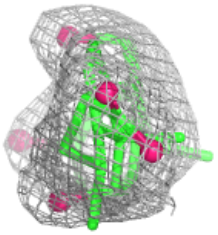




Electron density around CHD P 1271:

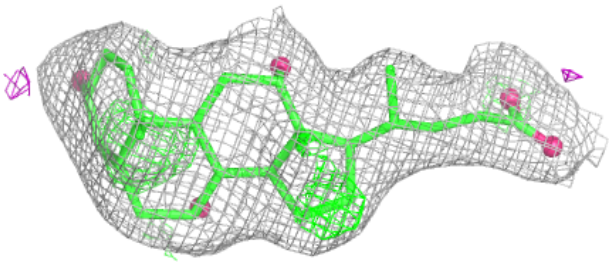
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

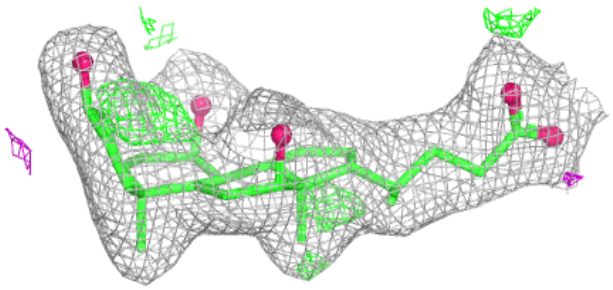


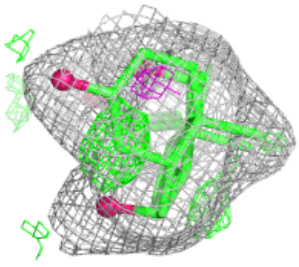


Electron density around CHD P 1525:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

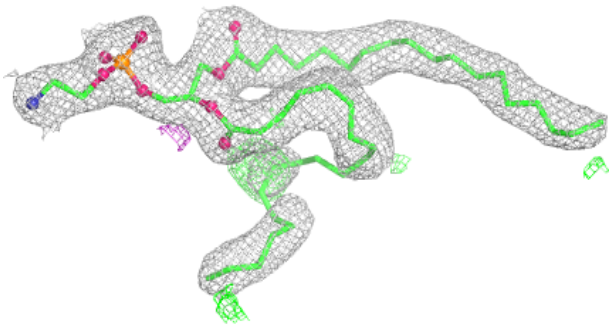


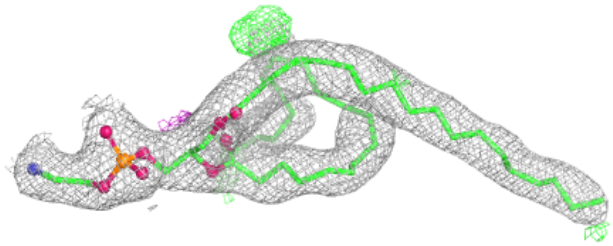


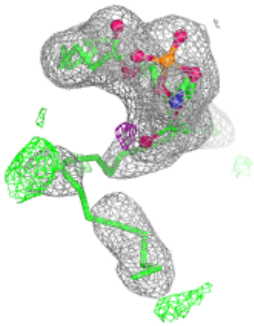


Electron density around PEK G 264:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

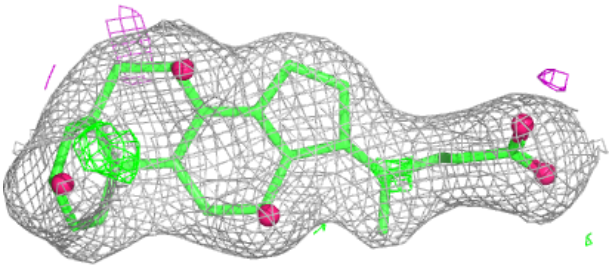


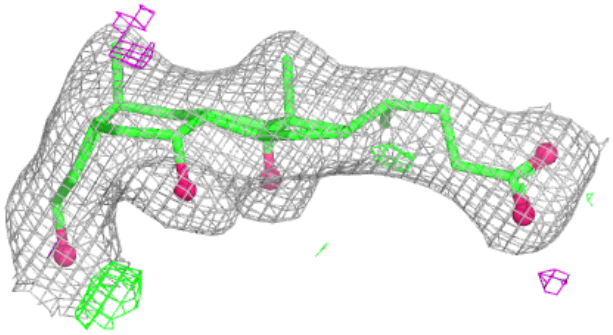


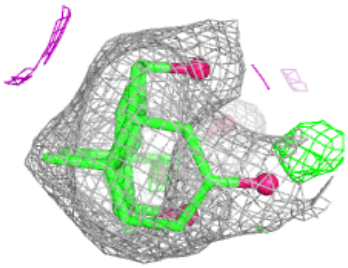


Electron density around CHD B 1085:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

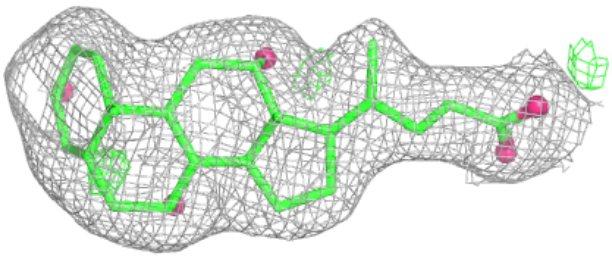


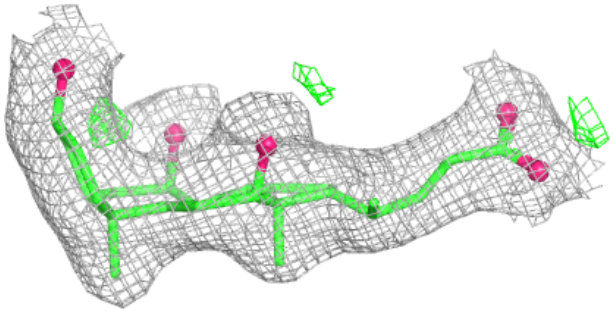


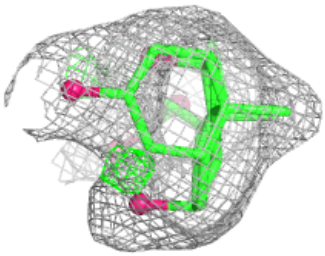


Electron density around CHD O 229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

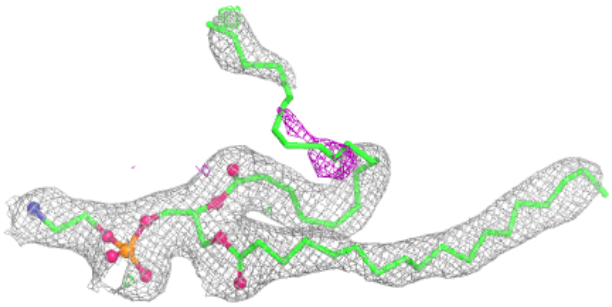


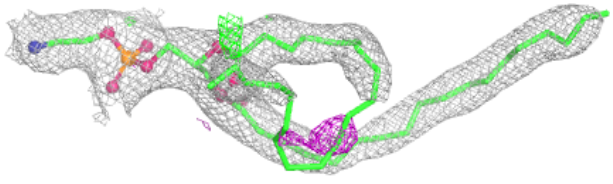


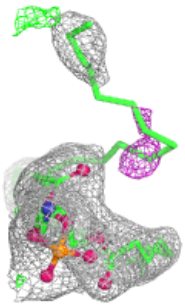


Electron density around PEK T 1264:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

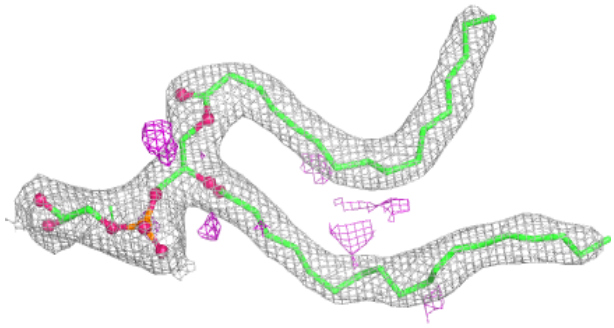


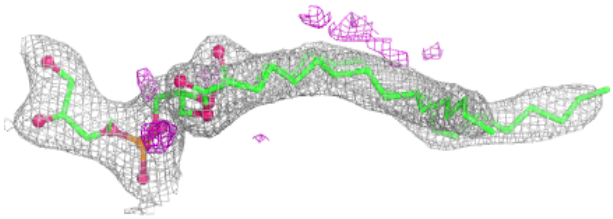


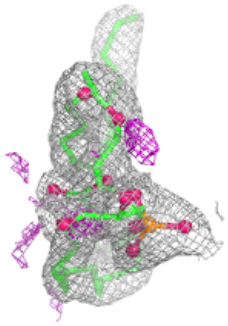


Electron density around PGV N 1266:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

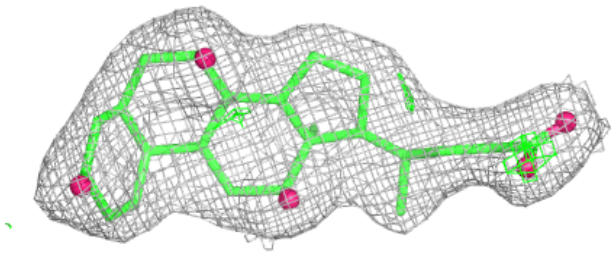


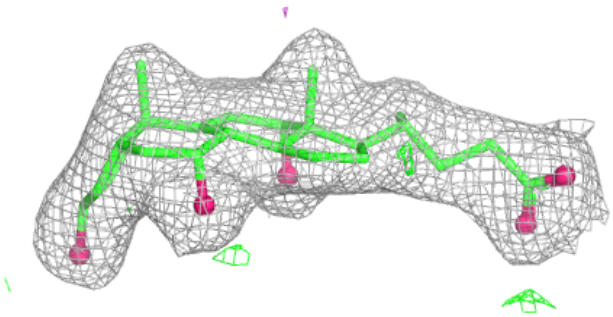


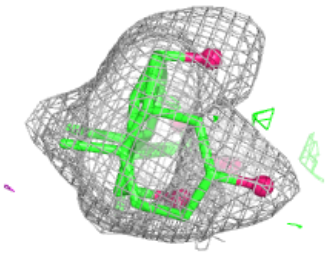


Electron density around CHD C 525:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

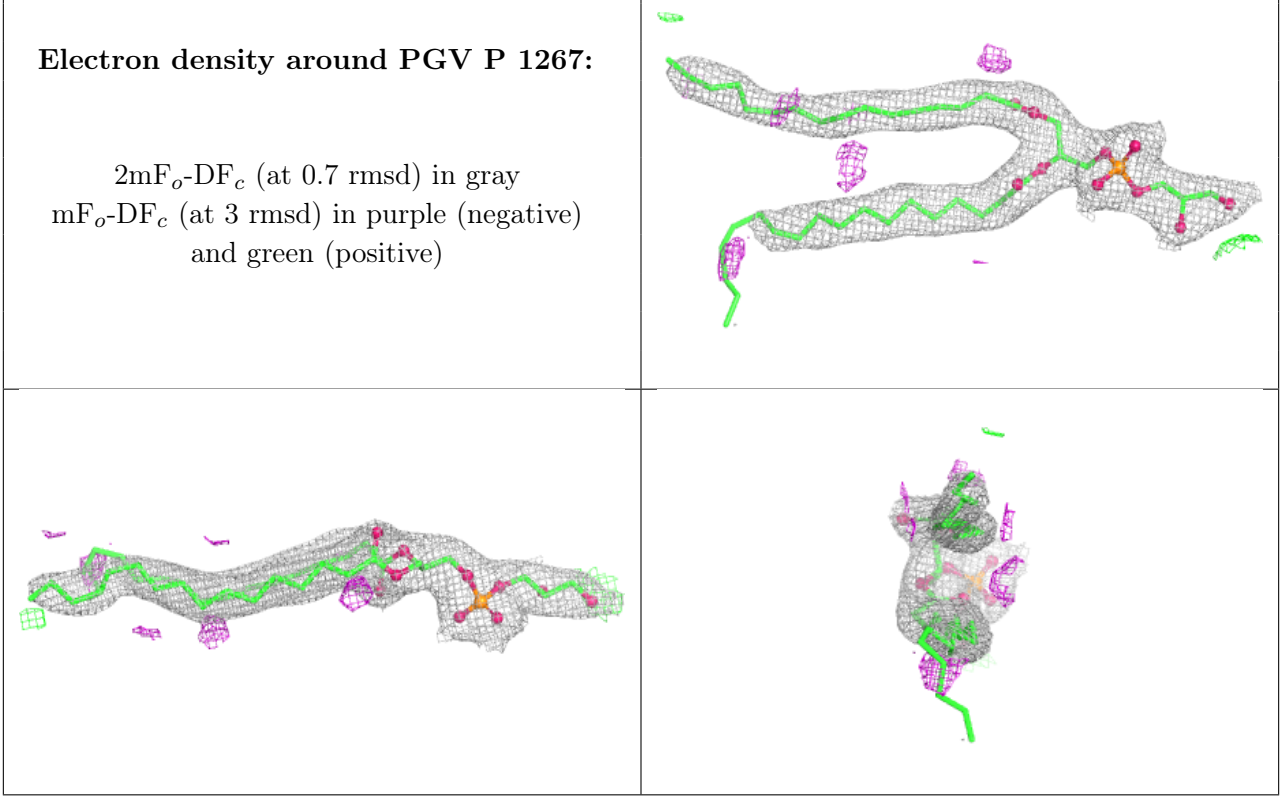






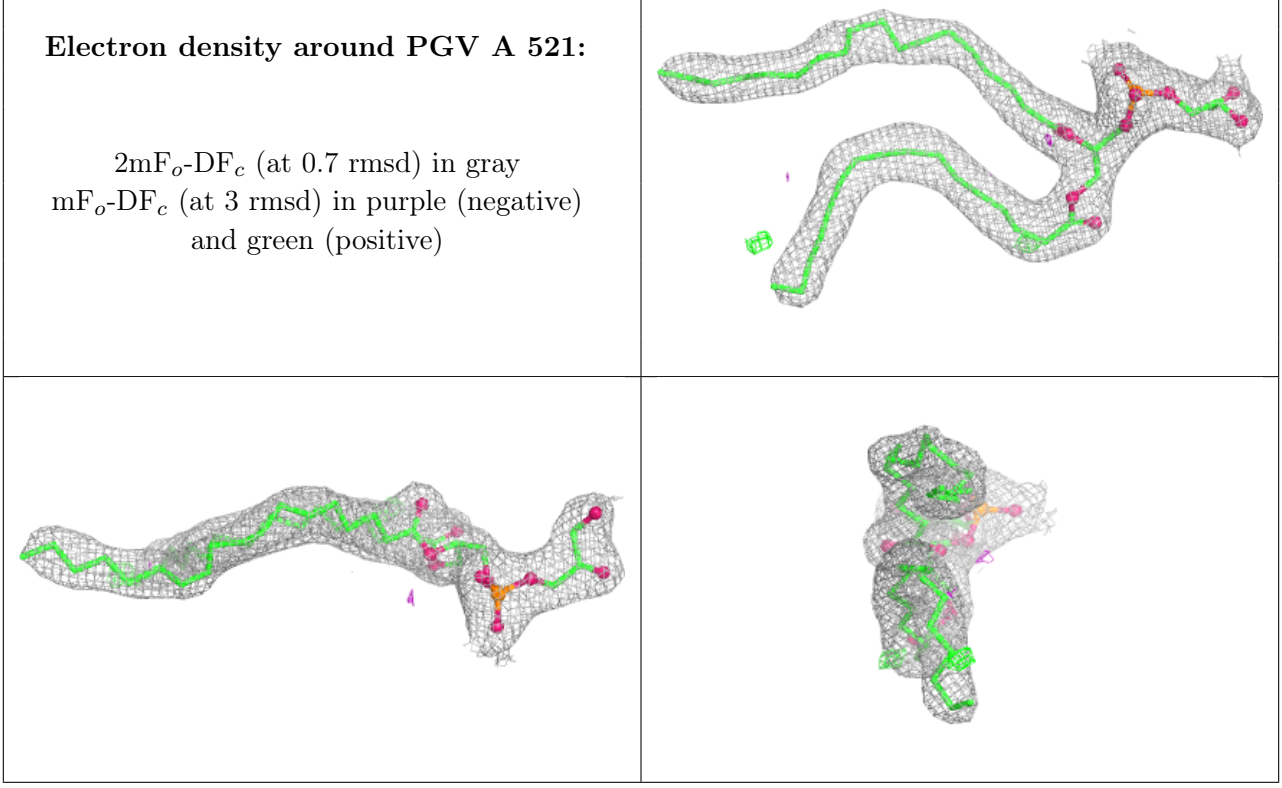
Electron density around PGV P 1267:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



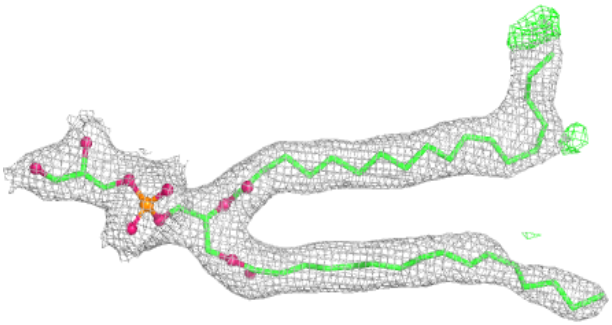
Electron density around PGV A 521:

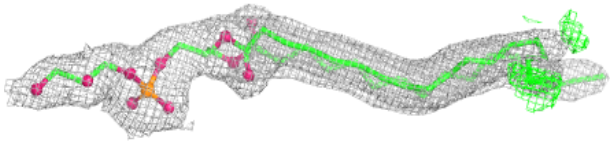
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

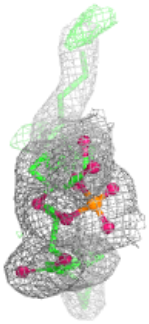


Electron density around PGV C 267:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

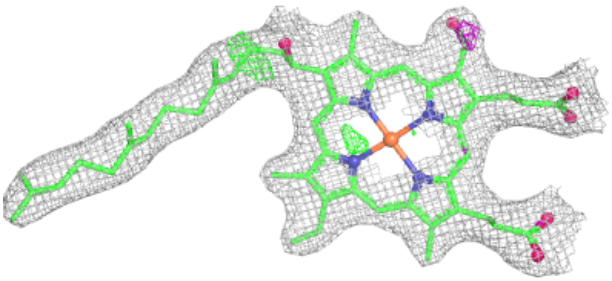


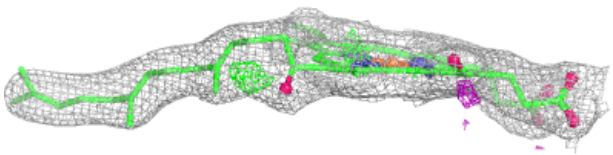




Electron density around HEA N 515:

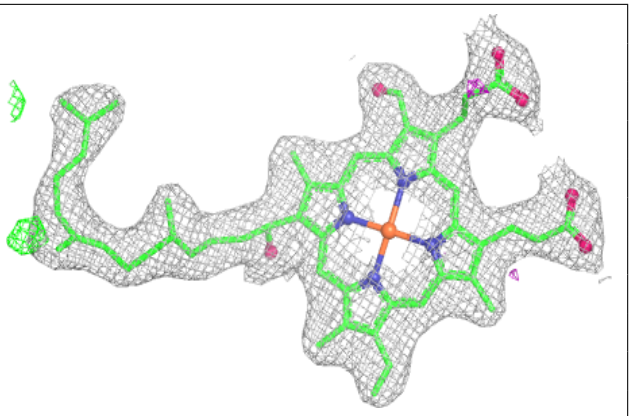
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

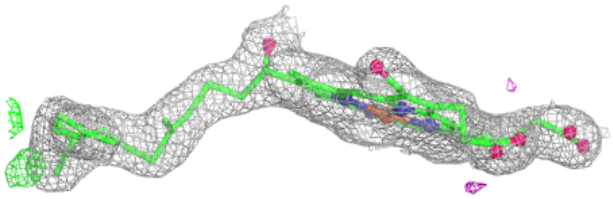




Electron density around HEA N 516:

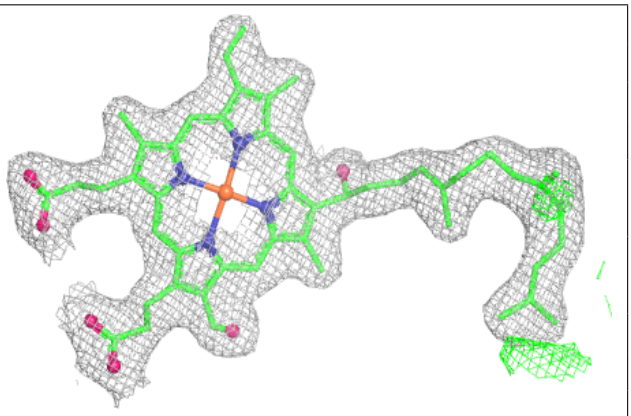
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

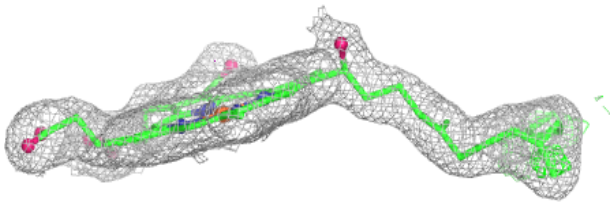


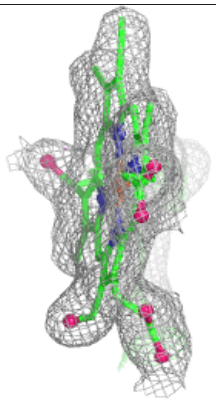


Electron density around HEA A 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

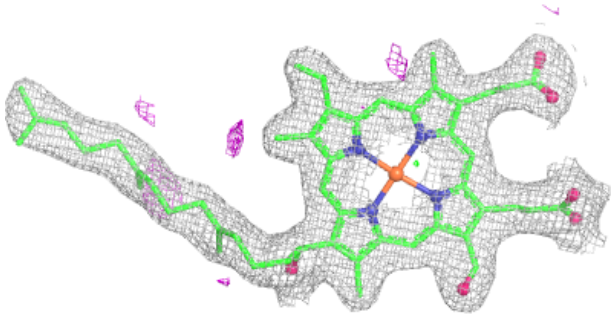


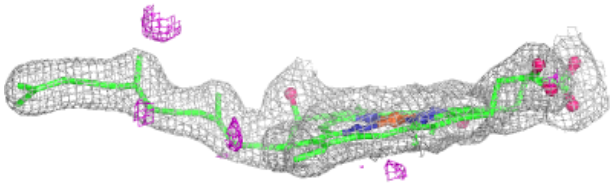


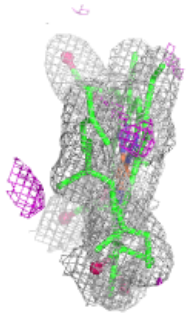


Electron density around HEA A 515:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.