Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:20 AM UTC

PDB ID	:	6WM2 / pdb_00006wm2
EMDB ID	:	EMD-21847
Title	:	Human V-ATPase in state 1 with SidK and ADP
Authors	:	Wang, L.; Wu, H.; Fu, T.M.
Deposited on	:	2020-04-20
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

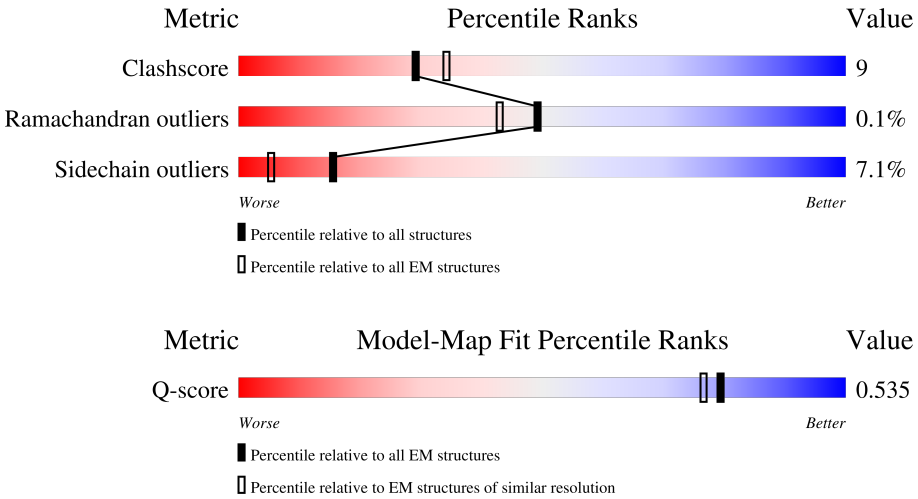
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	226	5% 70% 27%
1	I	226	7% 73% 27%
1	J	226	14% 76% 22%
2	K	118	13% 58% 36%

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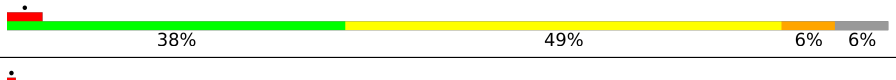
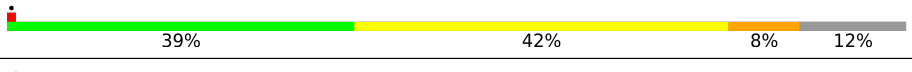
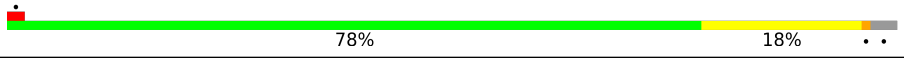
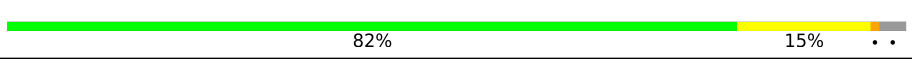
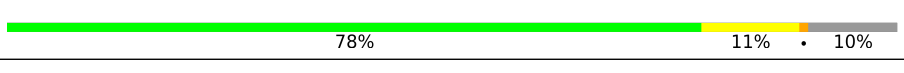
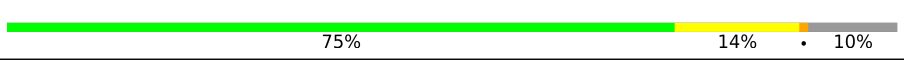
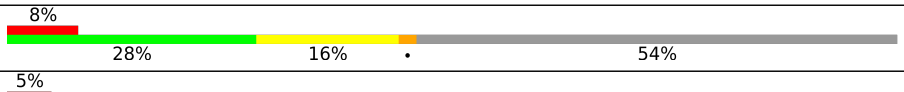
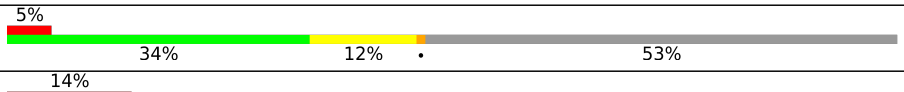
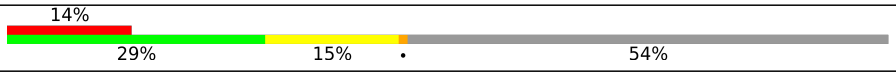
Mol	Chain	Length	Quality of chain
2	L	118	
2	M	118	
3	O	382	
4	P	483	
5	R	837	
6	A	617	
6	B	617	
6	C	617	
7	D	511	
7	E	511	
7	F	511	
8	X	573	
8	Y	573	
8	Z	573	
9	G	247	
10	N	119	
11	0	205	
12	1	155	
12	2	155	
12	3	155	
12	4	155	
12	5	155	
12	6	155	
12	7	155	
12	8	155	

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Mol	Chain	Length	Quality of chain
12	9	155	87% 8%
13	Q	351	81% 18%
14	S	81	77% 19% 5%
15	T	137	55% 6% 38%
16	U	470	30% 13% 56%
17	V	350	13% 86%
18	W	5	60% 40%
19	a	4	25% 75%
20	b	2	50% 50%
20	c	2	50% 50%
20	d	2	50% 50%
20	s	2	50% 50%
20	u	2	100%
21	r	11	36% 64%

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
19	NGA	a	2	X	-	-	-
21	NAG	r	1	X	-	-	-
21	MAN	r	11	X	-	-	-
24	PTY	0	307	X	-	-	-
24	PTY	R	904	X	-	-	-
24	PTY	U	503	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 73243 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
1	I	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		
1	J	225	Total	C	N	O	S	0	0
			1822	1143	322	347	10		

- Molecule 2 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
2	L	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
2	M	114	Total	C	N	O	S	0	0
			938	573	179	183	3		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	359	Total	C	N	O	S	0	0
			2916	1869	493	545	9		

- Molecule 4 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	427	Total	C	N	O	S	0	0
			3508	2228	605	648	27		

- Molecule 5 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	753	Total	C	N	O	S	0	0
			6141	4013	1020	1068	40		

- Molecule 6 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	600	Total	C	N	O	S	0	0
			4652	2949	785	890	28		
6	B	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
6	C	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 7 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	460	Total	C	N	O	S	0	0
			3600	2284	616	680	20		
7	E	460	Total	C	N	O	S	0	0
			3589	2278	616	676	19		
7	F	460	Total	C	N	O	S	0	0
			3596	2282	616	678	20		

- Molecule 8 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	262	Total	C	N	O	S	0	0
			2111	1339	354	408	10		
8	Y	267	Total	C	N	O	S	0	0
			2136	1355	359	411	11		
8	Z	262	Total	C	N	O	S	0	0
			2105	1333	354	408	10		

- Molecule 9 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	213	Total	C	N	O	S	0	0
			1713	1087	309	312	5		

- Molecule 10 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0	204	Total	C	N	O	S	0	0
			1495	988	238	259	10		

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	7	150	Total	C	N	O	S	0	0
			1059	695	166	191	7		
12	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
12	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 13 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	350	Total	C	N	O	S	0	0
			2829	1825	461	530	13		

- Molecule 14 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

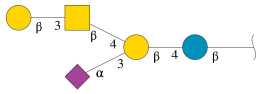
- Molecule 16 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	10		

- Molecule 17 is a protein called Renin receptor.

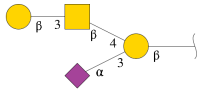
Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	50	Total	C	N	O	S	0	0
			417	283	58	73	3		

- Molecule 18 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	5	Total	C	N	O	0	0
			68	37	2	29		

- Molecule 19 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
19	a	4	Total	C	N	O	0	0
			56	31	2	23		

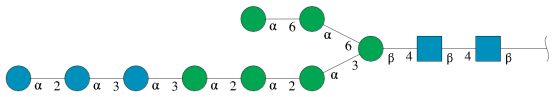
- Molecule 20 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



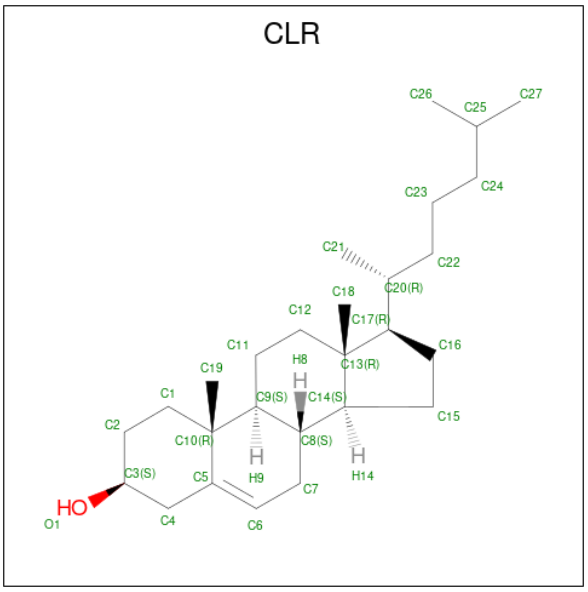
Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	2	Total	C	N	O	0	0
			28	16	2	10		
20	b	2	Total	C	N	O	0	0
			28	16	2	10		
20	c	2	Total	C	N	O	0	0
			28	16	2	10		
20	d	2	Total	C	N	O	0	0
			28	16	2	10		
20	s	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 21 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



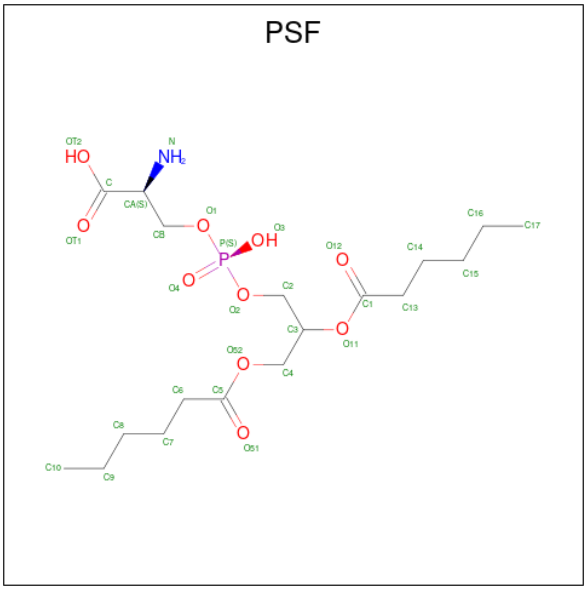
Mol	Chain	Residues	Atoms				AltConf	Trace
21	r	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 22 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



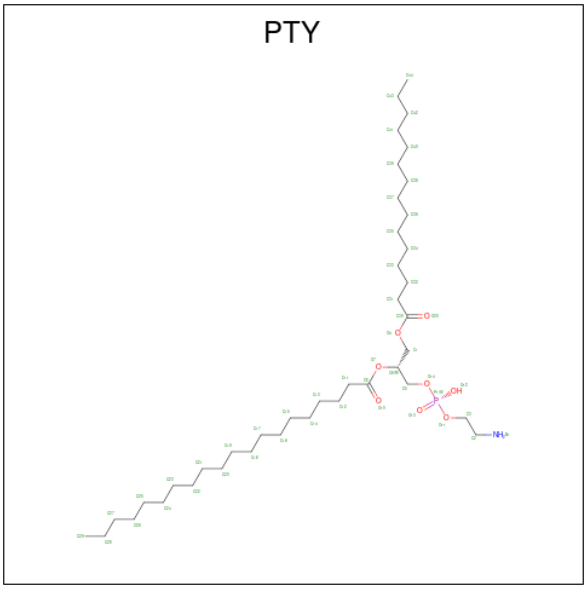
Mol	Chain	Residues	Atoms	AltConf
22	R	1	Total C O 28 27 1	0
22	0	1	Total C O 28 27 1	0
22	5	1	Total C O 28 27 1	0
22	V	1	Total C O 28 27 1	0

- Molecule 23 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
23	R	1	Total C N O P 30 18 1 10 1	0

- Molecule 24 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
24	R	1	Total C O 32 27 5	0
24	R	1	Total C N O P 29 20 1 7 1	0
24	0	1	Total C O P 17 9 7 1	0
24	0	1	Total C N O P 48 38 1 8 1	0
24	2	1	Total C N O P 29 20 1 7 1	0
24	5	1	Total C N O P 35 25 1 8 1	0
24	6	1	Total C O P 21 13 7 1	0
24	7	1	Total C N O P 42 32 1 8 1	0
24	8	1	Total C N O P 50 40 1 8 1	0
24	8	1	Total C O 33 28 5	0
24	Q	1	Total C N O P 30 20 1 8 1	0

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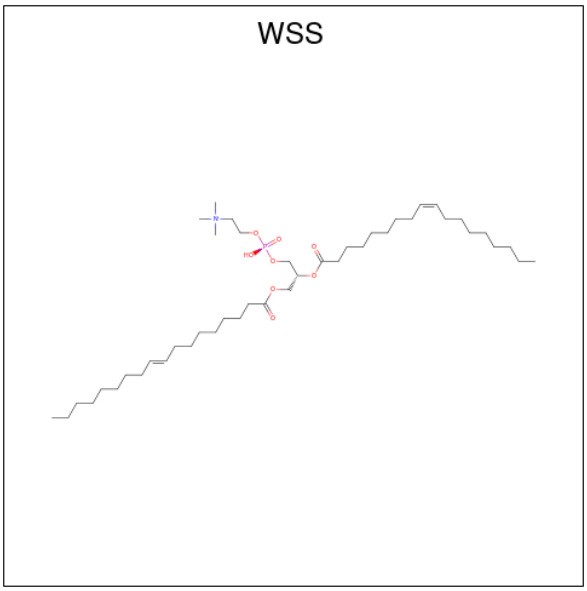
Mol	Chain	Residues	Atoms	AltConf
24	U	1	Total C O 26 21 5	0
24	V	1	Total C N O P 29 20 1 7 1	0

- Molecule 25 is tri(methyl)-[2-[[(2 {R})-2-[({Z})-octadec-9-enoyl]oxy-3-[({E})-1-oxidanylideneoctadec-9-enoxy]propoxy]-oxidanyl-phosphoryl]oxyethyl]azanium (CCD ID: WSS) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
25	R	1	Total C N O P 40 30 1 8 1	0
25	0	1	Total C N O P 44 34 1 8 1	0
25	0	1	Total C N O P 41 31 1 8 1	0
25	0	1	Total C N O P 26 16 1 8 1	0
25	0	1	Total C O P 31 22 8 1	0
25	1	1	Total C N O P 34 24 1 8 1	0
25	3	1	Total C O P 41 32 8 1	0
25	U	1	Total C N O P 39 29 1 8 1	0

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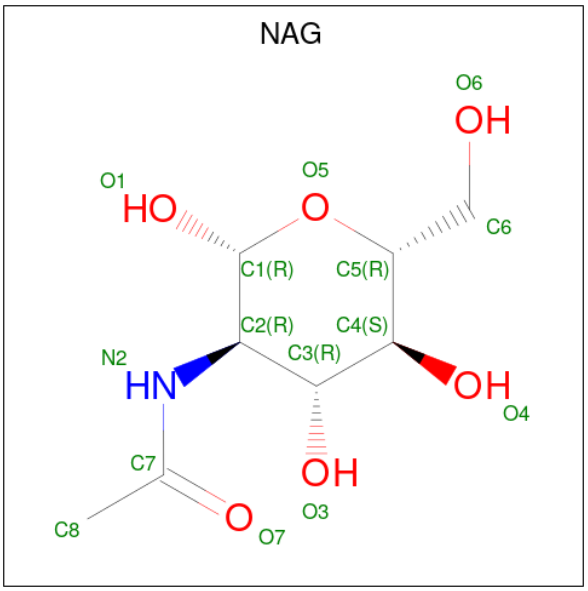
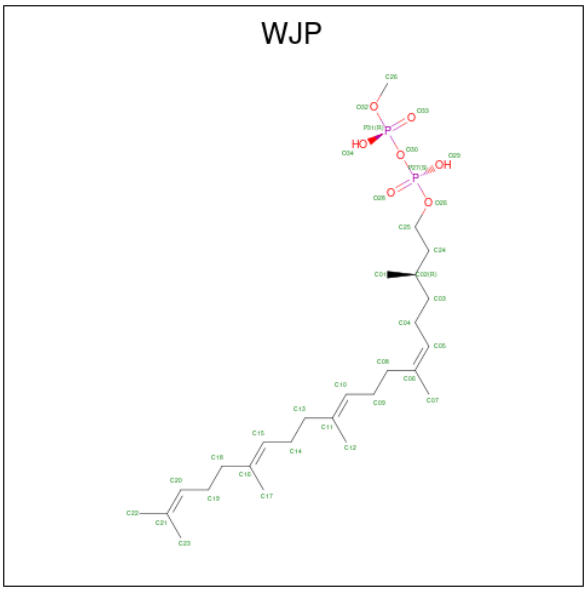
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	V	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 26 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



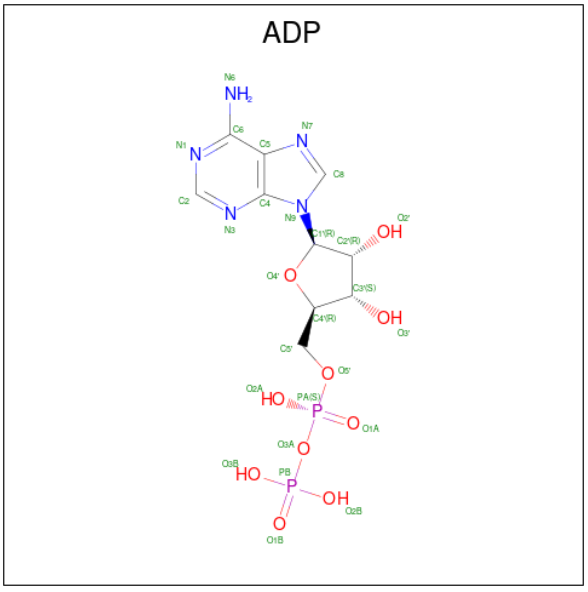
Mol	Chain	Residues	Atoms				AltConf
26	R	1	Total	C	N	O	0
			14	8	1	5	
26	U	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 27 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



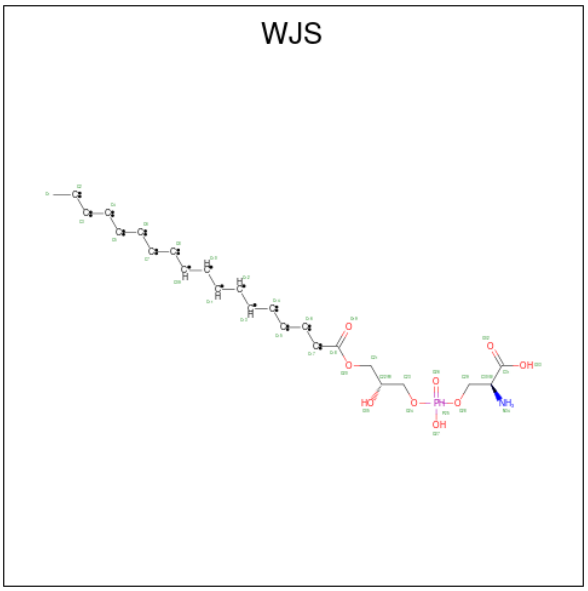
Mol	Chain	Residues	Atoms				AltConf
27	R	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
28	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 29 is (2 {S})-2-$l^{4}-azanyl-3-[[(2 {R})-3-octadecanoyloxy-2-oxidanyl-propoxy]-oxidanyl-oxidanylidene-$l^{6}-phosphanyl]oxy-propanoic acid (CCD ID: WJS) (formula: $C_{24}H_{20}NO_9P$).

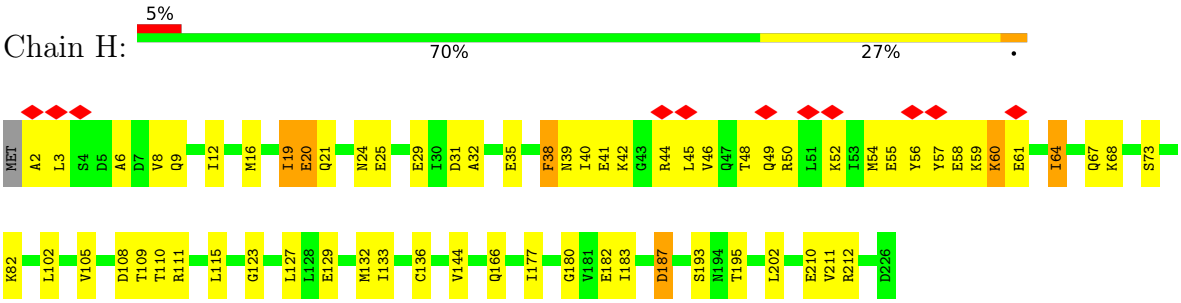


Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	N	O	P	0
			27	16	1	9	1	

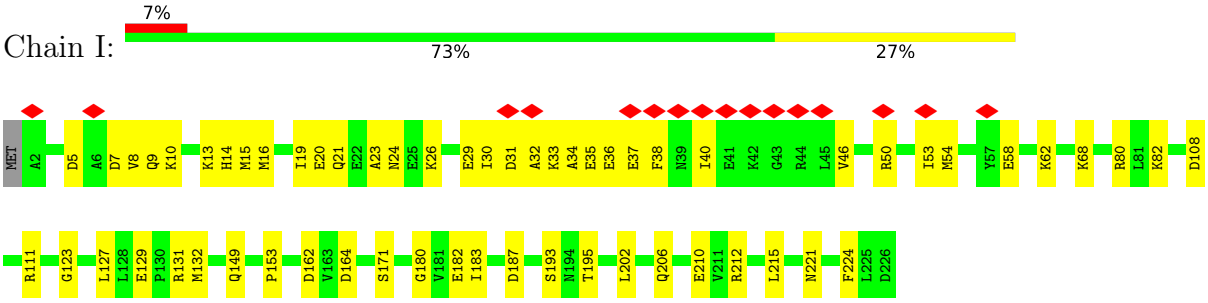
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

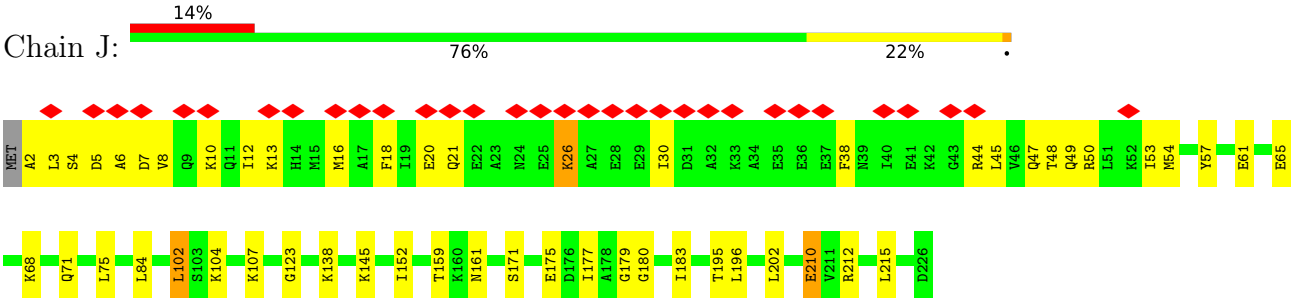
• Molecule 1: V-type proton ATPase subunit E 1



• Molecule 1: V-type proton ATPase subunit E 1

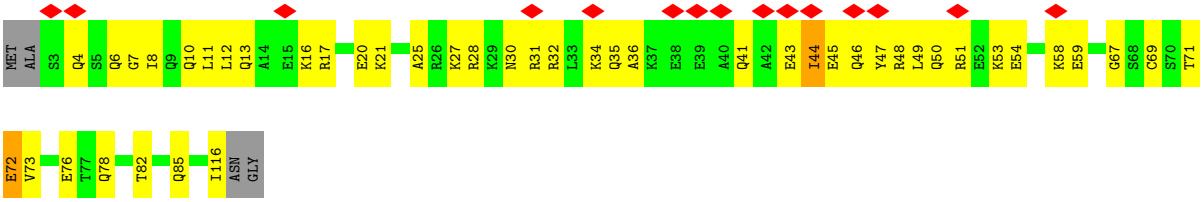


• Molecule 1: V-type proton ATPase subunit E 1



• Molecule 2: V-type proton ATPase subunit G 1

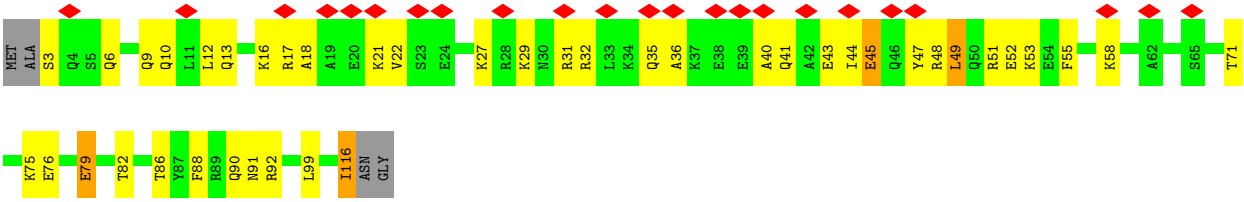




• Molecule 2: V-type proton ATPase subunit G 1

Chain L:

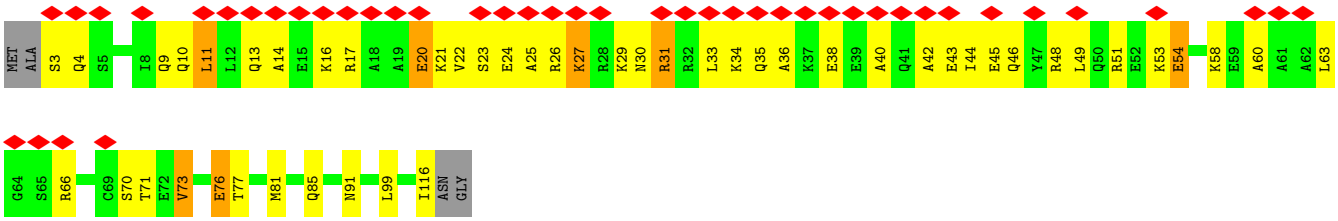




• Molecule 2: V-type proton ATPase subunit G 1

Chain M:

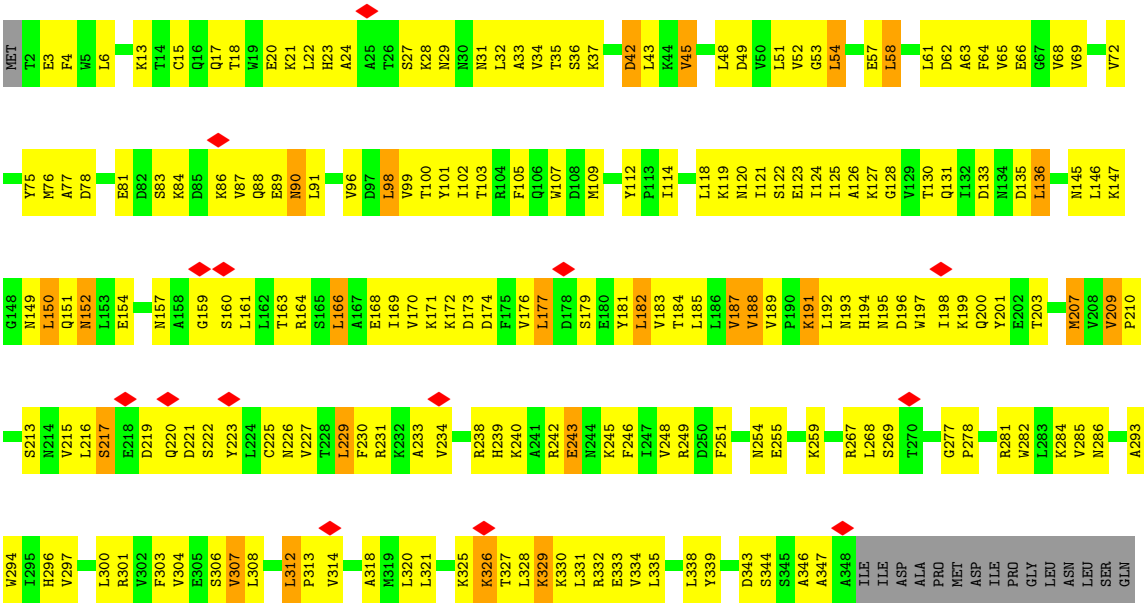


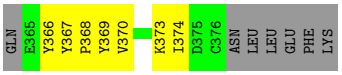


• Molecule 3: V-type proton ATPase subunit C 1

Chain O:



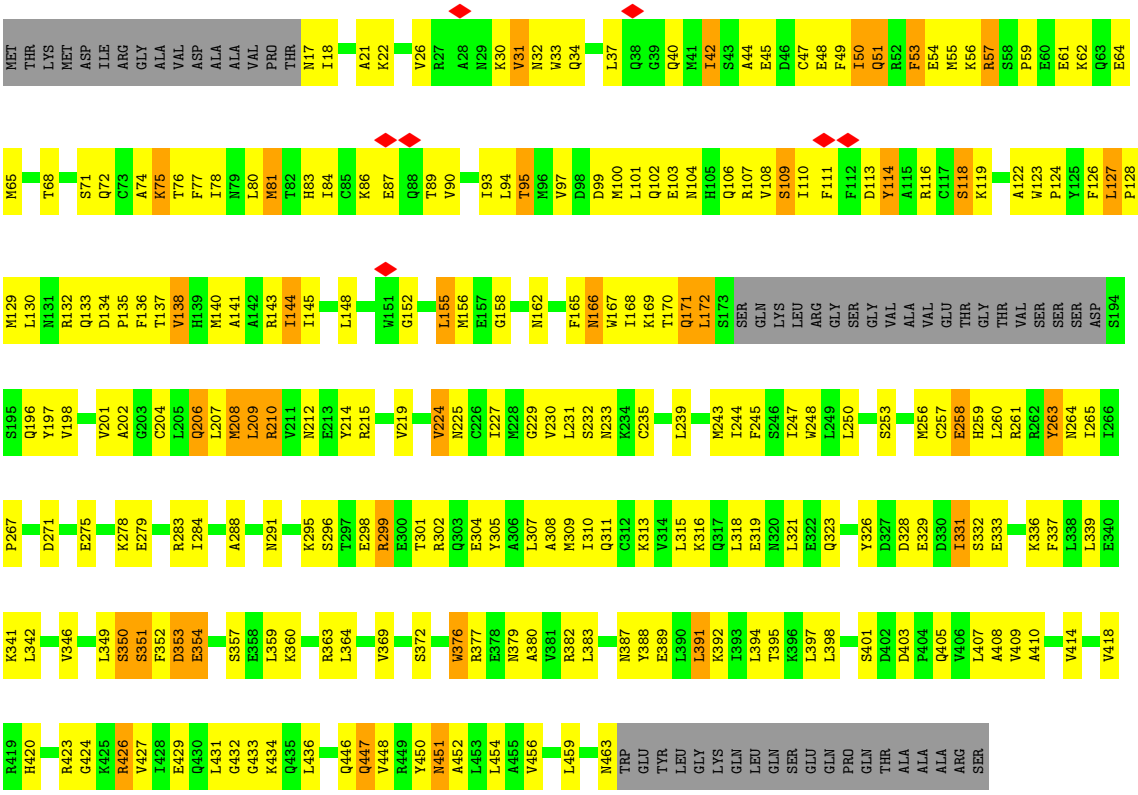




• Molecule 4: V-type proton ATPase subunit H

Chain P:

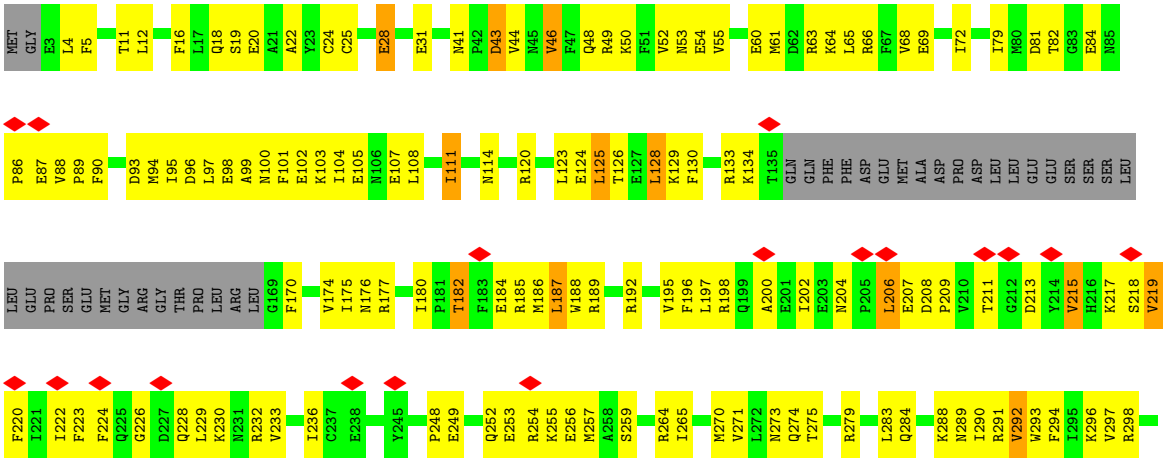


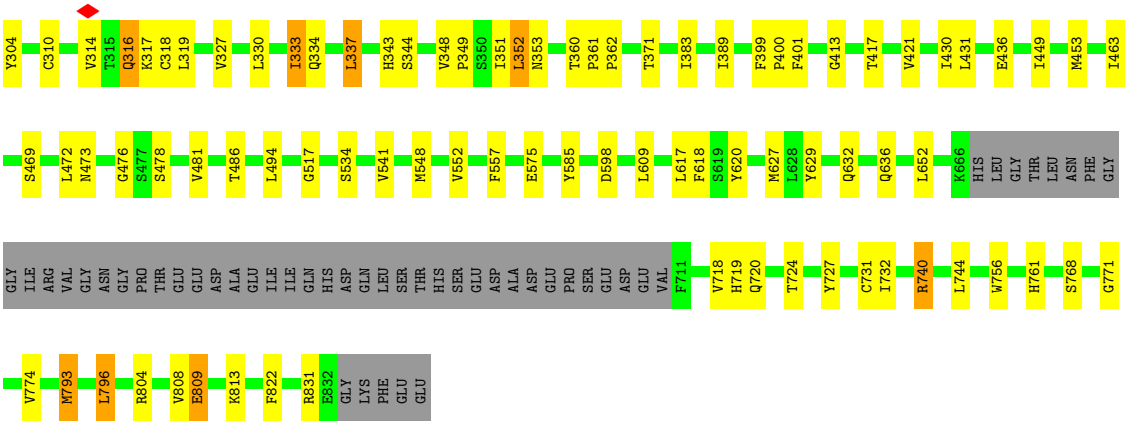


• Molecule 5: V-type proton ATPase 116 kDa subunit a isoform 1

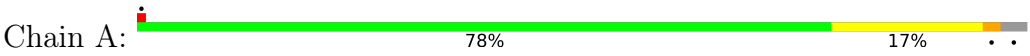
Chain R:

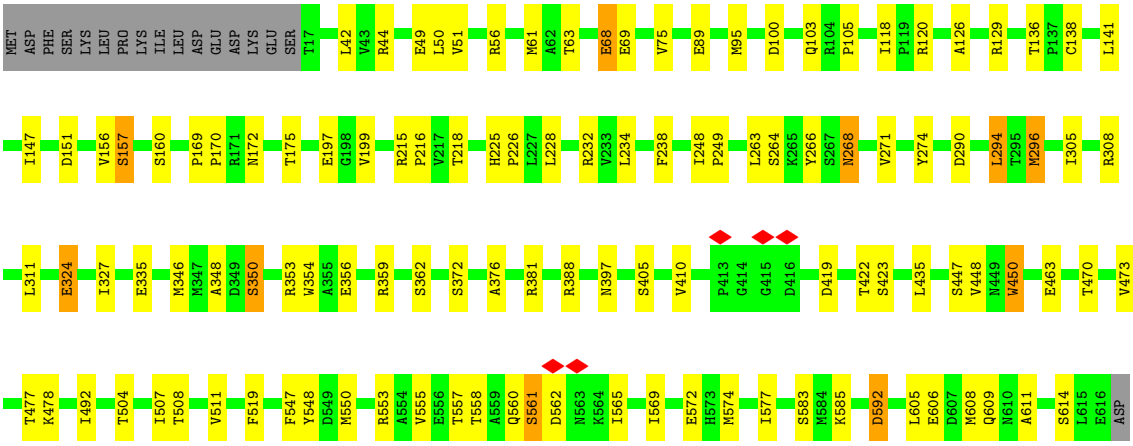




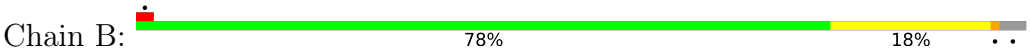


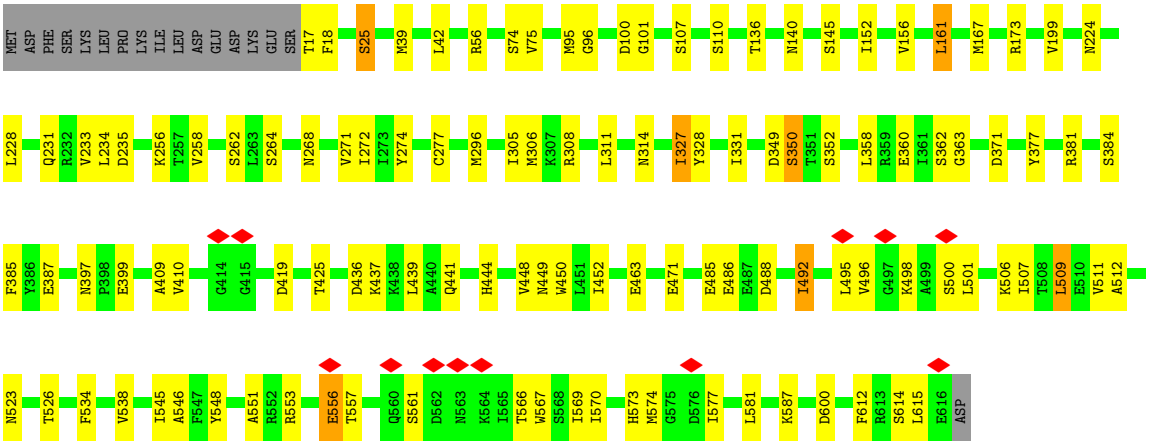
• Molecule 6: V-type proton ATPase catalytic subunit A





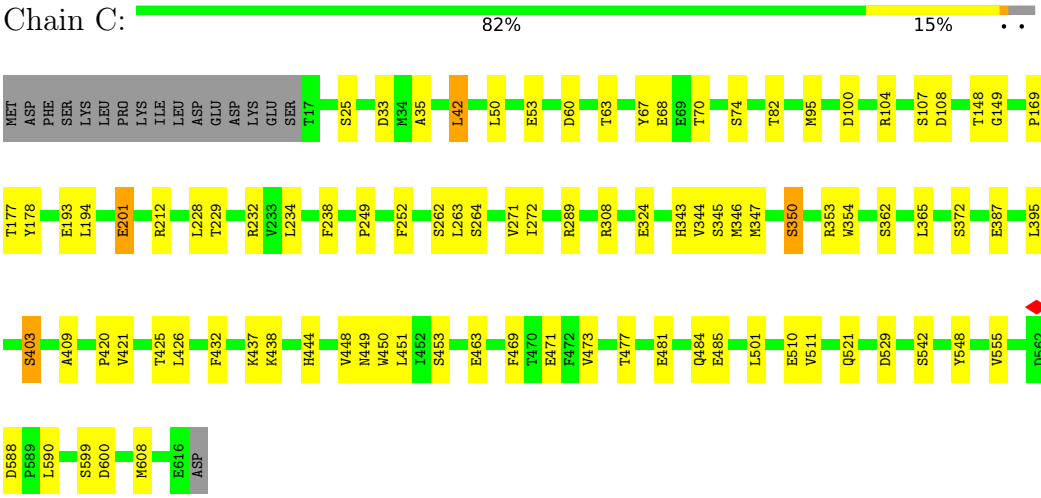
• Molecule 6: V-type proton ATPase catalytic subunit A





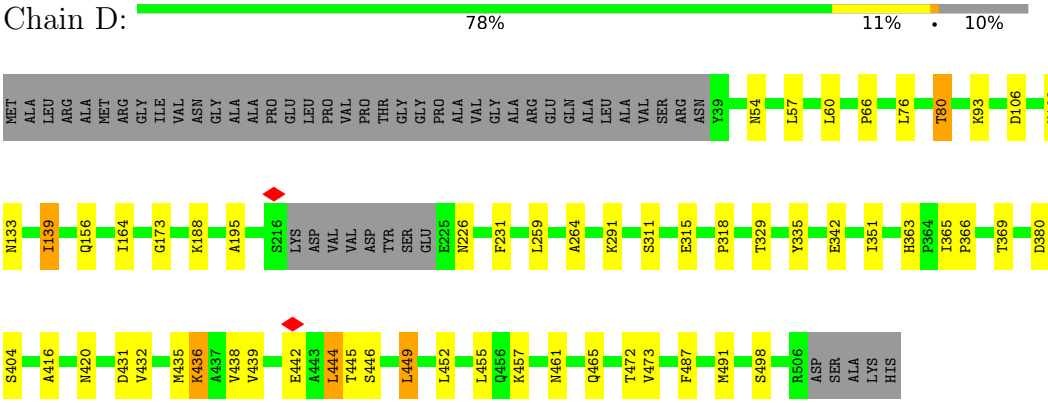
• Molecule 6: V-type proton ATPase catalytic subunit A

Chain C:



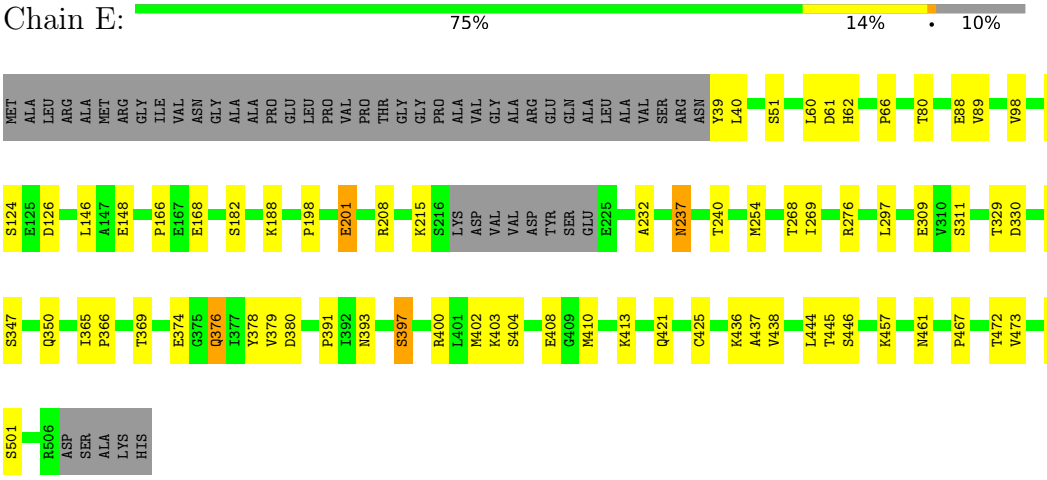
• Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain D:



• Molecule 7: V-type proton ATPase subunit B, brain isoform

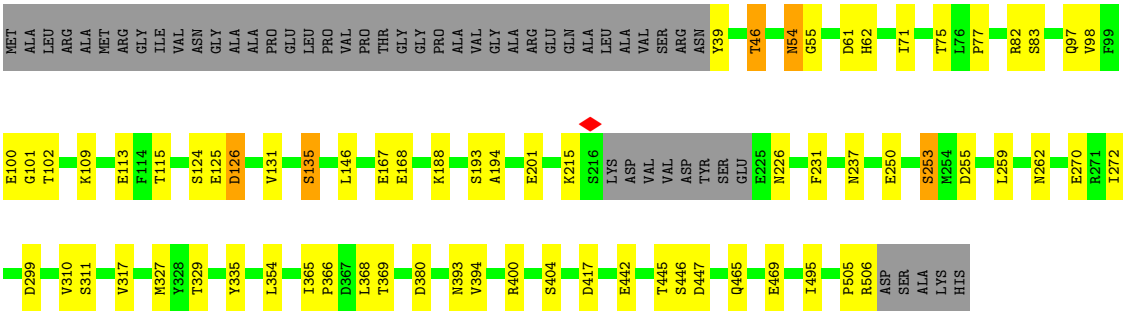
Chain E:



• Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain F:



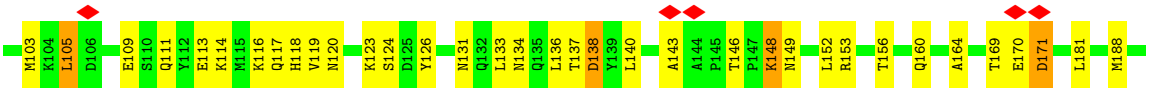


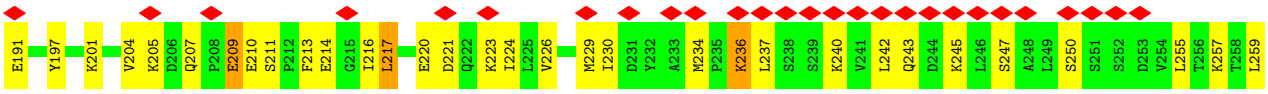
• Molecule 8: SidK

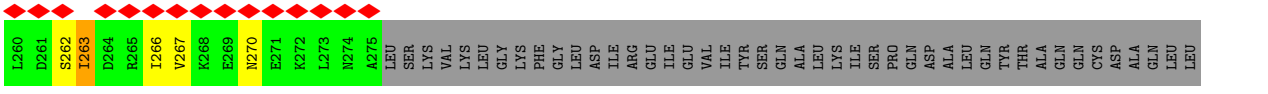
Chain X:

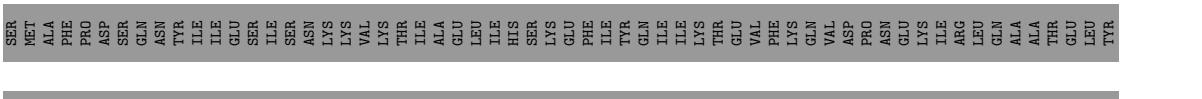


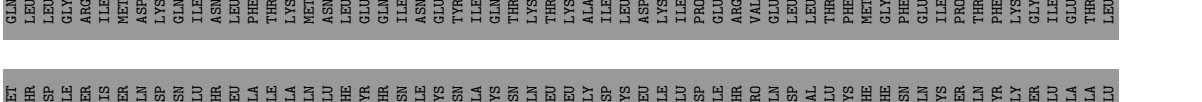


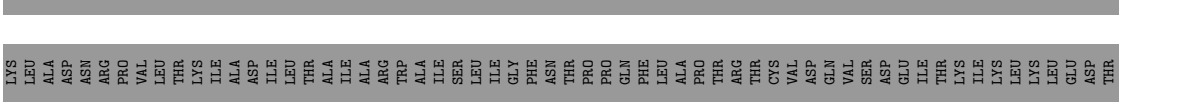




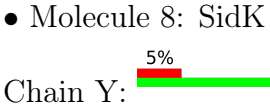








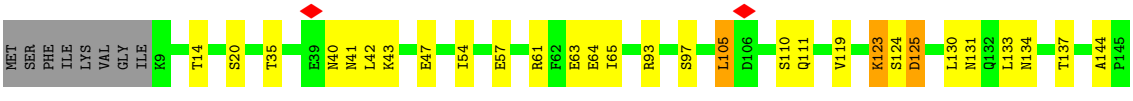


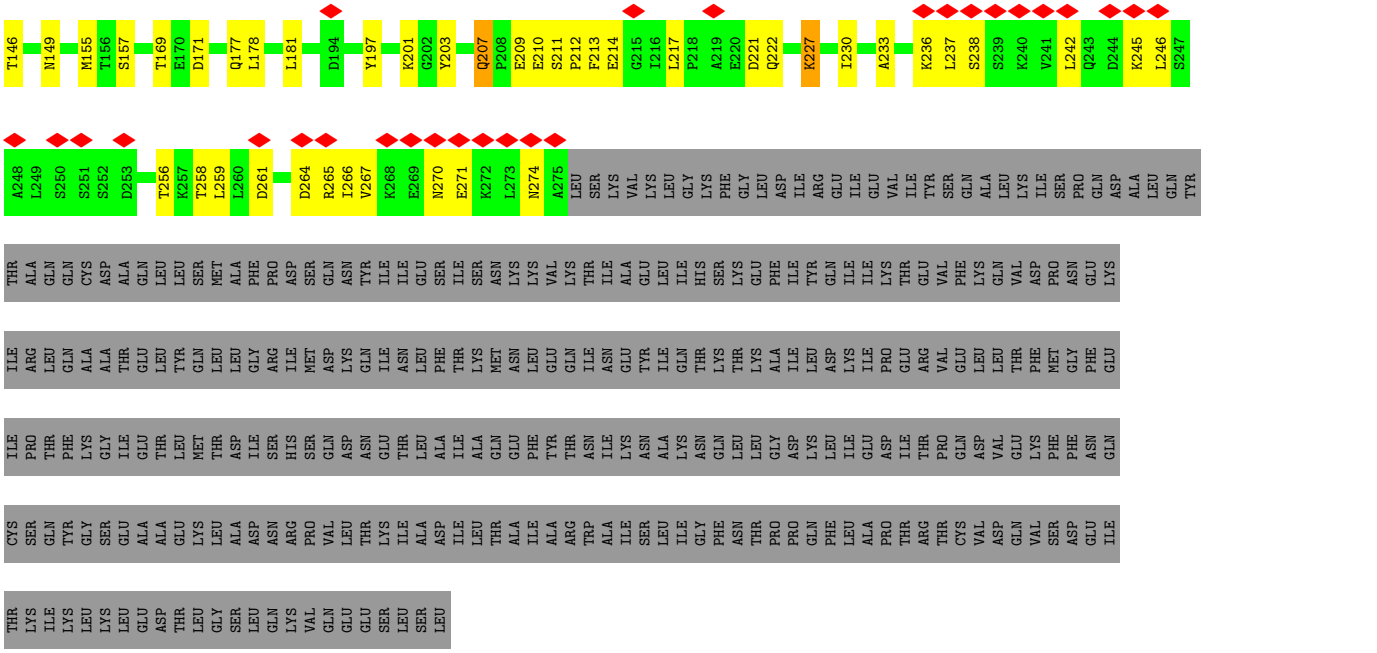


• Molecule 8: SidK

Chain Y:



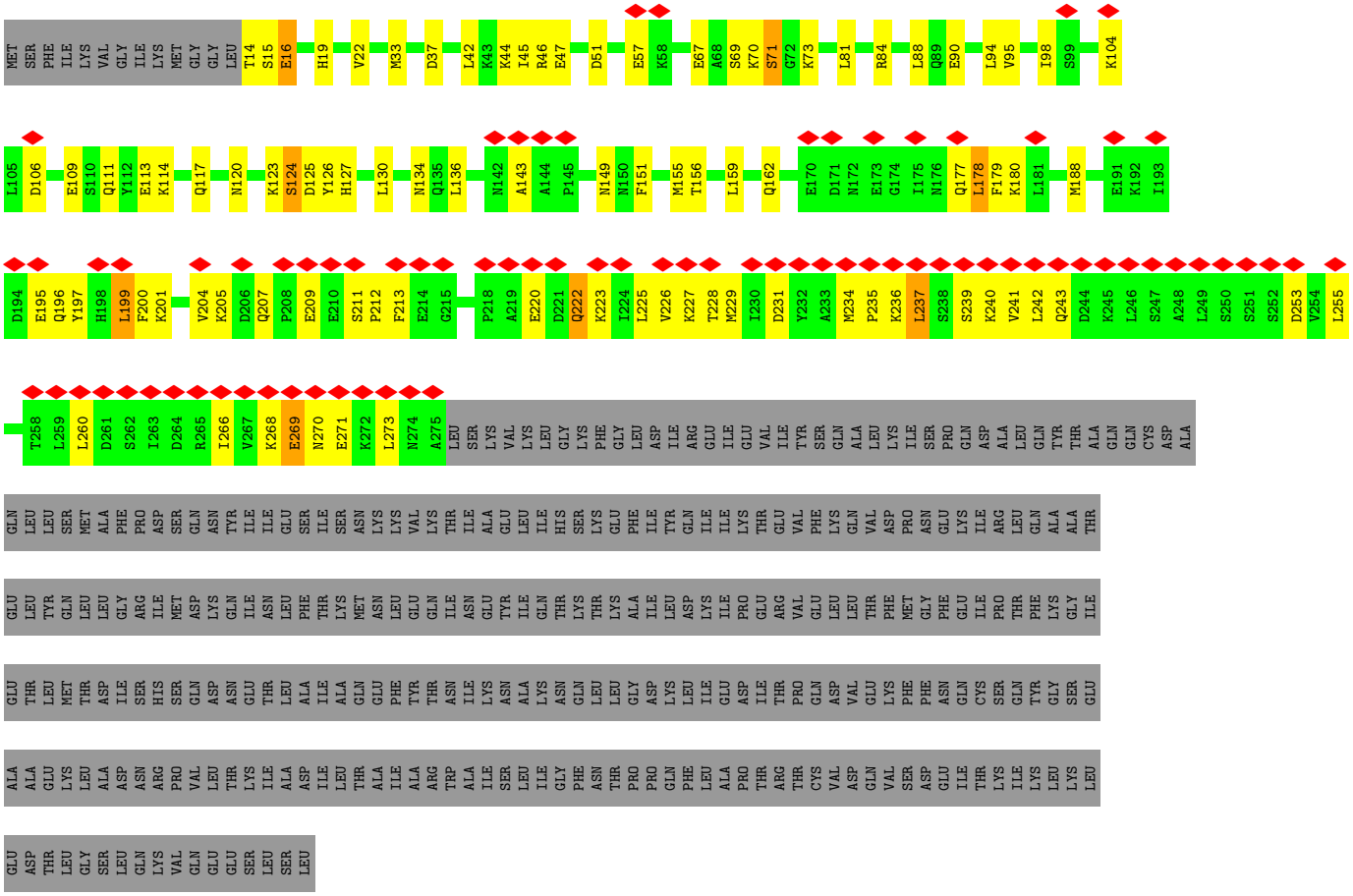




- Molecule 8: SidK

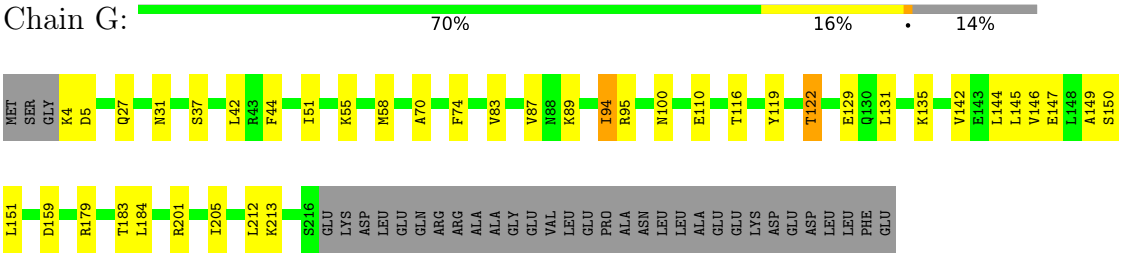
Chain Z:





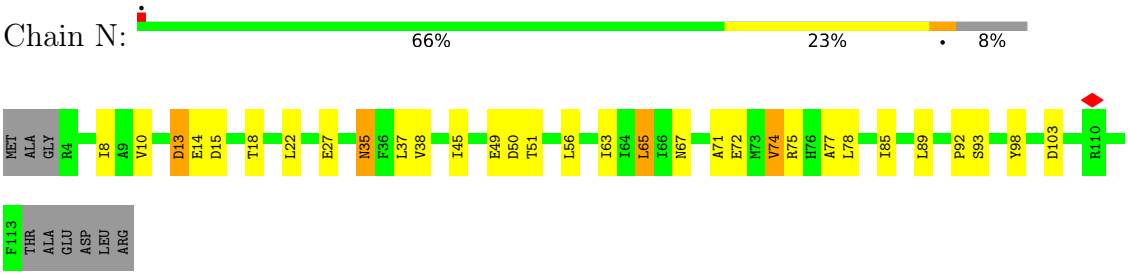
• Molecule 9: V-type proton ATPase subunit D

Chain G:



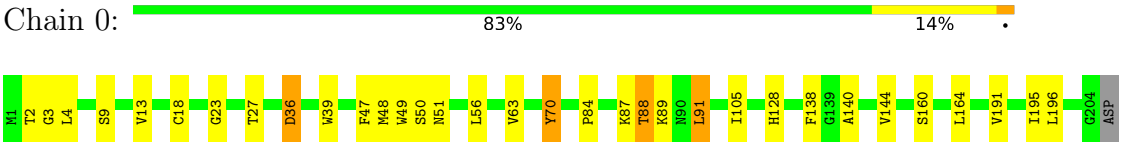
• Molecule 10: V-type proton ATPase subunit F

Chain N:



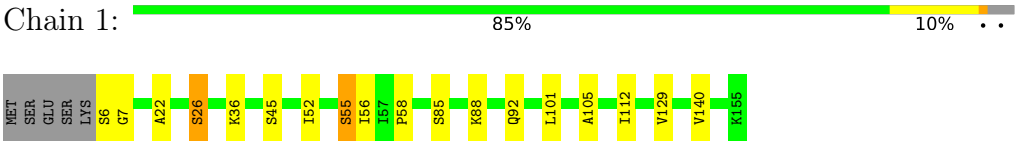
• Molecule 11: V-type proton ATPase 21 kDa proteolipid subunit

Chain 0:



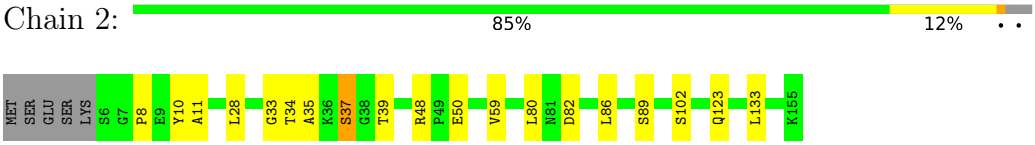
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 1:



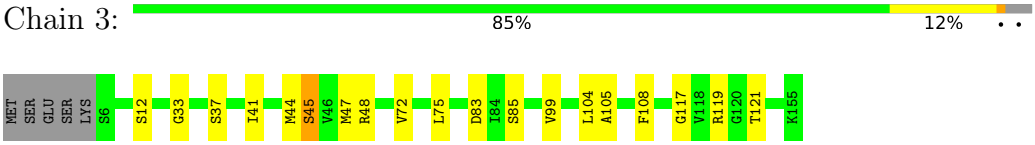
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:



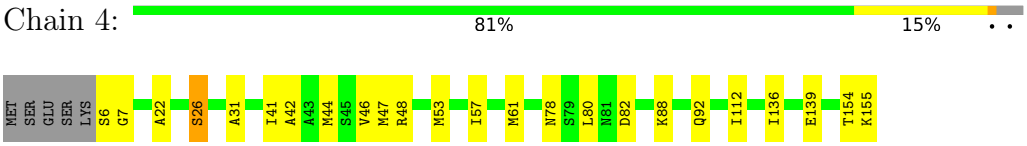
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 3:



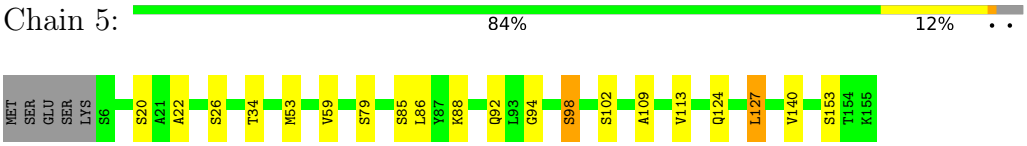
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:



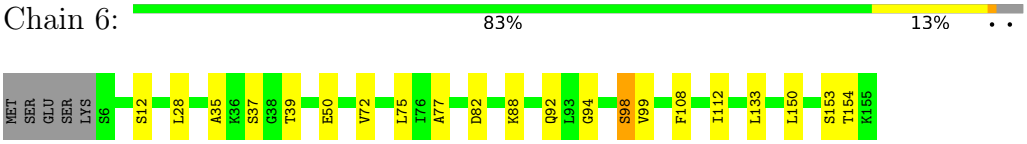
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



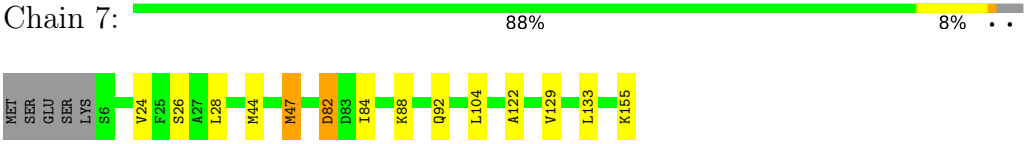
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



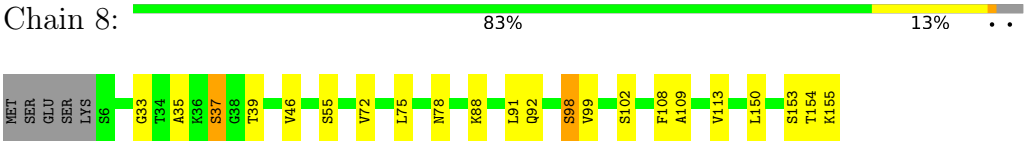
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:



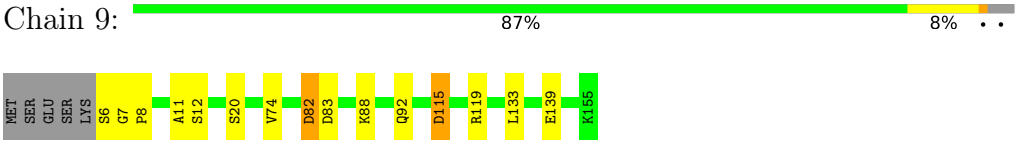
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:



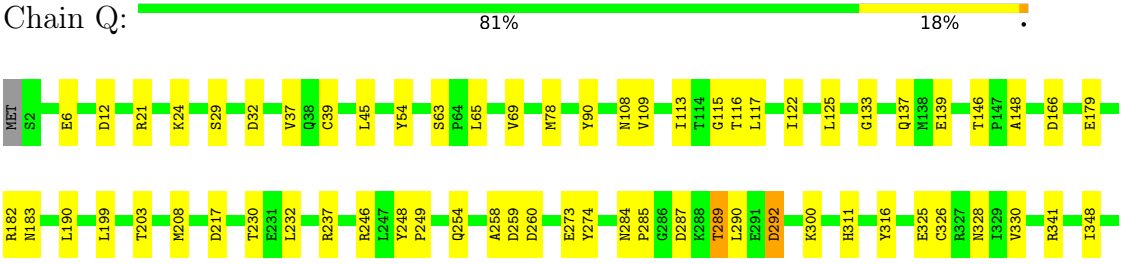
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9:



• Molecule 13: V-type proton ATPase subunit d 1

Chain Q:





• Molecule 14: V-type proton ATPase subunit e 1

Chain S:

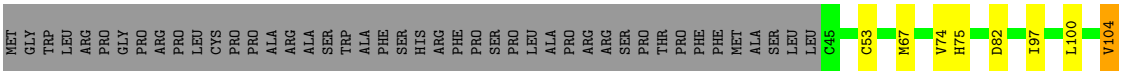


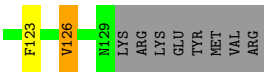


• Molecule 15: Ribonuclease kappa

Chain T:



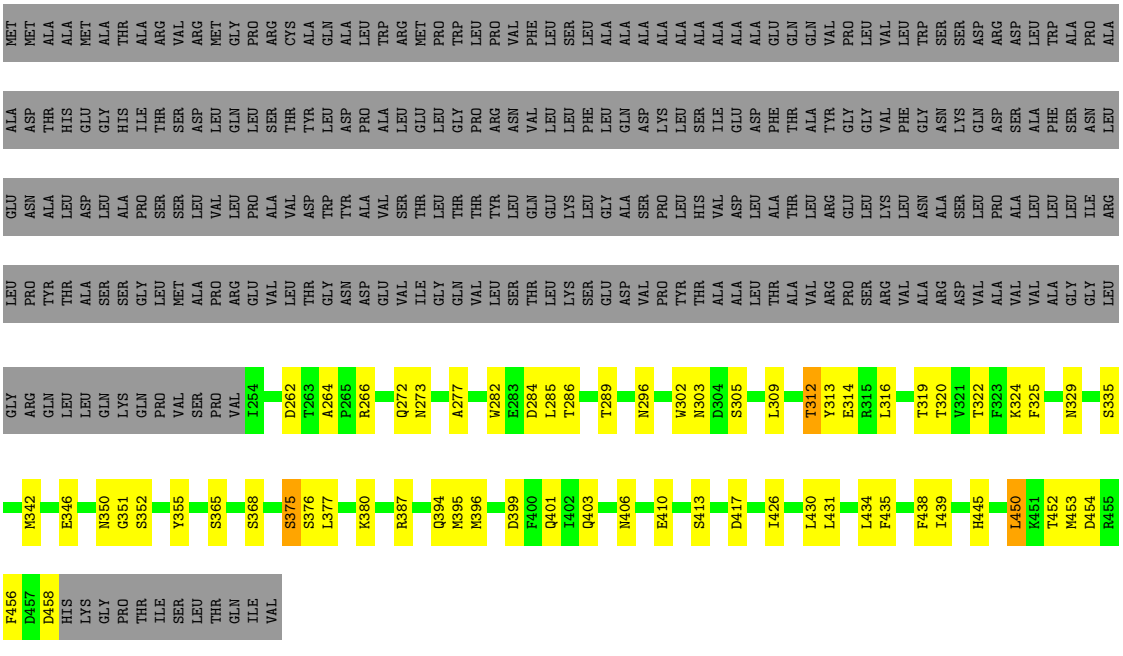




• Molecule 16: V-type proton ATPase subunit S1

Chain U:





• Molecule 17: Renin receptor

Chain V:

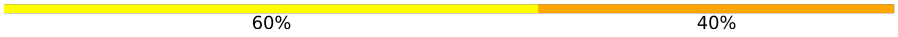






• Molecule 18: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:





• Molecule 19: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

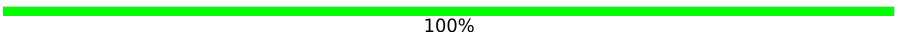
Chain a:





• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:





• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:





• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:





• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:





• Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

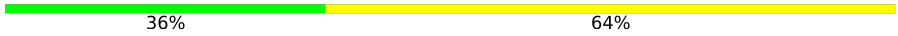
Chain s:

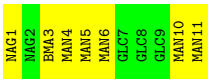




• Molecule 21: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.271	Depositor
Minimum map value	-15.824	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	2.8	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

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: PTY, ADP, BGC, WJP, BMA, WJS, NAG, MAN, SIA, PSF, GLC, NGA, WSS, CLR, GAL

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	H	0.25	0/1839	0.53	0/2462
1	I	0.25	0/1839	0.45	0/2462
1	J	0.24	0/1839	0.45	0/2462
2	K	0.24	0/945	0.53	0/1258
2	L	0.25	0/945	0.52	0/1258
2	M	0.27	0/945	0.54	0/1258
3	O	0.23	0/2970	0.55	0/4013
4	P	0.23	0/3576	0.52	0/4819
5	R	0.32	0/6299	0.47	0/8523
6	A	0.32	0/4748	0.37	0/6431
6	B	0.30	0/4752	0.39	0/6435
6	C	0.34	0/4752	0.38	0/6435
7	D	0.35	0/3671	0.39	0/4973
7	E	0.35	0/3660	0.39	0/4960
7	F	0.34	0/3667	0.38	0/4968
8	X	0.22	0/2145	0.43	0/2893
8	Y	0.19	0/2170	0.39	0/2926
8	Z	0.18	0/2138	0.40	0/2884
9	G	0.31	0/1731	0.50	0/2316
10	N	0.29	0/889	0.51	0/1200
11	0	0.39	0/1529	0.45	0/2079
12	1	0.42	0/1080	0.44	0/1461
12	2	0.40	0/1080	0.44	0/1461
12	3	0.40	0/1080	0.42	0/1461
12	4	0.41	0/1080	0.41	0/1461
12	5	0.41	0/1080	0.43	0/1461
12	6	0.38	0/1080	0.43	0/1461
12	7	0.37	0/1074	0.43	0/1454
12	8	0.39	0/1080	0.46	0/1461
12	9	0.40	0/1080	0.43	0/1461
13	Q	0.42	0/2895	0.42	0/3922
14	S	0.35	0/657	0.44	0/902

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
15	T	0.27	0/670	0.42	0/911
16	U	0.33	0/1718	0.42	0/2337
17	V	0.37	0/431	0.40	0/591
All	All	0.32	0/73134	0.44	0/98820

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
3	O	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	312	LEU	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	H	1822	0	1886	43	0
1	I	1822	0	1886	45	0
1	J	1822	0	1886	34	0
2	K	938	0	947	31	0
2	L	938	0	947	36	0
2	M	938	0	947	35	0
3	O	2916	0	2955	166	0
4	P	3508	0	3483	205	0
5	R	6141	0	6161	154	0
6	A	4652	0	4631	50	0
6	B	4656	0	4642	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	4656	0	4642	50	0
7	D	3600	0	3605	27	0
7	E	3589	0	3590	40	0
7	F	3596	0	3601	33	0
8	X	2111	0	2134	55	0
8	Y	2136	0	2158	41	0
8	Z	2105	0	2127	51	0
9	G	1713	0	1818	21	0
10	N	875	0	878	23	0
11	0	1495	0	1537	23	0
12	1	1065	0	1131	8	0
12	2	1065	0	1131	9	0
12	3	1065	0	1131	14	0
12	4	1065	0	1131	13	0
12	5	1065	0	1131	12	0
12	6	1065	0	1131	9	0
12	7	1059	0	1120	9	0
12	8	1065	0	1131	12	0
12	9	1065	0	1131	8	0
13	Q	2829	0	2757	33	0
14	S	631	0	646	11	0
15	T	654	0	641	5	0
16	U	1664	0	1584	55	0
17	V	417	0	405	5	0
18	W	68	0	58	6	0
19	a	56	0	47	6	0
20	b	28	0	25	1	0
20	c	28	0	25	1	0
20	d	28	0	25	4	0
20	s	28	0	25	0	0
20	u	28	0	25	0	0
21	r	127	0	106	1	0
22	0	28	0	46	1	0
22	5	28	0	46	16	0
22	R	28	0	46	1	0
22	V	28	0	46	11	0
23	R	30	0	32	0	0
24	0	65	0	85	4	0
24	2	29	0	40	1	0
24	5	35	0	46	6	0
24	6	21	0	19	7	0
24	7	42	0	60	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	8	83	0	129	10	0
24	Q	30	0	33	6	0
24	R	61	0	85	2	0
24	U	26	0	33	21	0
24	V	29	0	40	9	0
25	0	142	0	0	1	0
25	1	34	0	0	0	0
25	3	41	0	0	0	0
25	R	40	0	0	5	0
25	U	76	0	0	0	0
25	V	37	0	0	0	0
26	R	14	0	13	0	0
26	U	14	0	13	0	0
27	R	34	0	0	0	0
28	C	27	0	12	1	0
29	3	27	0	0	5	0
All	All	73243	0	73822	1374	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 9.

All (1374) 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)
16:U:273:ASN:ND2	20:d:1:NAG:C1	1.74	1.49
5:R:473:ASN:ND2	25:R:905:WSS:C4	1.82	1.39
16:U:273:ASN:HD21	20:d:1:NAG:C1	1.29	1.33
5:R:473:ASN:HD22	25:R:905:WSS:C4	1.38	1.33
16:U:438:PHE:CE2	24:U:503:PTY:H181	1.71	1.25
16:U:438:PHE:HE2	24:U:503:PTY:C18	1.56	1.17
24:6:201:PTY:O13	24:7:201:PTY:C2	1.95	1.14
22:5:201:CLR:C2	24:V:403:PTY:HC51	1.83	1.08
22:5:201:CLR:C1	24:V:403:PTY:HC51	1.83	1.08
24:6:201:PTY:O13	24:7:201:PTY:HC22	1.56	1.04
24:Q:401:PTY:H322	24:U:503:PTY:H321	1.37	1.02
4:P:37:LEU:HD11	4:P:48:GLU:HG2	1.43	1.00
22:5:201:CLR:H21	24:V:403:PTY:C5	1.90	1.00
24:6:201:PTY:O13	24:7:201:PTY:HC21	1.61	1.00
24:5:202:PTY:O13	24:6:201:PTY:C3	2.11	0.98
16:U:438:PHE:CE2	24:U:503:PTY:C18	2.39	0.98
24:5:202:PTY:H121	22:V:402:CLR:H193	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:438:PHE:HE2	24:U:503:PTY:H181	1.13	0.95
24:Q:401:PTY:H112	24:U:503:PTY:O10	1.65	0.94
22:5:201:CLR:H21	24:V:403:PTY:HC51	1.41	0.94
12:8:108:PHE:HB3	24:8:201:PTY:O13	1.71	0.91
12:3:108:PHE:CE2	29:3:202:WJS:O27	2.23	0.90
24:Q:401:PTY:C32	24:U:503:PTY:H321	2.00	0.90
1:I:14:HIS:HE2	3:O:312:LEU:H	1.18	0.89
12:8:108:PHE:HZ	24:8:202:PTY:H341	1.38	0.88
5:R:97:LEU:O	5:R:100:ASN:HB3	1.73	0.88
22:5:201:CLR:H11	24:V:403:PTY:HC51	1.55	0.88
12:3:108:PHE:CD2	29:3:202:WJS:O27	2.26	0.88
5:R:618:PHE:O	18:W:5:SIA:O1A	1.91	0.87
2:K:50:GLN:HA	2:K:53:LYS:HE2	1.57	0.85
16:U:438:PHE:HE2	24:U:503:PTY:H182	1.39	0.85
4:P:37:LEU:HD12	4:P:44:ALA:HA	1.58	0.84
4:P:26:VAL:HG21	4:P:95:THR:HB	1.60	0.83
4:P:51:GLN:HA	4:P:54:GLU:HB2	1.59	0.83
5:R:473:ASN:HD21	25:R:905:WSS:C4	1.89	0.82
4:P:267:PRO:HG3	4:P:311:GLN:HB3	1.61	0.82
4:P:158:GLY:O	4:P:162:ASN:HB2	1.81	0.81
16:U:273:ASN:HD22	20:d:1:NAG:C1	1.91	0.80
24:5:202:PTY:H121	22:V:402:CLR:C19	2.11	0.80
4:P:165:PHE:HB3	4:P:169:LYS:H	1.45	0.80
16:U:438:PHE:CD2	24:U:503:PTY:H181	2.17	0.79
2:M:4:GLN:NE2	3:O:210:PRO:O	2.16	0.79
4:P:307:LEU:O	4:P:311:GLN:N	2.17	0.78
4:P:86:LYS:O	4:P:90:VAL:N	2.15	0.78
12:6:108:PHE:HE2	24:6:201:PTY:HC6	1.47	0.78
5:R:24:CYS:HG	5:R:344:SER:HG	1.23	0.77
4:P:141:ALA:HA	4:P:144:ILE:HG22	1.66	0.77
11:0:13:VAL:HG11	24:0:306:PTY:H312	1.66	0.77
2:K:13:GLN:HA	2:K:16:LYS:HE2	1.66	0.76
1:H:61:GLU:OE1	2:K:58:LYS:NZ	2.16	0.76
8:Z:207:GLN:HE22	8:Z:212:PRO:HG3	1.51	0.76
1:H:19:ILE:HD12	5:R:316:GLN:HG2	1.68	0.76
4:P:31:VAL:HG21	4:P:33:TRP:CE2	2.21	0.75
5:R:473:ASN:ND2	25:R:905:WSS:C5	2.49	0.75
8:Y:264:ASP:HA	8:Y:267:VAL:HG12	1.66	0.75
3:O:183:VAL:HB	3:O:231:ARG:HE	1.51	0.75
2:L:27:LYS:HE3	2:L:31:ARG:HH22	1.52	0.75
7:E:208:ARG:NH2	7:E:467:PRO:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:140:MET:SD	4:P:141:ALA:N	2.60	0.74
6:B:410:VAL:HG11	6:B:425:THR:HG21	1.70	0.74
8:Z:37:ASP:HB3	8:Z:46:ARG:HH21	1.49	0.74
3:O:20:GLU:OE1	3:O:28:LYS:NZ	2.19	0.74
13:Q:230:THR:HG22	13:Q:232:LEU:H	1.53	0.74
1:H:49:GLN:HG3	2:K:44:ILE:HD13	1.70	0.74
4:P:395:THR:HA	4:P:398:LEU:HD12	1.69	0.74
12:8:108:PHE:CZ	24:8:202:PTY:H341	2.23	0.74
6:C:229:THR:HG22	6:C:263:LEU:HG	1.69	0.73
8:X:242:LEU:HD12	8:X:245:LYS:HE2	1.71	0.73
3:O:170:VAL:HA	3:O:216:LEU:HD11	1.70	0.73
1:I:34:ALA:HB2	2:L:29:LYS:HE2	1.69	0.73
5:R:294:PHE:HE2	5:R:298:ARG:HH11	1.33	0.73
5:R:66:ARG:HH12	5:R:294:PHE:HB2	1.54	0.72
4:P:451:ASN:OD1	4:P:451:ASN:N	2.20	0.72
6:A:95:MET:HE1	6:A:271:VAL:HG13	1.70	0.72
3:O:161:LEU:HD13	3:O:219:ASP:HB3	1.71	0.71
22:5:201:CLR:C2	24:V:403:PTY:C5	2.57	0.71
5:R:125:LEU:HD23	5:R:265:ILE:HG13	1.72	0.71
8:X:48:ASP:OD2	8:X:116:LYS:NZ	2.22	0.71
10:N:37:LEU:HG	10:N:51:THR:HG21	1.73	0.71
8:Z:177:GLN:HE22	8:Z:180:LYS:HE3	1.55	0.71
4:P:166:ASN:OD1	4:P:166:ASN:N	2.24	0.71
5:R:316:GLN:OE1	5:R:317:LYS:N	2.23	0.71
6:A:550:MET:HE1	6:A:609:GLN:HG2	1.73	0.71
3:O:163:THR:O	3:O:249:ARG:NH1	2.24	0.70
5:R:174:VAL:HA	5:R:219:VAL:HG21	1.72	0.70
4:P:446:GLN:NE2	4:P:447:GLN:OE1	2.24	0.70
4:P:74:ALA:HA	4:P:77:PHE:HD2	1.56	0.70
2:K:48:ARG:HE	2:K:49:LEU:HD22	1.56	0.70
4:P:74:ALA:HA	4:P:77:PHE:CD2	2.27	0.70
5:R:94:MET:HE3	5:R:98:GLU:HB3	1.74	0.70
12:1:36:LYS:HG3	16:U:450:LEU:HD21	1.72	0.70
2:L:3:SER:O	2:L:6:GLN:NE2	2.25	0.70
5:R:617:LEU:HB3	19:a:2:NGA:H81	1.73	0.70
6:A:138:CYS:HB2	6:A:141:LEU:HD12	1.72	0.69
6:C:95:MET:HE1	6:C:271:VAL:HG13	1.73	0.69
1:J:12:ILE:HG22	1:J:16:MET:HE1	1.74	0.69
12:3:108:PHE:HE2	29:3:202:WJS:O27	1.72	0.69
4:P:130:LEU:H	4:P:138:VAL:HB	1.58	0.69
8:Z:223:LYS:NZ	8:Z:253:ASP:OD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:249:GLU:H	5:R:254:ARG:HG2	1.56	0.68
5:R:100:ASN:O	5:R:103:LYS:HG3	1.94	0.68
3:O:33:ALA:HB1	3:O:321:LEU:HD11	1.75	0.68
10:N:35:ASN:N	10:N:35:ASN:OD1	2.27	0.68
6:A:565:ILE:HA	6:A:569:ILE:HD11	1.74	0.68
6:C:289:ARG:NH1	7:F:167:GLU:OE2	2.26	0.68
3:O:3:GLU:OE2	3:O:373:LYS:NZ	2.25	0.68
18:W:1:BGC:O4	18:W:1:BGC:O2	2.10	0.68
7:D:133:ASN:HB3	7:D:139:ILE:HD12	1.76	0.67
1:J:210:GLU:OE2	7:F:39:TYR:OH	2.12	0.67
4:P:202:ALA:O	4:P:206:GLN:NE2	2.28	0.67
5:R:473:ASN:HD22	25:R:905:WSS:C5	2.06	0.67
7:F:445:THR:HG22	7:F:446:SER:H	1.59	0.67
1:H:24:ASN:OD1	2:K:21:LYS:NZ	2.26	0.67
6:B:264:SER:O	6:B:308:ARG:NH2	2.28	0.67
2:M:51:ARG:NH2	2:M:54:GLU:OE1	2.22	0.67
4:P:353:ASP:N	4:P:353:ASP:OD1	2.27	0.67
1:H:180:GLY:HA3	1:H:195:THR:HA	1.76	0.67
3:O:335:LEU:HD22	3:O:369:TYR:CZ	2.30	0.67
6:A:419:ASP:HB3	6:A:422:THR:HG22	1.75	0.67
3:O:277:GLY:O	3:O:281:ARG:NH2	2.28	0.67
6:B:486:GLU:HG2	6:B:509:LEU:HD22	1.78	0.66
4:P:296:SER:HB2	4:P:302:ARG:HD3	1.75	0.66
1:J:180:GLY:HA3	1:J:195:THR:HA	1.77	0.66
3:O:45:VAL:HG23	3:O:51:LEU:HD11	1.78	0.66
4:P:102:GLN:HE21	4:P:140:MET:HA	1.61	0.66
6:A:264:SER:O	6:A:308:ARG:NH2	2.29	0.66
24:5:202:PTY:H312	24:5:202:PTY:H122	1.76	0.66
3:O:255:GLU:HG3	3:O:259:LYS:HD2	1.77	0.66
8:X:220:GLU:HA	8:X:223:LYS:HE3	1.78	0.66
4:P:350:SER:HA	4:P:369:VAL:HG12	1.77	0.66
6:B:17:THR:OG1	6:B:18:PHE:N	2.29	0.66
4:P:37:LEU:HD13	4:P:47:CYS:HB3	1.78	0.66
6:C:232:ARG:NH2	6:C:529:ASP:OD1	2.29	0.66
9:G:27:GLN:O	9:G:31:ASN:ND2	2.29	0.66
3:O:240:LYS:O	3:O:243:GLU:HB3	1.96	0.66
6:B:101:GLY:H	6:B:314:ASN:HD21	1.43	0.65
13:Q:39:CYS:O	13:Q:341:ARG:NH2	2.29	0.65
6:B:567:TRP:HA	6:B:570:ILE:HD12	1.78	0.65
3:O:160:SER:HB2	3:O:220:GLN:HE22	1.61	0.65
8:Y:111:GLN:NE2	8:Y:169:THR:OG1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:435:PHE:HE1	24:U:503:PTY:C20	2.10	0.65
16:U:319:THR:HG22	16:U:320:THR:H	1.61	0.65
2:M:31:ARG:O	2:M:35:GLN:HG3	1.97	0.65
4:P:55:MET:HB2	4:P:61:GLU:HG3	1.78	0.65
5:R:123:LEU:HD22	5:R:206:LEU:HD13	1.78	0.65
13:Q:179:GLU:OE1	13:Q:182:ARG:NH1	2.30	0.65
3:O:193:ASN:O	3:O:196:ASP:HB3	1.97	0.65
3:O:145:ASN:O	3:O:149:ASN:ND2	2.30	0.64
12:3:108:PHE:HD2	29:3:202:WJS:O27	1.80	0.64
3:O:332:ARG:HA	3:O:335:LEU:HD12	1.79	0.64
6:B:140:ASN:ND2	8:Y:35:THR:OG1	2.30	0.64
5:R:585:TYR:OH	5:R:629:TYR:OH	2.13	0.64
8:X:93:ARG:NH2	8:X:131:ASN:OD1	2.25	0.64
6:B:56:ARG:HD3	7:F:54:ASN:HD22	1.63	0.64
6:A:95:MET:HE3	6:A:308:ARG:HA	1.79	0.64
12:2:33:GLY:O	12:2:37:SER:OG	2.16	0.64
6:A:151:ASP:OD2	6:A:397:ASN:ND2	2.30	0.64
8:Z:111:GLN:HA	8:Z:114:LYS:HZ1	1.63	0.64
24:2:201:PTY:O12	29:3:202:WJS:C29	2.45	0.64
12:7:82:ASP:OD1	12:7:82:ASP:N	2.30	0.64
3:O:23:HIS:N	3:O:27:SER:OG	2.30	0.64
8:X:171:ASP:OD1	8:X:171:ASP:N	2.29	0.64
13:Q:108:ASN:ND2	13:Q:133:GLY:O	2.30	0.64
4:P:102:GLN:O	4:P:143:ARG:NH1	2.31	0.64
5:R:176:ASN:HD21	5:R:215:VAL:HG23	1.62	0.64
3:O:29:ASN:HB3	3:O:32:LEU:HB2	1.78	0.63
1:H:6:ALA:O	1:H:9:GLN:NE2	2.31	0.63
4:P:116:ARG:HH12	4:P:119:LYS:HD3	1.62	0.63
1:I:53:ILE:HD11	2:L:47:TYR:HD1	1.64	0.63
5:R:126:THR:O	5:R:129:LYS:HB2	1.98	0.63
2:L:55:PHE:HA	2:L:58:LYS:HZ1	1.63	0.63
3:O:185:LEU:HD11	3:O:248:VAL:HB	1.80	0.63
4:P:271:ASP:O	4:P:275:GLU:HB2	1.98	0.63
3:O:209:VAL:HG23	3:O:229:LEU:HA	1.79	0.63
4:P:328:ASP:HB3	4:P:331:ILE:HB	1.80	0.63
8:X:226:VAL:HG12	8:X:255:LEU:HD23	1.80	0.63
8:X:240:LYS:HG3	8:X:243:GLN:HG3	1.81	0.63
3:O:35:THR:HB	3:O:321:LEU:HD13	1.80	0.63
19:a:4:SIA:H112	19:a:4:SIA:O4	1.98	0.63
3:O:157:ASN:ND2	3:O:168:GLU:OE2	2.31	0.63
4:P:389:GLU:HA	4:P:392:LYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:GLU:HG2	1:H:44:ARG:HH11	1.63	0.62
4:P:224:VAL:HG21	4:P:260:LEU:HD21	1.81	0.62
22:5:201:CLR:H193	22:V:402:CLR:C19	2.29	0.62
1:H:123:GLY:HA3	1:H:183:ILE:HD13	1.80	0.62
12:7:47:MET:SD	13:Q:254:GLN:NE2	2.72	0.62
5:R:95:ILE:HA	5:R:98:GLU:HG2	1.80	0.62
8:X:236:LYS:NZ	8:X:236:LYS:HA	2.14	0.62
8:Y:93:ARG:NH2	8:Y:131:ASN:OD1	2.32	0.62
8:Y:213:PHE:O	8:Y:222:GLN:NE2	2.32	0.62
13:Q:29:SER:OG	13:Q:32:ASP:OD1	2.16	0.62
13:Q:208:MET:HE1	13:Q:316:TYR:CG	2.33	0.62
6:A:346:MET:HE2	6:A:348:ALA:HB2	1.80	0.62
10:N:67:ASN:ND2	10:N:93:SER:OG	2.33	0.62
5:R:81:ASP:HA	5:R:291:ARG:HB3	1.82	0.62
5:R:93:ASP:OD1	5:R:94:MET:N	2.32	0.62
8:Y:144:ALA:O	8:Y:149:ASN:ND2	2.31	0.62
8:Y:209:GLU:OE2	8:Y:210:GLU:N	2.33	0.62
13:Q:246:ARG:NH2	13:Q:273:GLU:OE2	2.32	0.62
5:R:108:LEU:HD21	5:R:283:LEU:HD13	1.81	0.62
1:H:2:ALA:HB2	5:R:337:LEU:HB3	1.82	0.62
3:O:150:LEU:HB2	3:O:268:LEU:HD13	1.81	0.62
3:O:125:ILE:HD11	3:O:293:ALA:HB1	1.81	0.61
5:R:96:ASP:OD2	5:R:97:LEU:N	2.33	0.61
5:R:134:LYS:HE3	5:R:200:ALA:HA	1.81	0.61
16:U:355:TYR:HB2	16:U:387:ARG:HG3	1.81	0.61
13:Q:146:THR:HG22	13:Q:148:ALA:H	1.64	0.61
5:R:413:GLY:O	5:R:417:THR:HG23	2.00	0.61
1:I:53:ILE:HD11	2:L:47:TYR:CD1	2.36	0.61
4:P:72:GLN:HA	4:P:76:THR:HG23	1.82	0.61
4:P:101:LEU:O	4:P:104:ASN:ND2	2.33	0.61
16:U:272:GLN:NE2	16:U:399:ASP:OD2	2.33	0.61
5:R:720:GLN:O	5:R:724:THR:HG23	2.00	0.61
22:5:201:CLR:H193	22:V:402:CLR:H191	1.83	0.61
4:P:307:LEU:HD13	4:P:311:GLN:HE21	1.66	0.61
5:R:94:MET:O	5:R:98:GLU:N	2.34	0.61
2:M:30:ASN:O	2:M:34:LYS:HD2	2.00	0.61
1:J:8:VAL:HB	3:O:210:PRO:HG2	1.82	0.61
8:X:25:LYS:HE3	8:X:82:SER:HB2	1.82	0.61
4:P:215:ARG:O	4:P:219:VAL:HG23	2.01	0.61
6:A:504:THR:O	6:A:508:THR:HG23	2.00	0.61
7:F:82:ARG:NH1	7:F:101:GLY:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:201:LYS:HB3	8:Z:205:LYS:HE3	1.83	0.61
5:R:49:ARG:NH2	5:R:310:CYS:O	2.34	0.60
24:5:202:PTY:H111	22:V:402:CLR:H22	1.82	0.60
4:P:279:GLU:OE2	4:P:326:TYR:OH	2.18	0.60
5:R:349:PRO:HB2	5:R:351:ILE:HG23	1.82	0.60
6:C:324:GLU:HG3	6:C:354:TRP:HE1	1.65	0.60
7:D:195:ALA:O	7:D:381:ARG:NH2	2.31	0.60
7:D:173:GLY:O	7:D:465:GLN:NE2	2.28	0.60
8:Z:227:LYS:NZ	8:Z:231:ASP:OD1	2.35	0.60
12:8:88:LYS:O	12:8:92:GLN:HG2	2.01	0.60
16:U:273:ASN:ND2	20:d:1:NAG:O5	2.29	0.60
5:R:65:LEU:HG	5:R:290:ILE:HD11	1.84	0.60
2:M:26:ARG:HH11	2:M:29:LYS:HD3	1.67	0.60
4:P:395:THR:HG21	4:P:431:LEU:HD22	1.84	0.60
16:U:458:ASP:N	16:U:458:ASP:OD1	2.35	0.60
3:O:62:ASP:OD2	3:O:63:ALA:N	2.33	0.60
3:O:321:LEU:HD21	3:O:331:LEU:HD11	1.82	0.60
5:R:177:ARG:HD2	5:R:218:SER:HB2	1.84	0.60
12:6:108:PHE:CE2	24:6:201:PTY:HC6	2.34	0.60
5:R:64:LYS:HE2	5:R:102:GLU:HG2	1.82	0.59
8:X:209:GLU:OE2	8:X:211:SER:N	2.35	0.59
12:2:8:PRO:HD2	12:2:11:ALA:HB2	1.84	0.59
3:O:194:HIS:O	3:O:198:ILE:HG13	2.02	0.59
7:D:318:PRO:HG3	9:G:201:ARG:HD2	1.85	0.59
12:4:22:ALA:O	12:4:26:SER:OG	2.18	0.59
4:P:104:ASN:O	4:P:109:SER:OG	2.21	0.59
4:P:283:ARG:HA	4:P:331:ILE:HD11	1.84	0.59
6:B:161:LEU:HD11	6:B:296:MET:HE1	1.84	0.59
6:B:296:MET:HG3	6:B:305:ILE:HG22	1.85	0.59
8:X:213:PHE:HB3	8:X:217:LEU:HD11	1.83	0.59
1:J:7:ASP:HA	1:J:10:LYS:HE3	1.84	0.59
3:O:328:LEU:HD23	3:O:328:LEU:H	1.68	0.59
4:P:423:ARG:HG2	4:P:426:ARG:HG2	1.85	0.59
8:Z:205:LYS:HE2	8:Z:260:LEU:HB3	1.84	0.59
4:P:108:VAL:O	4:P:110:ILE:HG12	2.03	0.59
4:P:224:VAL:HG11	4:P:260:LEU:HD11	1.84	0.59
5:R:362:PRO:HB2	5:R:822:PHE:HB2	1.84	0.59
8:X:14:THR:HG22	8:X:15:SER:H	1.68	0.59
8:Y:256:THR:HG22	8:Y:258:THR:H	1.67	0.59
1:H:8:VAL:O	1:H:12:ILE:HG13	2.03	0.59
9:G:95:ARG:NH1	9:G:110:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:79:HIS:NE2	15:T:75:HIS:O	2.35	0.59
16:U:445:HIS:CE1	24:U:503:PTY:H311	2.38	0.59
3:O:20:GLU:HA	3:O:27:SER:HA	1.84	0.59
3:O:150:LEU:HD12	3:O:268:LEU:HD13	1.85	0.59
4:P:75:LYS:C	4:P:75:LYS:HZ2	2.11	0.59
6:A:473:VAL:O	6:A:477:THR:HG23	2.03	0.59
1:J:71:GLN:HE22	2:M:66:ARG:HD2	1.68	0.59
4:P:77:PHE:HD1	4:P:80:LEU:HD13	1.67	0.59
8:Y:238:SER:O	8:Y:238:SER:OG	2.21	0.59
1:I:180:GLY:HA3	1:I:195:THR:HA	1.84	0.58
5:R:120:ARG:HG2	5:R:124:GLU:HG2	1.84	0.58
7:E:488:PRO:HD2	7:E:491:MET:HE3	1.85	0.58
2:K:8:ILE:O	2:K:12:LEU:HD12	2.03	0.58
5:R:61:MET:HE2	5:R:98:GLU:HB2	1.85	0.58
6:B:274:TYR:HB3	6:B:311:LEU:HD23	1.84	0.58
11:0:48:MET:HE1	16:U:431:LEU:HD12	1.84	0.58
4:P:424:GLY:HA2	4:P:427:VAL:HG12	1.85	0.58
8:Z:51:ASP:OD2	8:Z:84:ARG:NH1	2.30	0.58
1:I:108:ASP:OD2	1:I:111:ARG:NH2	2.36	0.58
2:M:40:ALA:O	2:M:44:ILE:HG13	2.02	0.58
3:O:118:LEU:HD21	3:O:303:PHE:HE1	1.68	0.58
7:E:403:LYS:H	7:E:403:LYS:HD2	1.69	0.58
9:G:149:ALA:HB2	10:N:89:LEU:HD11	1.84	0.58
16:U:303:ASN:HB3	16:U:305:SER:H	1.68	0.58
2:K:28:ARG:HA	2:K:31:ARG:HG2	1.85	0.58
1:I:5:ASP:HA	1:I:8:VAL:HG22	1.86	0.58
1:J:61:GLU:O	1:J:65:GLU:HG2	2.03	0.58
8:X:51:ASP:OD1	8:X:51:ASP:N	2.37	0.58
9:G:83:VAL:HG21	10:N:18:THR:HG23	1.86	0.58
9:G:119:TYR:O	9:G:135:LYS:NZ	2.37	0.58
1:I:16:MET:HG2	2:L:10:GLN:HG3	1.84	0.58
3:O:29:ASN:HD22	3:O:33:ALA:HB2	1.69	0.58
4:P:263:TYR:HB2	4:P:265:ILE:HD11	1.86	0.58
5:R:64:LYS:HE2	5:R:102:GLU:HA	1.85	0.58
8:Z:195:GLU:O	8:Z:199:LEU:HD23	2.04	0.58
5:R:632:GLN:HE21	5:R:636:GLN:NE2	2.02	0.58
6:A:169:PRO:HB2	6:A:172:ASN:HD22	1.69	0.58
6:B:233:VAL:HG13	6:B:234:LEU:HG	1.86	0.58
16:U:435:PHE:CE1	24:U:503:PTY:C20	2.87	0.57
2:K:28:ARG:HA	2:K:31:ARG:HE	1.69	0.57
4:P:22:LYS:O	4:P:26:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:125:LEU:O	5:R:128:LEU:HB2	2.04	0.57
8:X:230:ILE:HG21	8:X:250:SER:HB3	1.85	0.57
10:N:98:TYR:OH	10:N:103:ASP:OD2	2.22	0.57
13:Q:203:THR:HB	13:Q:311:HIS:HB3	1.86	0.57
8:Z:42:LEU:HD23	8:Z:45:ILE:HD12	1.85	0.57
8:Z:188:MET:HE3	8:Z:196:GLN:HG2	1.85	0.57
24:Q:401:PTY:C32	24:U:503:PTY:C32	2.79	0.57
1:H:16:MET:HA	1:H:19:ILE:HG22	1.86	0.57
6:A:89:GLU:OE1	6:A:129:ARG:NH2	2.37	0.57
5:R:20:GLU:OE2	5:R:20:GLU:N	2.37	0.57
8:Y:181:LEU:HD23	8:Y:203:TYR:HB2	1.86	0.57
3:O:98:LEU:H	3:O:98:LEU:HD12	1.70	0.57
3:O:367:TYR:HB3	3:O:369:TYR:CZ	2.40	0.57
5:R:11:THR:HG23	5:R:327:VAL:HG22	1.86	0.57
5:R:598:ASP:HA	14:S:61:ASN:HB3	1.87	0.57
8:Y:242:LEU:HA	8:Y:245:LYS:HB2	1.86	0.57
12:5:98:SER:O	12:5:102:SER:OG	2.21	0.57
16:U:329:ASN:ND2	16:U:365:SER:OG	2.37	0.57
6:C:421:VAL:O	6:C:425:THR:HG23	2.04	0.57
6:C:263:LEU:HD22	6:C:347:MET:HE1	1.86	0.56
7:F:55:GLY:O	7:F:102:THR:OG1	2.22	0.56
12:7:104:LEU:HD21	24:7:201:PTY:H322	1.86	0.56
12:9:12:SER:O	12:9:12:SER:OG	2.23	0.56
7:D:380:ASP:HB2	7:D:393:ASN:HB2	1.87	0.56
4:P:56:LYS:HZ2	4:P:57:ARG:HH21	1.52	0.56
5:R:28:GLU:O	5:R:31:GLU:HG3	2.06	0.56
6:C:100:ASP:OD1	6:C:100:ASP:N	2.36	0.56
16:U:368:SER:HB3	16:U:403:GLN:HB2	1.85	0.56
4:P:391:LEU:O	4:P:394:LEU:CB	2.54	0.56
5:R:87:GLU:HG3	5:R:89:PRO:HD3	1.86	0.56
5:R:99:ALA:O	5:R:102:GLU:HB2	2.06	0.56
4:P:108:VAL:C	4:P:110:ILE:H	2.13	0.56
4:P:387:ASN:HB3	4:P:389:GLU:HB2	1.87	0.56
5:R:18:GLN:NE2	5:R:20:GLU:OE2	2.34	0.56
5:R:100:ASN:HD22	5:R:101:PHE:HD1	1.54	0.56
2:K:78:GLN:O	2:K:82:THR:HG23	2.05	0.56
4:P:145:ILE:HD11	4:P:204:CYS:HB2	1.88	0.56
4:P:168:ILE:HA	4:P:171:GLN:OE1	2.06	0.56
8:Y:124:SER:OG	8:Y:125:ASP:N	2.39	0.56
18:W:5:SIA:H111	19:a:4:SIA:H31	1.87	0.56
4:P:17:ASN:O	4:P:21:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:88:LYS:O	12:1:92:GLN:HG2	2.06	0.56
5:R:793:MET:HE2	12:5:140:VAL:HG11	1.87	0.56
6:B:360:GLU:OE2	7:E:329:THR:OG1	2.15	0.56
9:G:131:LEU:O	9:G:135:LYS:HG2	2.06	0.56
24:Q:401:PTY:H321	24:U:503:PTY:H312	1.88	0.56
3:O:54:LEU:O	3:O:58:LEU:HB2	2.06	0.55
5:R:101:PHE:O	5:R:104:ILE:HB	2.06	0.55
6:C:463:GLU:N	6:C:463:GLU:OE1	2.39	0.55
13:Q:12:ASP:OD1	13:Q:12:ASP:N	2.38	0.55
6:A:50:LEU:HB3	6:A:68:GLU:HG3	1.88	0.55
7:F:82:ARG:HD3	7:F:100:GLU:HB2	1.89	0.55
11:0:56:LEU:HD21	16:U:435:PHE:CZ	2.41	0.55
12:1:22:ALA:O	12:1:26:SER:OG	2.23	0.55
3:O:126:ALA:O	3:O:130:THR:HG23	2.05	0.55
4:P:316:LYS:HE2	4:P:316:LYS:H	1.71	0.55
4:P:359:LEU:HA	4:P:364:LEU:HD11	1.88	0.55
5:R:44:VAL:HG13	5:R:48:GLN:HB2	1.89	0.55
8:X:105:LEU:HD22	8:X:105:LEU:H	1.71	0.55
1:H:49:GLN:N	1:H:49:GLN:OE1	2.39	0.55
3:O:220:GLN:HE21	3:O:221:ASP:CG	2.13	0.55
16:U:296:ASN:O	16:U:312:THR:OG1	2.24	0.55
3:O:29:ASN:O	3:O:32:LEU:HB2	2.07	0.55
3:O:306:SER:HB2	3:O:370:VAL:HG21	1.89	0.55
4:P:56:LYS:HZ3	4:P:57:ARG:HE	1.54	0.55
6:A:507:ILE:HD11	6:A:555:VAL:HG21	1.88	0.55
7:F:327:MET:HE2	7:F:368:LEU:HD12	1.88	0.55
6:B:231:GLN:O	6:B:235:ASP:HB2	2.06	0.55
8:X:201:LYS:HA	8:X:204:VAL:HG12	1.87	0.55
13:Q:179:GLU:O	13:Q:183:ASN:ND2	2.40	0.55
13:Q:217:ASP:OD2	13:Q:274:TYR:OH	2.16	0.55
4:P:408:ALA:HB2	4:P:448:VAL:HG12	1.89	0.55
6:A:561:SER:OG	6:A:562:ASP:N	2.39	0.55
8:Z:151:PHE:O	8:Z:155:MET:HG2	2.06	0.55
22:5:201:CLR:H121	22:V:402:CLR:H181	1.89	0.55
8:Z:237:LEU:HD13	8:Z:243:GLN:HA	1.89	0.55
24:8:201:PTY:H122	24:8:201:PTY:HC12	1.88	0.55
16:U:401:GLN:HE22	17:V:296:ALA:H	1.53	0.55
4:P:156:MET:HE2	4:P:156:MET:HA	1.89	0.55
4:P:329:GLU:H	4:P:329:GLU:CD	2.15	0.55
7:F:124:SER:OG	7:F:125:GLU:N	2.39	0.55
12:4:42:ALA:HA	12:5:127:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:49:ASP:OD2	5:R:228:GLN:HB2	2.06	0.55
6:B:511:VAL:HG11	6:B:548:TYR:CD1	2.42	0.55
9:G:4:LYS:HG2	9:G:5:ASP:H	1.71	0.55
1:I:8:VAL:HB	5:R:196:PHE:CE1	2.41	0.54
2:K:7:GLY:O	2:K:11:LEU:HG	2.07	0.54
3:O:4:PHE:HZ	3:O:99:VAL:HG12	1.72	0.54
4:P:405:GLN:O	4:P:409:VAL:HG23	2.08	0.54
8:Z:114:LYS:NZ	8:Z:114:LYS:HB3	2.22	0.54
1:H:55:GLU:O	1:H:59:LYS:HG2	2.08	0.54
2:M:11:LEU:HD22	3:O:182:LEU:HD11	1.89	0.54
8:X:207:GLN:NE2	8:X:209:GLU:O	2.40	0.54
2:K:41:GLN:HA	2:K:44:ILE:HG12	1.89	0.54
5:R:87:GLU:OE2	5:R:296:LYS:HE3	2.08	0.54
7:D:416:ALA:O	7:D:420:ASN:ND2	2.38	0.54
10:N:74:VAL:HG12	10:N:77:ALA:HB3	1.90	0.54
12:5:88:LYS:O	12:5:92:GLN:HG2	2.07	0.54
12:8:109:ALA:O	12:8:113:VAL:HG12	2.08	0.54
1:I:187:ASP:OD1	1:I:187:ASP:N	2.35	0.54
1:J:16:MET:HG3	2:M:14:ALA:HB2	1.89	0.54
4:P:145:ILE:HD13	4:P:208:MET:HG3	1.90	0.54
5:R:330:LEU:O	5:R:334:GLN:HG3	2.08	0.54
8:Z:237:LEU:HD13	8:Z:243:GLN:HG3	1.90	0.54
22:5:201:CLR:H212	22:V:402:CLR:H181	1.88	0.54
6:A:553:ARG:O	6:A:557:THR:HG23	2.06	0.54
8:X:152:LEU:O	8:X:156:THR:HG23	2.07	0.54
3:O:28:LYS:HE3	3:O:335:LEU:HD23	1.88	0.54
6:A:296:MET:HG2	6:A:305:ILE:HG22	1.90	0.54
6:C:484:GLN:O	6:C:484:GLN:NE2	2.41	0.54
8:X:148:LYS:NZ	8:X:188:MET:O	2.41	0.54
6:C:95:MET:HE3	6:C:308:ARG:HA	1.90	0.54
6:A:350:SER:HB3	6:A:353:ARG:HG3	1.89	0.54
6:C:178:TYR:HB3	6:C:193:GLU:HB3	1.90	0.54
8:Y:207:GLN:NE2	8:Y:212:PRO:HB3	2.23	0.54
12:8:72:VAL:HG11	12:8:99:VAL:HG11	1.89	0.54
4:P:127:LEU:HG	4:P:128:PRO:HD3	1.90	0.54
6:B:25:SER:O	6:B:25:SER:OG	2.26	0.54
6:B:397:ASN:O	6:B:399:GLU:N	2.41	0.54
4:P:99:ASP:HA	4:P:102:GLN:HB2	1.89	0.53
3:O:24:ALA:HA	3:O:31:ASN:HB2	1.89	0.53
4:P:108:VAL:O	4:P:110:ILE:N	2.42	0.53
4:P:244:ILE:HG22	4:P:284:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:299:ARG:O	4:P:299:ARG:NH1	2.42	0.53
6:A:372:SER:O	6:A:372:SER:OG	2.25	0.53
16:U:377:LEU:HB2	16:U:380:LYS:HB2	1.91	0.53
1:I:129:GLU:H	1:I:132:MET:HE2	1.73	0.53
3:O:300:LEU:HA	3:O:303:PHE:HB3	1.90	0.53
6:C:372:SER:O	6:C:372:SER:OG	2.25	0.53
2:M:23:SER:O	2:M:27:LYS:HE2	2.09	0.53
5:R:288:LYS:HG3	5:R:289:ASN:HD22	1.73	0.53
6:C:387:GLU:HG3	7:D:264:ALA:HB3	1.90	0.53
7:F:262:ASN:ND2	7:F:270:GLU:OE1	2.41	0.53
8:X:216:ILE:HB	8:X:217:LEU:HD23	1.91	0.53
3:O:216:LEU:HD23	3:O:217:SER:HB3	1.90	0.53
4:P:155:LEU:HD11	4:P:158:GLY:HA2	1.91	0.53
8:Y:63:GLU:OE2	8:Y:63:GLU:N	2.38	0.53
8:Z:143:ALA:HB1	8:Z:149:ASN:ND2	2.23	0.53
11:0:36:ASP:HB3	11:0:39:TRP:HB3	1.91	0.53
12:5:34:THR:HG23	12:5:59:VAL:HG13	1.90	0.53
2:L:41:GLN:HA	2:L:44:ILE:HD12	1.90	0.53
4:P:278:LYS:HA	5:R:20:GLU:OE1	2.09	0.53
9:G:70:ALA:O	9:G:74:PHE:HD2	1.92	0.53
4:P:71:SER:O	4:P:75:LYS:HE3	2.08	0.53
4:P:257:CYS:O	4:P:261:ARG:NH1	2.41	0.53
5:R:273:ASN:OD1	5:R:274:GLN:N	2.42	0.53
6:A:232:ARG:NH1	6:A:519:PHE:O	2.42	0.53
2:M:13:GLN:HA	2:M:16:LYS:HE3	1.91	0.53
2:M:60:ALA:HA	2:M:63:LEU:HD12	1.90	0.53
4:P:206:GLN:HG2	4:P:245:PHE:HD2	1.73	0.53
4:P:323:GLN:CD	5:R:53:ASN:HB2	2.33	0.53
5:R:18:GLN:O	5:R:22:ALA:N	2.41	0.53
7:F:365:ILE:HB	7:F:366:PRO:HD3	1.91	0.53
3:O:147:LYS:HA	3:O:150:LEU:HD22	1.91	0.52
4:P:261:ARG:NH2	4:P:301:THR:O	2.40	0.52
5:R:54:GLU:HG2	5:R:304:TYR:CZ	2.44	0.52
7:D:438:VAL:HG22	7:D:439:VAL:HG23	1.91	0.52
3:O:96:VAL:HG23	3:O:101:TYR:HB2	1.91	0.52
3:O:188:VAL:HG22	3:O:222:SER:OG	2.08	0.52
4:P:75:LYS:HA	4:P:78:ILE:HG13	1.90	0.52
7:F:193:SER:OG	7:F:194:ALA:N	2.43	0.52
9:G:94:ILE:HD13	10:N:63:ILE:HD12	1.92	0.52
9:G:179:ARG:O	9:G:183:THR:HG22	2.09	0.52
2:L:18:ALA:O	2:L:22:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:64:GLU:O	4:P:68:THR:HG23	2.09	0.52
4:P:108:VAL:HG13	4:P:113:ASP:H	1.74	0.52
4:P:145:ILE:O	4:P:148:LEU:HB2	2.09	0.52
5:R:808:VAL:HG21	12:4:136:ILE:HD11	1.91	0.52
8:Y:61:ARG:NH1	8:Y:64:GLU:OE2	2.42	0.52
12:5:109:ALA:O	12:5:113:VAL:HG12	2.08	0.52
3:O:66:GLU:HA	3:O:69:VAL:HG12	1.91	0.52
5:R:43:ASP:N	5:R:43:ASP:OD2	2.43	0.52
5:R:481:VAL:HG11	14:S:73:ILE:HG23	1.91	0.52
16:U:375:SER:HB2	16:U:396:MET:HA	1.90	0.52
3:O:234:VAL:O	3:O:238:ARG:N	2.34	0.52
6:A:324:GLU:HA	6:A:354:TRP:CD1	2.44	0.52
6:C:53:GLU:OE2	6:C:212:ARG:NH2	2.42	0.52
7:D:106:ASP:OD2	7:D:109:LYS:NZ	2.33	0.52
1:J:16:MET:O	1:J:20:GLU:HG2	2.09	0.52
6:B:350:SER:H	6:B:409:ALA:HB3	1.74	0.52
8:Y:238:SER:N	8:Y:270:ASN:HD21	2.08	0.52
8:Z:159:LEU:HB2	8:Z:178:LEU:HD22	1.91	0.52
18:W:5:SIA:C11	19:a:4:SIA:H31	2.39	0.52
1:H:129:GLU:H	1:H:132:MET:HE2	1.74	0.52
5:R:575:GLU:O	5:R:727:TYR:OH	2.27	0.52
8:Z:33:MET:HE2	8:Z:88:LEU:HD21	1.92	0.52
16:U:438:PHE:CE2	24:U:503:PTY:H182	2.31	0.52
1:I:16:MET:CG	2:L:10:GLN:HG3	2.40	0.52
4:P:351:SER:OG	4:P:354:GLU:OE2	2.28	0.52
7:D:365:ILE:HB	7:D:366:PRO:HD3	1.92	0.52
8:X:259:LEU:O	8:X:263:ILE:HD12	2.10	0.52
1:I:9:GLN:O	1:I:13:LYS:HD3	2.09	0.52
1:J:57:TYR:O	1:J:61:GLU:HG2	2.09	0.52
4:P:148:LEU:HD11	4:P:155:LEU:HD13	1.90	0.52
4:P:405:GLN:CD	4:P:405:GLN:H	2.18	0.52
6:B:553:ARG:O	6:B:557:THR:HG23	2.10	0.52
7:F:465:GLN:NE2	7:F:469:GLU:O	2.43	0.52
10:N:50:ASP:OD2	10:N:51:THR:N	2.43	0.52
11:0:18:CYS:SG	22:0:304:CLR:H273	2.50	0.52
12:4:6:SER:OG	12:4:7:GLY:N	2.41	0.52
4:P:111:PHE:CG	4:P:152:GLY:HA3	2.45	0.51
5:R:399:PHE:HB3	5:R:400:PRO:HD3	1.90	0.51
6:B:500:SER:O	6:B:500:SER:OG	2.28	0.51
7:F:253:SER:OG	7:F:255:ASP:OD1	2.22	0.51
17:V:329:TRP:CE3	24:V:403:PTY:O30	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:27:LYS:HD2	2:K:27:LYS:N	2.26	0.51
3:O:83:SER:HA	3:O:88:GLN:O	2.10	0.51
4:P:376:TRP:HA	4:P:376:TRP:CE3	2.44	0.51
7:D:442:GLU:CD	7:D:442:GLU:H	2.18	0.51
12:3:72:VAL:HG11	12:3:99:VAL:HG11	1.91	0.51
4:P:162:ASN:HA	4:P:167:TRP:CH2	2.46	0.51
16:U:445:HIS:CE1	24:U:503:PTY:C30	2.94	0.51
4:P:210:ARG:O	4:P:215:ARG:NH2	2.43	0.51
5:R:228:GLN:HB3	5:R:232:ARG:NH2	2.26	0.51
1:I:215:LEU:HD23	2:L:91:ASN:HB2	1.92	0.51
3:O:76:MET:HG2	3:O:91:LEU:HD11	1.93	0.51
4:P:257:CYS:O	4:P:261:ARG:HG2	2.10	0.51
4:P:307:LEU:O	4:P:310:ILE:N	2.44	0.51
4:P:450:TYR:OH	5:R:107:GLU:OE2	2.28	0.51
12:7:88:LYS:O	12:7:92:GLN:HG2	2.11	0.51
16:U:445:HIS:ND1	24:U:503:PTY:C30	2.74	0.51
3:O:187:VAL:HG11	3:O:197:TRP:CZ2	2.46	0.51
8:Y:54:ILE:HA	8:Y:57:GLU:HG2	1.92	0.51
8:Z:200:PHE:O	8:Z:204:VAL:HG12	2.11	0.51
2:M:22:VAL:O	2:M:26:ARG:HG2	2.11	0.51
3:O:102:ILE:HD12	3:O:103:THR:N	2.26	0.51
4:P:230:VAL:HG23	4:P:243:MET:HE1	1.91	0.51
4:P:247:ILE:HA	4:P:250:LEU:HD12	1.92	0.51
6:B:95:MET:HE1	6:B:271:VAL:HG13	1.91	0.51
8:X:83:ARG:NH1	8:X:119:VAL:O	2.33	0.51
2:K:6:GLN:O	2:K:10:GLN:HG2	2.11	0.51
4:P:47:CYS:HA	4:P:50:ILE:HD12	1.93	0.51
28:C:701:ADP:O1B	7:F:400:ARG:NH2	2.42	0.51
7:E:376:GLN:HG3	7:E:378:TYR:CE2	2.45	0.51
11:0:2:THR:HG22	11:0:3:GLY:H	1.75	0.51
13:Q:284:ASN:HD22	13:Q:285:PRO:HD2	1.76	0.51
1:I:20:GLU:O	1:I:24:ASN:ND2	2.43	0.51
1:J:2:ALA:HB2	3:O:203:THR:HG22	1.92	0.51
3:O:176:VAL:H	3:O:184:THR:HG1	1.59	0.51
6:A:75:VAL:HB	7:D:66:PRO:HD2	1.93	0.51
9:G:144:LEU:O	9:G:147:GLU:HG3	2.11	0.51
12:8:33:GLY:O	12:8:37:SER:OG	2.29	0.51
2:L:18:ALA:O	2:L:21:LYS:HG2	2.11	0.50
3:O:29:ASN:ND2	3:O:33:ALA:HB2	2.26	0.50
3:O:42:ASP:N	3:O:42:ASP:OD1	2.44	0.50
4:P:337:PHE:CZ	4:P:341:LYS:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:173:ARG:HD3	8:Y:20:SER:OG	2.11	0.50
6:C:398:PRO:O	6:C:400:ARG:HD3	2.11	0.50
1:I:149:GLN:O	1:I:153:PRO:HD2	2.12	0.50
4:P:162:ASN:HA	4:P:167:TRP:HH2	1.76	0.50
3:O:149:ASN:HA	3:O:152:ASN:OD1	2.12	0.50
6:B:511:VAL:HG11	6:B:548:TYR:HD1	1.74	0.50
6:B:566:THR:H	6:B:569:ILE:HD12	1.75	0.50
1:I:38:PHE:CD2	2:L:36:ALA:HB2	2.47	0.50
1:J:38:PHE:CD1	2:M:36:ALA:HB2	2.47	0.50
2:K:25:ALA:HA	2:K:28:ARG:NE	2.27	0.50
3:O:86:LYS:HE2	3:O:87:VAL:HG22	1.93	0.50
4:P:56:LYS:HB2	4:P:107:ARG:NH2	2.25	0.50
7:D:226:ASN:N	7:D:226:ASN:OD1	2.44	0.50
22:5:201:CLR:H261	22:V:402:CLR:H261	1.92	0.50
24:8:202:PTY:H332	24:8:202:PTY:C17	2.41	0.50
1:J:212:ARG:NH1	7:F:126:ASP:OD2	2.44	0.50
2:K:67:GLY:O	2:K:71:THR:HG23	2.12	0.50
9:G:145:LEU:HD23	10:N:65:LEU:HD23	1.93	0.50
4:P:77:PHE:HB3	4:P:81:MET:HE1	1.94	0.50
6:C:511:VAL:HG11	6:C:548:TYR:CD1	2.46	0.50
3:O:231:ARG:O	3:O:234:VAL:HG22	2.11	0.50
3:O:238:ARG:HG2	3:O:248:VAL:HG21	1.93	0.50
3:O:329:LYS:HG3	3:O:330:LYS:H	1.77	0.50
4:P:145:ILE:O	4:P:148:LEU:N	2.45	0.50
4:P:388:TYR:O	4:P:392:LYS:N	2.44	0.50
5:R:41:ASN:OD1	5:R:49:ARG:NH2	2.45	0.50
24:R:904:PTY:H181	14:S:40:MET:HB3	1.94	0.50
6:B:492:ILE:O	6:B:496:VAL:HG22	2.12	0.50
6:B:534:PHE:O	6:B:538:VAL:HG22	2.12	0.50
6:C:42:LEU:O	6:C:82:THR:OG1	2.30	0.50
12:6:88:LYS:O	12:6:92:GLN:HG2	2.11	0.50
1:J:48:THR:OG1	1:J:49:GLN:OE1	2.24	0.50
3:O:17:GLN:HE22	3:O:37:LYS:HG2	1.77	0.50
3:O:68:VAL:HB	3:O:133:ASP:OD2	2.12	0.50
4:P:37:LEU:H	4:P:37:LEU:HD23	1.76	0.50
4:P:72:GLN:N	4:P:72:GLN:OE1	2.45	0.50
5:R:46:VAL:HA	5:R:49:ARG:HB2	1.93	0.50
8:X:97:SER:O	8:X:160:GLN:NE2	2.45	0.50
12:9:88:LYS:O	12:9:92:GLN:HG2	2.11	0.50
1:I:14:HIS:HE2	3:O:312:LEU:N	1.98	0.50
4:P:65:MET:HA	4:P:68:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:170:GLU:CD	8:X:170:GLU:H	2.20	0.50
2:L:13:GLN:O	2:L:17:ARG:HG2	2.11	0.49
3:O:4:PHE:HB2	3:O:374:ILE:HG23	1.94	0.49
3:O:334:VAL:O	3:O:338:LEU:HB2	2.12	0.49
8:X:111:GLN:HG2	8:X:169:THR:HG23	1.93	0.49
2:M:13:GLN:HB3	2:M:17:ARG:HH11	1.77	0.49
3:O:278:PRO:HA	3:O:281:ARG:HH21	1.77	0.49
4:P:391:LEU:O	4:P:394:LEU:HB3	2.12	0.49
5:R:170:PHE:CD2	5:R:223:PHE:HB3	2.47	0.49
1:H:57:TYR:CE2	1:H:58:GLU:HG2	2.47	0.49
1:I:131:ARG:NH1	1:I:164:ASP:OD1	2.45	0.49
3:O:58:LEU:HB3	3:O:301:ARG:HG2	1.94	0.49
3:O:166:LEU:HD21	3:O:249:ARG:HG2	1.94	0.49
3:O:346:ALA:HB2	5:R:192:ARG:HD3	1.94	0.49
4:P:463:ASN:OD1	5:R:264:ARG:NH2	2.44	0.49
6:B:553:ARG:HA	6:B:556:GLU:OE2	2.12	0.49
8:Z:236:LYS:O	8:Z:236:LYS:HD3	2.12	0.49
8:Z:268:LYS:HA	8:Z:271:GLU:HB3	1.93	0.49
6:B:327:ILE:HG23	6:B:385:PHE:CE1	2.47	0.49
8:Y:214:GLU:O	8:Y:214:GLU:HG2	2.12	0.49
10:N:14:GLU:HG3	10:N:38:VAL:HG11	1.94	0.49
16:U:350:ASN:OD1	16:U:351:GLY:N	2.45	0.49
3:O:28:LYS:HE3	3:O:335:LEU:CD2	2.42	0.49
4:P:104:ASN:HB2	4:P:107:ARG:HB2	1.93	0.49
4:P:118:SER:O	4:P:122:ALA:N	2.45	0.49
4:P:230:VAL:CG2	4:P:243:MET:HE1	2.43	0.49
4:P:315:LEU:O	4:P:319:GLU:HG2	2.13	0.49
5:R:771:GLY:HA2	5:R:774:VAL:HG12	1.94	0.49
7:E:421:GLN:NE2	7:E:425:CYS:SG	2.84	0.49
12:1:6:SER:OG	12:1:7:GLY:N	2.44	0.49
4:P:316:LYS:HA	4:P:319:GLU:HG2	1.95	0.49
1:H:20:GLU:HG2	2:K:17:ARG:HD2	1.93	0.49
5:R:270:MET:HE3	5:R:274:GLN:HE21	1.78	0.49
22:5:201:CLR:H11	24:V:403:PTY:HC12	1.93	0.49
1:J:16:MET:HE3	2:M:10:GLN:HB3	1.94	0.49
3:O:173:ASP:OD1	3:O:173:ASP:N	2.45	0.49
4:P:394:LEU:HD12	4:P:397:LEU:HD11	1.95	0.49
6:A:583:SER:O	6:A:583:SER:OG	2.25	0.49
7:D:436:LYS:HB2	7:D:444:LEU:HD11	1.93	0.49
8:Z:239:SER:O	8:Z:243:GLN:N	2.46	0.49
11:0:47:PHE:O	11:0:51:ASN:ND2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:0:164:LEU:HD13	13:Q:21:ARG:HD2	1.95	0.49
1:H:136:CYS:SG	1:H:144:VAL:HG11	2.53	0.49
2:M:73:VAL:HA	2:M:76:GLU:CD	2.38	0.49
4:P:129:MET:HG2	4:P:137:THR:O	2.12	0.49
4:P:206:GLN:HG2	4:P:245:PHE:CD2	2.47	0.49
12:4:88:LYS:O	12:4:92:GLN:HG2	2.13	0.49
1:I:212:ARG:NH1	7:E:126:ASP:OD2	2.46	0.49
3:O:347:ALA:HA	3:O:366:TYR:HB3	1.95	0.49
1:H:29:GLU:OE2	4:P:283:ARG:NH1	2.46	0.48
1:H:39:ASN:O	1:H:42:LYS:HG3	2.13	0.48
3:O:207:MET:HE2	3:O:233:ALA:HB2	1.95	0.48
4:P:56:LYS:HD3	4:P:57:ARG:HE	1.78	0.48
4:P:90:VAL:O	4:P:94:LEU:HB2	2.13	0.48
7:D:487:PHE:HD2	7:D:491:MET:HE3	1.78	0.48
8:Z:143:ALA:HB1	8:Z:149:ASN:HD22	1.78	0.48
1:H:12:ILE:O	1:H:16:MET:HG2	2.13	0.48
1:H:127:LEU:HD12	1:H:183:ILE:HG22	1.95	0.48
12:2:28:LEU:HD23	12:3:105:ALA:HB2	1.94	0.48
12:3:47:MET:HG2	12:3:48:ARG:HG3	1.94	0.48
15:T:100:LEU:O	15:T:104:VAL:HG22	2.12	0.48
5:R:197:LEU:HD13	5:R:220:PHE:HB3	1.94	0.48
5:R:224:PHE:CD2	5:R:233:VAL:HB	2.47	0.48
7:D:231:PHE:HB3	7:D:259:LEU:HD23	1.94	0.48
12:8:35:ALA:O	12:8:39:THR:HG23	2.13	0.48
1:H:46:VAL:O	1:H:50:ARG:HB2	2.13	0.48
4:P:380:ALA:HA	4:P:383:LEU:HD23	1.96	0.48
12:5:53:MET:HE1	12:6:133:LEU:HD12	1.95	0.48
1:I:32:ALA:O	1:I:36:GLU:HG2	2.13	0.48
4:P:135:PRO:HB2	4:P:137:THR:HG23	1.96	0.48
5:R:334:GLN:HG2	5:R:352:LEU:HD21	1.95	0.48
5:R:494:LEU:O	14:S:70:ASN:ND2	2.41	0.48
8:X:98:ILE:HD12	8:X:164:ALA:HB2	1.94	0.48
19:a:4:SIA:O1A	19:a:4:SIA:H6	2.12	0.48
1:I:127:LEU:HD12	1:I:183:ILE:HG22	1.96	0.48
6:B:96:GLY:HA2	6:B:306:MET:HE3	1.96	0.48
1:I:206:GLN:NE2	7:E:40:LEU:O	2.43	0.48
2:M:34:LYS:O	2:M:38:GLU:HG2	2.14	0.48
8:Z:22:VAL:HG21	8:Z:69:SER:OG	2.13	0.48
8:Z:242:LEU:HD22	8:Z:269:GLU:HG3	1.96	0.48
12:8:150:LEU:O	12:8:154:THR:OG1	2.29	0.48
1:I:33:LYS:HA	1:I:36:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:45:GLU:O	4:P:49:PHE:HB2	2.13	0.48
6:C:587:LYS:HE3	6:C:600:ASP:HB3	1.96	0.48
7:E:365:ILE:HB	7:E:366:PRO:HD3	1.96	0.48
8:X:54:ILE:HA	8:X:57:GLU:HG2	1.96	0.48
22:5:201:CLR:H11	24:V:403:PTY:C1	2.44	0.48
3:O:151:GLN:O	3:O:154:GLU:HG2	2.13	0.48
13:Q:237:ARG:NH2	13:Q:258:ALA:O	2.46	0.48
1:H:187:ASP:OD2	1:H:187:ASP:N	2.47	0.48
3:O:131:GLN:NE2	3:O:135:ASP:OD1	2.47	0.48
4:P:54:GLU:HB3	4:P:55:MET:HE2	1.96	0.48
6:B:349:ASP:HA	6:B:409:ALA:HB3	1.95	0.48
8:Z:220:GLU:CD	8:Z:220:GLU:H	2.22	0.48
10:N:13:ASP:OD1	10:N:13:ASP:N	2.38	0.48
12:2:35:ALA:O	12:2:39:THR:HG23	2.14	0.48
1:H:61:GLU:O	1:H:64:ILE:HG13	2.14	0.47
9:G:119:TYR:HB3	9:G:122:THR:HG21	1.95	0.47
12:9:115:ASP:OD2	12:9:119:ARG:NH2	2.47	0.47
18:W:5:SIA:H112	19:a:1:GAL:H3	1.96	0.47
1:H:102:LEU:O	1:H:105:VAL:HG12	2.14	0.47
2:K:25:ALA:HA	2:K:28:ARG:HE	1.79	0.47
3:O:48:LEU:O	3:O:52:VAL:HG23	2.14	0.47
4:P:452:ALA:O	4:P:456:VAL:HG13	2.14	0.47
5:R:310:CYS:SG	5:R:319:LEU:HB3	2.54	0.47
5:R:831:ARG:HA	5:R:831:ARG:HH11	1.78	0.47
6:C:350:SER:HB3	6:C:353:ARG:HG2	1.95	0.47
8:Y:197:TYR:O	8:Y:201:LYS:HG3	2.14	0.47
8:Z:237:LEU:CD1	8:Z:243:GLN:HG3	2.44	0.47
16:U:266:ARG:HD2	16:U:302:TRP:CE3	2.49	0.47
16:U:410:GLU:OE2	20:b:1:NAG:O6	2.30	0.47
1:J:159:THR:OG1	1:J:161:ASN:OD1	2.21	0.47
3:O:120:ASN:O	3:O:124:ILE:HG23	2.14	0.47
8:Y:134:ASN:HA	8:Y:137:THR:HG22	1.96	0.47
12:2:10:TYR:HB2	17:V:309:MET:HE1	1.95	0.47
1:I:182:GLU:HG2	1:I:193:SER:HA	1.96	0.47
4:P:31:VAL:HG21	4:P:33:TRP:CD2	2.49	0.47
5:R:19:SER:HA	5:R:22:ALA:HB3	1.95	0.47
6:C:444:HIS:ND1	6:C:521:GLN:OE1	2.48	0.47
1:I:26:LYS:HA	1:I:29:GLU:HG2	1.96	0.47
3:O:193:ASN:HD22	3:O:245:LYS:HB2	1.79	0.47
5:R:170:PHE:HA	5:R:223:PHE:CD2	2.49	0.47
6:B:377:TYR:O	6:B:381:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:61:ASP:OD1	7:E:62:HIS:N	2.45	0.47
8:X:209:GLU:OE2	8:X:210:GLU:N	2.48	0.47
8:Z:225:LEU:HD12	8:Z:226:VAL:HG23	1.96	0.47
4:P:101:LEU:HA	4:P:104:ASN:HB3	1.96	0.47
4:P:198:VAL:HA	4:P:201:VAL:HG22	1.96	0.47
12:6:94:GLY:O	12:6:98:SER:OG	2.33	0.47
17:V:319:LEU:HD23	17:V:319:LEU:HA	1.74	0.47
1:J:177:ILE:HG22	1:J:179:GLY:H	1.79	0.47
4:P:230:VAL:O	4:P:233:ASN:HB2	2.14	0.47
4:P:333:GLU:OE2	4:P:333:GLU:HA	2.15	0.47
4:P:389:GLU:HA	4:P:392:LYS:CB	2.44	0.47
6:A:56:ARG:HB3	6:A:63:THR:HB	1.95	0.47
6:A:100:ASP:N	6:A:100:ASP:OD1	2.44	0.47
6:C:238:PHE:CZ	6:C:450:TRP:HA	2.50	0.47
8:Y:209:GLU:CD	8:Y:211:SER:H	2.22	0.47
8:Y:233:ALA:HA	8:Y:236:LYS:HD3	1.96	0.47
12:8:75:LEU:HD23	12:8:75:LEU:HA	1.79	0.47
16:U:324:LYS:HB2	16:U:346:GLU:HG3	1.97	0.47
2:K:50:GLN:O	2:K:54:GLU:HG2	2.14	0.47
2:L:12:LEU:O	2:L:16:LYS:HB2	2.15	0.47
3:O:159:GLY:C	3:O:164:ARG:HG2	2.39	0.47
5:R:232:ARG:O	5:R:236:ILE:HG12	2.15	0.47
14:S:28:ILE:O	14:S:34:ARG:NH1	2.47	0.47
1:H:182:GLU:HG2	1:H:193:SER:HA	1.96	0.47
1:I:46:VAL:O	1:I:50:ARG:HB2	2.15	0.47
1:J:44:ARG:HD2	1:J:45:LEU:HD22	1.97	0.47
3:O:332:ARG:NH2	3:O:333:GLU:OE1	2.48	0.47
4:P:426:ARG:O	4:P:429:GLU:HG2	2.14	0.47
6:A:592:ASP:N	6:A:592:ASP:OD1	2.47	0.47
7:E:457:LYS:O	7:E:461:ASN:HB2	2.15	0.47
3:O:90:ASN:HB3	3:O:98:LEU:HD11	1.97	0.47
3:O:282:TRP:CE2	3:O:286:ASN:ND2	2.83	0.47
4:P:209:LEU:HD22	4:P:215:ARG:HA	1.97	0.47
4:P:377:ARG:CZ	4:P:420:HIS:HE1	2.28	0.47
5:R:182:THR:O	5:R:186:MET:HG2	2.14	0.47
6:B:362:SER:OG	6:B:363:GLY:N	2.48	0.47
7:D:435:MET:HA	7:D:438:VAL:HG12	1.96	0.47
7:F:505:PRO:O	7:F:506:ARG:HG3	2.14	0.47
16:U:319:THR:HG21	16:U:350:ASN:HA	1.96	0.47
2:L:49:LEU:O	2:L:53:LYS:HG2	2.14	0.46
3:O:343:ASP:OD2	3:O:344:SER:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:33:TRP:HB2	4:P:47:CYS:SG	2.55	0.46
4:P:116:ARG:O	4:P:116:ARG:NH1	2.48	0.46
4:P:426:ARG:HA	4:P:429:GLU:CD	2.40	0.46
6:A:492:ILE:HG21	7:E:437:ALA:HB1	1.96	0.46
8:Y:246:LEU:HD12	8:Y:266:ILE:HD12	1.96	0.46
10:N:71:ALA:HB1	10:N:78:LEU:HD21	1.97	0.46
12:7:24:VAL:HG11	24:8:201:PTY:H392	1.97	0.46
1:J:6:ALA:O	1:J:10:LYS:HG3	2.15	0.46
2:K:10:GLN:O	2:K:13:GLN:HB2	2.15	0.46
2:L:12:LEU:HD12	2:L:13:GLN:N	2.30	0.46
2:L:79:GLU:O	2:L:82:THR:HG22	2.16	0.46
3:O:6:LEU:HB3	3:O:320:LEU:HD13	1.97	0.46
3:O:75:TYR:HA	3:O:78:ASP:OD1	2.14	0.46
3:O:249:ARG:O	3:O:251:PHE:N	2.48	0.46
1:H:50:ARG:O	1:H:54:MET:HG2	2.15	0.46
3:O:197:TRP:HB2	3:O:246:PHE:CE1	2.50	0.46
3:O:254:ASN:N	3:O:254:ASN:OD1	2.49	0.46
3:O:343:ASP:HB2	5:R:192:ARG:HH21	1.80	0.46
4:P:53:PHE:H	4:P:61:GLU:CD	2.23	0.46
7:F:380:ASP:HB2	7:F:393:ASN:HB2	1.96	0.46
12:3:117:GLY:O	12:3:121:THR:HG22	2.15	0.46
12:9:6:SER:OG	12:9:7:GLY:N	2.47	0.46
3:O:77:ALA:HA	3:O:83:SER:O	2.16	0.46
6:B:152:ILE:HG12	6:B:167:MET:HG2	1.97	0.46
6:C:481:GLU:O	6:C:485:GLU:HG3	2.16	0.46
7:F:237:ASN:H	7:F:237:ASN:ND2	2.13	0.46
12:6:35:ALA:O	12:6:39:THR:HG23	2.16	0.46
13:Q:260:ASP:N	13:Q:260:ASP:OD1	2.46	0.46
2:M:54:GLU:O	2:M:58:LYS:HE2	2.15	0.46
3:O:84:LYS:O	3:O:89:GLU:HA	2.15	0.46
5:R:175:ILE:HG22	5:R:219:VAL:HG13	1.97	0.46
5:R:188:TRP:HB3	5:R:192:ARG:HD2	1.96	0.46
7:E:436:LYS:HG3	7:E:444:LEU:HD11	1.97	0.46
12:7:28:LEU:HD22	24:8:201:PTY:HC11	1.98	0.46
3:O:183:VAL:HB	3:O:231:ARG:NE	2.27	0.46
5:R:111:ILE:HA	5:R:114:ASN:HB2	1.98	0.46
5:R:170:PHE:O	5:R:198:ARG:NH2	2.49	0.46
5:R:761:HIS:HD2	15:T:82:ASP:OD1	1.99	0.46
7:F:71:ILE:O	7:F:115:THR:OG1	2.31	0.46
8:Y:227:LYS:HB2	8:Y:227:LYS:HE2	1.48	0.46
16:U:262:ASP:C	16:U:264:ALA:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:36:SER:OG	3:O:37:LYS:N	2.48	0.46
3:O:62:ASP:HA	3:O:65:VAL:HG22	1.98	0.46
4:P:77:PHE:CD1	4:P:80:LEU:HD13	2.48	0.46
22:R:901:CLR:H213	24:R:904:PTY:H191	1.97	0.46
6:A:547:PHE:HB2	6:A:608:MET:SD	2.56	0.46
7:E:379:VAL:HG13	7:E:391:PRO:HG2	1.96	0.46
11:0:128:HIS:HB3	12:9:82:ASP:HB2	1.97	0.46
1:I:31:ASP:HA	2:L:32:ARG:NH1	2.30	0.46
2:L:32:ARG:O	2:L:35:GLN:HG2	2.15	0.46
4:P:87:GLU:HA	4:P:90:VAL:HG12	1.97	0.46
4:P:144:ILE:HD12	4:P:144:ILE:HA	1.74	0.46
4:P:376:TRP:HA	4:P:376:TRP:HE3	1.80	0.46
6:A:157:SER:O	6:A:157:SER:OG	2.32	0.46
6:B:463:GLU:OE2	6:B:463:GLU:N	2.46	0.46
6:B:523:ASN:O	6:B:526:THR:OG1	2.33	0.46
7:D:432:VAL:HG12	7:D:452:LEU:HD21	1.97	0.46
8:Y:207:GLN:HE21	8:Y:209:GLU:HB3	1.79	0.46
8:Z:19:HIS:CG	8:Z:70:LYS:HG3	2.51	0.46
5:R:90:PHE:HE2	5:R:343:HIS:CD2	2.34	0.46
5:R:740:ARG:NH2	12:4:139:GLU:OE1	2.49	0.46
8:X:17:GLN:O	8:X:21:GLN:HG2	2.15	0.46
8:X:72:GLY:HA2	8:X:76:ASN:ND2	2.30	0.46
8:X:220:GLU:O	8:X:224:ILE:HG13	2.16	0.46
8:Z:229:MET:HE2	8:Z:229:MET:HA	1.97	0.46
3:O:176:VAL:HG12	3:O:184:THR:OG1	2.16	0.46
4:P:315:LEU:HA	4:P:318:LEU:HD12	1.97	0.46
6:B:224:ASN:OD1	8:Y:123:LYS:NZ	2.49	0.46
8:X:250:SER:O	8:X:250:SER:OG	2.29	0.46
10:N:75:ARG:HA	10:N:75:ARG:HD2	1.72	0.46
11:0:191:VAL:O	11:0:195:ILE:HG13	2.16	0.46
4:P:313:LYS:HB2	4:P:313:LYS:HE2	1.76	0.45
4:P:351:SER:OG	4:P:353:ASP:OD1	2.32	0.45
4:P:379:ASN:HD21	4:P:382:ARG:HH11	1.64	0.45
6:C:234:LEU:HD21	6:C:448:VAL:HG21	1.97	0.45
2:L:10:GLN:O	2:L:13:GLN:HG3	2.16	0.45
2:M:81:MET:O	2:M:85:GLN:HG2	2.16	0.45
3:O:166:LEU:O	3:O:170:VAL:HG12	2.16	0.45
5:R:476:GLY:O	14:S:4:HIS:NE2	2.45	0.45
8:Z:270:ASN:O	8:Z:273:LEU:HB2	2.16	0.45
1:I:80:ARG:NH2	7:E:254:MET:O	2.49	0.45
3:O:304:VAL:HA	3:O:307:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:212:ASN:O	4:P:215:ARG:HB3	2.17	0.45
8:X:113:GLU:O	8:X:117:GLN:HG2	2.16	0.45
11:0:88:THR:OG1	11:0:89:LYS:N	2.50	0.45
24:5:202:PTY:O10	24:6:201:PTY:HC12	2.16	0.45
4:P:17:ASN:OD1	4:P:196:GLN:NE2	2.50	0.45
5:R:389:ILE:HD11	5:R:557:PHE:HB2	1.99	0.45
7:F:226:ASN:OD1	7:F:226:ASN:N	2.49	0.45
11:0:56:LEU:HD21	16:U:435:PHE:HZ	1.81	0.45
24:7:201:PTY:O10	24:7:201:PTY:HC12	2.16	0.45
1:I:68:LYS:HB3	1:I:68:LYS:HE3	1.77	0.45
3:O:171:LYS:HG3	3:O:172:LYS:H	1.82	0.45
4:P:59:PRO:O	4:P:62:LYS:HB2	2.17	0.45
4:P:81:MET:HE2	4:P:97:VAL:HG11	1.98	0.45
4:P:132:ARG:C	4:P:135:PRO:HD2	2.41	0.45
5:R:84:GLU:HG3	5:R:292:VAL:HB	1.98	0.45
6:B:545:ILE:HD12	6:B:546:ALA:N	2.32	0.45
6:C:42:LEU:HD23	6:C:53:GLU:HG3	1.99	0.45
6:C:169:PRO:HB2	6:C:172:ASN:HD22	1.82	0.45
7:D:363:HIS:HB3	7:D:366:PRO:HD2	1.99	0.45
7:F:131:VAL:HG22	7:F:259:LEU:HD12	1.99	0.45
8:Y:261:ASP:HA	8:Y:264:ASP:OD2	2.17	0.45
11:0:49:TRP:HB3	11:0:138:PHE:HB2	1.98	0.45
12:3:121:THR:O	12:3:121:THR:OG1	2.35	0.45
13:Q:115:GLY:HA3	13:Q:125:LEU:HD11	1.99	0.45
1:I:210:GLU:OE1	7:E:39:TYR:OH	2.30	0.45
2:K:32:ARG:HA	2:K:35:GLN:NE2	2.31	0.45
4:P:71:SER:O	4:P:75:LYS:HB3	2.17	0.45
7:E:380:ASP:HB2	7:E:393:ASN:HB2	1.98	0.45
7:F:417:ASP:HB3	7:F:495:ILE:HG23	1.99	0.45
9:G:55:LYS:NZ	10:N:103:ASP:OD2	2.42	0.45
12:7:133:LEU:HD23	12:7:133:LEU:HA	1.71	0.45
3:O:98:LEU:O	3:O:102:ILE:HG13	2.17	0.45
4:P:133:GLN:NE2	4:P:166:ASN:HA	2.32	0.45
4:P:363:ARG:HA	4:P:363:ARG:NH1	2.32	0.45
5:R:129:LYS:HD3	5:R:133:ARG:HH11	1.82	0.45
6:B:439:LEU:HD23	6:B:444:HIS:CD2	2.51	0.45
6:C:249:PRO:HG2	6:C:432:PHE:HE1	1.82	0.45
11:0:70:TYR:CD1	11:0:70:TYR:C	2.95	0.45
1:H:48:THR:HG23	1:H:49:GLN:H	1.82	0.45
3:O:107:TRP:HA	3:O:296:HIS:HE1	1.82	0.45
3:O:121:ILE:O	3:O:124:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:165:PHE:HD1	4:P:168:ILE:HB	1.82	0.45
6:A:376:ALA:HB1	7:E:309:GLU:HA	1.98	0.45
6:A:574:MET:HE3	6:A:611:ALA:HB3	1.98	0.45
7:E:350:GLN:HE21	7:E:350:GLN:HB3	1.51	0.45
7:E:393:ASN:O	7:E:397:SER:OG	2.28	0.45
8:Z:213:PHE:CE2	8:Z:255:LEU:HD22	2.52	0.45
12:6:150:LEU:O	12:6:154:THR:OG1	2.35	0.45
16:U:325:PHE:HB3	16:U:342:MET:HE2	1.98	0.45
3:O:284:LYS:HA	3:O:284:LYS:HD2	1.85	0.45
4:P:47:CYS:O	4:P:50:ILE:HB	2.17	0.45
4:P:114:TYR:CD1	4:P:114:TYR:N	2.85	0.45
4:P:197:TYR:O	4:P:201:VAL:HG13	2.17	0.45
5:R:620:TYR:HD1	5:R:627:MET:HE1	1.82	0.45
6:A:234:LEU:HD21	6:A:448:VAL:HG21	1.98	0.45
6:C:238:PHE:HZ	6:C:450:TRP:HA	1.81	0.45
7:D:445:THR:HG22	7:D:446:SER:N	2.32	0.45
7:F:231:PHE:HB3	7:F:259:LEU:HD23	1.99	0.45
8:Z:240:LYS:HA	8:Z:243:GLN:HB2	1.99	0.45
16:U:284:ASP:OD2	16:U:286:THR:HG22	2.16	0.45
3:O:4:PHE:CZ	3:O:99:VAL:HG12	2.51	0.45
3:O:66:GLU:HB3	3:O:294:TRP:NE1	2.32	0.45
3:O:195:ASN:HA	3:O:198:ILE:HD12	1.99	0.45
4:P:379:ASN:ND2	4:P:382:ARG:HG3	2.32	0.45
8:X:49:TYR:O	8:X:53:LEU:HB2	2.17	0.45
12:2:133:LEU:HA	12:2:133:LEU:HD23	1.74	0.45
16:U:289:THR:OG1	16:U:313:TYR:OH	2.21	0.45
1:H:38:PHE:CE1	2:K:36:ALA:HA	2.52	0.44
1:I:13:LYS:HG3	2:L:10:GLN:NE2	2.32	0.44
1:I:221:ASN:OD1	1:I:221:ASN:N	2.43	0.44
1:J:47:GLN:HE22	1:J:50:ARG:HH11	1.63	0.44
5:R:473:ASN:ND2	5:R:473:ASN:O	2.50	0.44
6:A:238:PHE:CZ	6:A:450:TRP:HA	2.52	0.44
6:A:356:GLU:OE2	6:A:359:ARG:NH2	2.41	0.44
6:C:63:THR:HG21	6:C:365:LEU:HD21	1.99	0.44
8:Z:44:LYS:O	8:Z:47:GLU:HG3	2.17	0.44
9:G:44:PHE:HE1	9:G:159:ASP:HB2	1.81	0.44
12:5:94:GLY:O	12:5:98:SER:OG	2.35	0.44
1:I:123:GLY:HA3	1:I:183:ILE:HD13	1.98	0.44
2:M:42:ALA:O	2:M:45:GLU:HB3	2.18	0.44
3:O:267:ARG:HB3	3:O:267:ARG:HH21	1.81	0.44
5:R:50:LYS:HB3	5:R:50:LYS:HE3	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:65:LEU:HA	5:R:68:VAL:HG12	2.00	0.44
7:F:335:TYR:CE2	7:F:369:THR:HG23	2.52	0.44
8:X:223:LYS:HA	8:X:226:VAL:HG22	1.98	0.44
8:Z:88:LEU:HD12	8:Z:88:LEU:HA	1.83	0.44
1:J:30:ILE:HG21	2:M:25:ALA:HB1	2.00	0.44
3:O:105:PHE:HE1	3:O:296:HIS:CE1	2.35	0.44
4:P:434:LYS:HE2	4:P:459:LEU:HD11	2.00	0.44
5:R:271:VAL:O	5:R:275:THR:HG22	2.18	0.44
7:E:201:GLU:H	7:E:201:GLU:HG2	1.41	0.44
7:E:376:GLN:HG3	7:E:378:TYR:HE2	1.82	0.44
13:Q:289:THR:OG1	13:Q:290:LEU:N	2.50	0.44
13:Q:292:ASP:OD1	13:Q:292:ASP:N	2.50	0.44
2:M:51:ARG:HD3	2:M:51:ARG:HA	1.74	0.44
2:M:73:VAL:O	2:M:77:THR:HG22	2.17	0.44
3:O:72:VAL:HG12	3:O:136:LEU:HG	1.99	0.44
3:O:166:LEU:HD12	3:O:169:ILE:HD12	1.98	0.44
3:O:335:LEU:HD13	3:O:369:TYR:OH	2.18	0.44
4:P:401:SER:HB3	4:P:407:LEU:HD12	1.99	0.44
8:Y:93:ARG:O	8:Y:97:SER:OG	2.33	0.44
20:c:1:NAG:O3	20:c:2:NAG:O5	2.33	0.44
2:L:86:THR:O	2:L:90:GLN:NE2	2.51	0.44
3:O:43:LEU:HB2	3:O:303:PHE:CZ	2.53	0.44
3:O:112:TYR:HE2	3:O:296:HIS:CD2	2.36	0.44
3:O:197:TRP:O	3:O:201:TYR:HD2	2.01	0.44
4:P:77:PHE:HE2	4:P:100:MET:HE1	1.83	0.44
4:P:291:ASN:O	4:P:295:LYS:HG2	2.18	0.44
5:R:69:GLU:HA	5:R:72:ILE:HG22	1.98	0.44
5:R:81:ASP:HA	5:R:291:ARG:CB	2.46	0.44
5:R:449:ILE:O	5:R:453:MET:HG3	2.18	0.44
5:R:517:GLY:O	14:S:59:GLN:NE2	2.51	0.44
5:R:756:TRP:CD1	5:R:756:TRP:C	2.95	0.44
6:C:469:PHE:O	6:C:471:GLU:N	2.50	0.44
8:Y:155:MET:HE1	8:Y:181:LEU:HB3	2.00	0.44
8:Z:234:MET:HG3	8:Z:235:PRO:HD3	1.99	0.44
1:I:58:GLU:O	1:I:62:LYS:HG2	2.18	0.44
2:L:10:GLN:NE2	2:L:13:GLN:HE21	2.15	0.44
3:O:18:THR:O	3:O:23:HIS:HB2	2.18	0.44
4:P:37:LEU:HB3	4:P:42:ILE:HB	1.99	0.44
9:G:89:LYS:HA	10:N:27:GLU:OE1	2.17	0.44
11:0:140:ALA:O	11:0:144:VAL:HG12	2.17	0.44
13:Q:284:ASN:HB3	13:Q:287:ASP:OD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:ALA:O	1:I:26:LYS:HG2	2.18	0.44
1:J:75:LEU:HD21	2:M:70:SER:HA	2.00	0.44
2:M:31:ARG:HD3	2:M:34:LYS:HB2	1.98	0.44
3:O:28:LYS:HB3	3:O:331:LEU:HG	1.99	0.44
4:P:134:ASP:HB3	4:P:135:PRO:HD3	1.99	0.44
6:A:605:LEU:O	6:A:609:GLN:HG3	2.17	0.44
8:X:143:ALA:HB1	8:X:149:ASN:OD1	2.18	0.44
8:Y:177:GLN:HG3	8:Y:178:LEU:N	2.32	0.44
12:4:41:ILE:O	12:4:44:MET:HG3	2.17	0.44
16:U:426:ILE:HG22	16:U:430:LEU:HD13	1.99	0.44
1:I:162:ASP:N	1:I:162:ASP:OD1	2.45	0.44
3:O:64:PHE:O	3:O:68:VAL:HG13	2.17	0.44
3:O:99:VAL:HG23	3:O:100:THR:H	1.83	0.44
3:O:112:TYR:HB3	3:O:121:ILE:HD12	1.99	0.44
5:R:60:GLU:O	5:R:63:ARG:HG3	2.18	0.44
5:R:176:ASN:ND2	5:R:215:VAL:HG23	2.29	0.44
5:R:224:PHE:CD2	5:R:229:LEU:HB3	2.53	0.44
5:R:534:SER:OG	21:r:1:NAG:H82	2.18	0.44
6:A:249:PRO:HG2	6:A:435:LEU:HB2	1.99	0.44
6:B:100:ASP:OD1	6:B:100:ASP:N	2.50	0.44
6:C:148:THR:OG1	6:C:149:GLY:N	2.49	0.44
8:X:140:LEU:HD13	8:X:153:ARG:HA	2.00	0.44
8:Z:94:LEU:HB2	8:Z:130:LEU:HD21	1.99	0.44
13:Q:113:ILE:O	13:Q:117:LEU:HG	2.16	0.44
16:U:365:SER:O	16:U:406:ASN:ND2	2.39	0.44
1:J:123:GLY:HA3	1:J:183:ILE:HD13	1.99	0.44
3:O:179:SER:OG	3:O:182:LEU:N	2.47	0.44
3:O:191:LYS:HB3	3:O:223:TYR:CD1	2.52	0.44
12:1:45:SER:HB2	12:1:52:ILE:HG12	2.00	0.44
2:L:6:GLN:O	2:L:10:GLN:HB2	2.18	0.43
2:L:75:LYS:NZ	2:L:79:GLU:HB3	2.33	0.43
4:P:212:ASN:HA	4:P:215:ARG:NE	2.33	0.43
4:P:342:LEU:HD23	4:P:342:LEU:HA	1.77	0.43
6:B:485:GLU:HA	6:B:488:ASP:OD2	2.18	0.43
6:C:438:LYS:HA	6:C:438:LYS:HD3	1.81	0.43
8:X:133:LEU:O	8:X:137:THR:HG22	2.18	0.43
12:2:86:LEU:HD12	12:2:86:LEU:HA	1.87	0.43
12:6:77:ALA:O	12:7:155:LYS:HE2	2.18	0.43
3:O:151:GLN:HA	3:O:154:GLU:OE2	2.18	0.43
4:P:165:PHE:HB3	4:P:169:LYS:N	2.22	0.43
4:P:235:CYS:HB3	4:P:239:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:185:ARG:O	5:R:189:ARG:HG3	2.18	0.43
6:C:473:VAL:O	6:C:477:THR:HG23	2.18	0.43
7:E:168:GLU:OE2	7:E:410:MET:HG2	2.19	0.43
8:Z:124:SER:OG	8:Z:125:ASP:N	2.52	0.43
1:J:65:GLU:HA	1:J:68:LYS:HG2	2.00	0.43
2:L:44:ILE:HA	2:L:47:TYR:CZ	2.53	0.43
3:O:61:LEU:O	3:O:65:VAL:HG13	2.18	0.43
3:O:213:SER:HA	3:O:226:ASN:O	2.17	0.43
4:P:357:SER:HA	4:P:360:LYS:HZ2	1.84	0.43
8:Z:209:GLU:HG2	8:Z:211:SER:H	1.83	0.43
16:U:277:ALA:HB2	16:U:282:TRP:CD2	2.53	0.43
3:O:339:TYR:O	3:O:368:PRO:HB2	2.17	0.43
4:P:263:TYR:HB2	4:P:265:ILE:CD1	2.48	0.43
6:C:511:VAL:HG11	6:C:548:TYR:HD1	1.83	0.43
7:E:335:TYR:CE2	7:E:369:THR:HG23	2.52	0.43
9:G:83:VAL:HG11	10:N:22:LEU:HD21	2.01	0.43
12:5:22:ALA:O	12:5:26:SER:OG	2.27	0.43
22:5:201:CLR:H121	22:V:402:CLR:C18	2.47	0.43
1:I:13:LYS:NZ	2:L:10:GLN:OE1	2.36	0.43
2:K:17:ARG:O	2:K:20:GLU:HG3	2.18	0.43
2:M:21:LYS:HE3	2:M:21:LYS:HB3	1.81	0.43
4:P:56:LYS:NZ	4:P:57:ARG:HH21	2.16	0.43
6:C:350:SER:H	6:C:409:ALA:HB3	1.84	0.43
7:E:269:ILE:HD12	7:E:269:ILE:H	1.83	0.43
8:Y:43:LYS:O	8:Y:47:GLU:HG2	2.19	0.43
9:G:145:LEU:HD23	10:N:65:LEU:CD2	2.49	0.43
12:6:72:VAL:HG11	12:6:99:VAL:HG11	2.00	0.43
12:9:8:PRO:HD2	12:9:11:ALA:HB2	2.00	0.43
1:H:60:LYS:HA	1:H:60:LYS:HD3	1.69	0.43
5:R:224:PHE:HD2	5:R:229:LEU:O	2.01	0.43
6:B:234:LEU:HD21	6:B:448:VAL:HG21	1.99	0.43
7:E:66:PRO:HB2	7:E:89:VAL:HG22	2.01	0.43
8:Y:270:ASN:O	8:Y:274:ASN:ND2	2.52	0.43
10:N:8:ILE:HG23	10:N:63:ILE:HB	2.00	0.43
12:4:47:MET:HG3	12:4:48:ARG:HG3	2.01	0.43
13:Q:190:LEU:HD12	13:Q:190:LEU:HA	1.82	0.43
2:M:11:LEU:HD22	3:O:182:LEU:CD1	2.49	0.43
5:R:188:TRP:CD1	5:R:222:ILE:HD11	2.54	0.43
24:0:307:PTY:H412	24:0:307:PTY:H161	2.00	0.43
24:8:202:PTY:HC6	24:8:202:PTY:H111	1.70	0.43
13:Q:139:GLU:CD	13:Q:139:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:395:MET:HE3	16:U:395:MET:HB3	1.87	0.43
1:H:108:ASP:OD2	1:H:111:ARG:HD3	2.19	0.43
1:I:26:LYS:O	1:I:30:ILE:HG12	2.19	0.43
1:J:26:LYS:HB3	2:M:21:LYS:HD3	2.00	0.43
2:M:29:LYS:HB3	2:M:29:LYS:HE2	1.72	0.43
3:O:325:LYS:C	3:O:326:LYS:HD3	2.44	0.43
4:P:426:ARG:HG3	4:P:427:VAL:N	2.34	0.43
6:C:252:PHE:O	6:C:437:LYS:NZ	2.51	0.43
11:0:9:SER:O	11:0:13:VAL:HG12	2.19	0.43
24:0:307:PTY:H112	24:0:307:PTY:C30	2.48	0.43
12:4:46:VAL:HA	12:5:124:GLN:HB2	2.01	0.43
1:H:82:LYS:HE2	1:H:82:LYS:HB3	1.82	0.43
2:K:43:GLU:O	2:K:46:GLN:HG3	2.19	0.43
2:M:53:LYS:HB3	2:M:53:LYS:HE3	1.69	0.43
3:O:196:ASP:O	3:O:199:LYS:HD3	2.19	0.43
3:O:215:VAL:HA	3:O:225:CYS:HB3	2.00	0.43
4:P:248:TRP:HD1	4:P:288:ALA:HA	1.84	0.43
6:A:511:VAL:HG11	6:A:548:TYR:HB2	2.01	0.43
6:A:574:MET:HE2	6:A:574:MET:HB3	1.93	0.43
6:B:511:VAL:HG21	6:B:548:TYR:HB2	2.01	0.43
8:X:136:LEU:HD13	8:X:156:THR:HG22	2.00	0.43
8:X:197:TYR:CE2	8:X:201:LYS:HD3	2.53	0.43
9:G:213:LYS:HB3	9:G:213:LYS:HE3	1.72	0.43
10:N:92:PRO:HB3	10:N:98:TYR:HB2	2.00	0.43
13:Q:326:CYS:O	13:Q:330:VAL:HG23	2.19	0.43
1:H:115:LEU:HD12	1:H:115:LEU:HA	1.91	0.43
1:I:15:MET:O	1:I:19:ILE:HG12	2.19	0.43
3:O:118:LEU:HD21	3:O:303:PHE:CE1	2.51	0.43
4:P:40:GLN:O	4:P:83:HIS:NE2	2.45	0.43
4:P:129:MET:HA	4:P:132:ARG:HH21	1.83	0.43
4:P:264:ASN:ND2	4:P:267:PRO:HG2	2.34	0.43
5:R:52:VAL:O	5:R:55:VAL:HG22	2.19	0.43
5:R:207:GLU:HB2	5:R:213:ASP:N	2.33	0.43
7:E:188:LYS:HE2	7:E:188:LYS:HB2	1.75	0.43
8:Y:181:LEU:CD2	8:Y:203:TYR:HB2	2.48	0.43
2:L:48:ARG:O	2:L:52:GLU:HG2	2.17	0.42
2:M:29:LYS:O	2:M:33:LEU:HG	2.19	0.42
4:P:264:ASN:HD21	4:P:267:PRO:HG2	1.83	0.42
5:R:180:ILE:O	5:R:184:GLU:HG2	2.19	0.42
6:B:574:MET:HB3	6:B:577:ILE:HB	1.99	0.42
6:C:510:GLU:HG3	6:C:567:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:134:ASN:O	8:X:138:ASP:HB2	2.18	0.42
8:Y:217:LEU:HB3	8:Y:221:ASP:OD1	2.19	0.42
13:Q:116:THR:HG22	13:Q:122:ILE:HD11	2.01	0.42
13:Q:248:TYR:HB3	13:Q:249:PRO:HD3	2.00	0.42
16:U:309:LEU:O	16:U:324:LYS:HA	2.20	0.42
3:O:76:MET:SD	3:O:81:GLU:HB3	2.59	0.42
3:O:304:VAL:O	3:O:308:LEU:HG	2.19	0.42
4:P:90:VAL:HA	4:P:93:ILE:HG13	2.01	0.42
5:R:84:GLU:HG2	5:R:87:GLU:HG2	2.00	0.42
6:A:105:PRO:HG3	6:A:126:ALA:HA	2.01	0.42
7:D:457:LYS:O	7:D:461:ASN:HB2	2.19	0.42
7:F:215:LYS:HE2	7:F:215:LYS:HB2	1.87	0.42
11:0:23:GLY:O	11:0:27:THR:HG22	2.19	0.42
13:Q:54:TYR:OH	13:Q:325:GLU:OE1	2.37	0.42
24:Q:401:PTY:H361	24:Q:401:PTY:H332	1.72	0.42
1:H:41:GLU:O	1:H:45:LEU:HG	2.18	0.42
3:O:114:ILE:HD12	3:O:114:ILE:HA	1.82	0.42
3:O:176:VAL:HG21	3:O:182:LEU:HD22	2.02	0.42
8:Z:106:ASP:OD2	8:Z:106:ASP:N	2.51	0.42
16:U:439:ILE:HG12	24:U:503:PTY:H192	2.01	0.42
1:J:4:SER:H	1:J:7:ASP:HB2	1.85	0.42
3:O:29:ASN:HB2	3:O:33:ALA:H	1.84	0.42
3:O:102:ILE:HD13	3:O:320:LEU:HD21	2.02	0.42
3:O:196:ASP:O	3:O:200:GLN:HB2	2.18	0.42
5:R:16:PHE:CZ	5:R:318:CYS:HB2	2.54	0.42
5:R:248:PRO:HA	5:R:254:ARG:HE	1.84	0.42
7:D:335:TYR:CE2	7:D:369:THR:HG23	2.54	0.42
8:X:245:LYS:HZ3	8:X:266:ILE:HG21	1.84	0.42
12:3:104:LEU:HD11	17:V:324:THR:HG21	2.02	0.42
12:4:57:ILE:O	12:4:61:MET:HG3	2.20	0.42
1:H:68:LYS:HA	1:H:68:LYS:HD3	1.73	0.42
1:I:33:LYS:O	1:I:37:GLU:HG2	2.19	0.42
1:J:104:LYS:HE2	1:J:104:LYS:HB2	1.78	0.42
3:O:177:LEU:HD12	3:O:177:LEU:HA	1.75	0.42
3:O:338:LEU:HD23	3:O:338:LEU:HA	1.91	0.42
3:O:347:ALA:HB1	3:O:367:TYR:N	2.33	0.42
4:P:37:LEU:CB	4:P:42:ILE:HB	2.49	0.42
5:R:187:LEU:HB3	5:R:222:ILE:HD12	2.00	0.42
6:A:290:ASP:O	6:A:294:LEU:HD13	2.19	0.42
6:B:498:LYS:HG2	6:B:501:LEU:HD22	2.01	0.42
8:X:263:ILE:O	8:X:266:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:8:98:SER:O	12:8:102:SER:OG	2.35	0.42
16:U:438:PHE:CE1	24:U:503:PTY:C36	3.03	0.42
1:H:32:ALA:HA	1:H:35:GLU:OE1	2.20	0.42
1:H:177:ILE:HD13	1:H:177:ILE:HA	1.89	0.42
4:P:126:PHE:O	4:P:129:MET:HB2	2.20	0.42
5:R:293:TRP:O	5:R:297:VAL:HG23	2.20	0.42
5:R:796:LEU:HD12	5:R:796:LEU:HA	1.83	0.42
7:E:408:GLU:HG2	7:E:413:LYS:HB3	2.01	0.42
7:F:272:ILE:HD11	7:F:310:VAL:HG11	2.01	0.42
8:X:61:ARG:H	8:X:64:GLU:HG3	1.85	0.42
8:X:205:LYS:HA	8:X:257:LYS:HD3	2.01	0.42
8:Z:222:GLN:O	8:Z:226:VAL:HG23	2.19	0.42
3:O:238:ARG:HB3	3:O:242:ARG:HH22	1.85	0.42
4:P:208:MET:C	4:P:210:ARG:H	2.28	0.42
4:P:299:ARG:NH1	4:P:302:ARG:O	2.53	0.42
5:R:279:ARG:O	5:R:283:LEU:HB2	2.20	0.42
7:E:198:PRO:HB2	7:E:201:GLU:HG3	2.02	0.42
7:F:188:LYS:HD3	7:F:335:TYR:O	2.19	0.42
8:Y:40:ASN:O	8:Y:41:ASN:ND2	2.51	0.42
12:2:48:ARG:NH2	12:2:50:GLU:OE2	2.53	0.42
12:4:31:ALA:HB1	12:5:109:ALA:HB2	2.02	0.42
16:U:376:SER:O	16:U:376:SER:OG	2.32	0.42
1:J:102:LEU:HG	1:J:196:LEU:HD13	2.01	0.42
2:K:4:GLN:H	5:R:353:ASN:ND2	2.18	0.42
3:O:297:VAL:O	3:O:300:LEU:HD23	2.19	0.42
4:P:108:VAL:C	4:P:110:ILE:N	2.76	0.42
4:P:108:VAL:HG22	4:P:113:ASP:OD1	2.20	0.42
4:P:410:ALA:O	4:P:414:VAL:HG12	2.19	0.42
6:B:486:GLU:HG3	6:B:512:ALA:HB3	2.00	0.42
6:B:507:ILE:O	6:B:511:VAL:HG12	2.20	0.42
6:B:566:THR:OG1	6:B:567:TRP:N	2.52	0.42
7:E:60:LEU:HD21	7:E:112:CYS:SG	2.60	0.42
16:U:277:ALA:HB3	16:U:394:GLN:HB2	2.02	0.42
3:O:119:LYS:HG3	3:O:123:GLU:OE2	2.20	0.42
3:O:191:LYS:HA	3:O:194:HIS:HB2	2.02	0.42
4:P:31:VAL:HG22	4:P:32:ASN:N	2.35	0.42
4:P:313:LYS:HE2	4:P:313:LYS:H	1.84	0.42
6:B:256:LYS:HB3	6:B:256:LYS:HE2	1.79	0.42
6:B:258:VAL:O	6:B:262:SER:OG	2.30	0.42
8:X:52:VAL:HG12	8:X:75:PRO:HG2	2.02	0.42
22:5:201:CLR:H261	22:V:402:CLR:C26	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:201:PTY:H432	24:8:201:PTY:H261	2.01	0.42
15:T:123:PHE:O	15:T:126:VAL:HG12	2.20	0.42
1:H:102:LEU:HD12	1:H:102:LEU:HA	1.83	0.42
3:O:37:LYS:HZ2	3:O:318:ALA:H	1.67	0.42
3:O:54:LEU:HA	3:O:57:GLU:HG3	2.02	0.42
3:O:127:LYS:HD2	3:O:128:GLY:N	2.34	0.42
4:P:231:LEU:O	4:P:231:LEU:HD23	2.20	0.42
4:P:395:THR:CA	4:P:398:LEU:HD12	2.45	0.42
4:P:432:GLY:O	4:P:436:LEU:HG	2.20	0.42
5:R:609:LEU:HD12	5:R:609:LEU:HA	1.87	0.42
6:A:169:PRO:HA	6:A:170:PRO:HD3	1.93	0.42
6:A:274:TYR:HB3	6:A:311:LEU:HD23	2.02	0.42
6:C:372:SER:HB3	6:C:420:PRO:HG2	2.01	0.42
7:E:146:LEU:HD12	7:E:146:LEU:HA	1.90	0.42
8:X:120:ASN:HD21	8:X:123:LYS:HB2	1.85	0.42
4:P:204:CYS:O	4:P:207:LEU:HG	2.20	0.41
4:P:394:LEU:O	4:P:398:LEU:N	2.53	0.41
5:R:64:LYS:HD3	5:R:105:GLU:HB2	2.02	0.41
6:A:225:HIS:HA	6:A:226:PRO:HD3	1.96	0.41
6:B:328:TYR:HA	6:B:331:ILE:HG22	2.02	0.41
6:C:108:ASP:OD1	6:C:108:ASP:N	2.52	0.41
7:F:77:PRO:HB3	7:F:109:LYS:HE2	2.02	0.41
8:Y:42:LEU:HD21	8:Y:105:LEU:HD12	2.02	0.41
24:0:307:PTY:HC11	24:U:503:PTY:H141	2.01	0.41
12:3:33:GLY:O	12:3:37:SER:OG	2.36	0.41
24:7:201:PTY:H392	24:8:201:PTY:H252	2.02	0.41
5:R:86:PRO:O	5:R:88:VAL:HG23	2.20	0.41
6:A:44:ARG:HD2	6:A:49:GLU:HB3	2.02	0.41
6:A:350:SER:HB3	6:A:353:ARG:CG	2.49	0.41
6:B:449:ASN:HD22	6:B:452:ILE:HG12	1.84	0.41
6:C:264:SER:HB2	6:C:272:ILE:HG21	2.02	0.41
15:T:67:MET:HE3	15:T:67:MET:HB2	1.88	0.41
1:J:5:ASP:HA	1:J:8:VAL:HG22	2.01	0.41
1:J:49:GLN:O	1:J:53:ILE:HG12	2.20	0.41
2:L:116:ILE:H	2:L:116:ILE:HG12	1.64	0.41
4:P:94:LEU:HD12	4:P:136:PHE:HB3	2.02	0.41
5:R:333:ILE:HG13	5:R:334:GLN:N	2.35	0.41
5:R:431:LEU:HD12	5:R:431:LEU:HA	1.86	0.41
6:A:268:ASN:OD1	6:A:268:ASN:N	2.46	0.41
6:B:501:LEU:HB3	6:B:506:LYS:HE2	2.02	0.41
7:E:445:THR:HG22	7:E:446:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:146:LEU:HD12	7:F:146:LEU:HA	1.85	0.41
8:X:72:GLY:HA2	8:X:76:ASN:HD21	1.85	0.41
8:Z:90:GLU:OE1	8:Z:127:HIS:ND1	2.53	0.41
10:N:72:GLU:HA	10:N:75:ARG:HG2	2.02	0.41
13:Q:24:LYS:O	13:Q:24:LYS:HG2	2.20	0.41
1:J:10:LYS:HA	1:J:13:LYS:HB2	2.03	0.41
1:J:54:MET:HE2	1:J:54:MET:HA	2.02	0.41
2:K:30:ASN:O	2:K:34:LYS:HE3	2.19	0.41
2:K:45:GLU:O	2:K:49:LEU:HD23	2.20	0.41
2:L:88:PHE:CZ	2:L:92:ARG:HD3	2.55	0.41
3:O:53:GLY:O	3:O:57:GLU:HG3	2.20	0.41
4:P:259:HIS:CG	4:P:260:LEU:N	2.87	0.41
5:R:18:GLN:NE2	5:R:20:GLU:HB2	2.35	0.41
5:R:430:ILE:H	5:R:430:ILE:HG13	1.68	0.41
6:C:50:LEU:HB3	6:C:68:GLU:HG3	2.02	0.41
7:D:60:LEU:HD21	7:D:112:CYS:SG	2.59	0.41
7:D:291:LYS:HE2	7:D:291:LYS:HB3	1.78	0.41
8:X:58:LYS:HE2	8:X:58:LYS:HB2	1.72	0.41
8:X:118:HIS:CE1	8:X:124:SER:HB3	2.56	0.41
8:Y:133:LEU:O	8:Y:137:THR:HG22	2.19	0.41
13:Q:284:ASN:HD22	13:Q:285:PRO:CD	2.33	0.41
2:K:72:GLU:HG3	2:K:73:VAL:N	2.34	0.41
3:O:150:LEU:HD23	3:O:151:GLN:N	2.36	0.41
4:P:45:GLU:HG2	4:P:49:PHE:HD2	1.86	0.41
4:P:162:ASN:O	4:P:168:ILE:HG13	2.21	0.41
4:P:172:LEU:O	4:P:172:LEU:HD13	2.20	0.41
5:R:252:GLN:HE22	5:R:255:LYS:HD2	1.86	0.41
8:Z:120:ASN:ND2	8:Z:123:LYS:HB2	2.36	0.41
8:Z:222:GLN:HA	8:Z:225:LEU:HG	2.01	0.41
22:5:201:CLR:C26	22:V:402:CLR:C26	2.98	0.41
12:9:83:ASP:OD1	12:9:83:ASP:N	2.49	0.41
3:O:65:VAL:HA	3:O:68:VAL:HG22	2.02	0.41
5:R:24:CYS:SG	5:R:344:SER:OG	2.53	0.41
5:R:360:THR:HB	5:R:361:PRO:N	2.36	0.41
6:B:39:MET:HE3	6:B:39:MET:HB3	1.91	0.41
6:B:587:LYS:NZ	6:B:600:ASP:OD1	2.52	0.41
6:C:173:ARG:NH1	8:Z:16:GLU:OE1	2.42	0.41
7:F:46:THR:HG23	7:F:113:GLU:HB2	2.03	0.41
8:X:36:ILE:HG13	8:X:95:VAL:HG21	2.02	0.41
8:Y:61:ARG:O	8:Y:65:ILE:HG13	2.21	0.41
8:Y:130:LEU:HD23	8:Y:130:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:56:LEU:HD23	10:N:56:LEU:HA	1.87	0.41
11:0:4:LEU:HD23	11:0:4:LEU:HA	1.84	0.41
13:Q:12:ASP:HB2	13:Q:90:TYR:CD2	2.56	0.41
13:Q:328:ASN:ND2	13:Q:348:ILE:O	2.48	0.41
1:I:21:GLN:NE2	3:O:45:VAL:HG13	2.35	0.41
3:O:325:LYS:HD2	3:O:325:LYS:HA	1.61	0.41
4:P:123:TRP:HB2	4:P:124:PRO:HD3	2.03	0.41
4:P:298:GLU:O	4:P:301:THR:OG1	2.30	0.41
6:A:335:GLU:OE1	6:A:388:ARG:NH1	2.48	0.41
6:B:573:HIS:CG	6:B:615:LEU:HD13	2.55	0.41
7:E:374:GLU:HA	7:E:400:ARG:HD2	2.02	0.41
7:F:135:SER:O	7:F:135:SER:OG	2.38	0.41
14:S:72:THR:O	14:S:76:LEU:HG	2.21	0.41
4:P:414:VAL:O	4:P:418:VAL:HG22	2.21	0.41
5:R:208:ASP:OD1	5:R:209:PRO:HD2	2.21	0.41
6:C:194:LEU:HD23	6:C:201:GLU:HB3	2.03	0.41
8:Z:113:GLU:O	8:Z:117:GLN:HG2	2.21	0.41
10:N:45:ILE:O	10:N:49:GLU:HG2	2.20	0.41
11:0:63:VAL:HG22	12:1:105:ALA:HB2	2.02	0.41
11:0:91:LEU:HD12	11:0:91:LEU:HA	1.83	0.41
12:3:41:ILE:O	12:3:45:SER:HB3	2.21	0.41
16:U:312:THR:HG22	16:U:322:THR:OG1	2.21	0.41
18:W:5:SIA:O7	18:W:5:SIA:H113	2.21	0.41
1:H:127:LEU:HD23	1:H:127:LEU:HA	1.92	0.41
2:L:40:ALA:O	2:L:43:GLU:HG2	2.21	0.41
3:O:163:THR:HA	3:O:249:ARG:NH2	2.34	0.41
3:O:281:ARG:O	3:O:285:VAL:HG22	2.21	0.41
4:P:258:GLU:H	4:P:258:GLU:HG3	1.38	0.41
4:P:433:GLY:HA2	4:P:436:LEU:HD12	2.02	0.41
5:R:61:MET:SD	5:R:64:LYS:HE3	2.61	0.41
6:B:437:LYS:O	6:B:441:GLN:HG3	2.20	0.41
6:C:426:LEU:HD23	6:C:426:LEU:HA	1.90	0.41
6:C:511:VAL:HG21	6:C:548:TYR:HB2	2.03	0.41
7:D:164:ILE:HD11	7:D:342:GLU:HA	2.02	0.41
8:X:45:ILE:C	8:X:47:GLU:H	2.29	0.41
8:Z:241:VAL:HG13	8:Z:242:LEU:HG	2.03	0.41
11:0:3:GLY:HA3	25:0:305:WSS:C1	2.50	0.41
11:0:84:PRO:O	11:0:87:LYS:HG2	2.21	0.41
12:1:55:SER:O	12:1:58:PRO:HD2	2.21	0.41
12:3:44:MET:HG2	12:3:119:ARG:HA	2.03	0.41
12:4:154:THR:O	12:4:154:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:179:GLU:H	13:Q:179:GLU:HG2	1.72	0.41
16:U:284:ASP:O	16:U:285:LEU:HD23	2.21	0.41
16:U:314:GLU:H	16:U:314:GLU:CD	2.29	0.41
1:H:21:GLN:O	1:H:25:GLU:HG2	2.20	0.41
1:H:31:ASP:OD2	1:H:32:ALA:N	2.54	0.41
3:O:63:ALA:O	3:O:66:GLU:HG2	2.20	0.41
4:P:229:GLY:O	4:P:233:ASN:ND2	2.47	0.41
4:P:336:LYS:O	4:P:339:LEU:HG	2.21	0.41
6:C:449:ASN:C	6:C:451:LEU:H	2.29	0.41
8:X:242:LEU:HD23	8:X:242:LEU:H	1.86	0.41
12:1:101:LEU:HD23	12:1:101:LEU:HA	1.89	0.41
12:2:34:THR:HG23	12:2:59:VAL:HG13	2.03	0.41
14:S:13:MET:HE3	14:S:13:MET:HB3	1.99	0.41
1:H:133:ILE:HA	1:H:166:GLN:O	2.22	0.40
1:I:82:LYS:HB3	1:I:82:LYS:HE3	1.76	0.40
2:K:47:TYR:HA	2:K:50:GLN:HG2	2.04	0.40
2:L:76:GLU:O	2:L:79:GLU:HG3	2.20	0.40
2:M:20:GLU:OE1	2:M:21:LYS:N	2.53	0.40
3:O:181:TYR:HD2	3:O:230:PHE:CE1	2.39	0.40
4:P:304:GLU:O	4:P:308:ALA:HB3	2.21	0.40
5:R:84:GLU:HG2	5:R:87:GLU:CD	2.46	0.40
5:R:130:PHE:HB3	5:R:202:ILE:HG12	2.03	0.40
6:C:104:ARG:HE	6:C:104:ARG:HB2	1.66	0.40
6:C:271:VAL:HB	6:C:344:VAL:HG22	2.03	0.40
7:D:444:LEU:HD23	7:D:449:LEU:HG	2.03	0.40
16:U:445:HIS:CE1	24:U:503:PTY:C31	3.03	0.40
16:U:453:MET:SD	16:U:453:MET:N	2.92	0.40
1:I:202:LEU:O	1:I:206:GLN:HG2	2.21	0.40
1:J:215:LEU:HD23	2:M:91:ASN:HB2	2.04	0.40
3:O:13:LYS:HB2	3:O:13:LYS:HE2	1.77	0.40
4:P:253:SER:OG	4:P:256:MET:HE2	2.21	0.40
5:R:22:ALA:HA	5:R:25:CYS:SG	2.61	0.40
5:R:188:TRP:HB3	5:R:192:ARG:HE	1.87	0.40
5:R:226:GLY:O	5:R:230:LYS:N	2.46	0.40
5:R:253:GLU:HA	5:R:256:GLU:OE1	2.21	0.40
5:R:257:MET:HB3	5:R:257:MET:HE3	1.73	0.40
5:R:401:PHE:HZ	14:S:51:PHE:HB2	1.86	0.40
6:B:551:ALA:HB2	6:B:612:PHE:HZ	1.86	0.40
7:E:232:ALA:HB3	7:E:297:LEU:HD23	2.02	0.40
7:E:237:ASN:ND2	7:E:240:THR:H	2.19	0.40
8:X:263:ILE:O	8:X:267:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:71:SER:OG	8:Z:73:LYS:HD2	2.22	0.40
12:7:44:MET:HB2	12:7:122:ALA:HB2	2.03	0.40
2:M:43:GLU:O	2:M:46:GLN:HB2	2.22	0.40
5:R:793:MET:HE3	5:R:793:MET:HB3	1.74	0.40
6:A:197:GLU:C	6:A:199:VAL:H	2.29	0.40
7:D:76:LEU:HB2	7:D:80:THR:HG23	2.04	0.40
7:F:61:ASP:OD1	7:F:62:HIS:N	2.50	0.40
8:Z:98:ILE:H	8:Z:98:ILE:HG12	1.79	0.40
12:4:80:LEU:HD23	12:4:80:LEU:HA	1.88	0.40
2:L:18:ALA:HA	2:L:21:LYS:HD3	2.03	0.40
2:L:45:GLU:O	2:L:49:LEU:HD22	2.22	0.40
3:O:21:LYS:HG3	3:O:22:LEU:H	1.86	0.40
3:O:150:LEU:HB2	3:O:268:LEU:HD22	2.02	0.40
4:P:130:LEU:O	4:P:133:GLN:NE2	2.49	0.40
4:P:309:MET:HE1	4:P:315:LEU:HB2	2.04	0.40
5:R:202:ILE:HB	5:R:217:LYS:HB2	2.03	0.40
6:A:215:ARG:HA	6:A:216:PRO:HD3	1.94	0.40
6:C:67:TYR:C	6:C:68:GLU:HG2	2.46	0.40
7:E:166:PRO:HA	7:E:340:ARG:HD3	2.02	0.40
7:E:182:SER:HB2	7:E:402:MET:HG3	2.03	0.40
7:E:445:THR:HG22	7:E:446:SER:N	2.37	0.40
8:Y:171:ASP:OD2	8:Y:171:ASP:N	2.54	0.40
9:G:131:LEU:HD23	9:G:131:LEU:HA	1.86	0.40
11:0:196:LEU:HD12	12:9:74:VAL:HG22	2.02	0.40
12:8:91:LEU:HD13	12:8:155:LYS:HB3	2.03	0.40
1:H:57:TYR:CE1	2:K:51:ARG:HD2	2.57	0.40
1:I:8:VAL:HB	5:R:196:PHE:HE1	1.87	0.40
1:J:18:PHE:O	1:J:21:GLN:HB2	2.22	0.40
2:K:69:CYS:O	2:K:73:VAL:HG23	2.22	0.40
2:L:9:GLN:HA	2:L:12:LEU:HG	2.02	0.40
3:O:325:LYS:C	3:O:327:THR:H	2.29	0.40
4:P:103:GLU:O	4:P:104:ASN:ND2	2.54	0.40
4:P:394:LEU:HD12	4:P:394:LEU:HA	1.89	0.40
5:R:12:LEU:HD12	5:R:12:LEU:HA	1.87	0.40
5:R:548:MET:HG2	5:R:813:LYS:HE2	2.04	0.40
5:R:804:ARG:NH1	5:R:809:GLU:OE2	2.52	0.40
6:B:25:SER:HB2	7:E:88:GLU:HG3	2.04	0.40
6:B:167:MET:HE3	6:B:167:MET:HB2	1.92	0.40
6:C:343:HIS:ND1	6:C:403:SER:HB3	2.36	0.40
7:E:124:SER:HA	7:E:148:GLU:HB2	2.04	0.40
8:X:103:MET:HE1	8:X:111:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:197:TYR:CD1	8:Z:229:MET:HE1	2.57	0.40
12:3:83:ASP:OD2	12:3:83:ASP:N	2.55	0.40
12:5:86:LEU:HD12	12:5:86:LEU:HA	1.87	0.40
16:U:453:MET:HE2	16:U:456:PHE:CZ	2.56	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 PDB entries followed by that with respect to all EM entries.

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	H	223/226 (99%)	213 (96%)	10 (4%)	0	100	100
1	I	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
1	J	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
2	K	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	L	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
2	M	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	O	355/382 (93%)	325 (92%)	29 (8%)	1 (0%)	36	67
4	P	423/483 (88%)	379 (90%)	41 (10%)	3 (1%)	18	49
5	R	745/837 (89%)	698 (94%)	47 (6%)	0	100	100
6	A	598/617 (97%)	572 (96%)	26 (4%)	0	100	100
6	B	598/617 (97%)	562 (94%)	36 (6%)	0	100	100
6	C	598/617 (97%)	567 (95%)	30 (5%)	1 (0%)	43	73
7	D	456/511 (89%)	432 (95%)	24 (5%)	0	100	100
7	E	456/511 (89%)	434 (95%)	22 (5%)	0	100	100
7	F	456/511 (89%)	440 (96%)	16 (4%)	0	100	100
8	X	260/573 (45%)	248 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Y	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
8	Z	260/573 (45%)	238 (92%)	22 (8%)	0	100	100
9	G	211/247 (85%)	201 (95%)	10 (5%)	0	100	100
10	N	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
11	0	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
12	1	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	2	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	3	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	4	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	5	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	6	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
12	7	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
12	8	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
13	Q	348/351 (99%)	333 (96%)	15 (4%)	0	100	100
14	S	75/81 (93%)	70 (93%)	5 (7%)	0	100	100
15	T	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
16	U	203/470 (43%)	187 (92%)	16 (8%)	0	100	100
17	V	48/350 (14%)	44 (92%)	4 (8%)	0	100	100
All	All	9085/11192 (81%)	8610 (95%)	470 (5%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	109	SER
4	P	30	LYS
6	C	35	ALA
3	O	313	PRO
4	P	31	VAL

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 PDB entries followed by that with respect to all EM entries.

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	H	198/199 (100%)	180 (91%)	18 (9%)	9 32
1	I	198/199 (100%)	191 (96%)	7 (4%)	32 62
1	J	198/199 (100%)	186 (94%)	12 (6%)	17 46
2	K	99/101 (98%)	93 (94%)	6 (6%)	17 46
2	L	99/101 (98%)	92 (93%)	7 (7%)	13 41
2	M	99/101 (98%)	84 (85%)	15 (15%)	3 13
3	O	323/344 (94%)	288 (89%)	35 (11%)	6 25
4	P	385/429 (90%)	331 (86%)	54 (14%)	3 15
5	R	673/746 (90%)	624 (93%)	49 (7%)	13 40
6	A	507/525 (97%)	463 (91%)	44 (9%)	9 34
6	B	508/525 (97%)	475 (94%)	33 (6%)	15 44
6	C	508/525 (97%)	483 (95%)	25 (5%)	22 53
7	D	393/430 (91%)	373 (95%)	20 (5%)	21 52
7	E	390/430 (91%)	371 (95%)	19 (5%)	22 53
7	F	392/430 (91%)	371 (95%)	21 (5%)	20 50
8	X	238/519 (46%)	211 (89%)	27 (11%)	5 23
8	Y	239/519 (46%)	224 (94%)	15 (6%)	16 45
8	Z	237/519 (46%)	213 (90%)	24 (10%)	7 28
9	G	183/212 (86%)	166 (91%)	17 (9%)	8 31
10	N	94/100 (94%)	87 (93%)	7 (7%)	13 40
11	0	153/155 (99%)	146 (95%)	7 (5%)	24 55
12	1	107/112 (96%)	100 (94%)	7 (6%)	15 44
12	2	107/112 (96%)	101 (94%)	6 (6%)	19 49
12	3	107/112 (96%)	103 (96%)	4 (4%)	30 61
12	4	107/112 (96%)	101 (94%)	6 (6%)	19 49
12	5	107/112 (96%)	101 (94%)	6 (6%)	19 49
12	6	107/112 (96%)	98 (92%)	9 (8%)	10 35
12	7	106/112 (95%)	101 (95%)	5 (5%)	23 55
12	8	107/112 (96%)	101 (94%)	6 (6%)	19 49
12	9	107/112 (96%)	102 (95%)	5 (5%)	23 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	Q	303/306 (99%)	288 (95%)	15 (5%)	22 53
14	S	69/72 (96%)	67 (97%)	2 (3%)	37 66
15	T	70/116 (60%)	65 (93%)	5 (7%)	13 41
16	U	182/397 (46%)	171 (94%)	11 (6%)	17 47
17	V	45/308 (15%)	44 (98%)	1 (2%)	45 71
All	All	7745/9515 (81%)	7195 (93%)	550 (7%)	15 41

All (550) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	LEU
1	H	19	ILE
1	H	20	GLU
1	H	38	PHE
1	H	40	ILE
1	H	52	LYS
1	H	56	TYR
1	H	60	LYS
1	H	64	ILE
1	H	67	GLN
1	H	73	SER
1	H	109	THR
1	H	110	THR
1	H	187	ASP
1	H	202	LEU
1	H	210	GLU
1	H	211	VAL
1	H	212	ARG
1	I	7	ASP
1	I	10	LYS
1	I	35	GLU
1	I	40	ILE
1	I	54	MET
1	I	171	SER
1	I	224	PHE
1	J	3	LEU
1	J	26	LYS
1	J	84	LEU
1	J	102	LEU
1	J	107	LYS

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Mol	Chain	Res	Type
1	J	138	LYS
1	J	145	LYS
1	J	152	ILE
1	J	171	SER
1	J	175	GLU
1	J	202	LEU
1	J	210	GLU
2	K	44	ILE
2	K	59	GLU
2	K	72	GLU
2	K	76	GLU
2	K	85	GLN
2	K	116	ILE
2	L	45	GLU
2	L	49	LEU
2	L	51	ARG
2	L	71	THR
2	L	79	GLU
2	L	99	LEU
2	L	116	ILE
2	M	3	SER
2	M	9	GLN
2	M	11	LEU
2	M	20	GLU
2	M	24	GLU
2	M	27	LYS
2	M	31	ARG
2	M	48	ARG
2	M	49	LEU
2	M	54	GLU
2	M	71	THR
2	M	73	VAL
2	M	76	GLU
2	M	99	LEU
2	M	116	ILE
3	O	15	CYS
3	O	34	VAL
3	O	42	ASP
3	O	45	VAL
3	O	54	LEU
3	O	58	LEU
3	O	90	ASN

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Mol	Chain	Res	Type
3	O	98	LEU
3	O	109	MET
3	O	122	SER
3	O	136	LEU
3	O	146	LEU
3	O	150	LEU
3	O	152	ASN
3	O	166	LEU
3	O	174	ASP
3	O	177	LEU
3	O	182	LEU
3	O	187	VAL
3	O	188	VAL
3	O	189	VAL
3	O	191	LYS
3	O	192	LEU
3	O	207	MET
3	O	209	VAL
3	O	217	SER
3	O	227	VAL
3	O	229	LEU
3	O	239	HIS
3	O	243	GLU
3	O	269	SER
3	O	307	VAL
3	O	314	VAL
3	O	326	LYS
3	O	329	LYS
4	P	18	ILE
4	P	34	GLN
4	P	42	ILE
4	P	50	ILE
4	P	51	GLN
4	P	53	PHE
4	P	57	ARG
4	P	75	LYS
4	P	81	MET
4	P	84	ILE
4	P	89	THR
4	P	95	THR
4	P	106	GLN
4	P	114	TYR

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Mol	Chain	Res	Type
4	P	118	SER
4	P	127	LEU
4	P	138	VAL
4	P	144	ILE
4	P	155	LEU
4	P	166	ASN
4	P	170	THR
4	P	171	GLN
4	P	172	LEU
4	P	206	GLN
4	P	208	MET
4	P	209	LEU
4	P	210	ARG
4	P	214	TYR
4	P	224	VAL
4	P	225	ASN
4	P	227	ILE
4	P	232	SER
4	P	258	GLU
4	P	263	TYR
4	P	299	ARG
4	P	305	TYR
4	P	321	LEU
4	P	331	ILE
4	P	332	SER
4	P	346	VAL
4	P	349	LEU
4	P	350	SER
4	P	351	SER
4	P	352	PHE
4	P	353	ASP
4	P	354	GLU
4	P	372	SER
4	P	376	TRP
4	P	391	LEU
4	P	403	ASP
4	P	426	ARG
4	P	447	GLN
4	P	451	ASN
4	P	454	LEU
5	R	4	LEU
5	R	5	PHE

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Mol	Chain	Res	Type
5	R	28	GLU
5	R	43	ASP
5	R	46	VAL
5	R	79	ILE
5	R	82	THR
5	R	111	ILE
5	R	125	LEU
5	R	128	LEU
5	R	182	THR
5	R	187	LEU
5	R	195	VAL
5	R	204	ASN
5	R	206	LEU
5	R	211	THR
5	R	215	VAL
5	R	219	VAL
5	R	259	SER
5	R	284	GLN
5	R	292	VAL
5	R	314	VAL
5	R	316	GLN
5	R	333	ILE
5	R	337	LEU
5	R	348	VAL
5	R	352	LEU
5	R	371	THR
5	R	383	ILE
5	R	421	VAL
5	R	436	GLU
5	R	463	ILE
5	R	469	SER
5	R	472	LEU
5	R	478	SER
5	R	486	THR
5	R	541	VAL
5	R	552	VAL
5	R	652	LEU
5	R	718	VAL
5	R	719	HIS
5	R	731	CYS
5	R	732	ILE
5	R	740	ARG

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Mol	Chain	Res	Type
5	R	744	LEU
5	R	768	SER
5	R	793	MET
5	R	796	LEU
5	R	809	GLU
6	A	42	LEU
6	A	51	VAL
6	A	61	MET
6	A	68	GLU
6	A	69	GLU
6	A	103	GLN
6	A	118	ILE
6	A	120	ARG
6	A	136	THR
6	A	147	ILE
6	A	156	VAL
6	A	157	SER
6	A	160	SER
6	A	175	THR
6	A	218	THR
6	A	228	LEU
6	A	248	ILE
6	A	263	LEU
6	A	266	TYR
6	A	268	ASN
6	A	294	LEU
6	A	296	MET
6	A	324	GLU
6	A	327	ILE
6	A	350	SER
6	A	362	SER
6	A	381	ARG
6	A	405	SER
6	A	410	VAL
6	A	423	SER
6	A	447	SER
6	A	450	TRP
6	A	463	GLU
6	A	470	THR
6	A	478	LYS
6	A	558	THR
6	A	560	GLN

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Mol	Chain	Res	Type
6	A	561	SER
6	A	572	GLU
6	A	577	ILE
6	A	585	LYS
6	A	592	ASP
6	A	606	GLU
6	A	614	SER
6	B	25	SER
6	B	42	LEU
6	B	74	SER
6	B	75	VAL
6	B	107	SER
6	B	110	SER
6	B	136	THR
6	B	145	SER
6	B	156	VAL
6	B	161	LEU
6	B	199	VAL
6	B	228	LEU
6	B	268	ASN
6	B	272	ILE
6	B	277	CYS
6	B	327	ILE
6	B	350	SER
6	B	352	SER
6	B	358	LEU
6	B	371	ASP
6	B	384	SER
6	B	387	GLU
6	B	419	ASP
6	B	436	ASP
6	B	450	TRP
6	B	471	GLU
6	B	492	ILE
6	B	495	LEU
6	B	509	LEU
6	B	556	GLU
6	B	561	SER
6	B	581	LEU
6	B	614	SER
6	C	25	SER
6	C	33	ASP

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Mol	Chain	Res	Type
6	C	42	LEU
6	C	60	ASP
6	C	70	THR
6	C	74	SER
6	C	107	SER
6	C	177	THR
6	C	201	GLU
6	C	228	LEU
6	C	262	SER
6	C	345	SER
6	C	346	MET
6	C	350	SER
6	C	362	SER
6	C	395	LEU
6	C	403	SER
6	C	453	SER
6	C	501	LEU
6	C	542	SER
6	C	555	VAL
6	C	588	ASP
6	C	590	LEU
6	C	599	SER
6	C	608	MET
7	D	54	ASN
7	D	57	LEU
7	D	80	THR
7	D	93	LYS
7	D	139	ILE
7	D	156	GLN
7	D	188	LYS
7	D	311	SER
7	D	315	GLU
7	D	329	THR
7	D	351	ILE
7	D	404	SER
7	D	431	ASP
7	D	436	LYS
7	D	444	LEU
7	D	449	LEU
7	D	455	LEU
7	D	472	THR
7	D	473	VAL

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Mol	Chain	Res	Type
7	D	498	SER
7	E	51	SER
7	E	80	THR
7	E	98	VAL
7	E	103	SER
7	E	201	GLU
7	E	215	LYS
7	E	237	ASN
7	E	268	THR
7	E	276	ARG
7	E	311	SER
7	E	330	ASP
7	E	347	SER
7	E	376	GLN
7	E	397	SER
7	E	404	SER
7	E	438	VAL
7	E	472	THR
7	E	473	VAL
7	E	501	SER
7	F	46	THR
7	F	54	ASN
7	F	75	THR
7	F	83	SER
7	F	97	GLN
7	F	98	VAL
7	F	126	ASP
7	F	135	SER
7	F	168	GLU
7	F	201	GLU
7	F	250	GLU
7	F	253	SER
7	F	299	ASP
7	F	311	SER
7	F	317	VAL
7	F	329	THR
7	F	354	LEU
7	F	394	VAL
7	F	404	SER
7	F	442	GLU
7	F	447	ASP
8	X	16	GLU

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Mol	Chain	Res	Type
8	X	32	CYS
8	X	58	LYS
8	X	71	SER
8	X	81	LEU
8	X	105	LEU
8	X	109	GLU
8	X	114	LYS
8	X	126	TYR
8	X	138	ASP
8	X	146	THR
8	X	148	LYS
8	X	171	ASP
8	X	181	LEU
8	X	191	GLU
8	X	209	GLU
8	X	214	GLU
8	X	217	LEU
8	X	221	ASP
8	X	229	MET
8	X	234	MET
8	X	236	LYS
8	X	237	LEU
8	X	247	SER
8	X	262	SER
8	X	263	ILE
8	X	270	ASN
8	Y	14	THR
8	Y	105	LEU
8	Y	110	SER
8	Y	119	VAL
8	Y	123	LYS
8	Y	125	ASP
8	Y	146	THR
8	Y	157	SER
8	Y	207	GLN
8	Y	227	LYS
8	Y	230	ILE
8	Y	237	LEU
8	Y	259	LEU
8	Y	265	ARG
8	Y	271	GLU
8	Z	14	THR

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Mol	Chain	Res	Type
8	Z	15	SER
8	Z	16	GLU
8	Z	57	GLU
8	Z	67	GLU
8	Z	71	SER
8	Z	81	LEU
8	Z	95	VAL
8	Z	104	LYS
8	Z	109	GLU
8	Z	124	SER
8	Z	126	TYR
8	Z	134	ASN
8	Z	136	LEU
8	Z	156	THR
8	Z	162	GLN
8	Z	178	LEU
8	Z	179	PHE
8	Z	199	LEU
8	Z	222	GLN
8	Z	228	THR
8	Z	237	LEU
8	Z	266	ILE
8	Z	269	GLU
9	G	37	SER
9	G	42	LEU
9	G	51	ILE
9	G	58	MET
9	G	87	VAL
9	G	94	ILE
9	G	100	ASN
9	G	116	THR
9	G	122	THR
9	G	129	GLU
9	G	142	VAL
9	G	146	VAL
9	G	150	SER
9	G	151	LEU
9	G	184	LEU
9	G	205	ILE
9	G	212	LEU
10	N	10	VAL
10	N	13	ASP

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Mol	Chain	Res	Type
10	N	15	ASP
10	N	35	ASN
10	N	65	LEU
10	N	74	VAL
10	N	85	ILE
11	0	36	ASP
11	0	50	SER
11	0	70	TYR
11	0	88	THR
11	0	91	LEU
11	0	105	ILE
11	0	160	SER
12	1	26	SER
12	1	55	SER
12	1	56	ILE
12	1	85	SER
12	1	112	ILE
12	1	129	VAL
12	1	140	VAL
12	2	37	SER
12	2	80	LEU
12	2	82	ASP
12	2	89	SER
12	2	102	SER
12	2	123	GLN
12	3	12	SER
12	3	45	SER
12	3	75	LEU
12	3	85	SER
12	4	26	SER
12	4	53	MET
12	4	78	ASN
12	4	82	ASP
12	4	112	ILE
12	4	155	LYS
12	5	20	SER
12	5	79	SER
12	5	85	SER
12	5	98	SER
12	5	127	LEU
12	5	153	SER
12	6	12	SER

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Mol	Chain	Res	Type
12	6	28	LEU
12	6	37	SER
12	6	50	GLU
12	6	75	LEU
12	6	82	ASP
12	6	98	SER
12	6	112	ILE
12	6	153	SER
12	7	26	SER
12	7	47	MET
12	7	82	ASP
12	7	84	ILE
12	7	129	VAL
12	8	37	SER
12	8	46	VAL
12	8	55	SER
12	8	78	ASN
12	8	98	SER
12	8	153	SER
12	9	20	SER
12	9	82	ASP
12	9	115	ASP
12	9	133	LEU
12	9	139	GLU
13	Q	6	GLU
13	Q	37	VAL
13	Q	45	LEU
13	Q	63	SER
13	Q	65	LEU
13	Q	69	VAL
13	Q	78	MET
13	Q	109	VAL
13	Q	137	GLN
13	Q	166	ASP
13	Q	199	LEU
13	Q	259	ASP
13	Q	289	THR
13	Q	292	ASP
13	Q	300	LYS
14	S	24	VAL
14	S	57	LEU
15	T	53	CYS

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Mol	Chain	Res	Type
15	T	74	VAL
15	T	97	ILE
15	T	104	VAL
15	T	126	VAL
16	U	312	THR
16	U	316	LEU
16	U	335	SER
16	U	352	SER
16	U	375	SER
16	U	413	SER
16	U	417	ASP
16	U	434	LEU
16	U	450	LEU
16	U	452	THR
16	U	454	ASP
17	V	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	100	GLN
1	H	126	GLN
1	H	139	GLN
1	H	166	GLN
1	H	219	ASN
1	I	11	GLN
1	I	24	ASN
1	I	47	GLN
1	I	66	GLN
1	I	67	GLN
1	I	126	GLN
1	I	149	GLN
1	I	219	ASN
1	J	21	GLN
1	J	24	ASN
1	J	39	ASN
1	J	47	GLN
1	J	63	GLN
1	J	74	ASN
1	J	77	ASN
1	J	100	GLN
1	J	149	GLN

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Mol	Chain	Res	Type
1	J	219	ASN
2	K	10	GLN
2	K	35	GLN
2	K	46	GLN
2	K	50	GLN
2	K	85	GLN
2	L	4	GLN
2	L	13	GLN
2	M	10	GLN
3	O	17	GLN
3	O	29	ASN
3	O	94	ASN
3	O	134	ASN
3	O	157	ASN
3	O	220	GLN
3	O	252	GLN
3	O	296	HIS
3	O	317	GLN
4	P	17	ASN
4	P	32	ASN
4	P	40	GLN
4	P	102	GLN
4	P	104	ASN
4	P	106	GLN
4	P	196	GLN
4	P	242	GLN
4	P	291	ASN
4	P	379	ASN
4	P	420	HIS
4	P	430	GLN
4	P	439	ASN
4	P	457	GLN
5	R	100	ASN
5	R	176	ASN
5	R	274	GLN
5	R	289	ASN
5	R	308	ASN
5	R	433	GLN
5	R	473	ASN
5	R	497	ASN
5	R	547	HIS
5	R	558	ASN

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Mol	Chain	Res	Type
5	R	604	ASN
5	R	636	GLN
5	R	734	ASN
5	R	761	HIS
6	A	172	ASN
6	A	213	GLN
6	A	343	HIS
6	A	430	GLN
6	A	441	GLN
6	B	47	HIS
6	B	65	GLN
6	B	140	ASN
6	B	164	HIS
6	B	172	ASN
6	B	261	GLN
6	B	314	ASN
6	B	521	GLN
6	B	560	GLN
6	C	47	HIS
6	C	140	ASN
6	C	164	HIS
6	C	172	ASN
6	C	225	HIS
6	C	242	GLN
6	C	261	GLN
6	C	441	GLN
6	C	609	GLN
7	D	42	GLN
7	D	97	GLN
7	D	156	GLN
7	D	171	GLN
7	D	205	GLN
7	D	209	GLN
7	D	265	ASN
7	D	350	GLN
7	E	42	GLN
7	E	156	GLN
7	E	205	GLN
7	E	209	GLN
7	E	237	ASN
7	E	256	ASN
7	E	350	GLN

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Mol	Chain	Res	Type
7	E	363	HIS
7	E	382	GLN
7	E	470	ASN
7	F	42	GLN
7	F	54	ASN
7	F	85	GLN
7	F	97	GLN
7	F	237	ASN
7	F	345	ASN
7	F	350	GLN
8	X	59	ASN
8	X	120	ASN
8	X	184	HIS
8	X	198	HIS
8	X	222	GLN
8	X	243	GLN
8	Y	41	ASN
8	Y	59	ASN
8	Y	184	HIS
8	Y	196	GLN
8	Y	207	GLN
8	Y	270	ASN
8	Z	40	ASN
8	Z	41	ASN
8	Z	120	ASN
8	Z	149	ASN
8	Z	150	ASN
8	Z	162	GLN
8	Z	177	GLN
8	Z	207	GLN
8	Z	243	GLN
8	Z	274	ASN
9	G	31	ASN
9	G	85	GLN
9	G	88	ASN
9	G	91	GLN
9	G	152	GLN
9	G	206	GLN
10	N	67	ASN
10	N	68	GLN
10	N	83	GLN
11	0	132	HIS

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Mol	Chain	Res	Type
12	1	78	ASN
12	1	123	GLN
12	3	124	GLN
12	4	92	GLN
12	4	124	GLN
12	5	51	GLN
12	5	78	ASN
12	5	81	ASN
12	6	92	GLN
12	6	124	GLN
12	8	124	GLN
12	9	78	ASN
12	9	92	GLN
13	Q	50	GLN
13	Q	56	ASN
13	Q	137	GLN
13	Q	165	GLN
13	Q	284	ASN
13	Q	338	GLN
15	T	99	ASN
15	T	107	ASN
16	U	272	GLN
16	U	329	ASN
16	U	338	HIS
16	U	348	HIS
16	U	370	HIS
16	U	398	GLN
16	U	401	GLN
16	U	411	GLN
16	U	445	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

30 monosaccharides 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	$\#\|Z\| > 2$
18	BGC	W	1	18	12,12,12	0.55	0	17,17,17	1.38	3 (17%)
18	GAL	W	2	18	11,11,12	0.74	0	15,15,17	1.34	1 (6%)
18	NGA	W	3	18	14,14,15	0.43	0	17,19,21	2.00	6 (35%)
18	GAL	W	4	18	11,11,12	0.32	0	15,15,17	0.74	1 (6%)
18	SIA	W	5	18	20,20,21	0.61	0	21,28,31	1.45	2 (9%)
19	GAL	a	1	19	11,11,12	0.57	0	15,15,17	1.31	2 (13%)
19	NGA	a	2	19	14,14,15	0.70	0	17,19,21	1.90	4 (23%)
19	GAL	a	3	19	11,11,12	0.57	0	15,15,17	1.64	2 (13%)
19	SIA	a	4	19	20,20,21	0.74	1 (5%)	21,28,31	1.15	2 (9%)
20	NAG	b	1	20,16	14,14,15	0.22	0	17,19,21	0.53	0
20	NAG	b	2	20	14,14,15	0.28	0	17,19,21	0.49	0
20	NAG	c	1	20,16	14,14,15	0.53	0	17,19,21	0.77	0
20	NAG	c	2	20	14,14,15	0.24	0	17,19,21	0.87	1 (5%)
20	NAG	d	1	20	14,14,15	0.42	0	17,19,21	0.35	0
20	NAG	d	2	20	14,14,15	0.18	0	17,19,21	0.46	0
21	NAG	r	1	27,21	14,14,15	0.36	0	17,19,21	0.51	0
21	MAN	r	10	21	11,11,12	0.54	0	15,15,17	1.04	1 (6%)
21	MAN	r	11	21	11,11,12	0.36	0	15,15,17	0.77	1 (6%)
21	NAG	r	2	21	14,14,15	0.41	0	17,19,21	0.51	0
21	BMA	r	3	21	11,11,12	0.83	0	15,15,17	0.99	1 (6%)
21	MAN	r	4	21	11,11,12	0.87	1 (9%)	15,15,17	1.03	1 (6%)
21	MAN	r	5	21	11,11,12	0.90	0	15,15,17	1.20	2 (13%)
21	MAN	r	6	21	11,11,12	0.82	1 (9%)	15,15,17	0.88	1 (6%)
21	GLC	r	7	21	11,11,12	0.76	0	15,15,17	0.74	0
21	GLC	r	8	21	11,11,12	0.63	0	15,15,17	0.75	0
21	GLC	r	9	21	11,11,12	0.65	0	15,15,17	0.61	0
20	NAG	s	1	20,14	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
20	NAG	s	2	20	14,14,15	0.22	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	NAG	u	1	20,16	14,14,15	0.21	0	17,19,21	0.55	0
20	NAG	u	2	20	14,14,15	0.31	0	17,19,21	0.49	0

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
18	BGC	W	1	18	-	1/2/22/22	0/1/1/1
18	GAL	W	2	18	-	0/2/19/22	0/1/1/1
18	NGA	W	3	18	-	2/6/23/26	0/1/1/1
18	GAL	W	4	18	-	1/2/19/22	0/1/1/1
18	SIA	W	5	18	-	2/18/34/38	0/1/1/1
19	GAL	a	1	19	-	0/2/19/22	0/1/1/1
19	NGA	a	2	19	1/1/5/7	3/6/23/26	0/1/1/1
19	GAL	a	3	19	-	1/2/19/22	0/1/1/1
19	SIA	a	4	19	-	13/18/34/38	0/1/1/1
20	NAG	b	1	20,16	-	1/6/23/26	0/1/1/1
20	NAG	b	2	20	-	4/6/23/26	0/1/1/1
20	NAG	c	1	20,16	-	3/6/23/26	0/1/1/1
20	NAG	c	2	20	-	2/6/23/26	0/1/1/1
20	NAG	d	1	20	-	2/6/23/26	0/1/1/1
20	NAG	d	2	20	-	2/6/23/26	0/1/1/1
21	NAG	r	1	27,21	1/1/5/7	2/6/23/26	0/1/1/1
21	MAN	r	10	21	-	2/2/19/22	0/1/1/1
21	MAN	r	11	21	1/1/4/5	0/2/19/22	0/1/1/1
21	NAG	r	2	21	-	2/6/23/26	0/1/1/1
21	BMA	r	3	21	-	0/2/19/22	0/1/1/1
21	MAN	r	4	21	-	2/2/19/22	0/1/1/1
21	MAN	r	5	21	-	2/2/19/22	0/1/1/1
21	MAN	r	6	21	-	2/2/19/22	0/1/1/1
21	GLC	r	7	21	-	1/2/19/22	0/1/1/1
21	GLC	r	8	21	-	0/2/19/22	0/1/1/1
21	GLC	r	9	21	-	0/2/19/22	0/1/1/1
20	NAG	s	1	20,14	-	2/6/23/26	0/1/1/1
20	NAG	s	2	20	-	4/6/23/26	0/1/1/1
20	NAG	u	1	20,16	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	NAG	u	2	20	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	4	SIA	O1B-C1	-2.94	1.21	1.30
21	r	6	MAN	O5-C1	-2.48	1.39	1.43
21	r	4	MAN	O5-C1	-2.41	1.39	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	2	NGA	C1-O5-C5	4.87	118.72	112.19
19	a	3	GAL	C1-O5-C5	4.08	117.66	112.19
18	W	3	NGA	C1-C2-N2	4.05	116.82	110.43
19	a	2	NGA	C2-N2-C7	-3.94	117.62	122.90
19	a	3	GAL	C1-C2-C3	3.82	115.20	109.64
18	W	5	SIA	C11-C10-N5	3.77	122.37	116.12
18	W	3	NGA	O5-C1-C2	-3.74	105.51	111.29
18	W	3	NGA	C4-C3-C2	-3.32	106.15	111.02
19	a	4	SIA	O6-C2-C3	-3.26	106.17	110.56
20	c	2	NAG	C1-O5-C5	3.19	116.46	112.19
21	r	5	MAN	O2-C2-C3	-3.00	103.94	110.15
18	W	3	NGA	C1-O5-C5	2.98	116.18	112.19
19	a	2	NGA	C1-C2-N2	2.66	114.62	110.43
21	r	4	MAN	O2-C2-C3	-2.64	104.69	110.15
21	r	3	BMA	O2-C2-C3	-2.62	104.72	110.15
18	W	5	SIA	O9-C9-C8	-2.61	105.67	111.16
18	W	2	GAL	O4-C4-C3	2.54	116.37	110.38
19	a	4	SIA	O1B-C1-C2	2.54	119.31	112.71
19	a	1	GAL	C1-O5-C5	-2.50	108.83	112.19
18	W	1	BGC	O5-C5-C6	2.50	112.63	106.44
18	W	1	BGC	C4-C3-C2	-2.49	106.46	110.83
19	a	1	GAL	C1-C2-C3	2.37	113.10	109.64
21	r	10	MAN	O2-C2-C3	-2.37	105.25	110.15
18	W	3	NGA	O3-C3-C2	2.36	114.30	109.40
19	a	2	NGA	O3-C3-C2	-2.34	104.54	109.40
21	r	11	MAN	C1-O5-C5	-2.34	109.05	112.19
21	r	6	MAN	O2-C2-C3	-2.33	105.33	110.15
18	W	1	BGC	O2-C2-C1	-2.29	103.96	109.25
20	s	1	NAG	C1-O5-C5	2.29	115.25	112.19
18	W	4	GAL	C1-C2-C3	2.19	112.83	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	r	5	MAN	C1-O5-C5	2.18	115.11	112.19
18	W	3	NGA	O3-C3-C4	-2.01	105.63	110.38

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	a	2	NGA	C1
21	r	1	NAG	C1
21	r	11	MAN	C1

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	W	3	NGA	C8-C7-N2-C2
18	W	3	NGA	O7-C7-N2-C2
19	a	4	SIA	C5-C6-C7-C8
19	a	4	SIA	C5-C6-C7-O7
19	a	4	SIA	O6-C6-C7-C8
19	a	4	SIA	O6-C6-C7-O7
19	a	4	SIA	C6-C7-C8-C9
19	a	4	SIA	C7-C8-C9-O9
20	s	2	NAG	C4-C5-C6-O6
21	r	10	MAN	O5-C5-C6-O6
19	a	4	SIA	O8-C8-C9-O9
20	b	2	NAG	O5-C5-C6-O6
20	d	1	NAG	O5-C5-C6-O6
20	c	2	NAG	O5-C5-C6-O6
21	r	4	MAN	O5-C5-C6-O6
19	a	4	SIA	O7-C7-C8-O8
21	r	4	MAN	C4-C5-C6-O6
21	r	10	MAN	C4-C5-C6-O6
19	a	4	SIA	C6-C7-C8-O8
20	b	2	NAG	C4-C5-C6-O6
20	d	1	NAG	C4-C5-C6-O6
20	s	2	NAG	O5-C5-C6-O6
19	a	4	SIA	O7-C7-C8-C9
21	r	1	NAG	O5-C5-C6-O6
21	r	6	MAN	O5-C5-C6-O6
20	s	1	NAG	O5-C5-C6-O6
21	r	1	NAG	C4-C5-C6-O6
20	u	1	NAG	C4-C5-C6-O6
19	a	4	SIA	C11-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
19	a	4	SIA	O10-C10-N5-C5
20	s	1	NAG	C4-C5-C6-O6
20	c	2	NAG	C4-C5-C6-O6
21	r	6	MAN	C4-C5-C6-O6
18	W	5	SIA	C11-C10-N5-C5
18	W	5	SIA	O10-C10-N5-C5
19	a	2	NGA	C8-C7-N2-C2
20	b	2	NAG	C8-C7-N2-C2
20	b	2	NAG	O7-C7-N2-C2
20	d	2	NAG	C8-C7-N2-C2
20	d	2	NAG	O7-C7-N2-C2
20	u	1	NAG	O5-C5-C6-O6
20	c	1	NAG	O5-C5-C6-O6
21	r	5	MAN	O5-C5-C6-O6
19	a	2	NGA	O7-C7-N2-C2
21	r	5	MAN	C4-C5-C6-O6
18	W	4	GAL	O5-C5-C6-O6
20	u	2	NAG	O5-C5-C6-O6
20	b	1	NAG	O5-C5-C6-O6
21	r	7	GLC	O5-C5-C6-O6
20	c	1	NAG	C3-C2-N2-C7
20	c	1	NAG	C4-C5-C6-O6
20	u	2	NAG	C1-C2-N2-C7
19	a	2	NGA	C4-C5-C6-O6
21	r	2	NAG	C4-C5-C6-O6
19	a	3	GAL	O5-C5-C6-O6
20	s	2	NAG	C3-C2-N2-C7
19	a	4	SIA	O1A-C1-C2-O6
21	r	2	NAG	O5-C5-C6-O6
18	W	1	BGC	O5-C5-C6-O6
20	s	2	NAG	C1-C2-N2-C7
20	u	2	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	c	1	NAG	1	0
19	a	2	NGA	1	0
20	d	1	NAG	4	0
20	b	1	NAG	1	0
19	a	1	GAL	1	0

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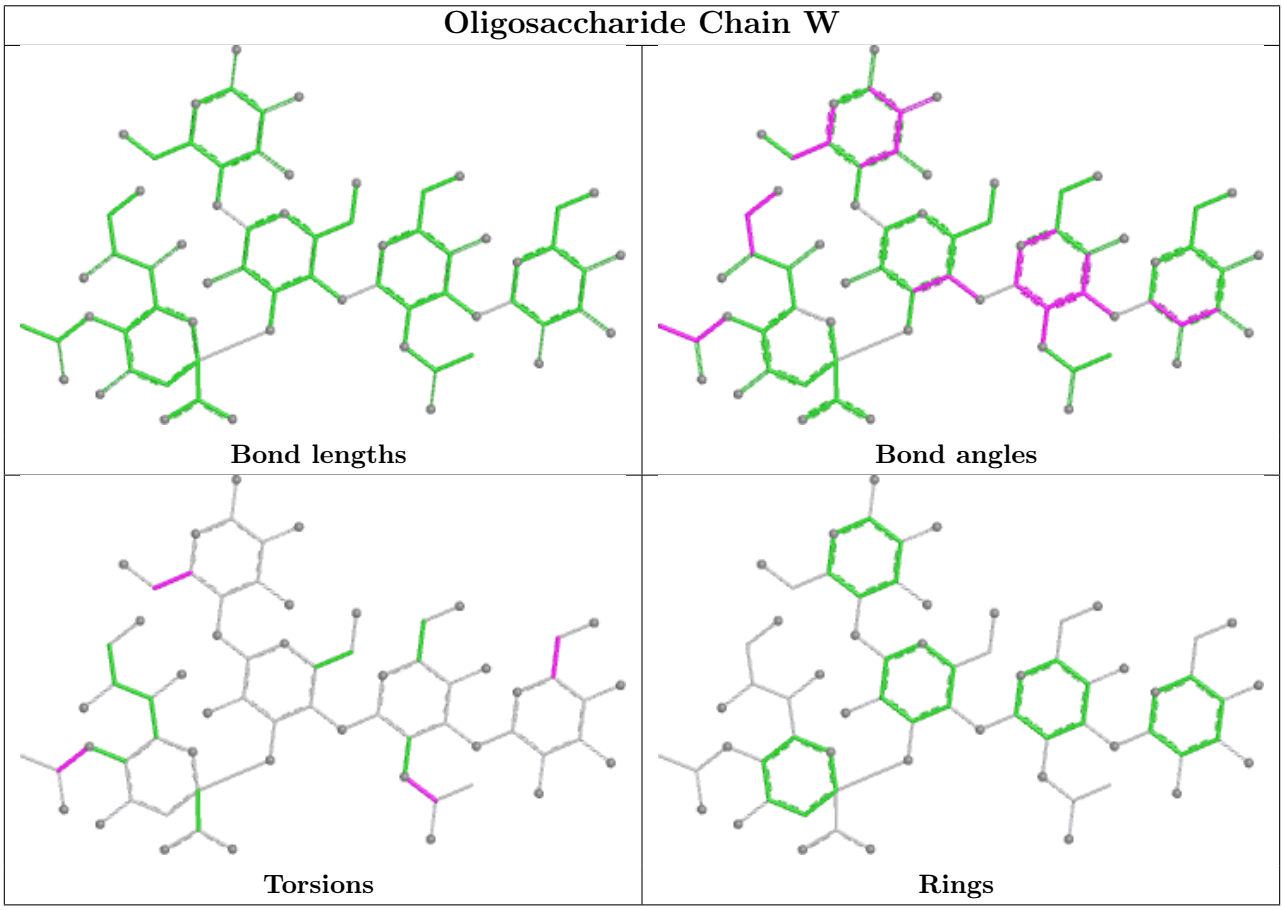
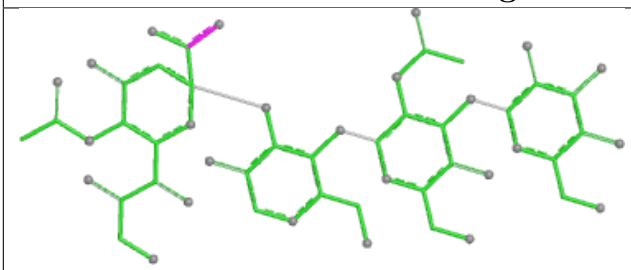
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	4	SIA	4	0
18	W	5	SIA	5	0
21	r	1	NAG	1	0
20	c	2	NAG	1	0
18	W	1	BGC	1	0

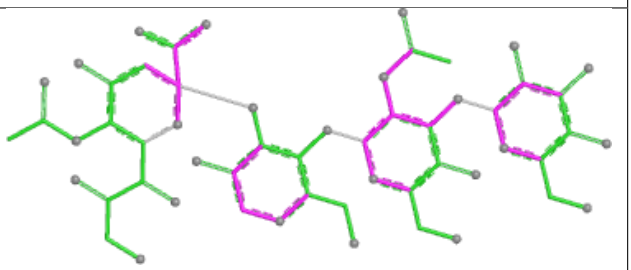
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



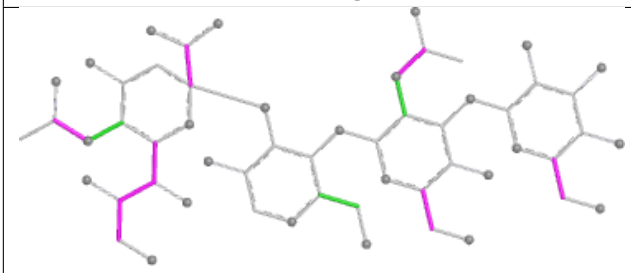
Oligosaccharide Chain a



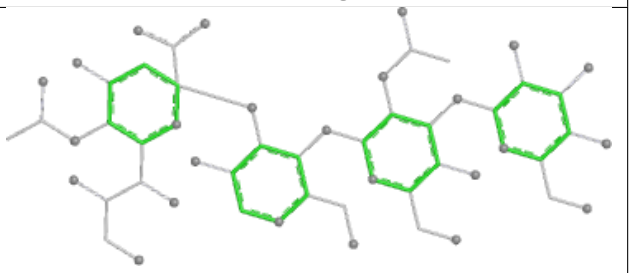
Bond lengths



Bond angles

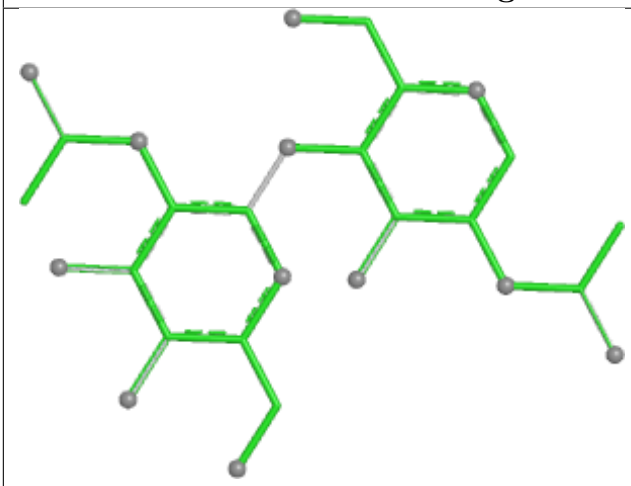


Torsions

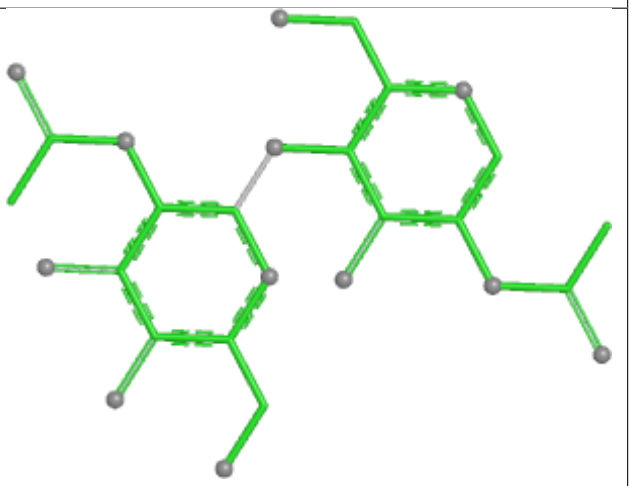


Rings

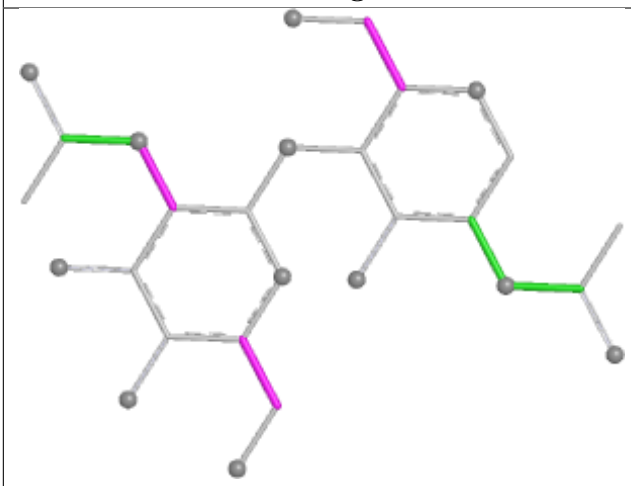
Oligosaccharide Chain u



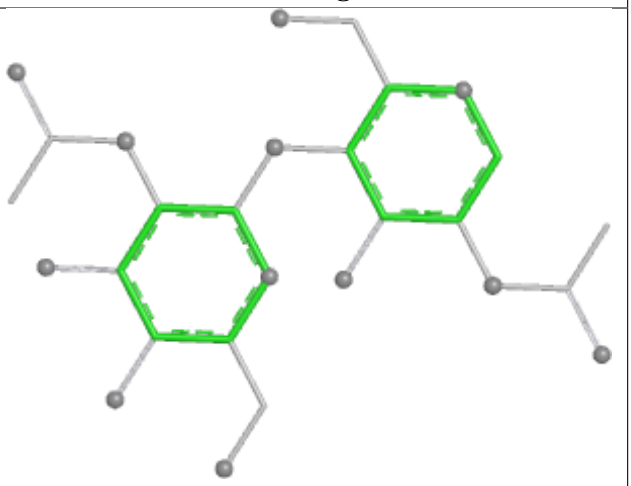
Bond lengths



Bond angles

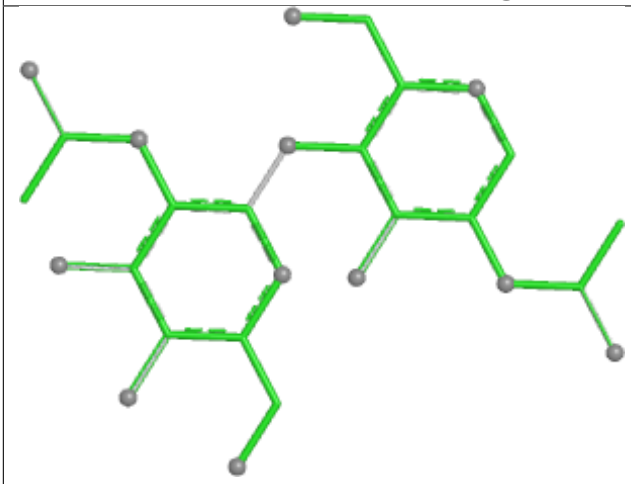


Torsions

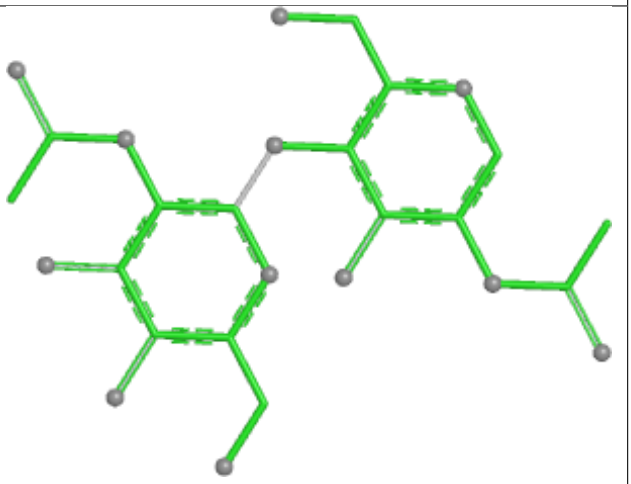


Rings

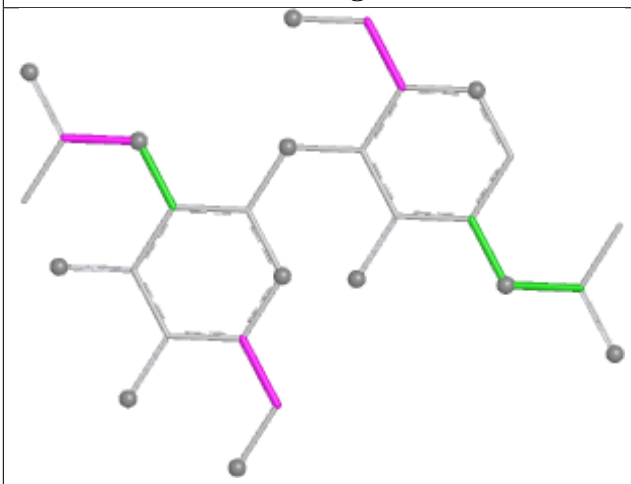
Oligosaccharide Chain b



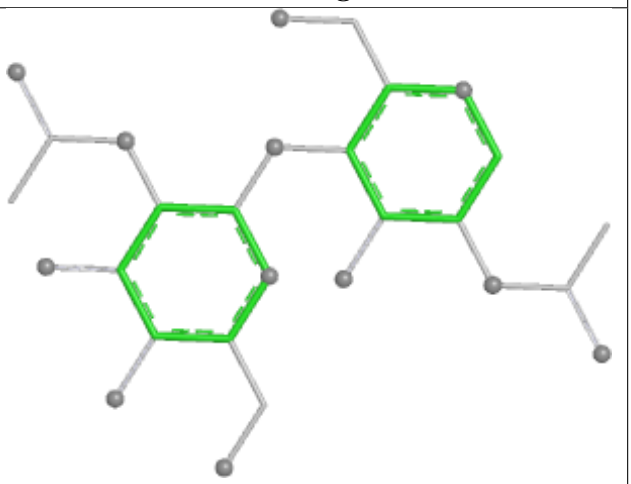
Bond lengths



Bond angles

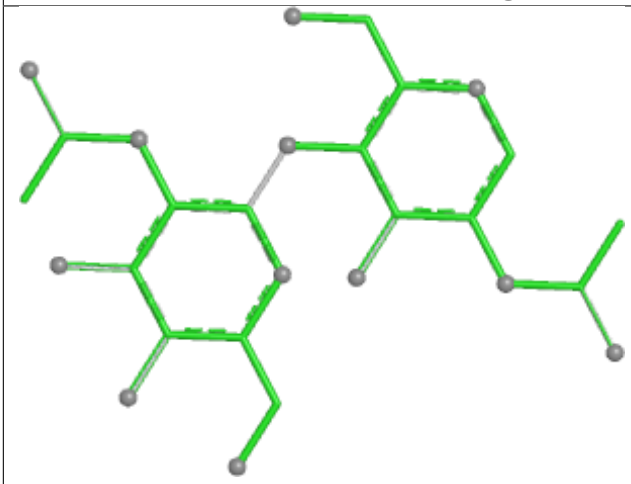


Torsions

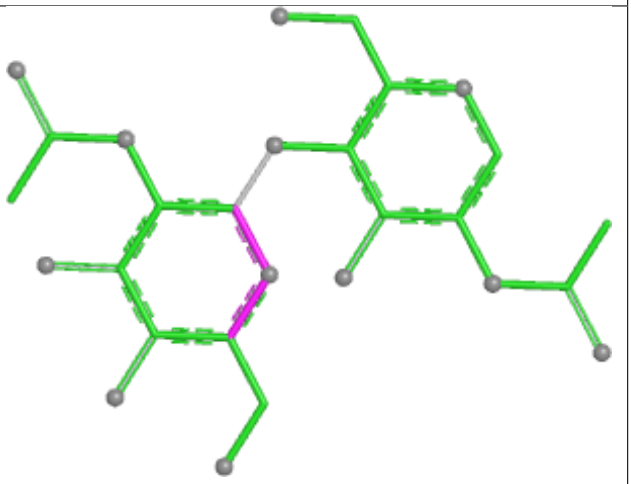


Rings

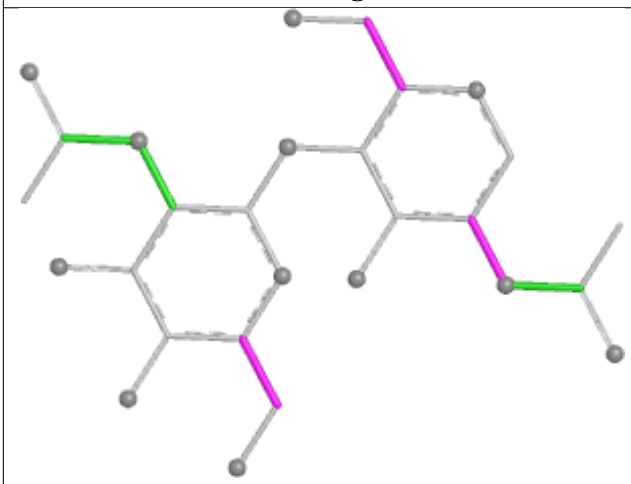
Oligosaccharide Chain c



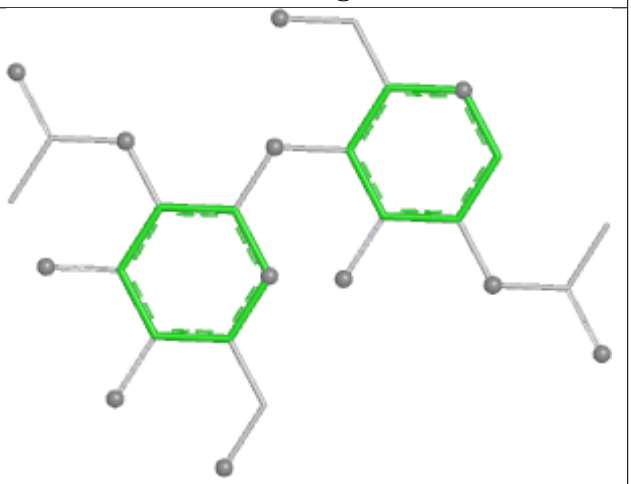
Bond lengths



Bond angles

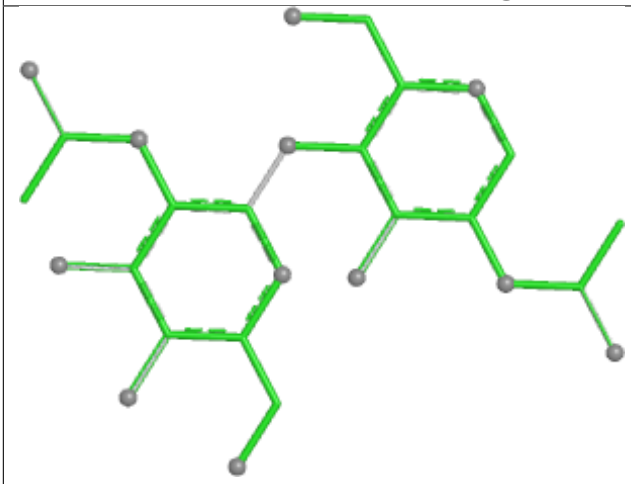


Torsions

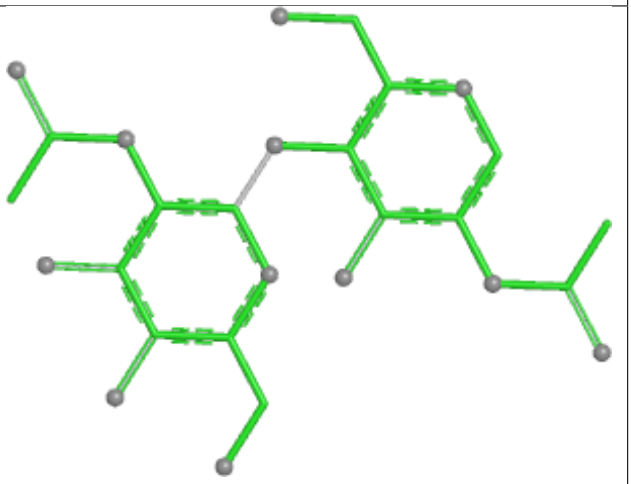


Rings

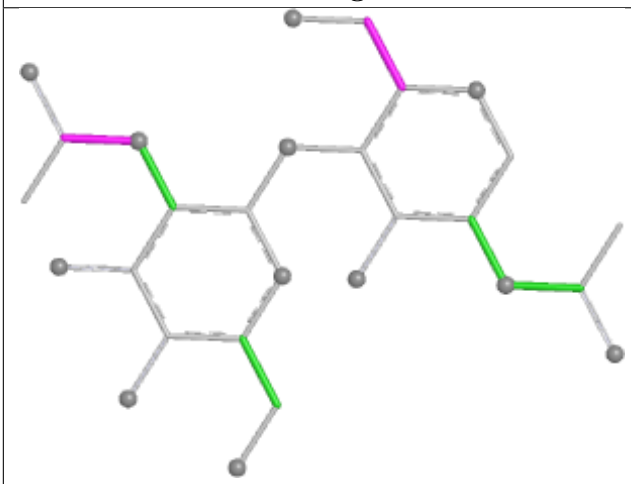
Oligosaccharide Chain d



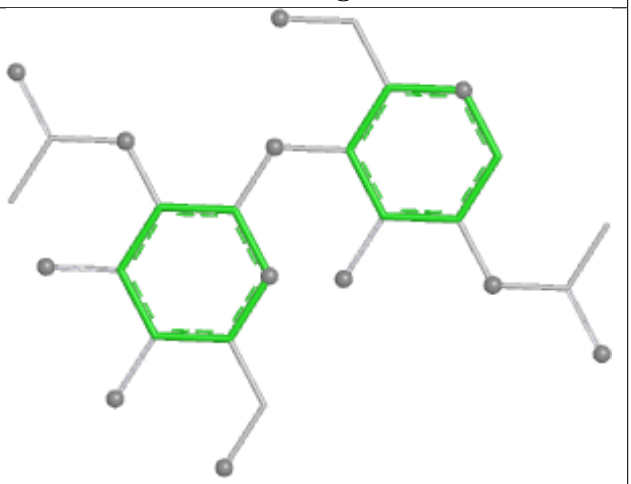
Bond lengths



Bond angles

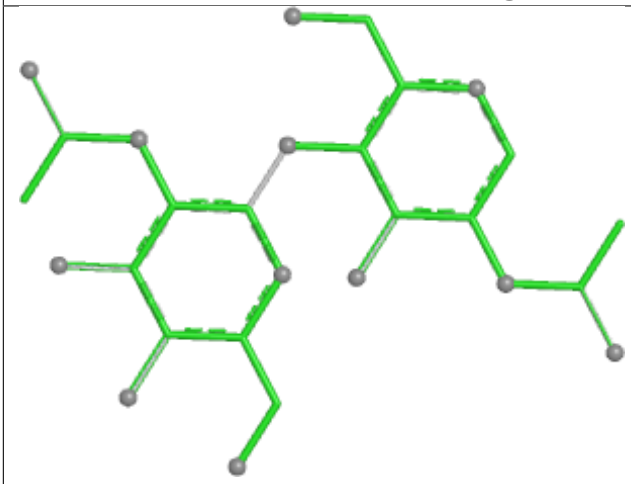


Torsions

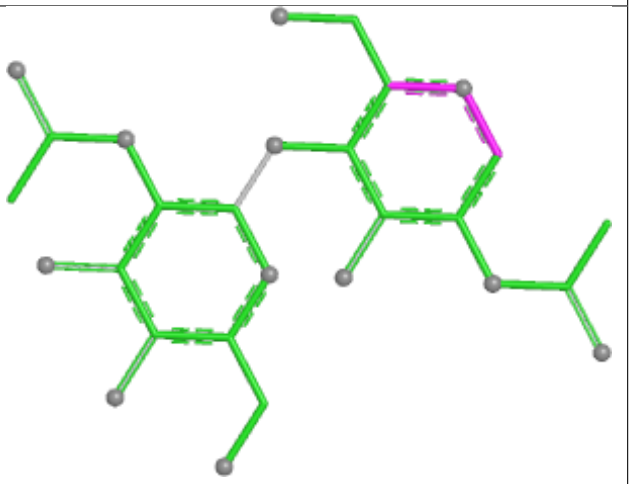


Rings

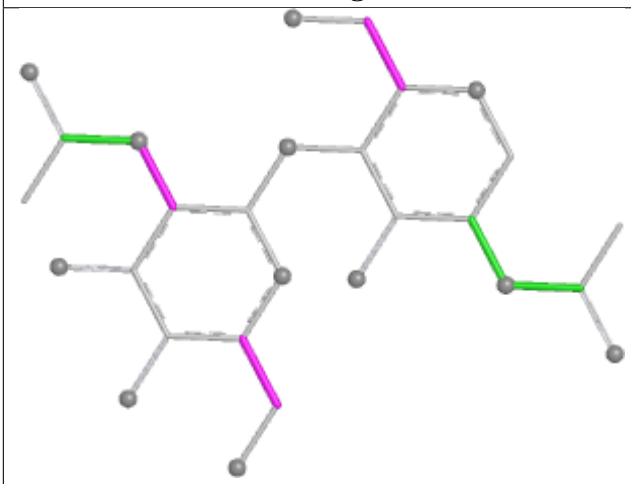
Oligosaccharide Chain s



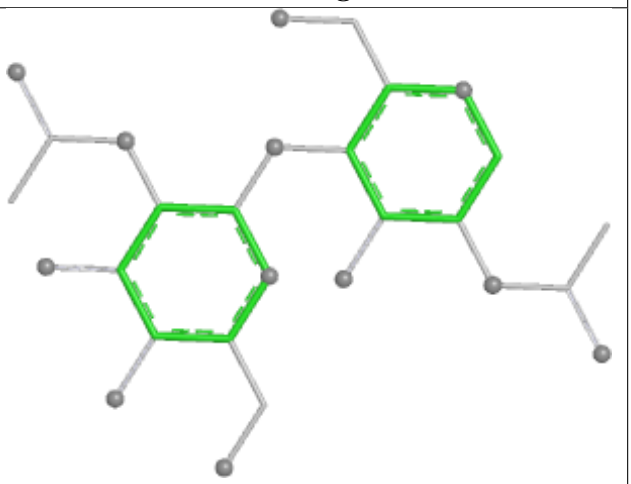
Bond lengths



Bond angles

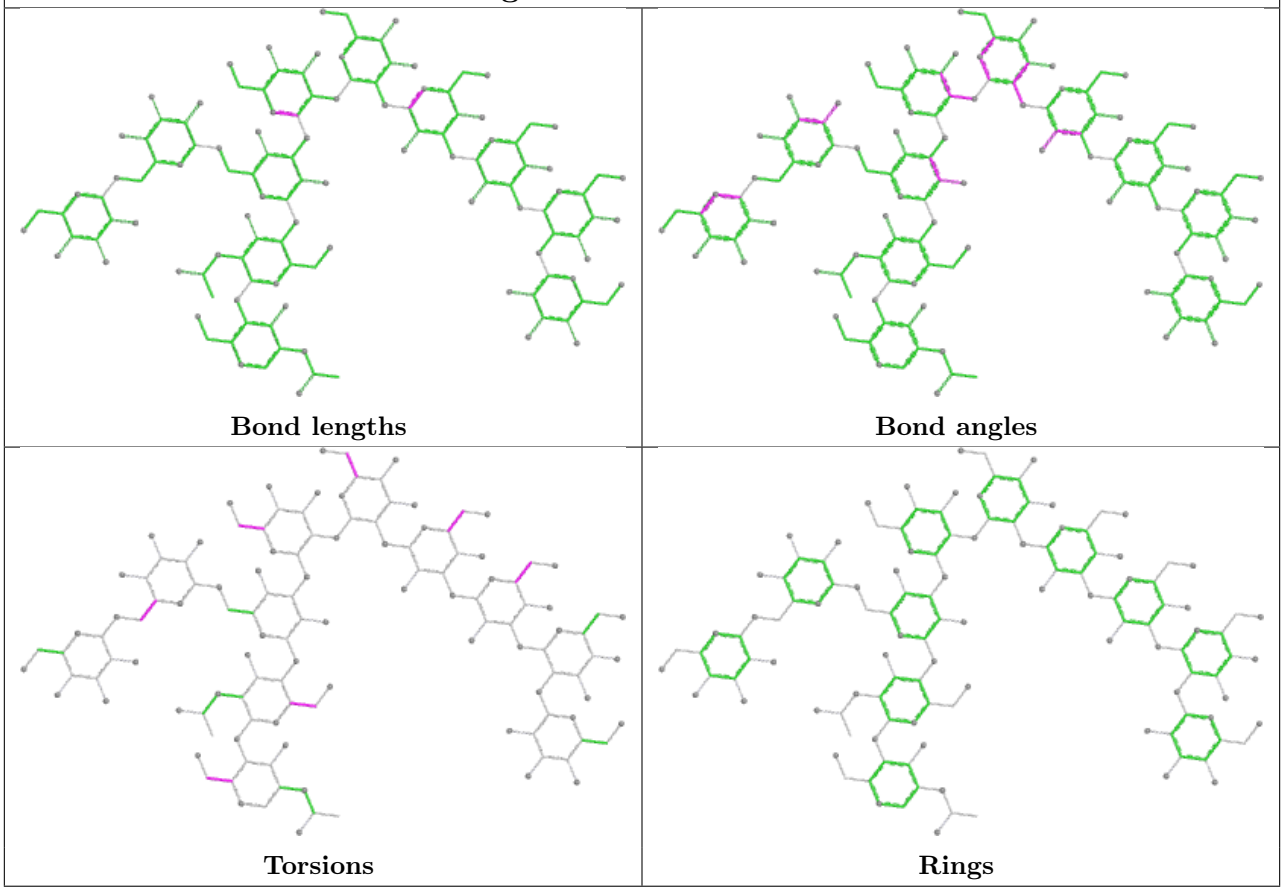


Torsions



Rings

Oligosaccharide Chain r



5.6 Ligand geometry (i)

33 ligands 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	$\#\|Z\| > 2$
25	WSS	3	201	-	40,40,53	0.46	0	43,45,61	0.69	1 (2%)
22	CLR	R	901	-	31,31,31	0.28	0	48,48,48	0.49	0
29	WJS	3	202	-	25,26,34	1.44	2 (8%)	26,32,40	1.53	2 (7%)
24	PTY	V	403	-	28,28,49	0.36	0	30,32,54	0.41	0
24	PTY	U	503	-	25,25,49	0.34	0	27,27,54	0.33	0
22	CLR	5	201	-	31,31,31	0.30	0	48,48,48	0.66	1 (2%)
22	CLR	0	304	-	31,31,31	0.32	0	48,48,48	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	WSS	0	302	-	40,40,53	0.34	0	46,48,61	0.40	0
24	PTY	5	202	-	34,34,49	0.36	0	37,39,54	0.44	0
26	NAG	R	906	5	14,14,15	0.44	0	17,19,21	0.49	0
25	WSS	U	502	-	36,36,53	0.39	0	42,44,61	0.54	0
25	WSS	R	905	-	39,39,53	0.35	0	45,47,61	0.39	0
25	WSS	1	201	-	33,33,53	0.38	0	39,41,61	0.67	1 (2%)
27	WJP	R	907	21	32,33,34	1.64	6 (18%)	39,43,44	1.94	10 (25%)
24	PTY	R	904	-	28,28,49	0.32	0	30,32,54	0.46	0
23	PSF	R	902	-	28,29,29	0.52	0	30,36,36	0.49	0
25	WSS	0	303	-	25,25,53	0.39	0	31,33,61	0.82	1 (3%)
24	PTY	0	306	-	16,16,49	0.59	0	18,20,54	0.74	1 (5%)
26	NAG	U	504	16	14,14,15	0.20	0	17,19,21	0.44	0
22	CLR	V	402	-	31,31,31	0.53	0	48,48,48	0.62	0
24	PTY	8	201	-	49,49,49	0.30	0	52,54,54	0.31	0
24	PTY	6	201	-	20,20,49	0.44	0	22,24,54	0.44	0
24	PTY	8	202	-	32,32,49	0.28	0	34,34,54	0.44	0
24	PTY	2	201	-	28,28,49	0.35	0	30,32,54	0.48	0
25	WSS	0	305	-	30,30,53	0.47	0	33,35,61	0.63	1 (3%)
25	WSS	0	301	-	43,43,53	0.35	0	49,51,61	0.81	1 (2%)
24	PTY	7	201	-	41,41,49	0.31	0	44,46,54	0.38	0
24	PTY	Q	401	-	29,29,49	0.36	0	32,34,54	0.46	0
25	WSS	V	401	-	36,36,53	0.35	0	42,44,61	0.48	0
24	PTY	0	307	-	47,47,49	0.29	0	50,52,54	0.35	0
28	ADP	C	701	-	28,29,29	1.40	5 (17%)	43,45,45	1.81	8 (18%)
25	WSS	U	501	-	38,38,53	0.38	0	44,46,61	0.35	0
24	PTY	R	903	-	31,31,49	0.31	0	33,33,54	0.33	0

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	WSS	3	201	-	-	9/44/44/57	-
22	CLR	R	901	-	-	6/10/68/68	0/4/4/4
29	WJS	3	202	-	-	10/30/30/38	-
24	PTY	V	403	-	-	18/30/30/53	-
24	PTY	U	503	-	-	10/27/27/53	-
22	CLR	5	201	-	-	0/10/68/68	0/4/4/4
22	CLR	0	304	-	-	0/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	WSS	0	302	-	-	12/44/44/57	-
24	PTY	5	202	-	-	23/38/38/53	-
26	NAG	R	906	5	-	3/6/23/26	0/1/1/1
25	WSS	U	502	-	-	4/40/40/57	-
25	WSS	R	905	-	-	18/43/43/57	-
25	WSS	1	201	-	-	3/37/37/57	-
27	WJP	R	907	21	-	11/37/37/40	-
24	PTY	R	904	-	1/1/3/4	19/31/31/53	-
23	PSF	R	902	-	-	15/35/35/35	-
25	WSS	0	303	-	-	6/29/29/57	-
24	PTY	0	306	-	-	6/16/16/53	-
26	NAG	U	504	16	-	2/6/23/26	0/1/1/1
22	CLR	V	402	-	-	0/10/68/68	0/4/4/4
24	PTY	8	201	-	-	28/53/53/53	-
24	PTY	6	201	-	-	11/22/22/53	-
24	PTY	8	202	-	-	17/34/34/53	-
24	PTY	2	201	-	-	11/30/30/53	-
25	WSS	0	305	-	-	8/32/32/57	-
25	WSS	0	301	-	-	15/47/47/57	-
24	PTY	7	201	-	-	22/45/45/53	-
24	PTY	Q	401	-	-	15/33/33/53	-
25	WSS	V	401	-	-	6/40/40/57	-
24	PTY	0	307	-	1/1/4/4	34/51/51/53	-
28	ADP	C	701	-	-	2/16/32/32	0/3/3/3
25	WSS	U	501	-	-	3/42/42/57	-
24	PTY	R	903	-	-	19/33/33/53	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	907	WJP	P31-O34	4.87	1.72	1.54
29	3	202	WJS	P25-O24	4.41	1.76	1.59
28	C	701	ADP	C5-C4	4.29	1.46	1.39
27	R	907	WJP	P27-O26	3.08	1.71	1.59
27	R	907	WJP	C15-C16	3.07	1.40	1.33
27	R	907	WJP	C10-C11	2.96	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	907	WJP	P27-O30	-2.96	1.56	1.59
28	C	701	ADP	C5-N7	-2.60	1.34	1.39
28	C	701	ADP	C5-C6	2.43	1.47	1.41
27	R	907	WJP	C12-C11	-2.42	1.44	1.50
28	C	701	ADP	C8-N7	2.17	1.35	1.31
29	3	202	WJS	C29-C30	2.16	1.58	1.52
28	C	701	ADP	C4-N9	-2.15	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	202	WJS	O28-C29-C30	6.21	113.47	108.06
28	C	701	ADP	C5-C4-N3	-5.85	118.66	126.72
27	R	907	WJP	C12-C11-C13	5.34	124.50	115.23
27	R	907	WJP	C04-C05-C06	-5.22	115.68	127.62
28	C	701	ADP	N3-C4-N9	4.48	134.79	127.17
27	R	907	WJP	C17-C16-C18	4.28	122.65	115.23
25	0	301	WSS	O2-C31-C32	4.04	120.22	111.48
28	C	701	ADP	C2-N3-C4	3.62	120.67	111.83
28	C	701	ADP	C4-C5-N7	-3.42	106.67	110.58
25	0	303	WSS	O2-C31-C32	3.34	118.70	111.48
25	3	201	WSS	O2-C31-C32	3.08	118.15	111.48
28	C	701	ADP	N3-C2-N1	-3.03	124.00	128.58
27	R	907	WJP	C03-C04-C05	2.87	119.70	112.16
25	1	201	WSS	O2-C31-C32	2.73	117.39	111.48
27	R	907	WJP	C17-C16-C15	-2.54	117.10	123.63
29	3	202	WJS	O27-P25-O26	2.45	123.82	112.44
25	0	305	WSS	O2P-P-O1P	2.41	120.23	110.83
24	0	306	PTY	O12-P1-O13	2.40	120.18	110.83
28	C	701	ADP	C3'-C2'-C1'	2.37	105.95	101.46
28	C	701	ADP	C4-N9-C8	2.36	108.22	105.74
28	C	701	ADP	C5-N7-C8	2.36	107.15	103.45
22	5	201	CLR	C15-C14-C13	2.35	106.60	103.84
27	R	907	WJP	O34-P31-O30	2.30	112.36	104.64
27	R	907	WJP	O26-P27-O28	-2.24	100.06	108.94
27	R	907	WJP	C07-C06-C05	2.19	129.25	123.63
27	R	907	WJP	C08-C06-C05	-2.08	116.50	121.17
27	R	907	WJP	C12-C11-C10	-2.06	118.35	123.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	R	904	PTY	C6
24	0	307	PTY	C6

All (366) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	R	902	PSF	C2-O2-P-O1
23	R	902	PSF	C2-O2-P-O4
23	R	902	PSF	C2-O2-P-O3
23	R	902	PSF	C13-C1-O11-C3
24	R	903	PTY	C11-C8-O7-C6
24	R	904	PTY	C11-C8-O7-C6
24	R	904	PTY	C3-O11-P1-O14
24	R	904	PTY	C5-O14-P1-O11
24	R	904	PTY	C5-O14-P1-O12
24	R	904	PTY	C5-O14-P1-O13
24	0	306	PTY	C5-O14-P1-O11
24	0	307	PTY	O4-C1-C6-O7
24	0	307	PTY	O10-C8-O7-C6
24	0	307	PTY	C11-C8-O7-C6
24	0	307	PTY	C3-O11-P1-O12
24	0	307	PTY	C3-O11-P1-O14
24	0	307	PTY	C5-O14-P1-O11
24	2	201	PTY	N1-C2-C3-O11
24	2	201	PTY	O14-C5-C6-C1
24	2	201	PTY	C5-O14-P1-O11
24	2	201	PTY	C5-O14-P1-O12
24	2	201	PTY	C5-O14-P1-O13
24	5	202	PTY	N1-C2-C3-O11
24	5	202	PTY	C3-O11-P1-O12
24	5	202	PTY	C3-O11-P1-O13
24	5	202	PTY	C5-O14-P1-O11
24	5	202	PTY	C5-O14-P1-O12
24	6	201	PTY	C5-O14-P1-O11
24	6	201	PTY	C5-O14-P1-O12
24	7	201	PTY	N1-C2-C3-O11
24	7	201	PTY	C3-O11-P1-O12
24	7	201	PTY	C3-O11-P1-O14
24	7	201	PTY	C5-O14-P1-O11
24	7	201	PTY	C5-O14-P1-O12
24	8	201	PTY	N1-C2-C3-O11
24	8	202	PTY	O10-C8-O7-C6
24	8	202	PTY	C11-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
24	Q	401	PTY	O30-C30-O4-C1
24	U	503	PTY	O14-C5-C6-C1
24	U	503	PTY	O14-C5-C6-O7
24	V	403	PTY	O4-C1-C6-O7
24	V	403	PTY	C3-O11-P1-O12
24	V	403	PTY	C3-O11-P1-O14
24	V	403	PTY	C5-O14-P1-O11
24	V	403	PTY	C5-O14-P1-O13
25	0	301	WSS	C32-C31-O2-C2
25	0	301	WSS	O31-C31-O2-C2
25	0	301	WSS	C39-C40-C41-C42
25	0	301	WSS	C1-O3P-P-O1P
25	0	301	WSS	C1-O3P-P-O4P
25	0	301	WSS	C4-O4P-P-O1P
25	0	301	WSS	C4-O4P-P-O3P
25	0	302	WSS	C5-C4-O4P-P
25	0	302	WSS	C1-O3P-P-O2P
25	0	302	WSS	C1-O3P-P-O4P
25	0	302	WSS	C4-O4P-P-O2P
25	0	302	WSS	C4-O4P-P-O3P
25	0	303	WSS	C32-C31-O2-C2
25	0	303	WSS	O31-C31-O2-C2
25	0	305	WSS	C39-C40-C41-C42
25	1	201	WSS	O31-C31-O2-C2
25	3	201	WSS	C32-C31-O2-C2
25	3	201	WSS	O31-C31-O2-C2
25	U	501	WSS	C1-O3P-P-O4P
25	V	401	WSS	C1-O3P-P-O2P
25	V	401	WSS	C1-O3P-P-O4P
27	R	907	WJP	C02-C03-C04-C05
29	3	202	WJS	C29-O28-P25-O24
29	3	202	WJS	C29-O28-P25-O26
29	3	202	WJS	C30-C29-O28-P25
29	3	202	WJS	O28-C29-C30-C31
29	3	202	WJS	O28-C29-C30-N34
24	8	201	PTY	O30-C30-O4-C1
26	R	906	NAG	O5-C5-C6-O6
23	R	902	PSF	O12-C1-O11-C3
24	R	903	PTY	O10-C8-O7-C6
24	R	904	PTY	O10-C8-O7-C6
24	8	201	PTY	C31-C30-O4-C1
24	Q	401	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
25	1	201	WSS	C32-C31-O2-C2
24	8	202	PTY	O30-C30-O4-C1
24	R	903	PTY	O30-C30-O4-C1
29	3	202	WJS	O20-C21-C22-O35
25	R	905	WSS	C32-C31-O2-C2
24	R	903	PTY	C31-C30-O4-C1
24	8	202	PTY	C31-C30-O4-C1
26	R	906	NAG	C4-C5-C6-O6
24	0	307	PTY	C33-C34-C35-C36
23	R	902	PSF	OT2-C-CA-N
29	3	202	WJS	C12-C13-C14-C15
24	V	403	PTY	O14-C5-C6-C1
24	6	201	PTY	C31-C30-O4-C1
22	R	901	CLR	C13-C17-C20-C22
27	R	907	WJP	C01-C02-C03-C04
24	0	307	PTY	C17-C18-C19-C20
24	0	306	PTY	C30-C31-C32-C33
24	V	403	PTY	C30-C31-C32-C33
24	0	307	PTY	C36-C37-C38-C39
26	U	504	NAG	C8-C7-N2-C2
26	U	504	NAG	O7-C7-N2-C2
24	8	202	PTY	C32-C33-C34-C35
29	3	202	WJS	C10-C11-C12-C13
25	R	905	WSS	O31-C31-O2-C2
27	R	907	WJP	C16-C18-C19-C20
24	0	307	PTY	C30-C31-C32-C33
24	8	202	PTY	C8-C11-C12-C13
24	8	202	PTY	C30-C31-C32-C33
24	7	201	PTY	C30-C31-C32-C33
24	8	201	PTY	C8-C11-C12-C13
24	6	201	PTY	O30-C30-O4-C1
24	2	201	PTY	O14-C5-C6-O7
24	V	403	PTY	O14-C5-C6-O7
24	U	503	PTY	C31-C30-O4-C1
22	R	901	CLR	C13-C17-C20-C21
22	R	901	CLR	C22-C23-C24-C25
24	8	201	PTY	C11-C8-O7-C6
25	V	401	WSS	C31-C32-C33-C34
24	U	503	PTY	O30-C30-O4-C1
24	8	201	PTY	O10-C8-O7-C6
24	0	307	PTY	C14-C15-C16-C17
24	8	201	PTY	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	R	902	PSF	C6-C5-O52-C4
24	2	201	PTY	C31-C30-O4-C1
24	7	201	PTY	C37-C38-C39-C40
25	R	905	WSS	C32-C33-C34-C35
25	0	305	WSS	C34-C35-C36-C37
24	R	903	PTY	C36-C37-C38-C39
24	R	904	PTY	C20-C21-C22-C23
24	8	201	PTY	C31-C32-C33-C34
24	8	201	PTY	C39-C40-C41-C42
24	0	307	PTY	C23-C24-C25-C26
24	2	201	PTY	C31-C32-C33-C34
24	7	201	PTY	C34-C35-C36-C37
24	8	202	PTY	C40-C41-C42-C43
24	Q	401	PTY	C35-C36-C37-C38
24	R	903	PTY	C14-C15-C16-C17
25	R	905	WSS	C11-C12-C13-C14
24	0	307	PTY	C35-C36-C37-C38
24	R	903	PTY	O4-C1-C6-C5
24	5	202	PTY	C39-C40-C41-C42
29	3	202	WJS	C13-C14-C15-C16
24	8	201	PTY	C30-C31-C32-C33
24	R	904	PTY	C19-C20-C21-C22
24	0	307	PTY	C31-C32-C33-C34
24	U	503	PTY	C32-C33-C34-C35
25	R	905	WSS	C38-C39-C40-C41
22	R	901	CLR	C16-C17-C20-C21
24	R	904	PTY	C11-C12-C13-C14
24	5	202	PTY	C31-C30-O4-C1
24	7	201	PTY	C31-C30-O4-C1
23	R	902	PSF	O51-C5-O52-C4
24	8	201	PTY	C12-C13-C14-C15
24	8	201	PTY	C32-C33-C34-C35
24	8	202	PTY	C34-C35-C36-C37
24	R	903	PTY	C12-C13-C14-C15
24	V	403	PTY	C31-C30-O4-C1
24	Q	401	PTY	C11-C8-O7-C6
24	5	202	PTY	C11-C12-C13-C14
24	0	307	PTY	C21-C22-C23-C24
24	R	904	PTY	C18-C19-C20-C21
24	0	307	PTY	C19-C20-C21-C22
24	0	307	PTY	C16-C17-C18-C19
25	R	905	WSS	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
24	0	307	PTY	C12-C13-C14-C15
24	5	202	PTY	O30-C30-O4-C1
24	2	201	PTY	O30-C30-O4-C1
24	V	403	PTY	C31-C32-C33-C34
25	R	905	WSS	C43-C44-C45-C46
24	0	307	PTY	C6-C5-O14-P1
24	Q	401	PTY	O10-C8-O7-C6
24	R	903	PTY	C32-C33-C34-C35
24	5	202	PTY	C32-C33-C34-C35
24	V	403	PTY	C36-C37-C38-C39
24	0	306	PTY	C31-C32-C33-C34
24	R	904	PTY	O14-C5-C6-C1
25	0	301	WSS	O3P-C1-C2-C3
22	R	901	CLR	C20-C22-C23-C24
24	7	201	PTY	O30-C30-O4-C1
22	R	901	CLR	C16-C17-C20-C22
24	V	403	PTY	C39-C40-C41-C42
24	5	202	PTY	C40-C41-C42-C43
24	0	307	PTY	O4-C1-C6-C5
25	0	305	WSS	C1-C2-C3-O3
24	R	903	PTY	C35-C36-C37-C38
24	7	201	PTY	C36-C37-C38-C39
24	7	201	PTY	C13-C14-C15-C16
24	0	307	PTY	C15-C16-C17-C18
24	V	403	PTY	O30-C30-O4-C1
24	R	904	PTY	C15-C16-C17-C18
24	0	306	PTY	C5-O14-P1-O13
24	R	904	PTY	C13-C14-C15-C16
24	2	201	PTY	C30-C31-C32-C33
24	7	201	PTY	C12-C13-C14-C15
25	0	301	WSS	C1-C2-O2-C31
24	8	201	PTY	C23-C24-C25-C26
24	U	503	PTY	C11-C12-C13-C14
24	0	307	PTY	C20-C21-C22-C23
24	7	201	PTY	C39-C40-C41-C42
24	0	306	PTY	C32-C33-C34-C35
24	0	307	PTY	C32-C33-C34-C35
24	0	307	PTY	C38-C39-C40-C41
24	8	201	PTY	C22-C23-C24-C25
24	Q	401	PTY	C11-C12-C13-C14
24	5	202	PTY	O4-C1-C6-O7
25	0	303	WSS	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	R	903	PTY	C15-C16-C17-C18
25	R	905	WSS	C35-C36-C37-C38
23	R	902	PSF	C7-C8-C9-C10
24	8	202	PTY	C41-C42-C43-C44
24	7	201	PTY	C41-C42-C43-C44
24	8	202	PTY	C36-C37-C38-C39
24	8	202	PTY	C15-C16-C17-C18
24	Q	401	PTY	C36-C37-C38-C39
24	7	201	PTY	C6-C5-O14-P1
24	6	201	PTY	C31-C32-C33-C34
24	R	903	PTY	C37-C38-C39-C40
25	R	905	WSS	C41-C42-C43-C44
24	0	307	PTY	O14-C5-C6-C1
24	R	904	PTY	C21-C22-C23-C24
23	R	902	PSF	C1-C13-C14-C15
24	8	201	PTY	C25-C26-C27-C28
24	8	201	PTY	C24-C25-C26-C27
23	R	902	PSF	OT1-C-CA-N
24	8	202	PTY	C33-C34-C35-C36
24	8	201	PTY	C17-C18-C19-C20
24	0	307	PTY	O14-C5-C6-O7
25	0	301	WSS	O3P-C1-C2-O2
25	0	303	WSS	O3P-C1-C2-O2
24	Q	401	PTY	C33-C34-C35-C36
24	5	202	PTY	C30-C31-C32-C33
24	8	202	PTY	C14-C15-C16-C17
24	8	201	PTY	C26-C27-C28-C29
27	R	907	WJP	C17-C16-C18-C19
23	R	902	PSF	C13-C14-C15-C16
24	8	202	PTY	C11-C12-C13-C14
24	6	201	PTY	C30-C31-C32-C33
25	0	302	WSS	C31-C32-C33-C34
25	0	302	WSS	C33-C34-C35-C36
24	V	403	PTY	O4-C1-C6-C5
27	R	907	WJP	P31-O30-P27-O26
24	8	202	PTY	C37-C38-C39-C40
24	Q	401	PTY	C31-C32-C33-C34
25	0	305	WSS	C37-C38-C39-C40
27	R	907	WJP	C15-C16-C18-C19
24	R	903	PTY	C41-C42-C43-C44
24	5	202	PTY	O14-C5-C6-C1
24	Q	401	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
25	3	201	WSS	C19-C20-C21-C22
27	R	907	WJP	C24-C02-C03-C04
24	6	201	PTY	C32-C33-C34-C35
24	5	202	PTY	C37-C38-C39-C40
24	0	307	PTY	C18-C19-C20-C21
24	Q	401	PTY	C1-C6-O7-C8
25	U	502	WSS	C17-C18-C19-C20
24	R	904	PTY	O14-C5-C6-O7
24	Q	401	PTY	O14-C5-C6-O7
24	8	201	PTY	C35-C36-C37-C38
24	5	202	PTY	O4-C1-C6-C5
24	7	201	PTY	O4-C1-C6-C5
24	Q	401	PTY	O4-C1-C6-C5
25	3	201	WSS	C1-C2-C3-O3
25	U	502	WSS	C5-C4-O4P-P
24	5	202	PTY	C36-C37-C38-C39
24	5	202	PTY	C31-C32-C33-C34
24	R	903	PTY	O4-C1-C6-O7
25	3	201	WSS	O2-C2-C3-O3
24	8	201	PTY	C33-C34-C35-C36
25	R	905	WSS	C4-C5-N1-C8
24	0	307	PTY	C31-C30-O4-C1
23	R	902	PSF	N-CA-CB-O1
25	0	302	WSS	O4P-C4-C5-N1
25	U	502	WSS	O4P-C4-C5-N1
25	3	201	WSS	C17-C18-C19-C20
24	R	903	PTY	C11-C12-C13-C14
25	0	302	WSS	C11-C12-C13-C14
24	5	202	PTY	C34-C35-C36-C37
25	0	301	WSS	C17-C18-C19-C20
24	7	201	PTY	C40-C41-C42-C43
25	0	301	WSS	C2-C1-O3P-P
24	0	307	PTY	O30-C30-O4-C1
25	R	905	WSS	C4-C5-N1-C7
25	0	305	WSS	O2-C2-C3-O3
24	V	403	PTY	C41-C42-C43-C44
23	R	902	PSF	CB-O1-P-O4
24	0	307	PTY	C5-O14-P1-O13
24	5	202	PTY	C3-O11-P1-O14
24	5	202	PTY	C5-O14-P1-O13
24	6	201	PTY	C5-O14-P1-O13
24	V	403	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
25	R	905	WSS	C1-O3P-P-O1P
25	0	301	WSS	C1-O3P-P-O2P
25	1	201	WSS	C4-O4P-P-O1P
27	R	907	WJP	C25-O26-P27-O30
24	8	201	PTY	C6-C5-O14-P1
23	R	902	PSF	C5-C6-C7-C8
25	0	301	WSS	C19-C20-C21-C22
24	6	201	PTY	C3-O11-P1-O13
24	R	903	PTY	C5-C6-O7-C8
24	7	201	PTY	C1-C6-O7-C8
25	3	201	WSS	C36-C37-C38-C39
25	0	301	WSS	C12-C13-C14-C15
24	6	201	PTY	O14-C5-C6-C1
29	3	202	WJS	C21-C22-C23-O24
24	5	202	PTY	O14-C5-C6-O7
24	7	201	PTY	C14-C15-C16-C17
25	U	501	WSS	C2-C1-O3P-P
24	Q	401	PTY	O4-C1-C6-O7
25	0	302	WSS	C19-C20-C21-C22
25	0	303	WSS	C1-C2-C3-O3
24	7	201	PTY	C33-C34-C35-C36
24	6	201	PTY	C33-C34-C35-C36
24	7	201	PTY	C35-C36-C37-C38
24	8	201	PTY	C20-C21-C22-C23
24	V	403	PTY	C37-C38-C39-C40
24	0	307	PTY	C37-C38-C39-C40
25	U	501	WSS	C17-C18-C19-C20
24	8	201	PTY	O4-C1-C6-O7
24	U	503	PTY	C12-C13-C14-C15
25	R	905	WSS	C34-C35-C36-C37
25	V	401	WSS	C13-C14-C15-C16
24	U	503	PTY	C6-C1-O4-C30
25	R	905	WSS	C4-C5-N1-C9
24	U	503	PTY	C13-C14-C15-C16
24	R	904	PTY	O4-C1-C6-C5
24	5	202	PTY	C35-C36-C37-C38
24	0	307	PTY	C40-C41-C42-C43
24	8	201	PTY	C34-C35-C36-C37
25	0	302	WSS	C37-C38-C39-C40
24	Q	401	PTY	C34-C35-C36-C37
27	R	907	WJP	C12-C11-C13-C14
24	R	904	PTY	O4-C1-C6-O7

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Mol	Chain	Res	Type	Atoms
25	R	905	WSS	O11-C11-O3-C3
26	R	906	NAG	C3-C2-N2-C7
24	R	903	PTY	C39-C40-C41-C42
25	0	303	WSS	O3P-C1-C2-C3
25	3	201	WSS	C39-C40-C41-C42
24	0	306	PTY	C6-C5-O14-P1
24	0	307	PTY	C13-C14-C15-C16
25	R	905	WSS	C12-C11-O3-C3
25	R	905	WSS	C37-C38-C39-C40
25	0	302	WSS	C17-C18-C19-C20
24	R	904	PTY	C12-C13-C14-C15
24	8	201	PTY	O4-C1-C6-C5
24	2	201	PTY	C33-C34-C35-C36
24	0	307	PTY	C41-C42-C43-C44
25	U	502	WSS	C2-C1-O3P-P
27	R	907	WJP	P31-O30-P27-O28
25	3	201	WSS	C37-C38-C39-C40
25	0	305	WSS	O3-C11-C12-C13
24	R	903	PTY	C38-C39-C40-C41
25	V	401	WSS	C14-C15-C16-C17
24	R	903	PTY	C13-C14-C15-C16
24	V	403	PTY	C33-C34-C35-C36
28	C	701	ADP	O4'-C4'-C5'-O5'
27	R	907	WJP	C10-C11-C13-C14
25	V	401	WSS	O3P-C1-C2-O2
24	R	904	PTY	C17-C18-C19-C20
25	R	905	WSS	C31-C32-C33-C34
24	8	201	PTY	C38-C39-C40-C41
24	8	201	PTY	C41-C42-C43-C44
24	8	202	PTY	C12-C11-C8-O7
24	U	503	PTY	C15-C16-C17-C18
25	0	305	WSS	O11-C11-C12-C13
24	8	201	PTY	C12-C11-C8-O7
25	0	305	WSS	O2-C31-C32-C33
28	C	701	ADP	PB-O3A-PA-O2A

There are no ring outliers.

20 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	901	CLR	1	0
29	3	202	WJS	5	0

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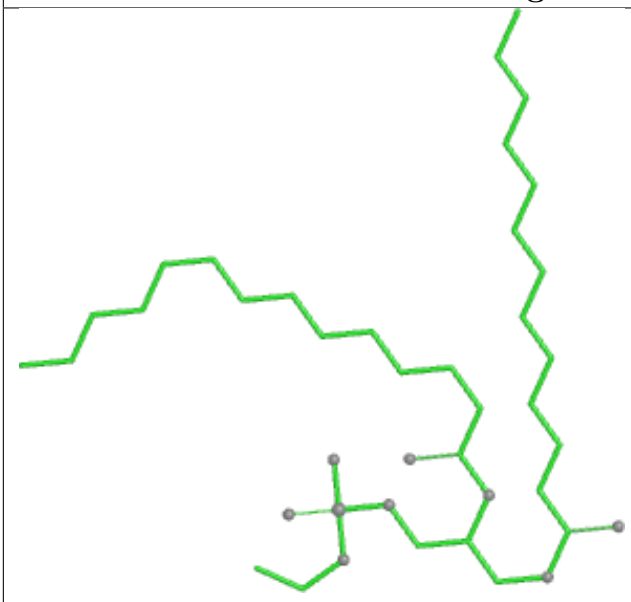
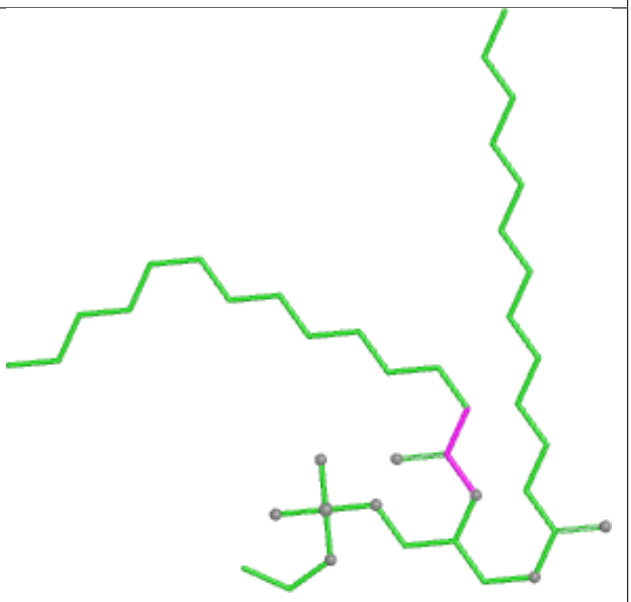
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	V	403	PTY	9	0
24	U	503	PTY	21	0
22	5	201	CLR	16	0
22	0	304	CLR	1	0
24	5	202	PTY	6	0
25	R	905	WSS	5	0
24	R	904	PTY	2	0
24	0	306	PTY	1	0
22	V	402	CLR	11	0
24	8	201	PTY	6	0
24	6	201	PTY	7	0
24	8	202	PTY	4	0
24	2	201	PTY	1	0
25	0	305	WSS	1	0
24	7	201	PTY	7	0
24	Q	401	PTY	6	0
24	0	307	PTY	3	0
28	C	701	ADP	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.

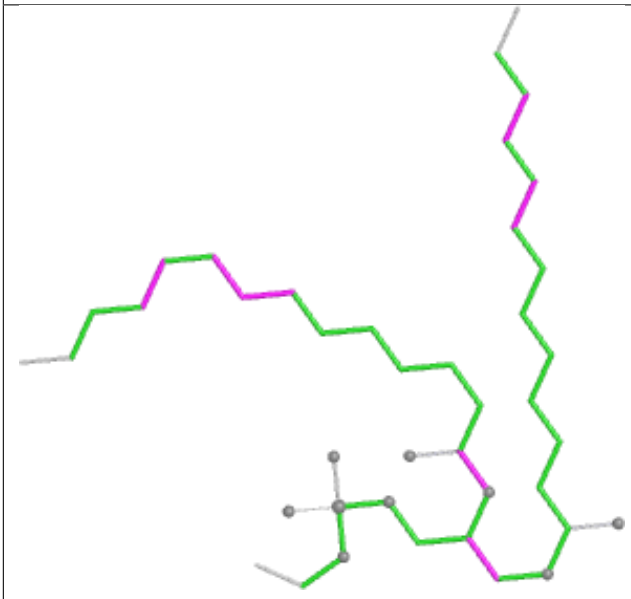
Ligand WSS 3 201



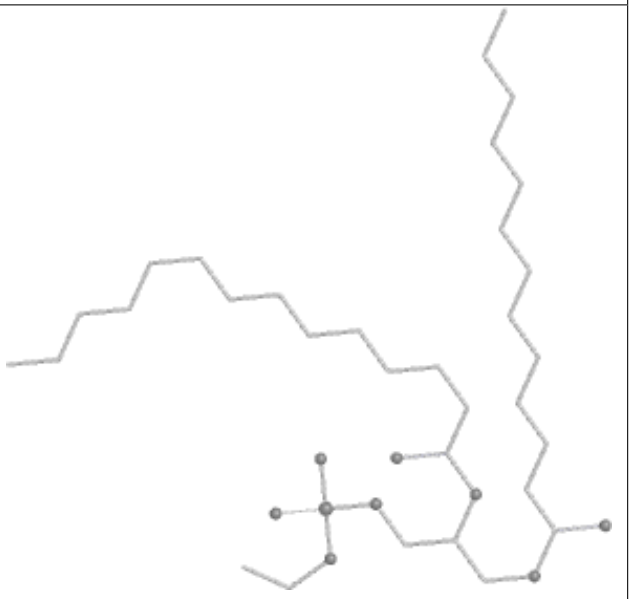
Bond lengths



Bond angles

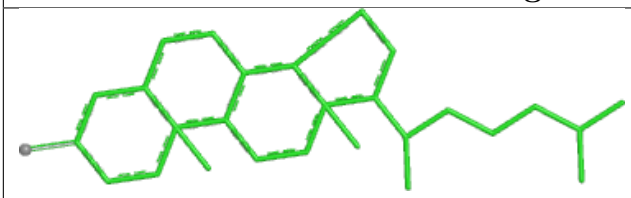


Torsions

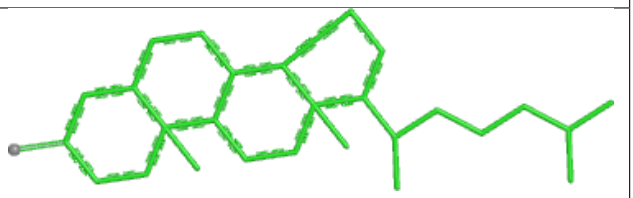


Rings

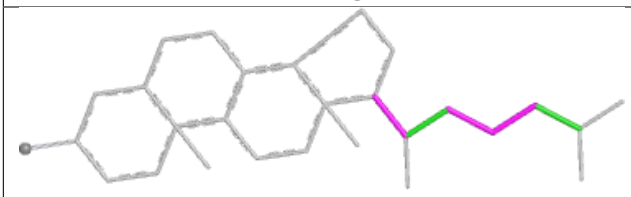
Ligand CLR R 901



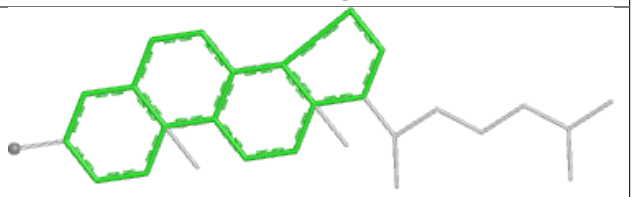
Bond lengths



Bond angles

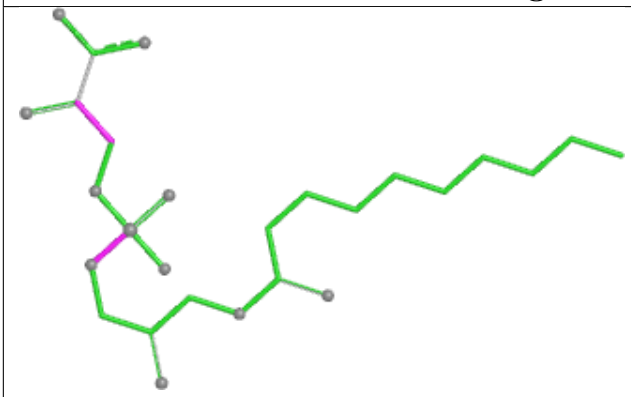


Torsions

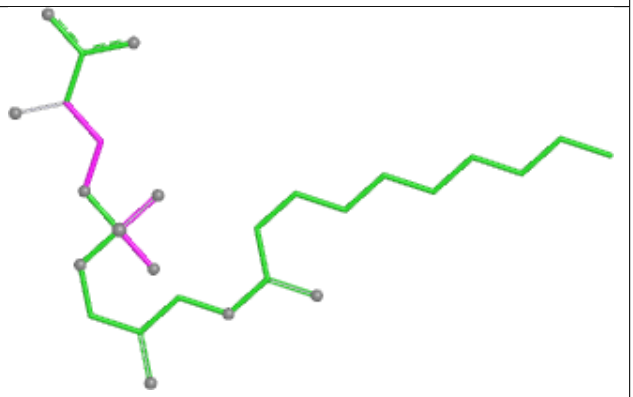


Rings

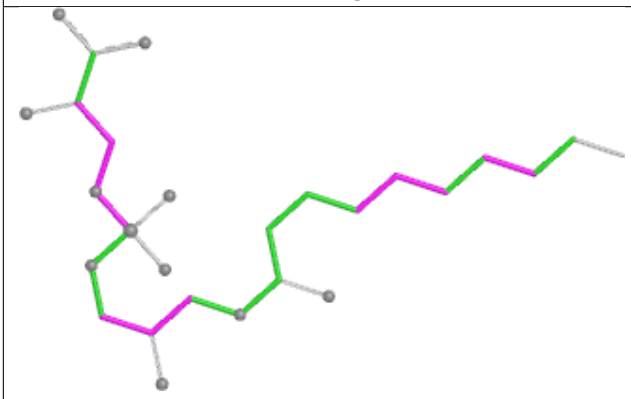
Ligand WJS 3 202



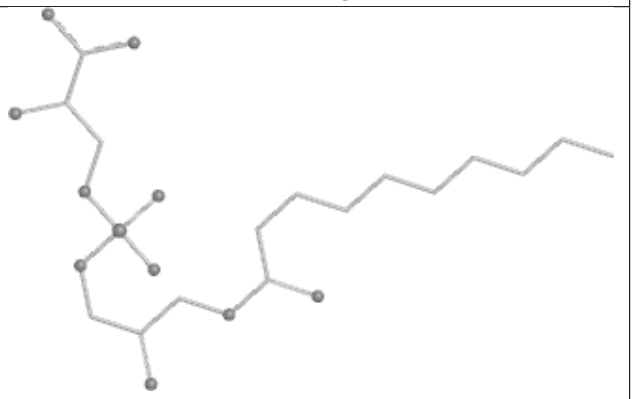
Bond lengths



Bond angles

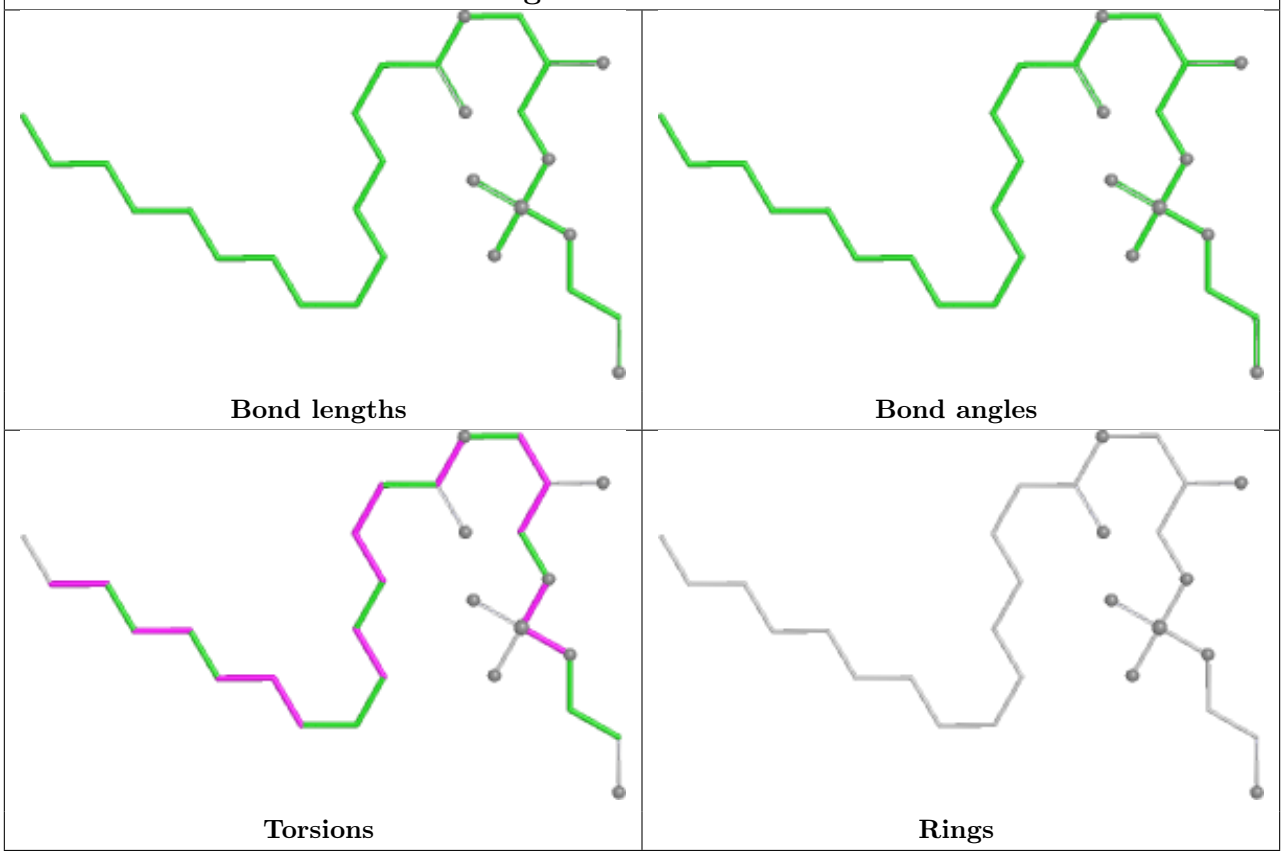


Torsions

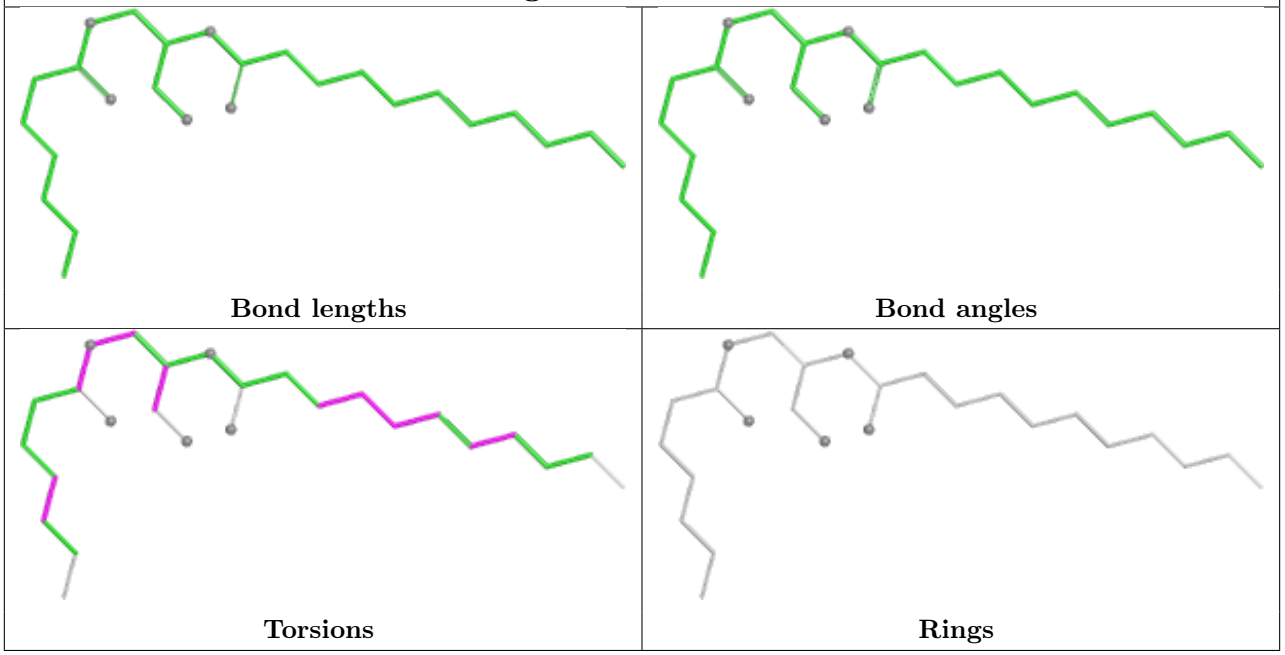


Rings

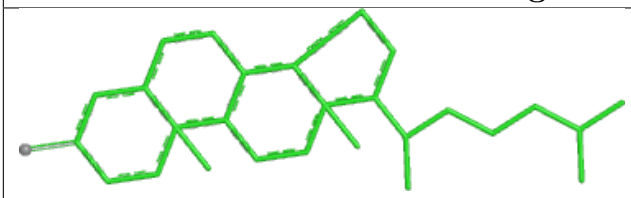
Ligand PTY V 403



Ligand PTY U 503



Ligand CLR 5 201



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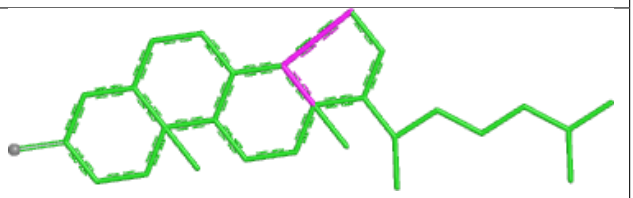

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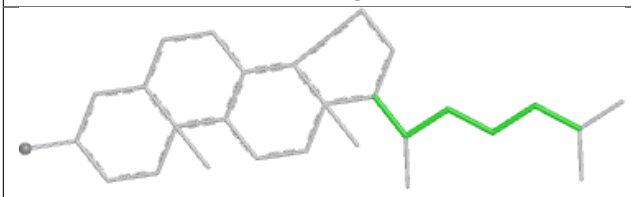

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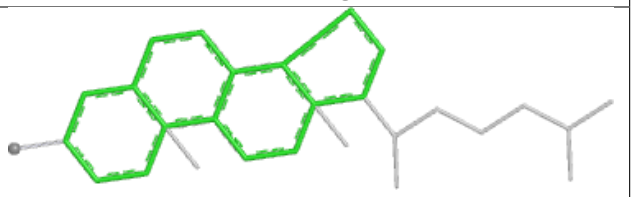
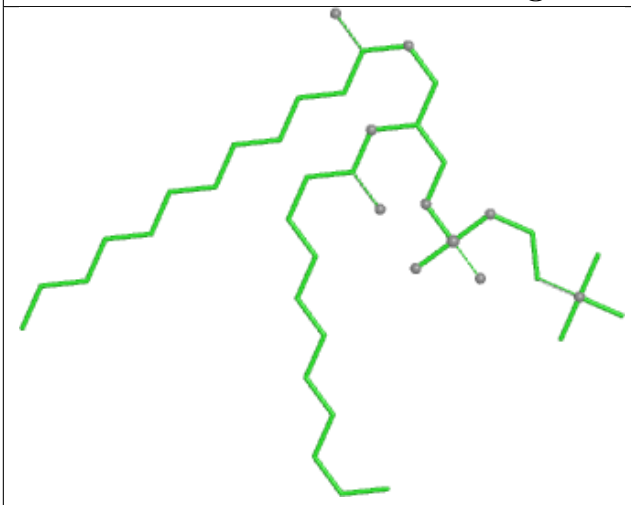


Rings

Ligand WSS 0 302



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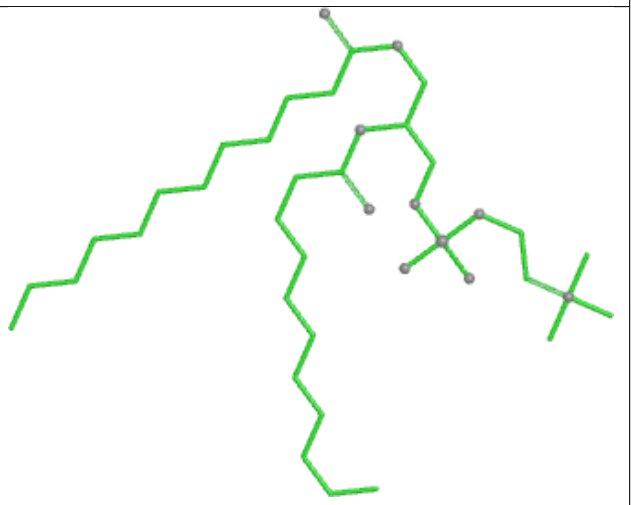

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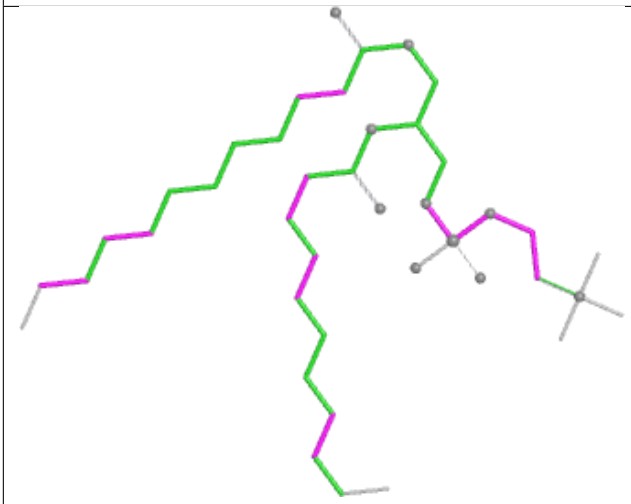

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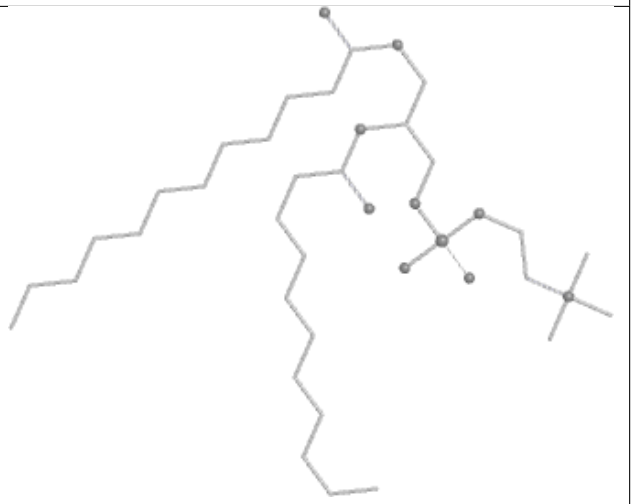

Rings

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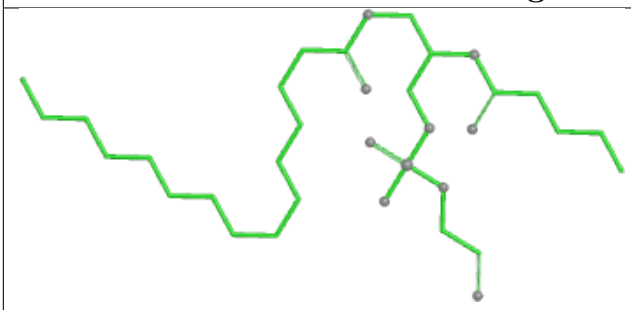

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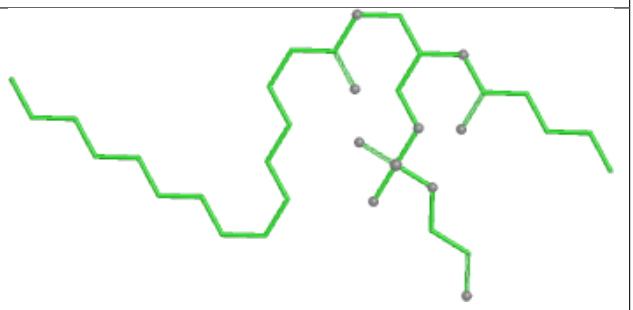

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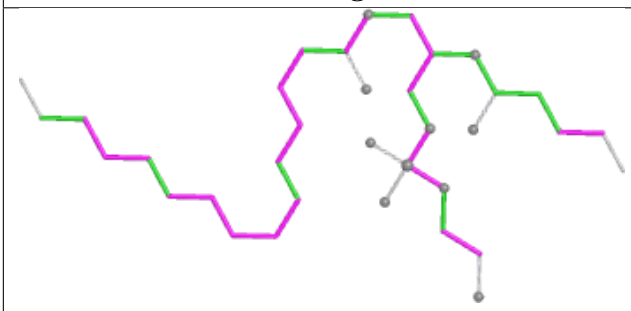

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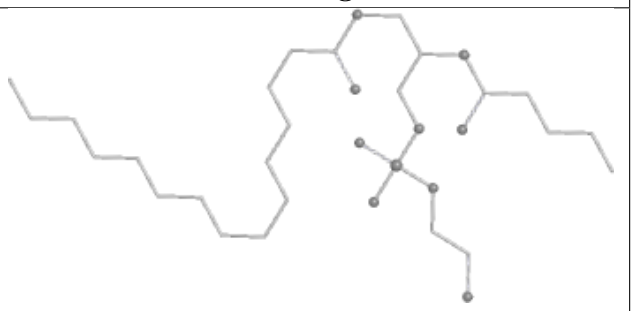
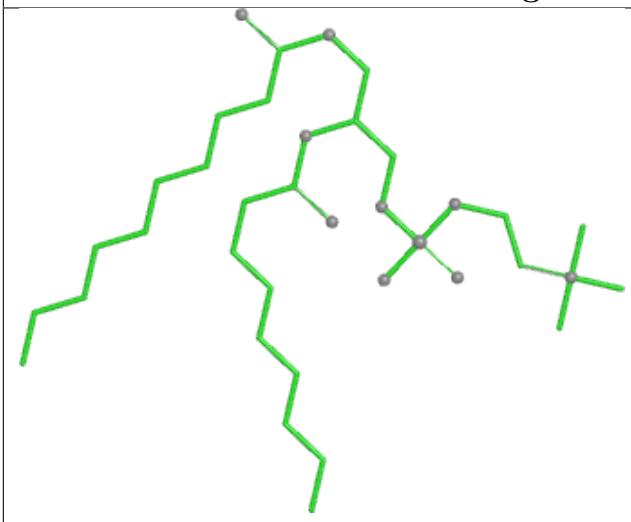


Rings

Ligand WSS U 502



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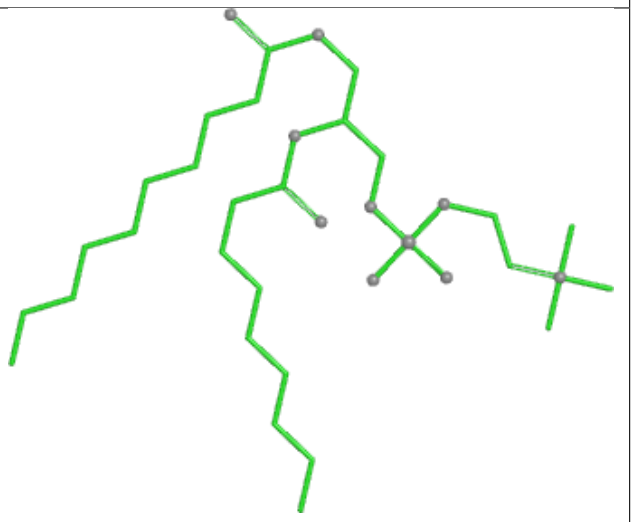

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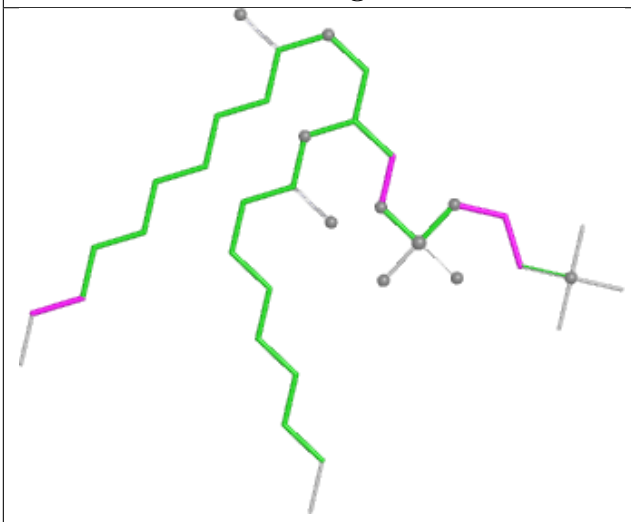

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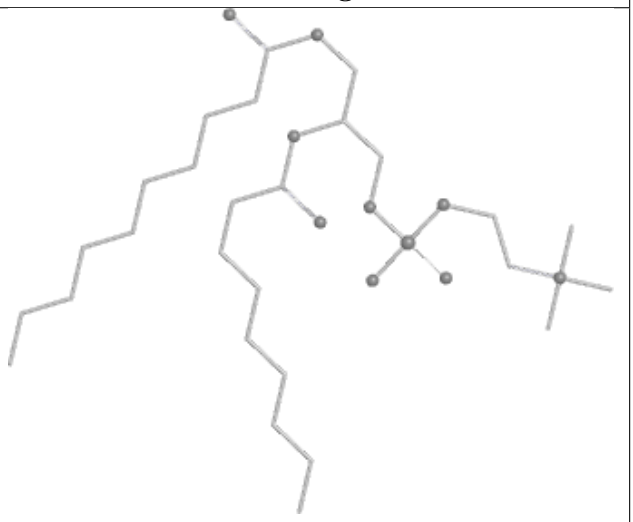
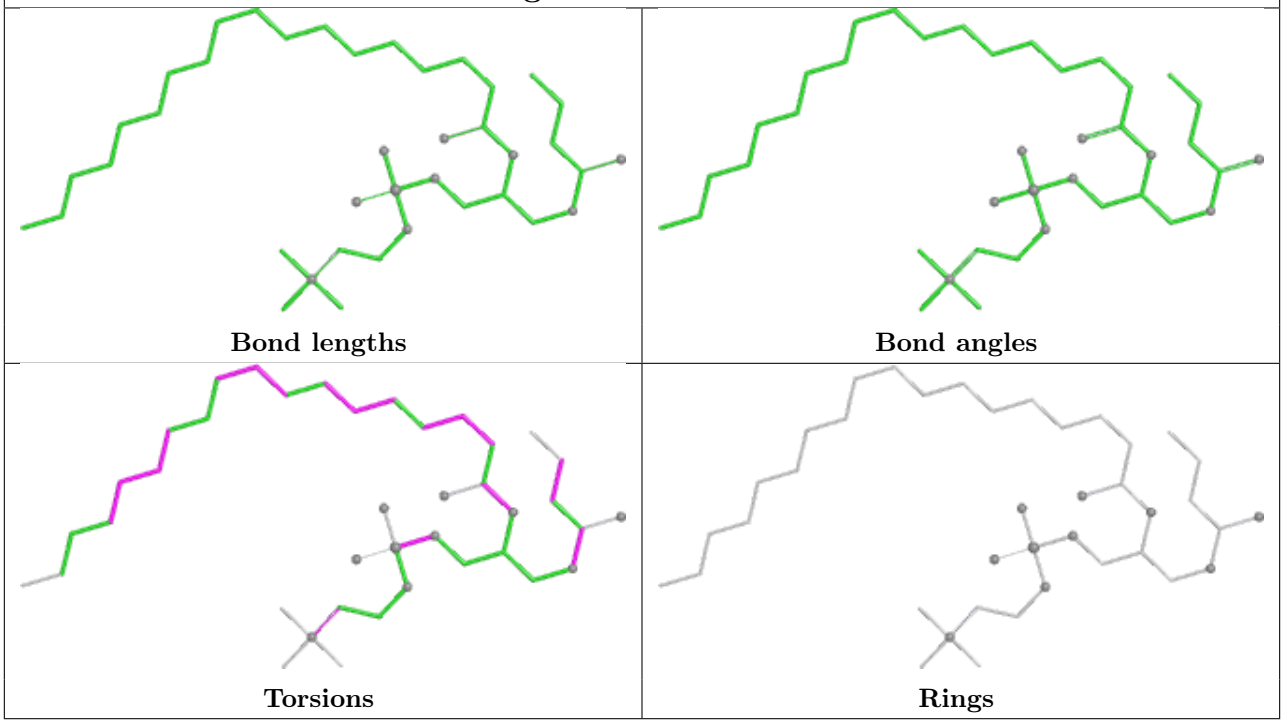
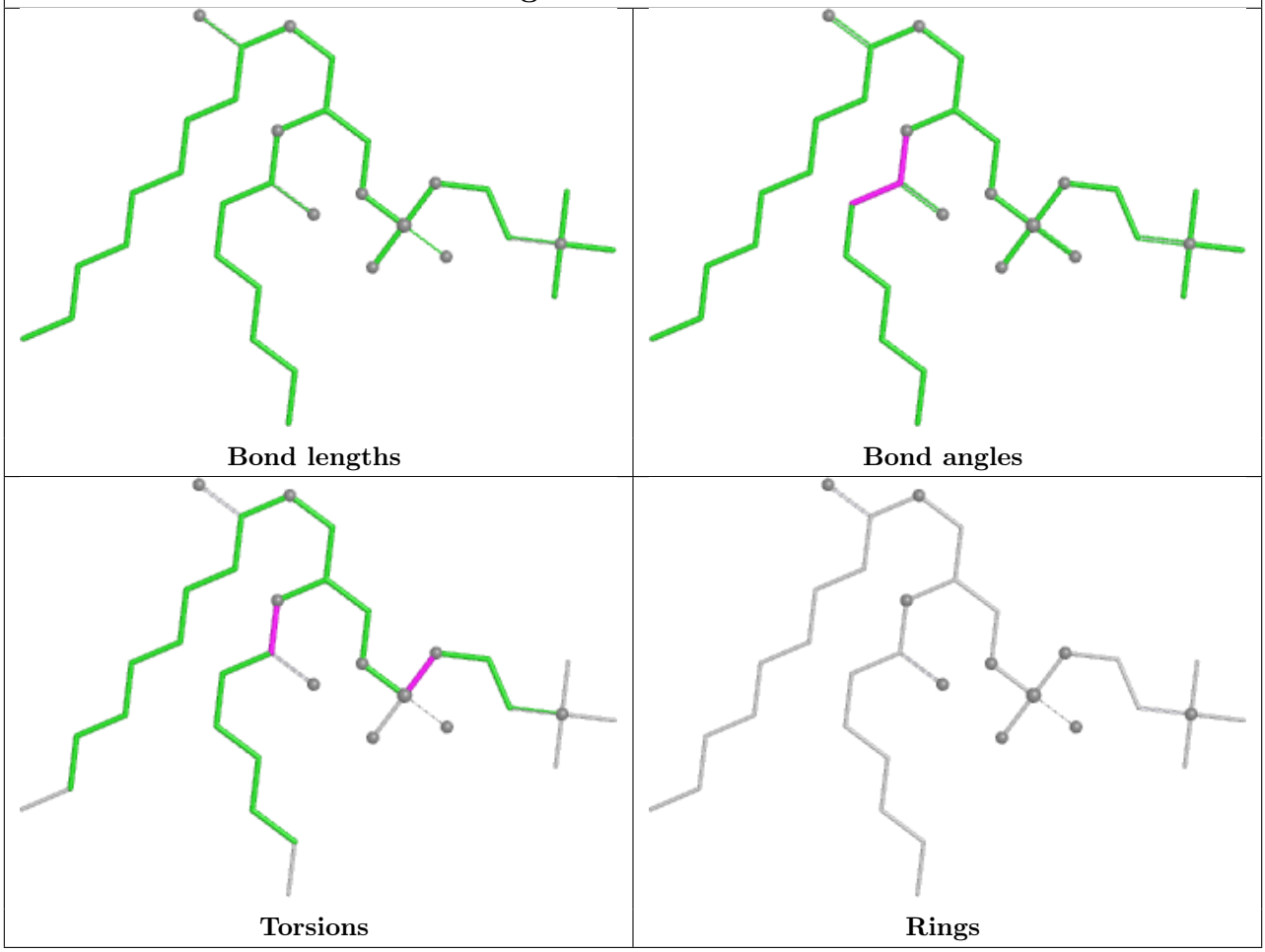


Rings

Ligand WSS R 905



Ligand WSS 1 201



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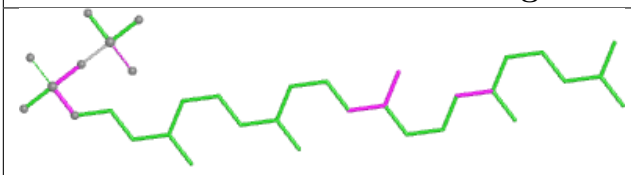

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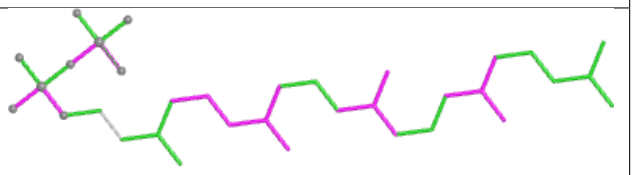
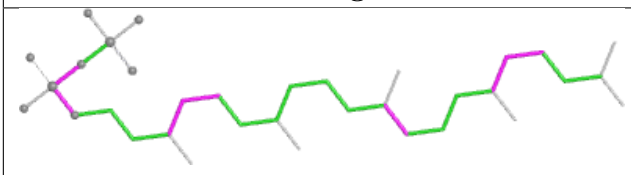


Bond angles



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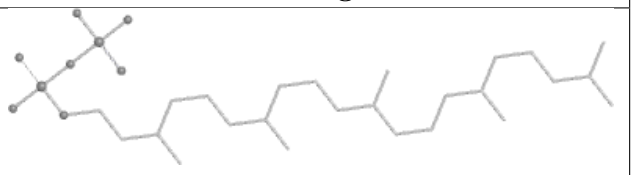
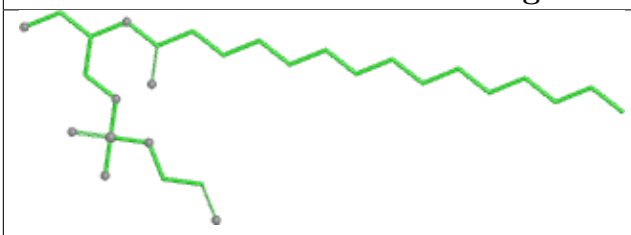


Rings

Ligand PTY R 904



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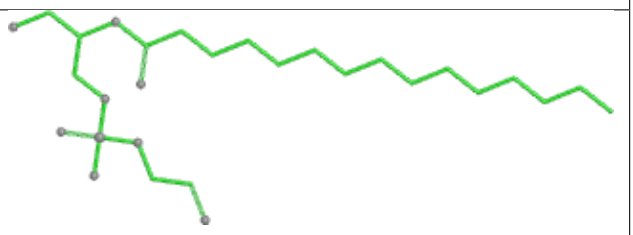

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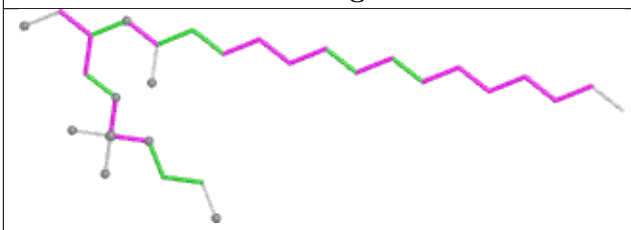

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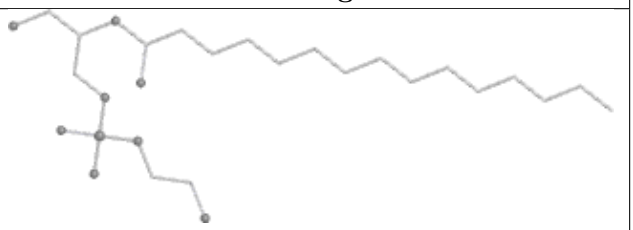
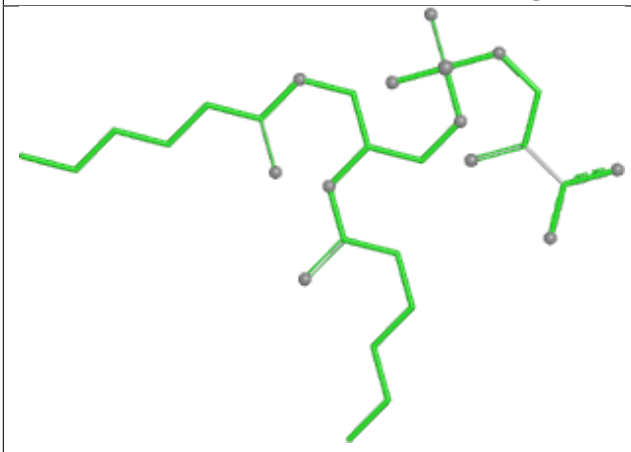


Rings

Ligand PSF R 902



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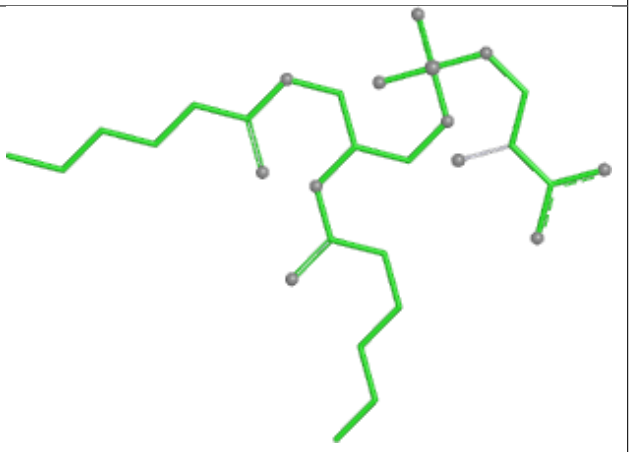
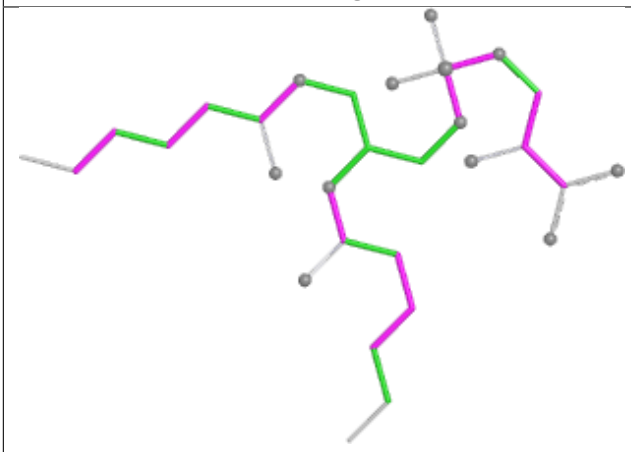


Bond angles



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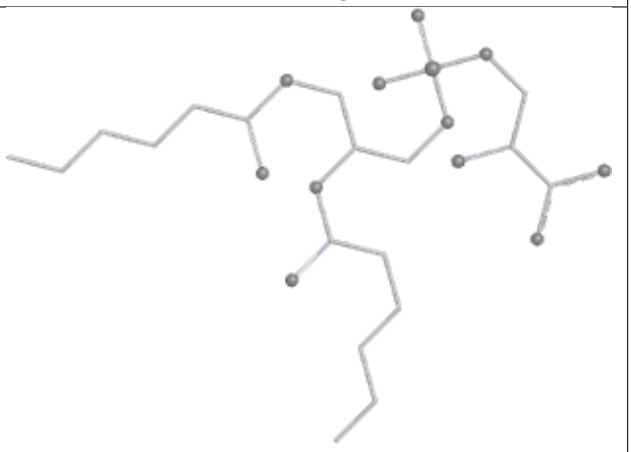
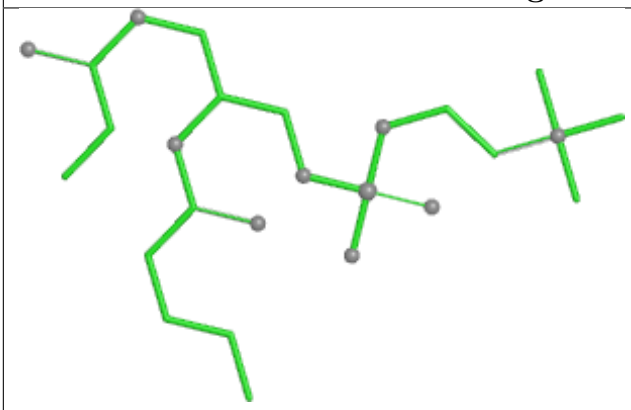


Rings

Ligand WSS 0 303



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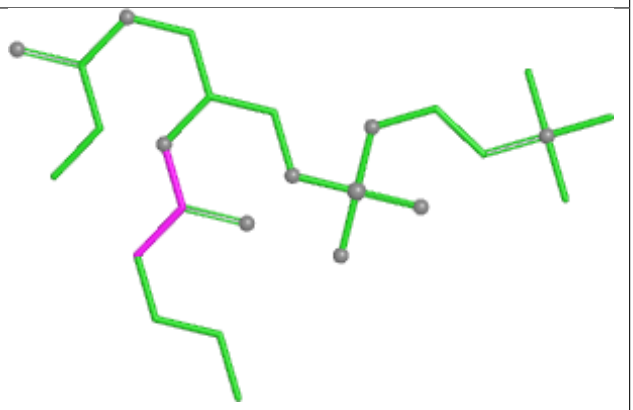
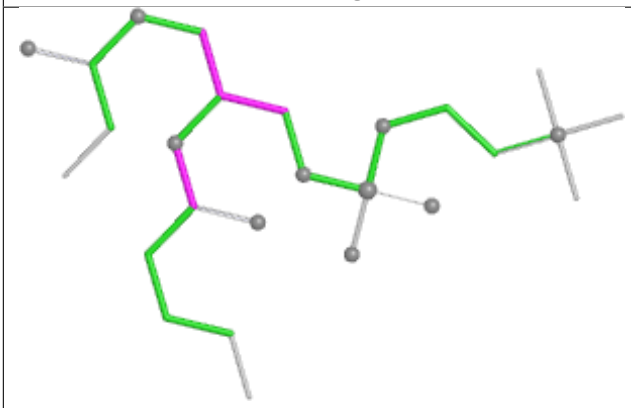


Bond angles



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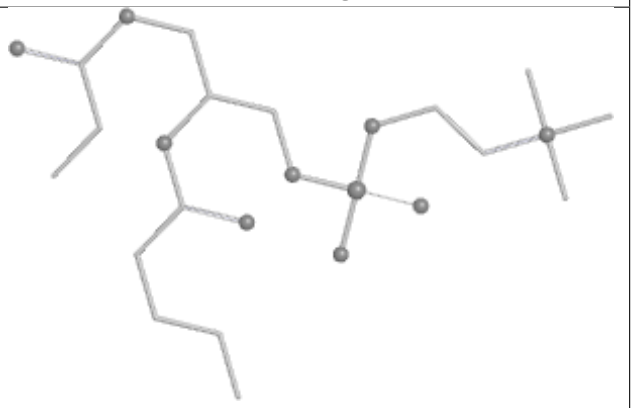
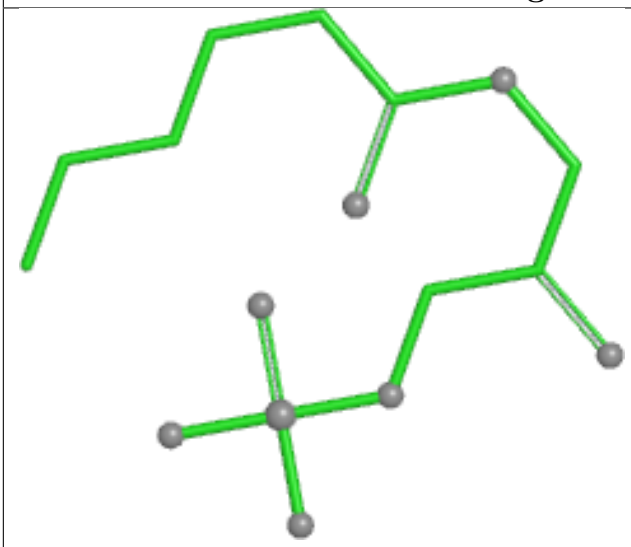


Rings

Ligand PTY 0 306



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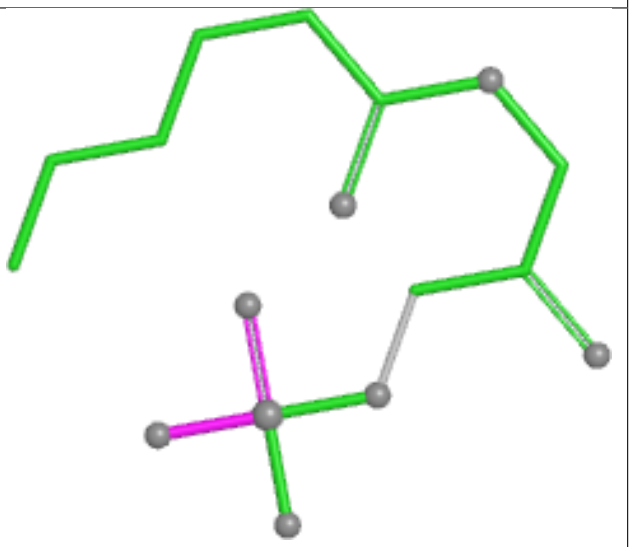

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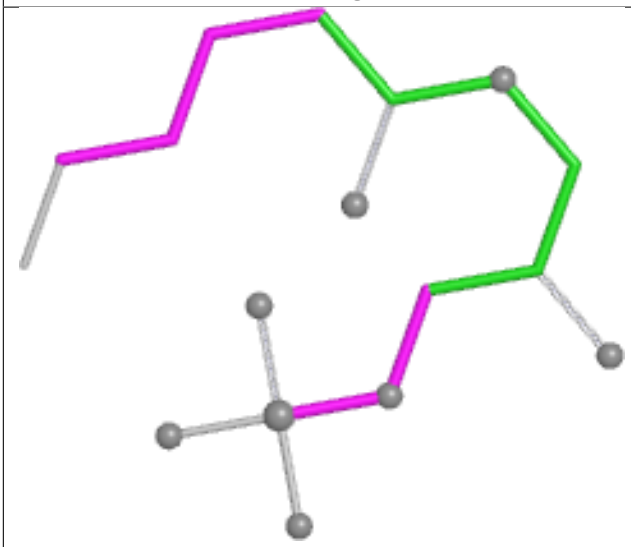

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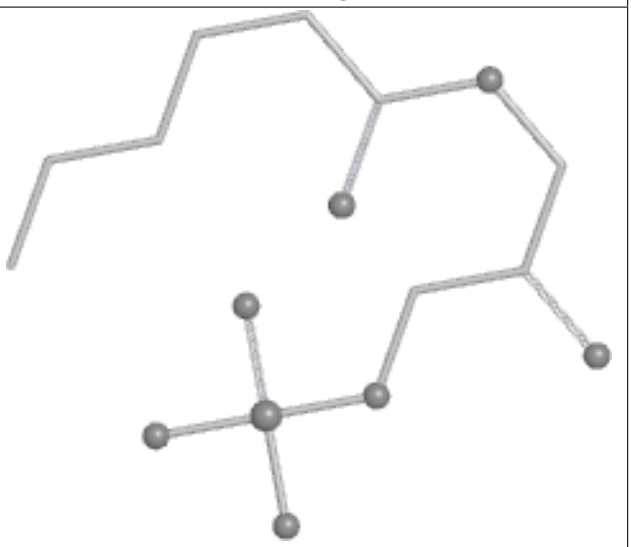
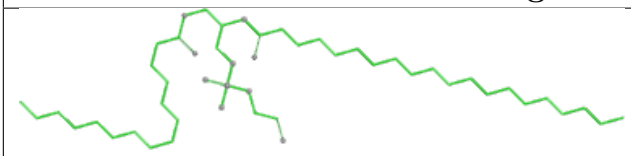


Rings

Ligand PTY 8 201



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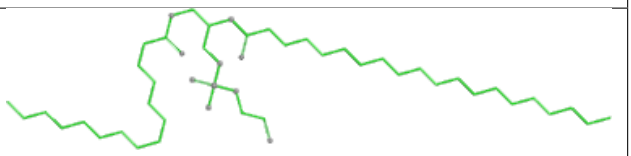

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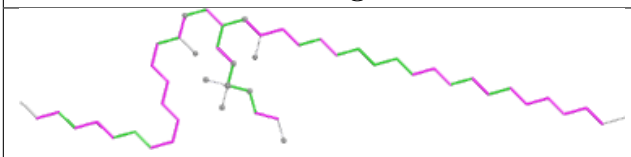

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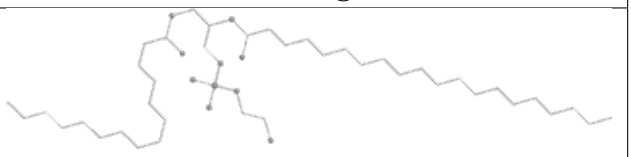
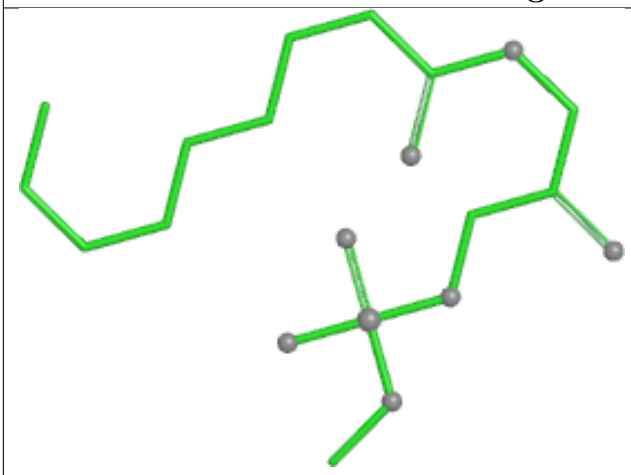


Rings

Ligand PTY 6 201



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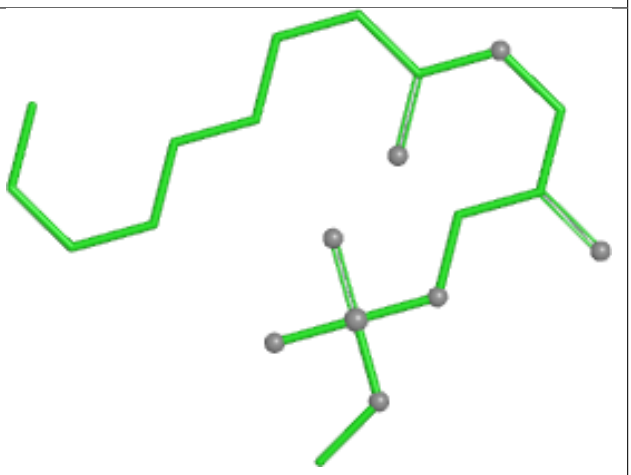

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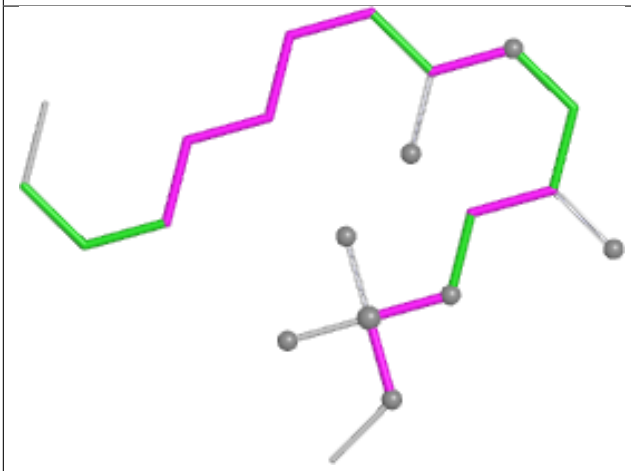

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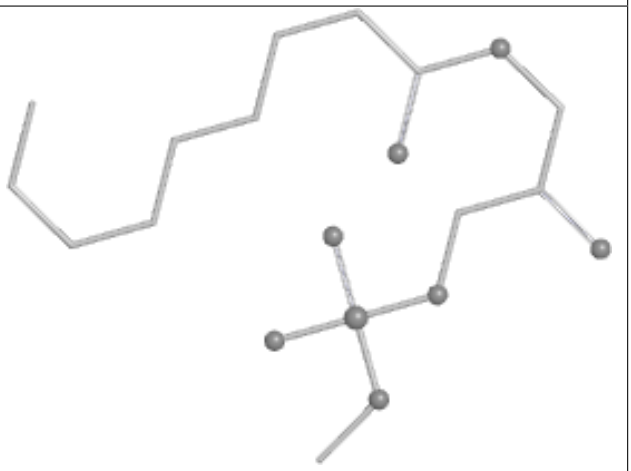
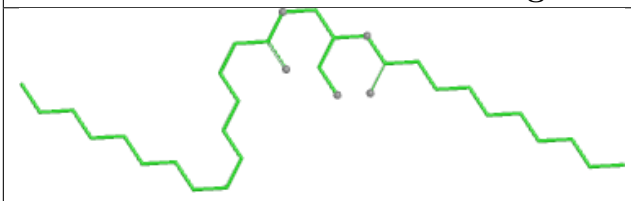


Rings

Ligand PTY 8 202



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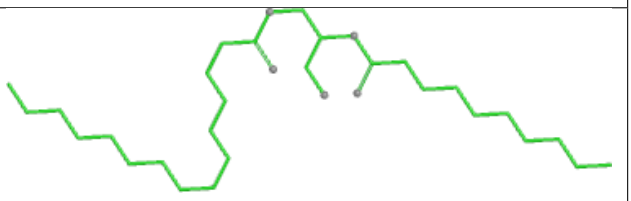

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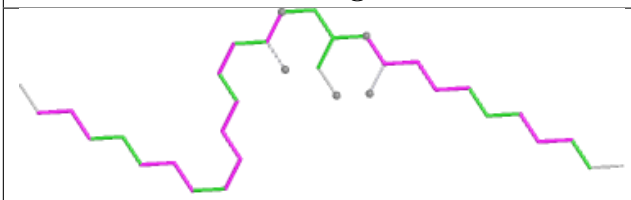

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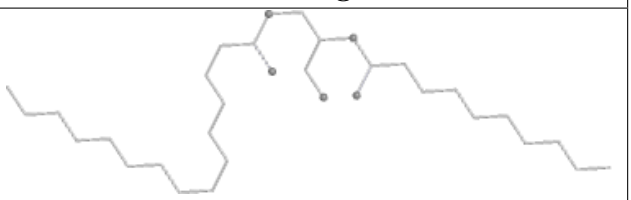
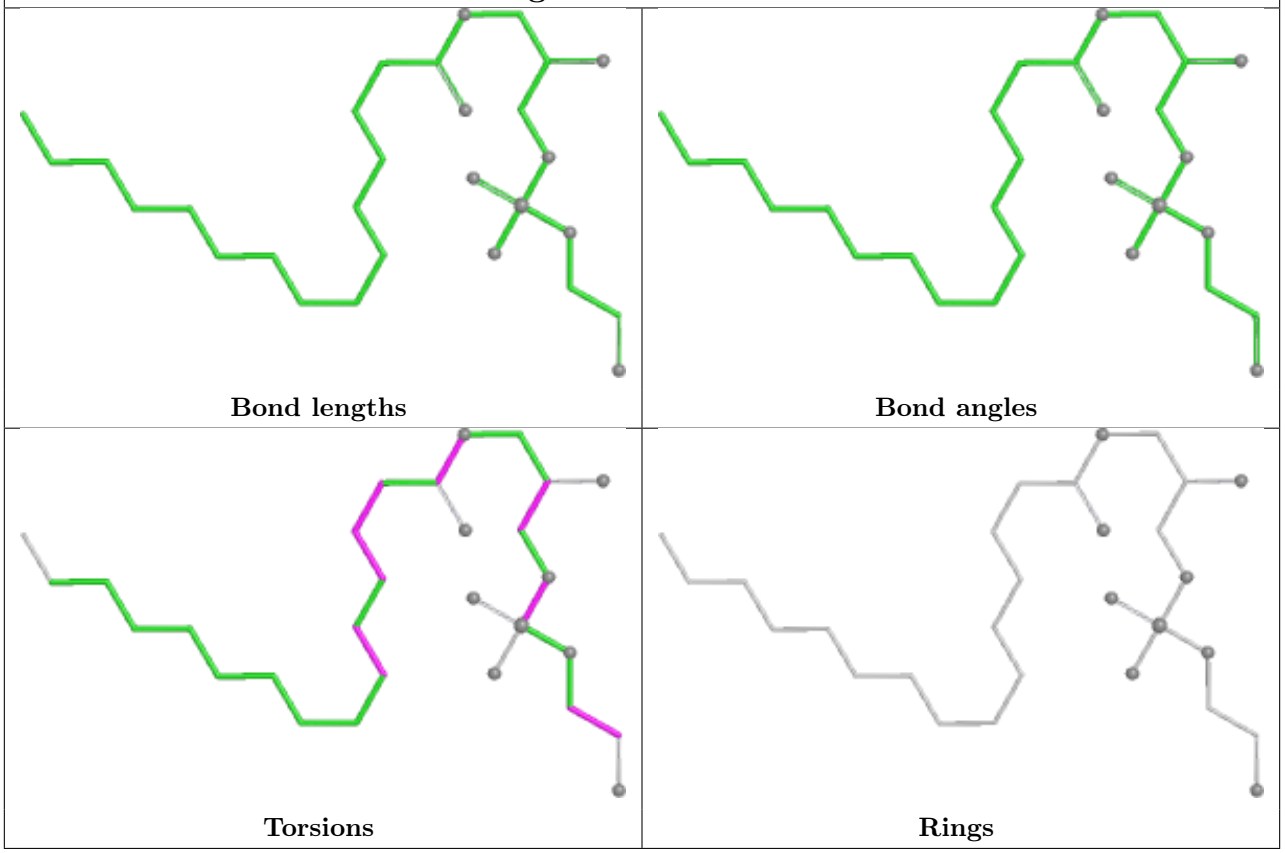
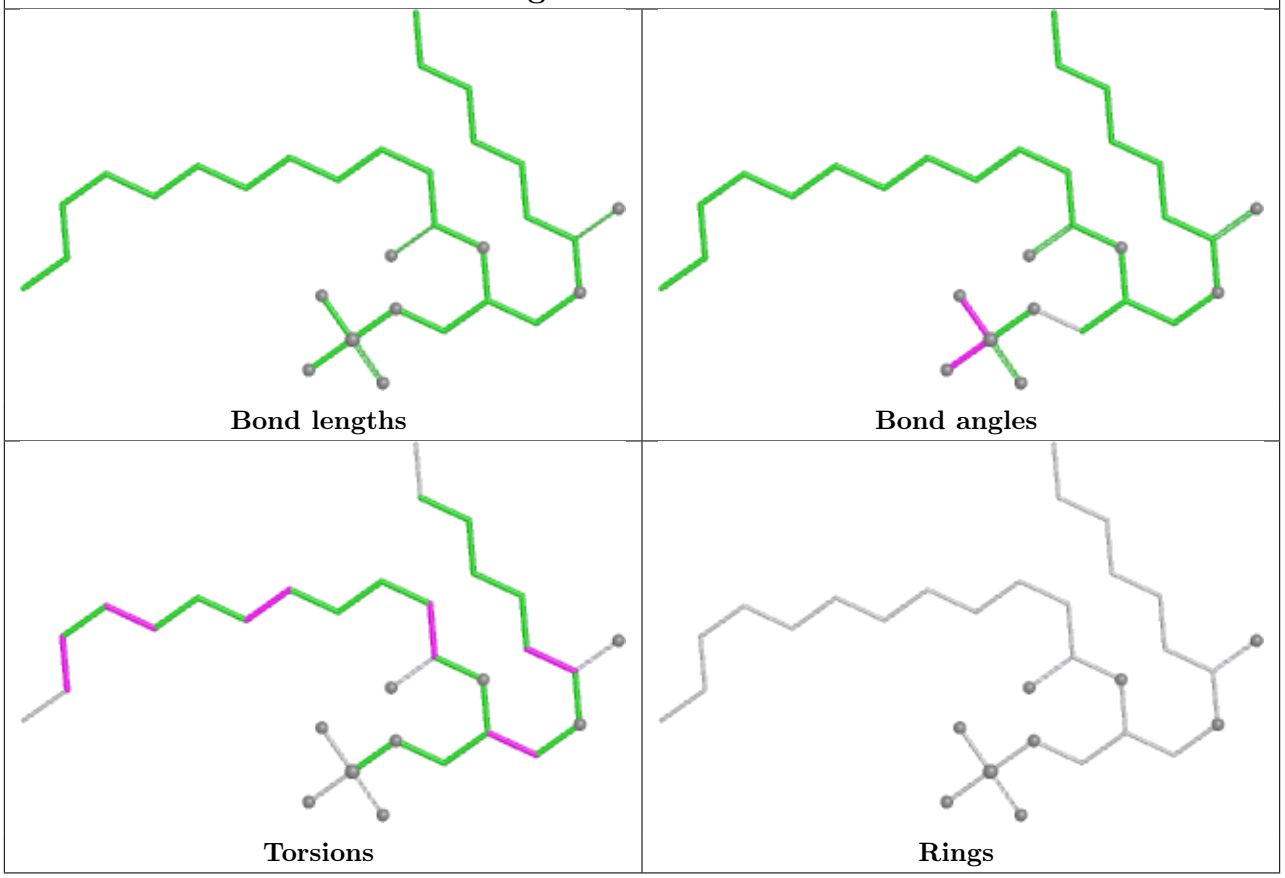


Rings

Ligand PTY 2 201



Ligand WSS 0 305



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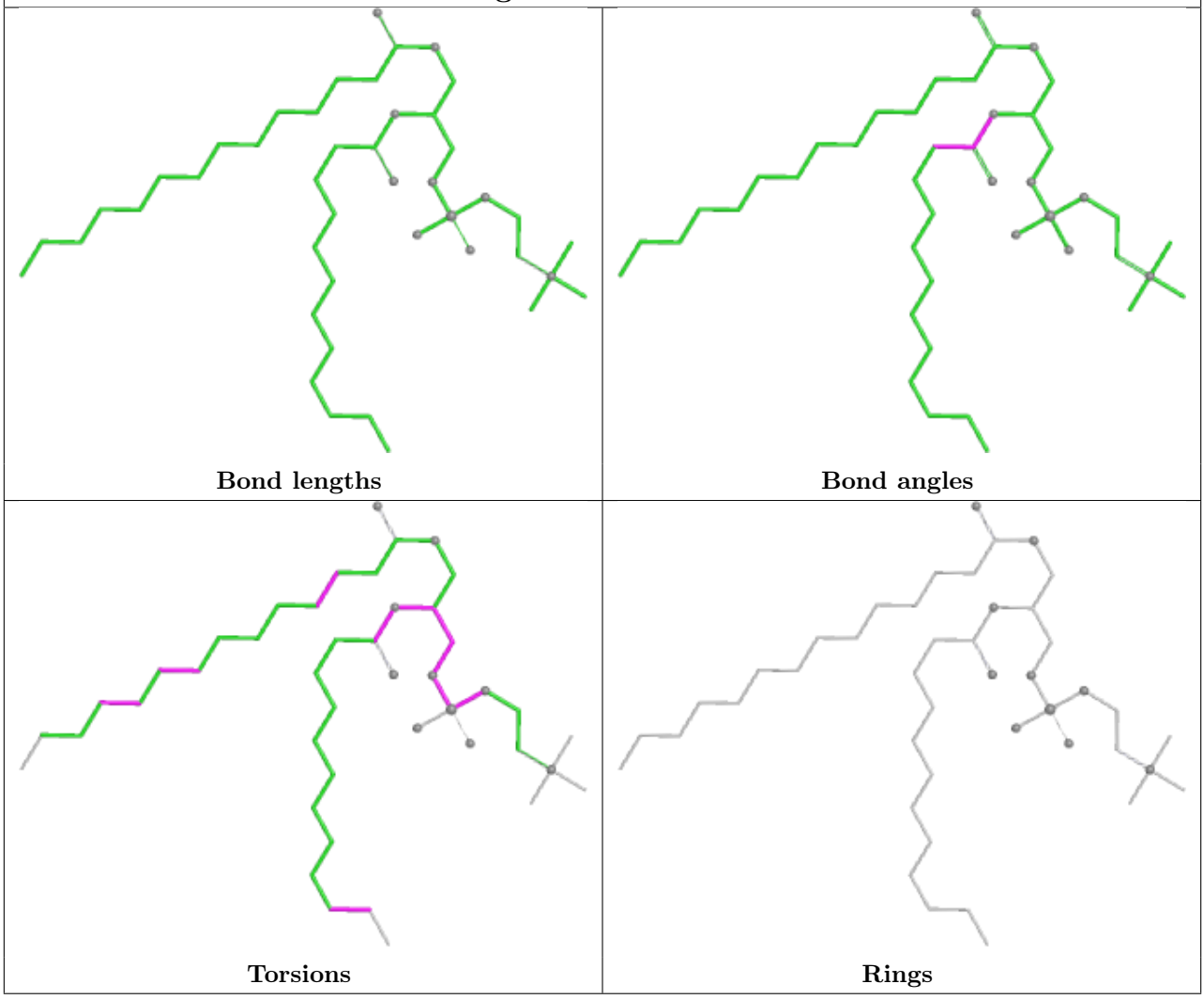
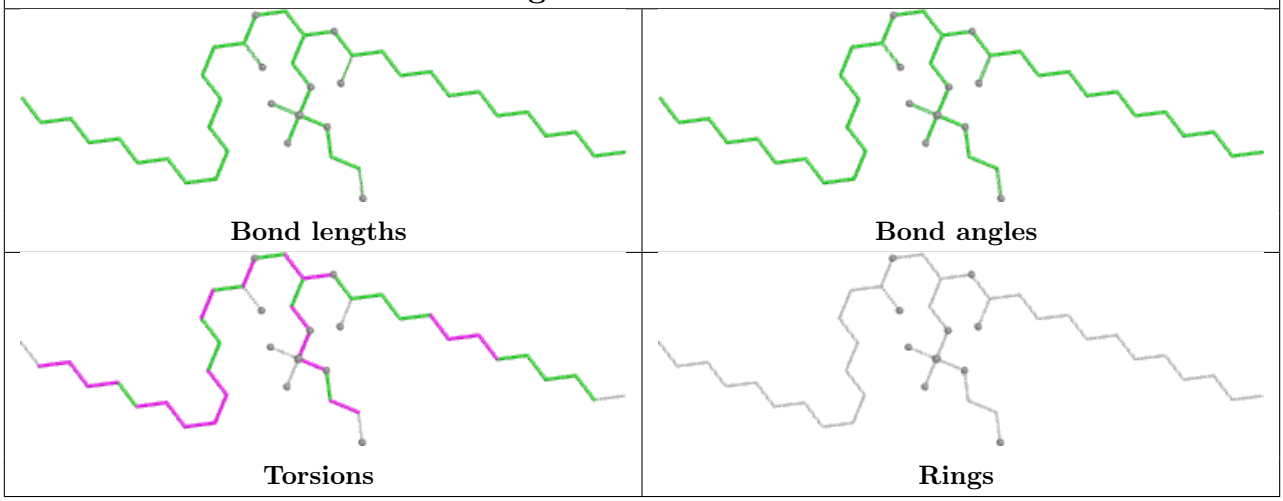
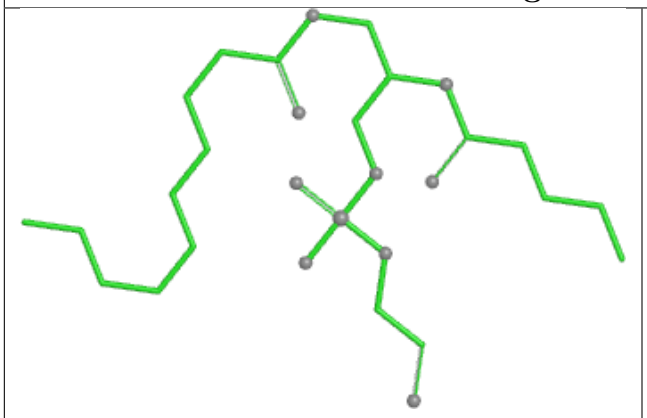


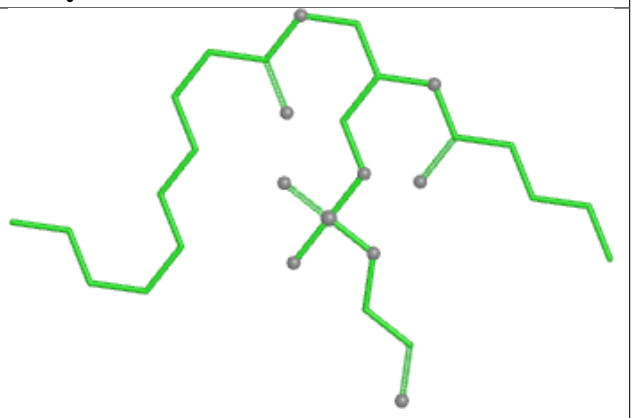
Ligand PTY 7 201



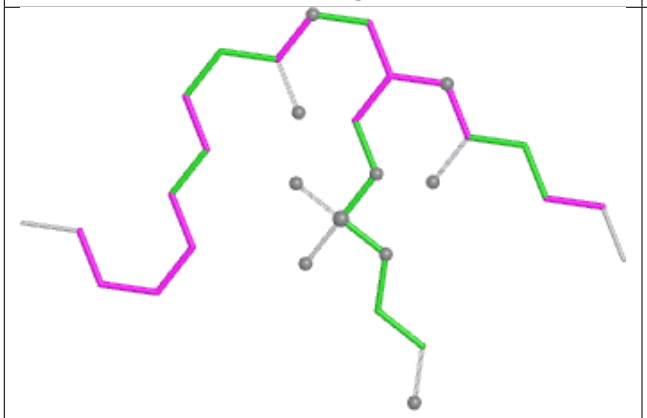
Ligand PTY Q 401



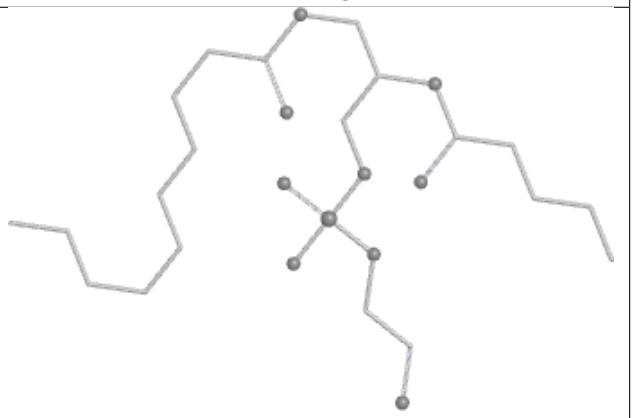
Bond lengths



Bond angles

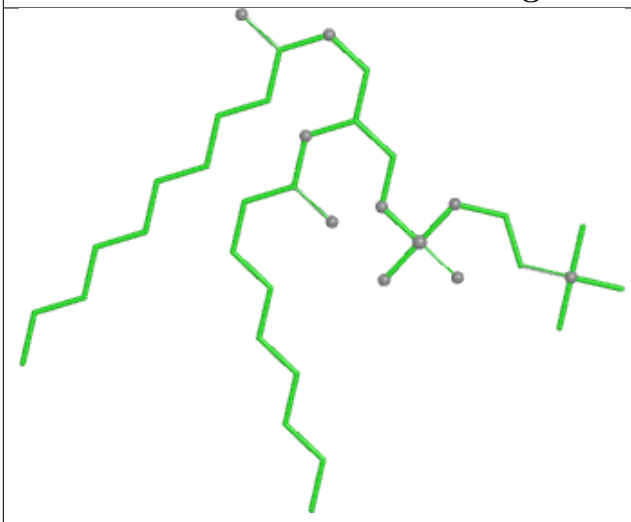


Torsions

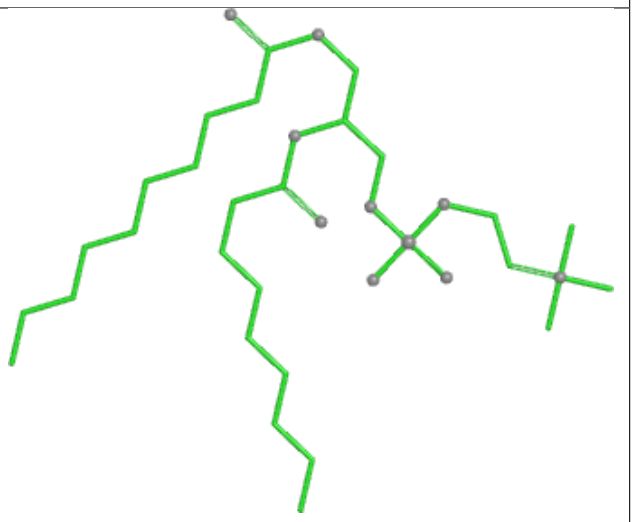


Rings

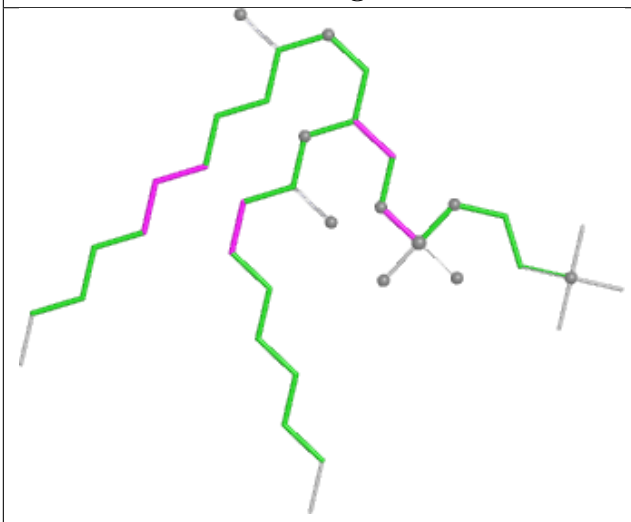
Ligand WSS V 401



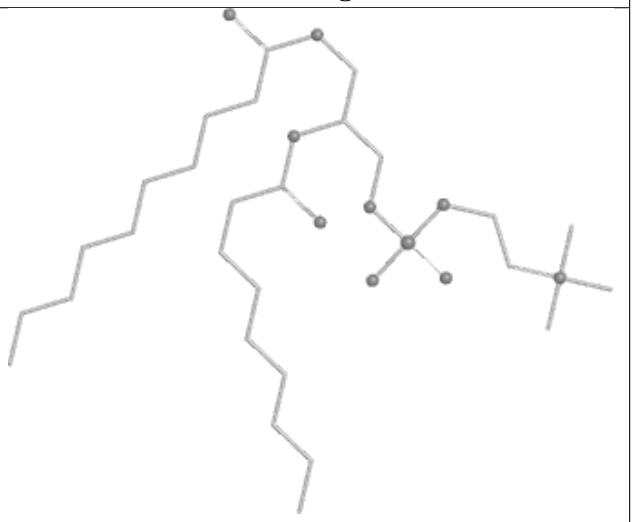
Bond lengths



Bond angles

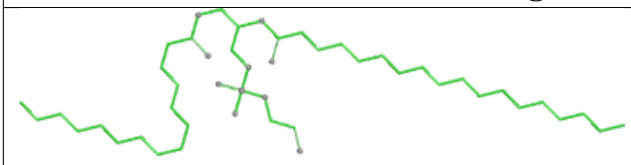


Torsions

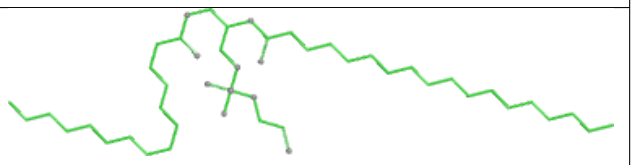


Rings

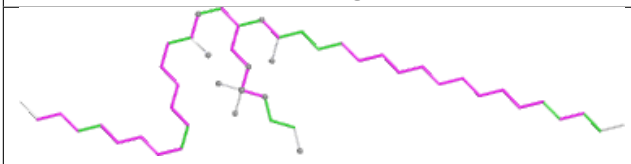
Ligand PTY 0 307



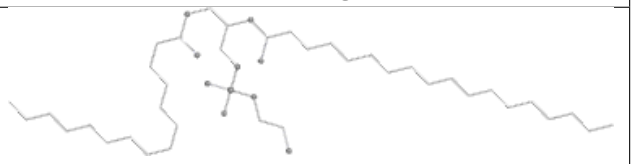
Bond lengths



Bond angles

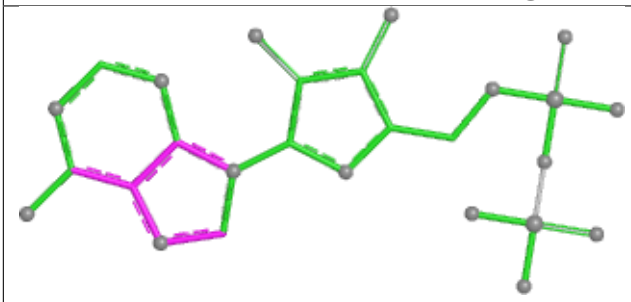


Torsions

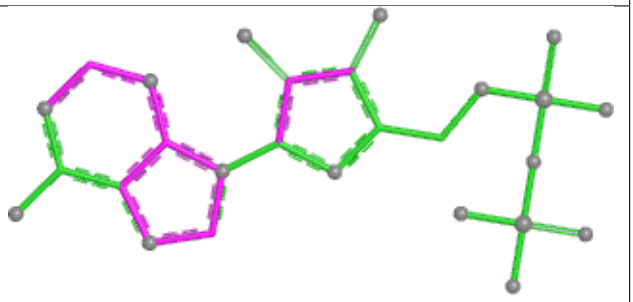


Rings

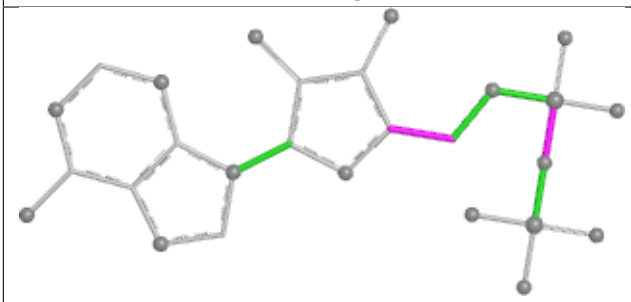
Ligand ADP C 701



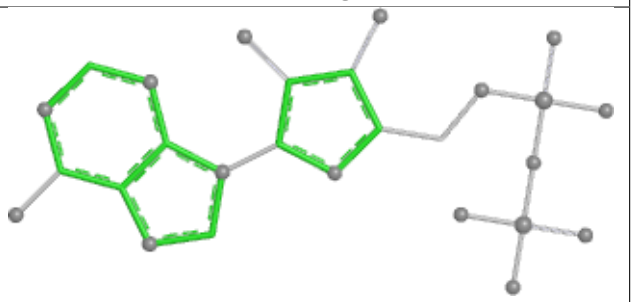
Bond lengths



Bond angles

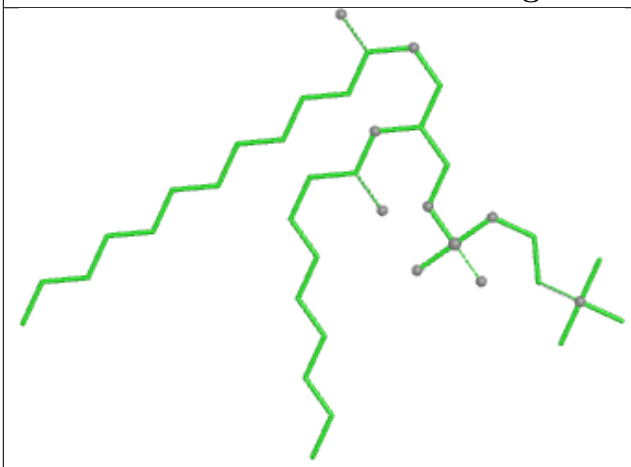


Torsions

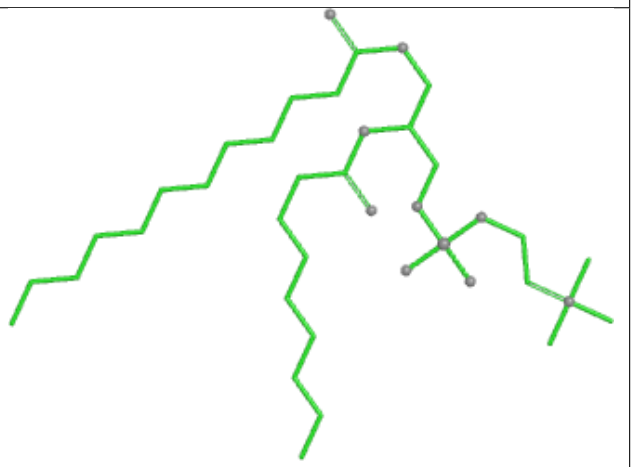


Rings

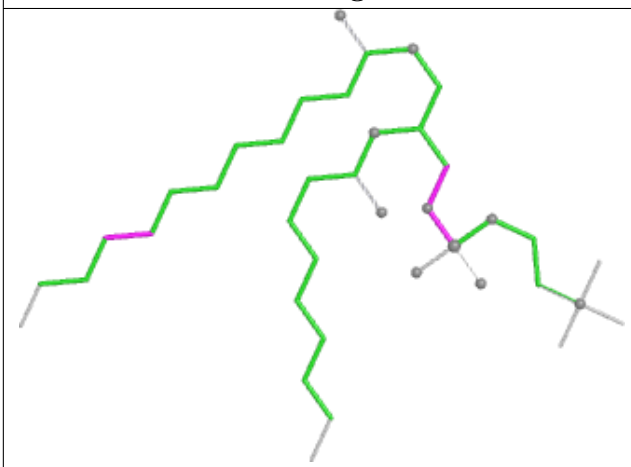
Ligand WSS U 501



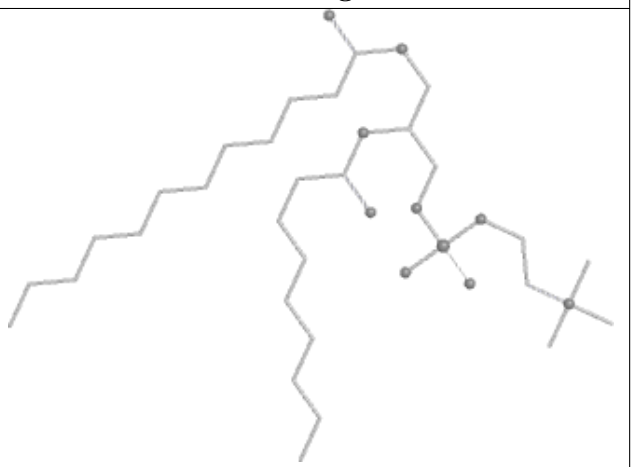
Bond lengths



Bond angles

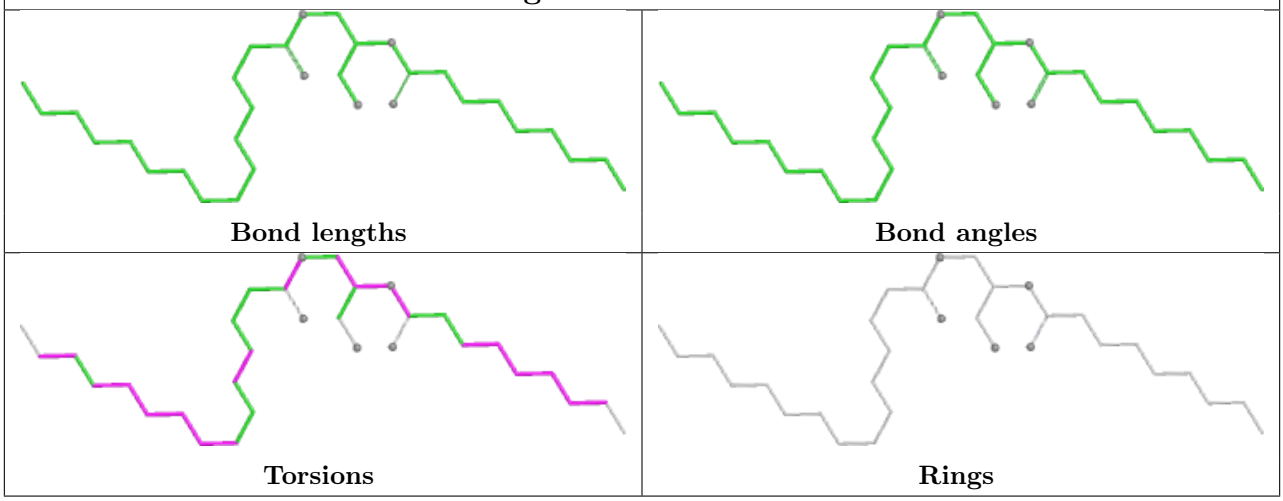


Torsions



Rings

Ligand PTY R 903



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	360:THR	C	361:PRO	N	5.02

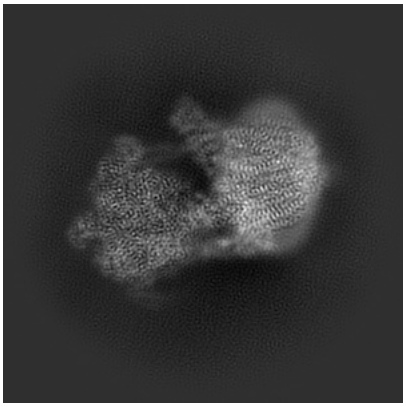
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21847. These allow visual inspection of the internal detail of the map and identification of artifacts.

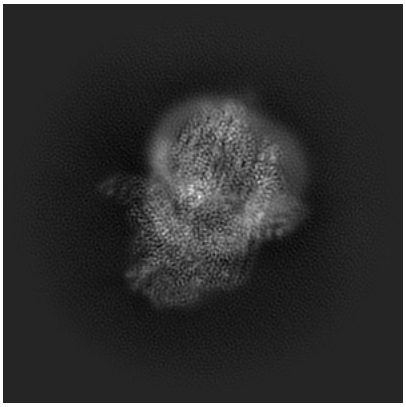
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

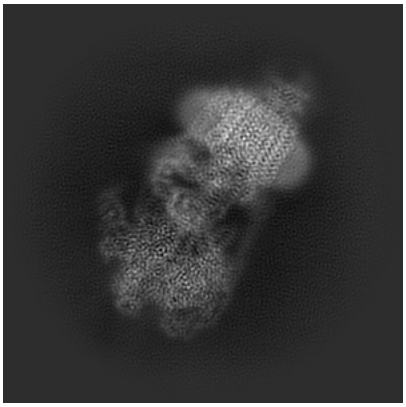
6.1.1 Primary map



X



Y

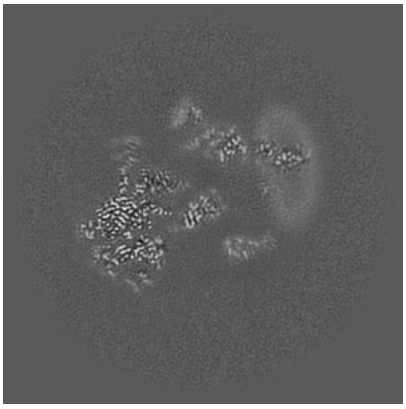


Z

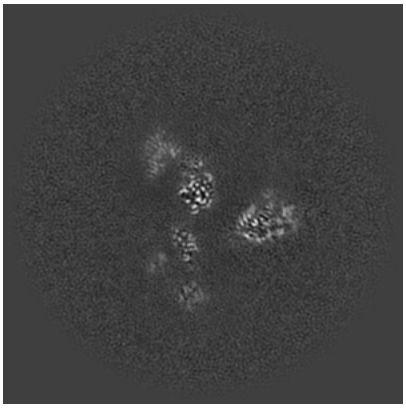
The images above show the map projected in three orthogonal directions.

6.2 Central slices

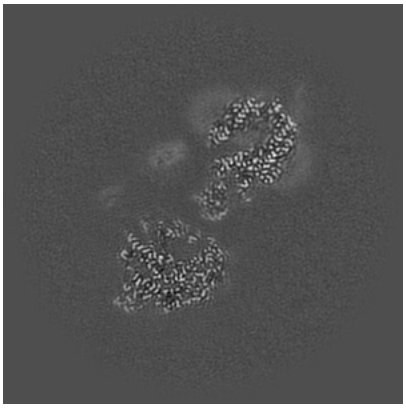
6.2.1 Primary map



X Index: 180



Y Index: 180

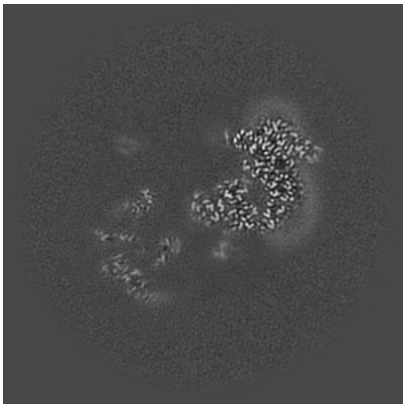


Z Index: 180

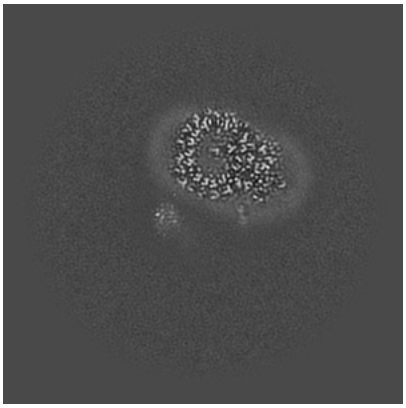
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

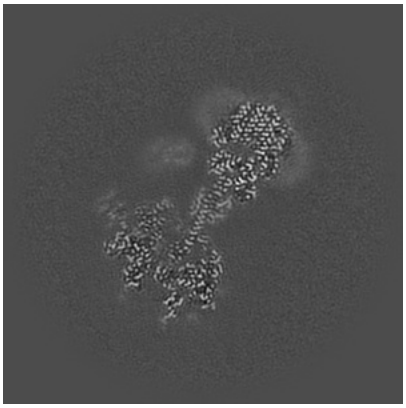
6.3.1 Primary map



X Index: 199



Y Index: 242

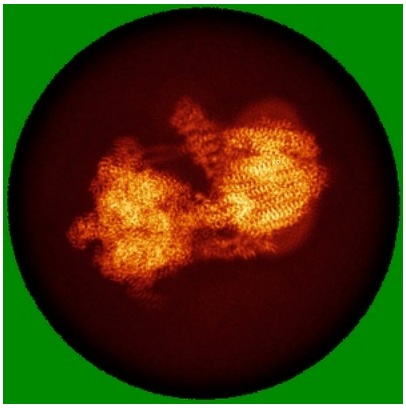


Z Index: 170

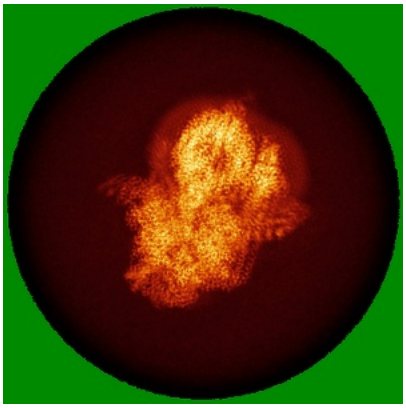
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

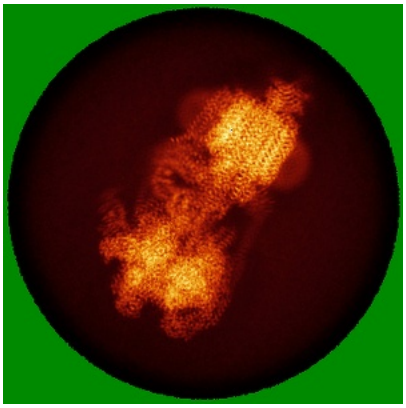
6.4.1 Primary map



X



Y

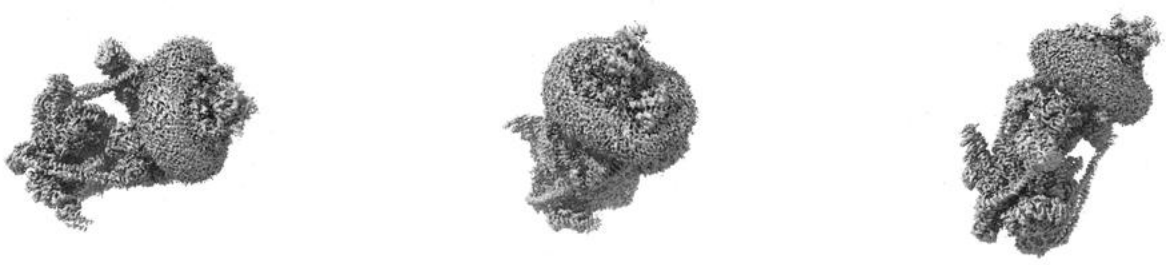


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

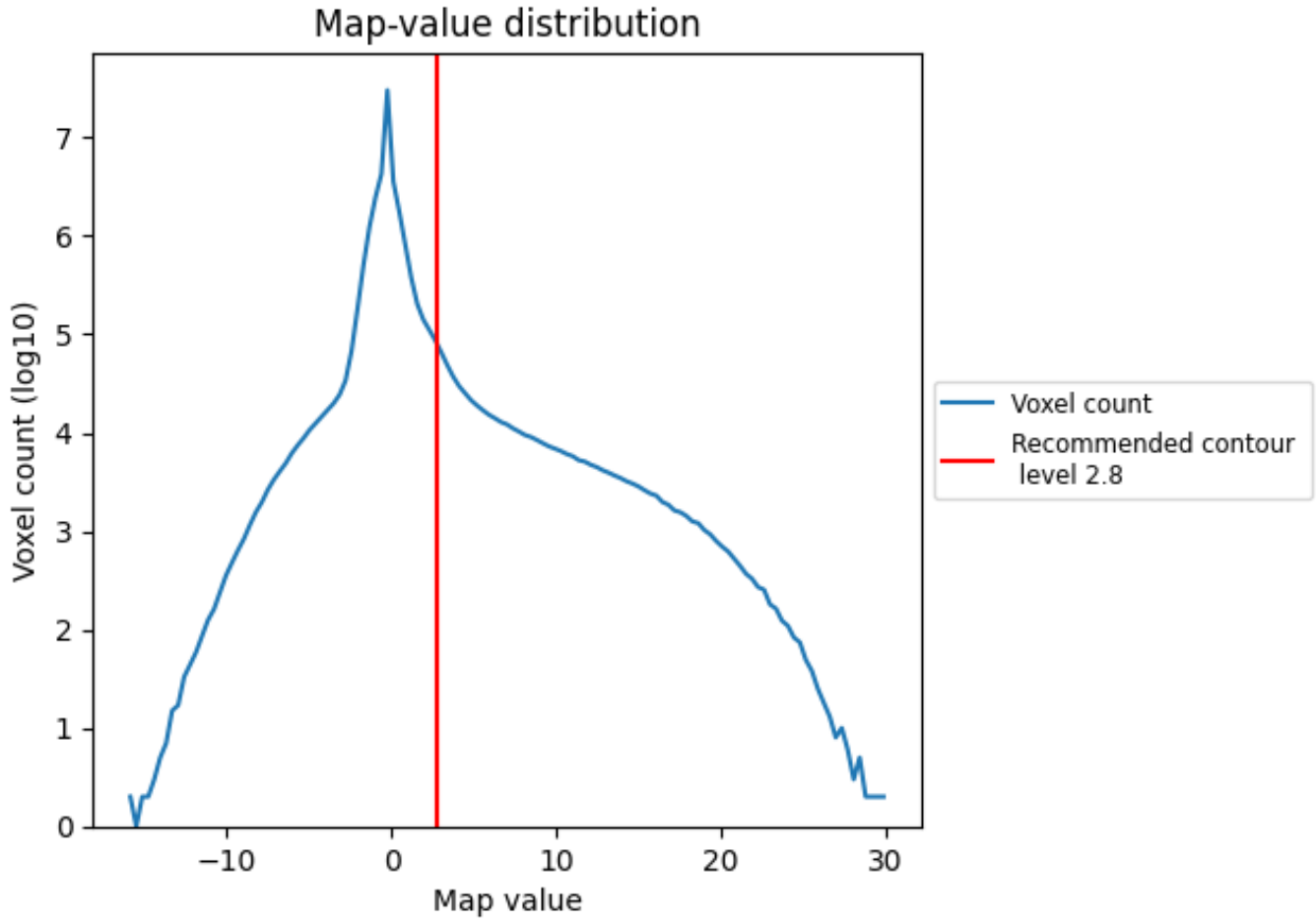
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

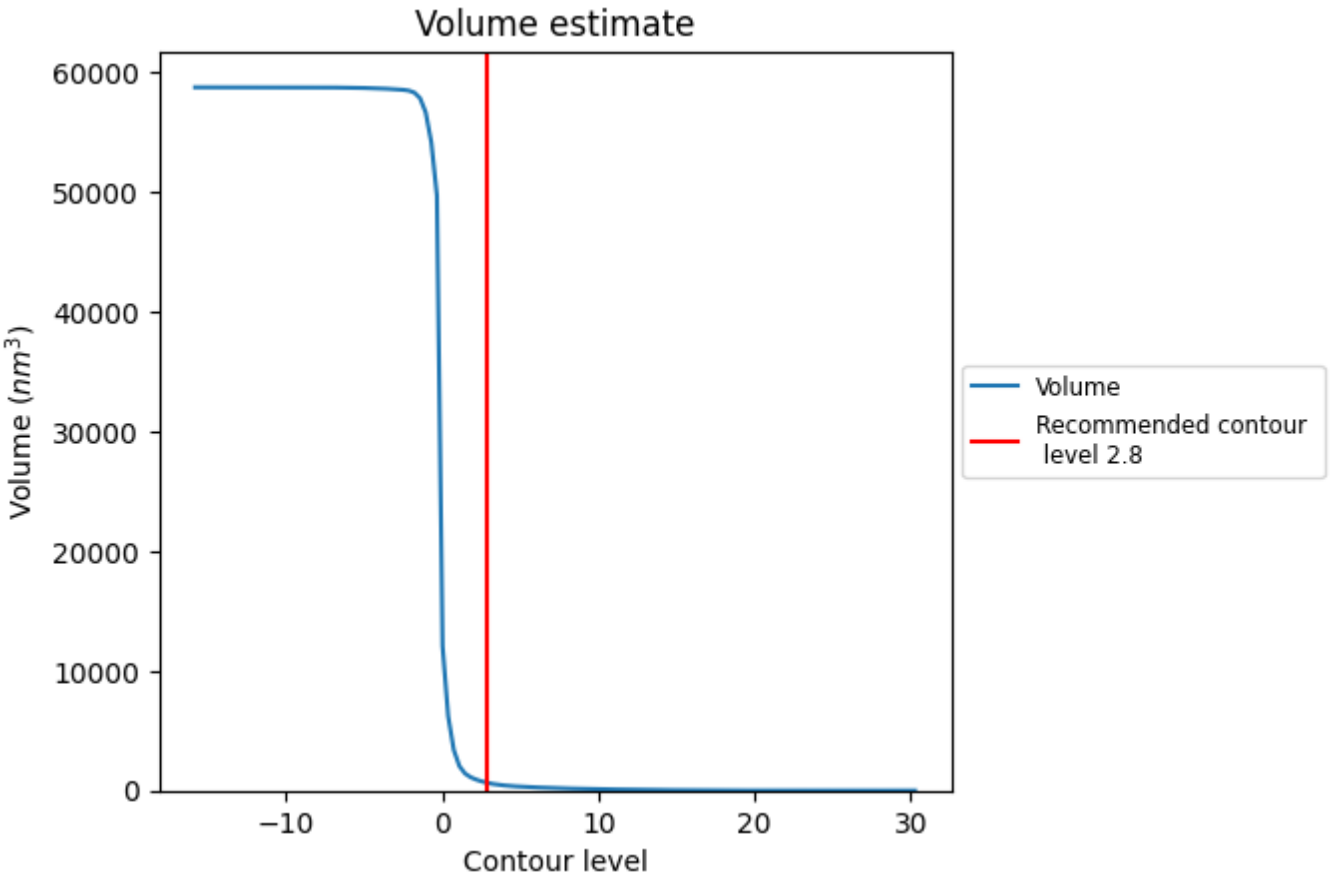
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

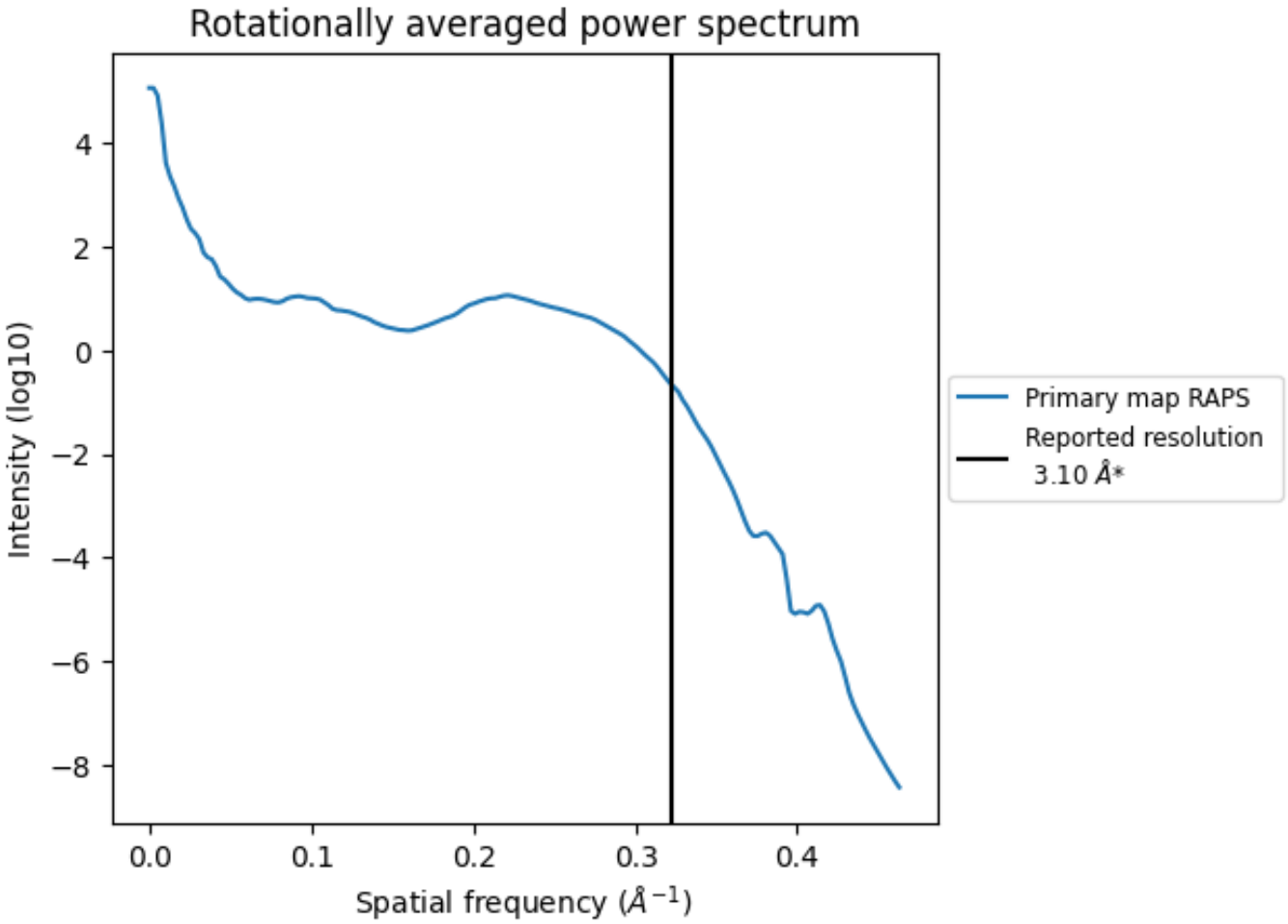
7.2 Volume estimate



The volume at the recommended contour level is 675 nm^3; this corresponds to an approximate mass of 610 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

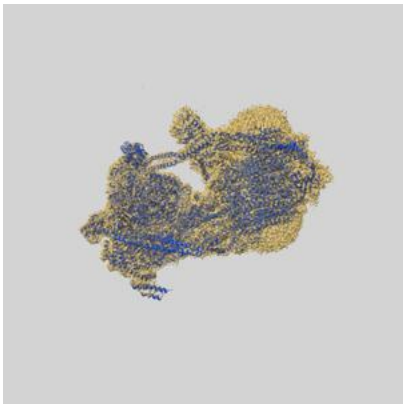
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

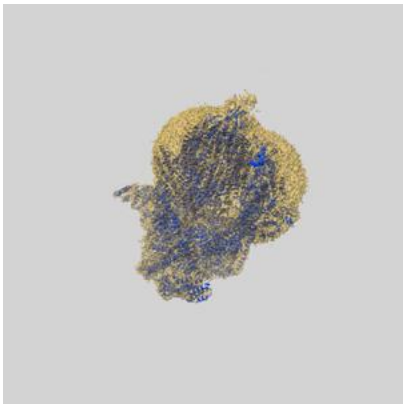
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21847 and PDB model 6WM2. Per-residue inclusion information can be found in section 3 on page 16.

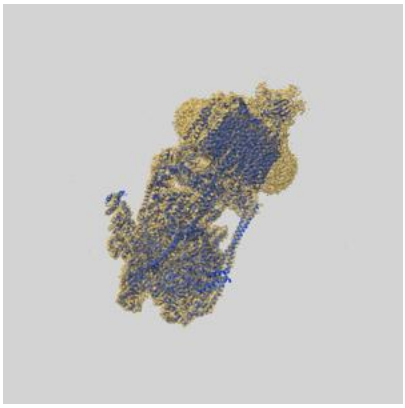
9.1 Map-model overlay



X



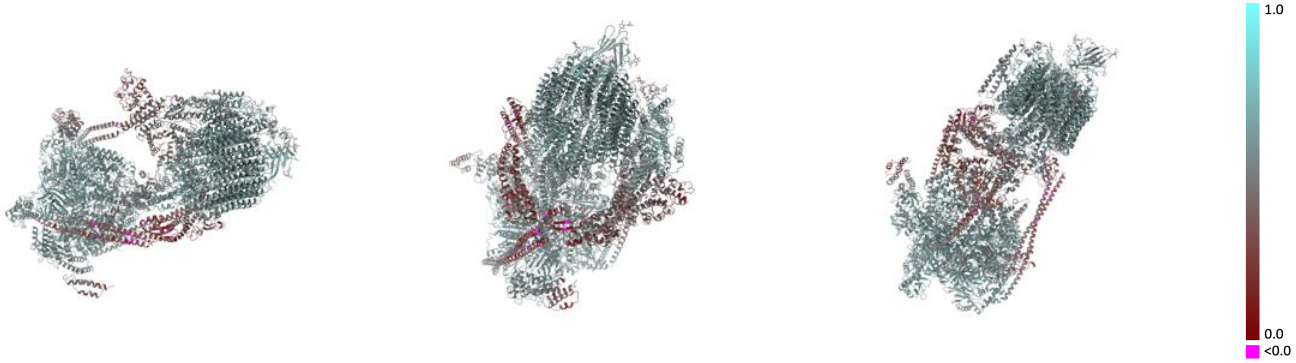
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

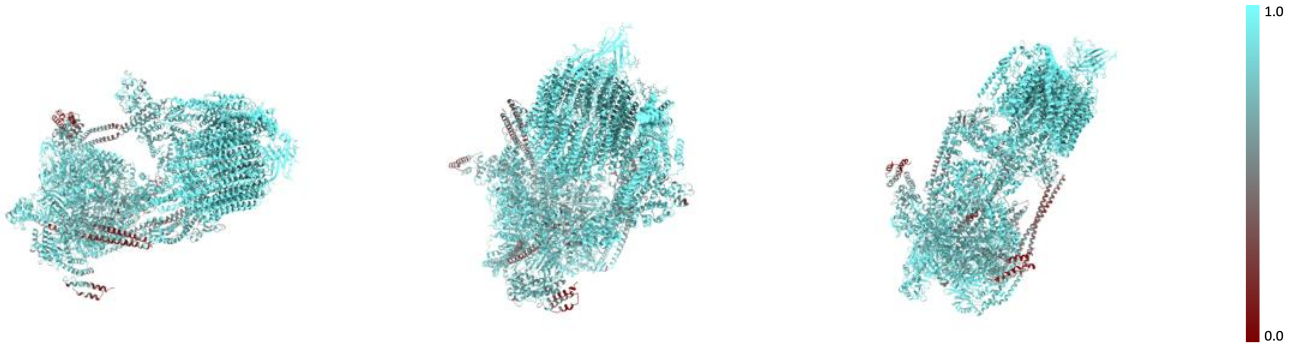
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

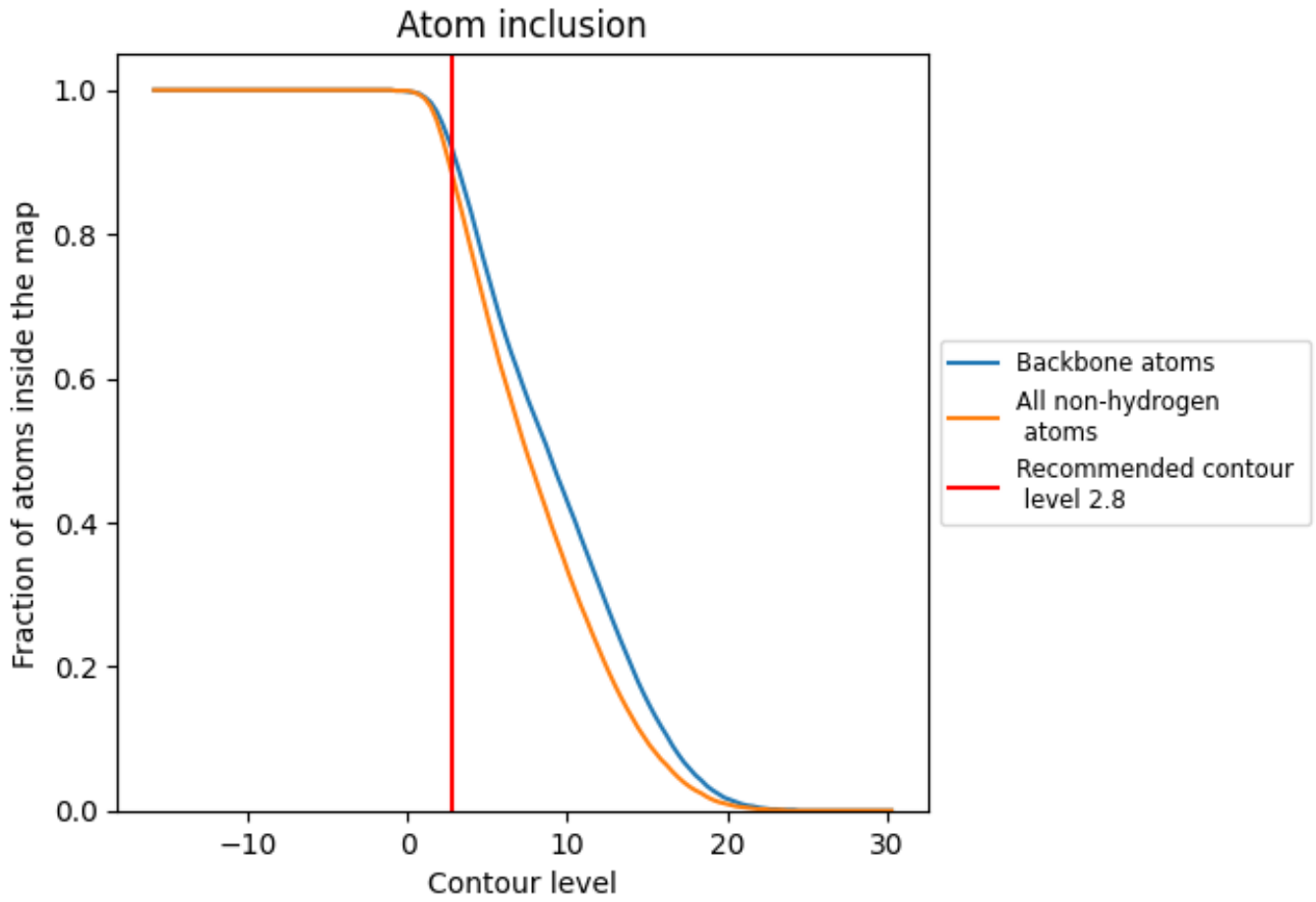
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5350
0	0.9820	0.5860
1	0.9880	0.5870
2	0.9780	0.5800
3	0.9790	0.5880
4	0.9800	0.5790
5	0.9720	0.5780
6	0.9670	0.5770
7	0.9750	0.5750
8	0.9720	0.5750
9	0.9820	0.5840
A	0.9160	0.5980
B	0.9000	0.5860
C	0.9370	0.6080
D	0.9440	0.6150
E	0.9540	0.6120
F	0.9490	0.6160
G	0.8910	0.5490
H	0.8270	0.5230
I	0.8100	0.4800
J	0.7490	0.4990
K	0.6960	0.4500
L	0.6740	0.3890
M	0.5590	0.3840
N	0.9080	0.5140
O	0.7840	0.2890
P	0.8720	0.3600
Q	0.9640	0.5850
R	0.8990	0.4760
S	0.9650	0.5650
T	0.9570	0.5230
U	0.9870	0.5750
V	0.9740	0.5780
W	0.8090	0.3900
X	0.6600	0.4920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.7310	0.5200
Z	0.5670	0.4900
a	0.8570	0.4310
b	0.8930	0.4270
c	0.9290	0.4260
d	0.8570	0.4170
r	0.9840	0.5560
s	1.0000	0.5130
u	0.9290	0.4320