Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 04:48 am BST

PDB ID	:	2UX4 / pdb_00002ux4
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the charge-separated state, 2nd dataset
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-26
Resolution	:	2.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

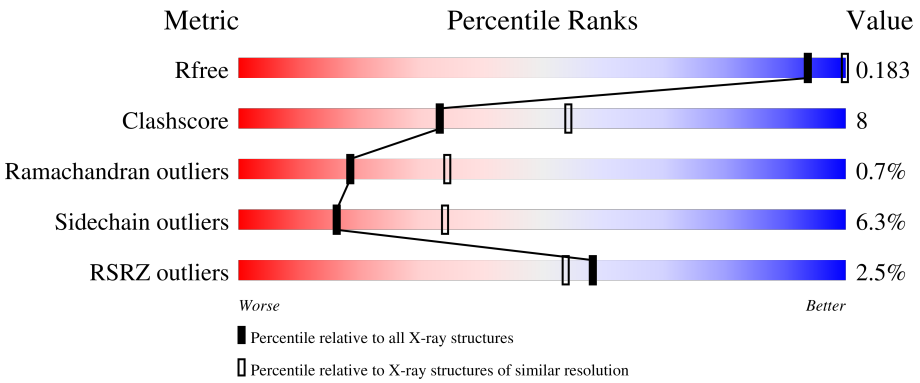
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	H	260	3% 83% 7% • 7%
2	L	281	% 87% 12% •
3	M	307	3% 80% 16% • •

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
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	M	1309	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	241	1846	1181	319	337	9	0	3	1

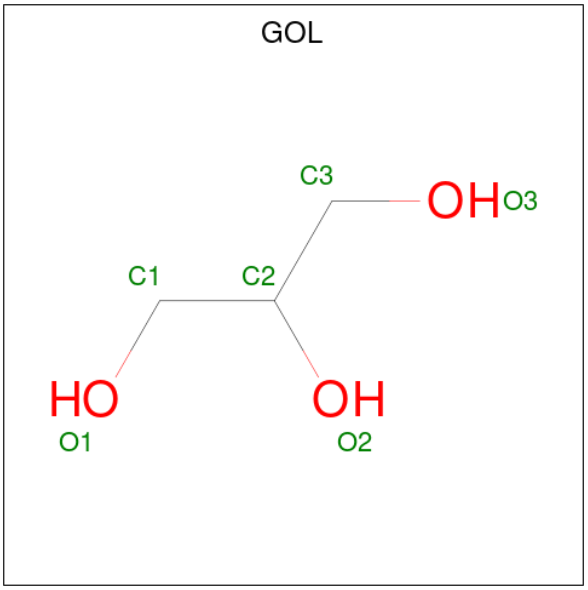
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2232	1507	355	362	8	0	0	0

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

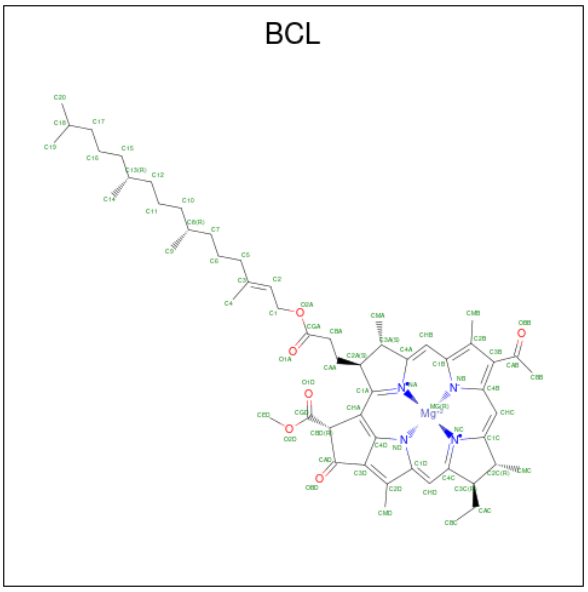
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



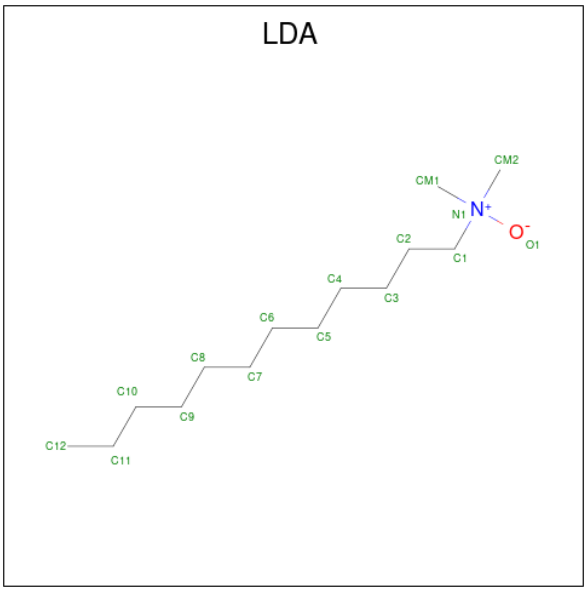
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	O		0	0
			6	3	3			
4	H	1	Total	C	O		0	0
			6	3	3			
4	H	1	Total	C	O		0	0
			6	3	3			
4	H	1	Total	C	O		0	0
			6	3	3			
4	L	1	Total	C	O		0	0
			6	3	3			
4	L	1	Total	C	O		0	0
			6	3	3			
4	M	1	Total	C	O		0	0
			6	3	3			

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



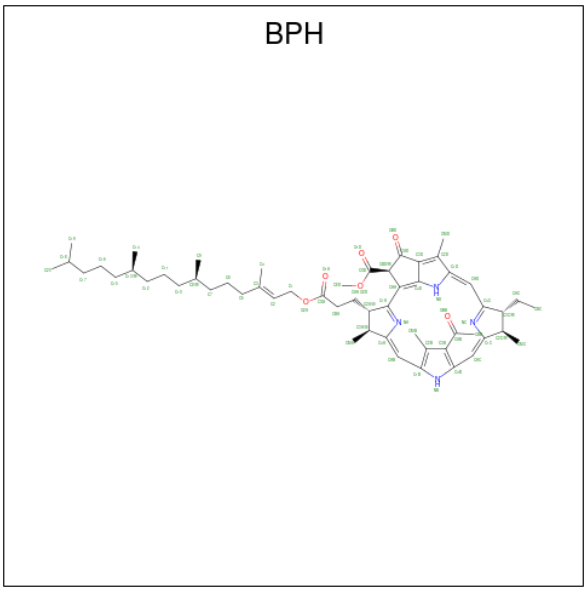
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



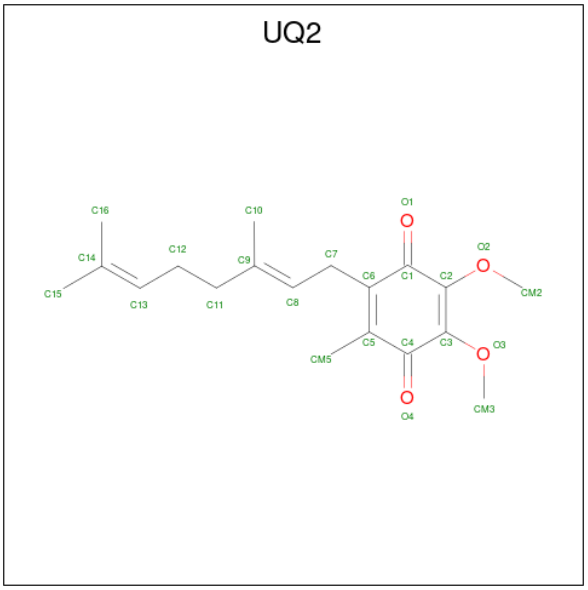
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



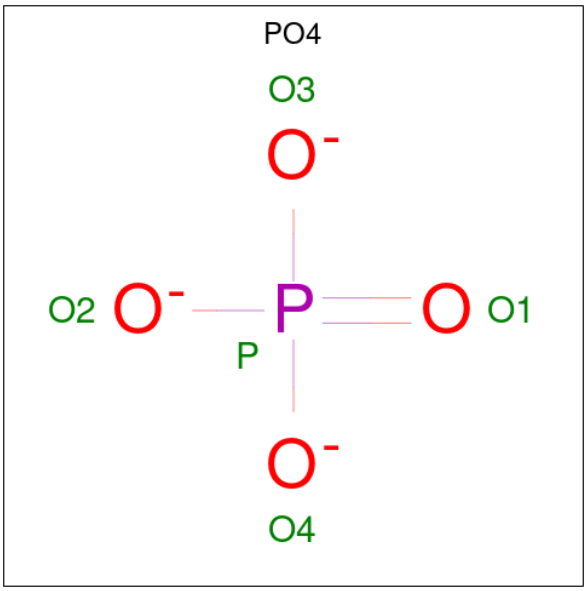
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	65	55	4	6	0	0

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



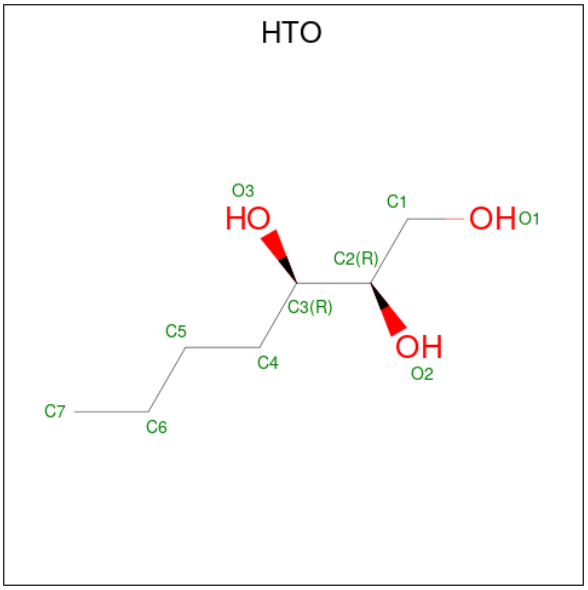
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total O P 5 4 1	0	0

- Molecule 10 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).

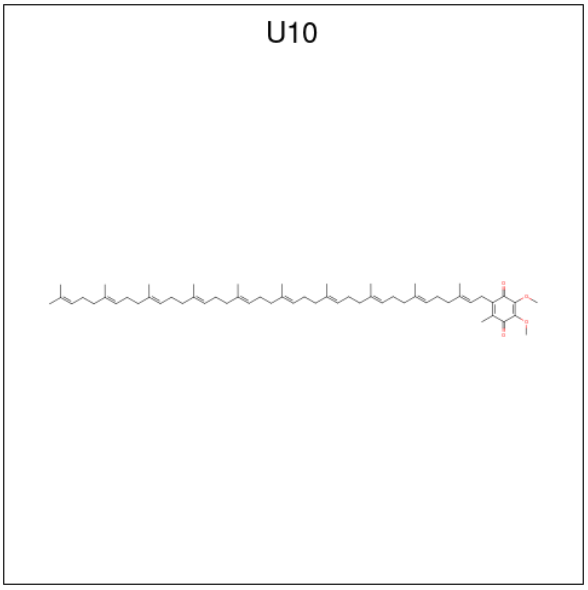


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

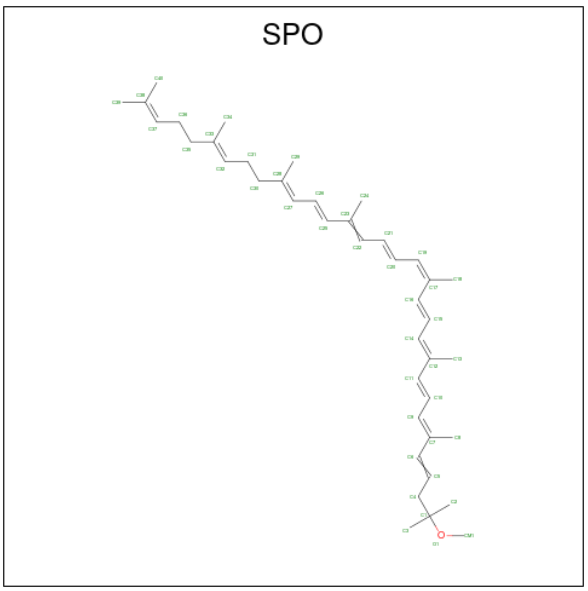
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
11	M	1	1	1	0	0

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



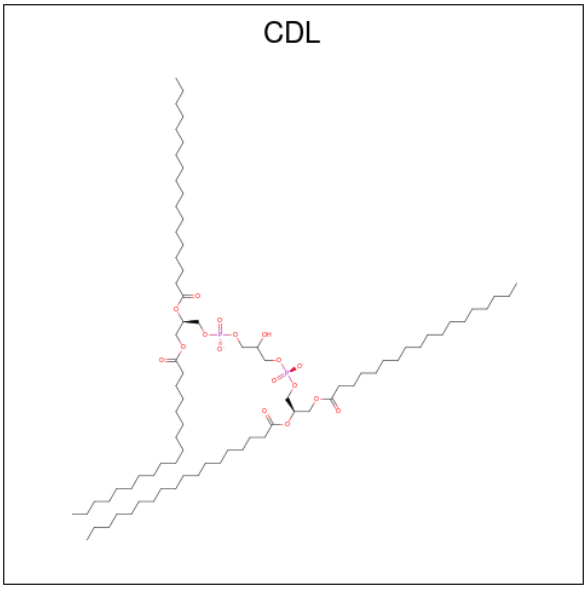
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	M	1	48	44	4	0	0

- Molecule 13 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	M	1	42	41	1	0	0

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
14	M	1	81	62	17	2	0	0

- Molecule 15 is water.

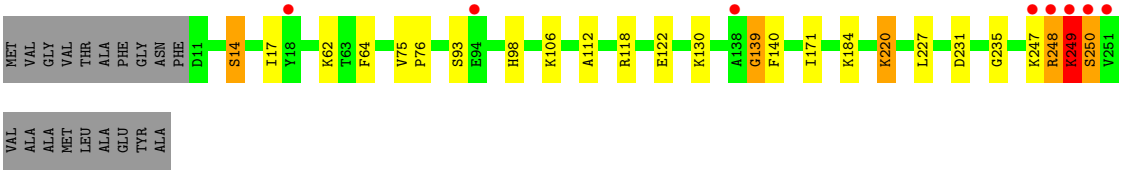
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	H	149	149	149	0	0
			Total	O		
15	L	111	111	111	0	0
			Total	O		
15	M	111	111	111	0	0

3 Residue-property plots (i)

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

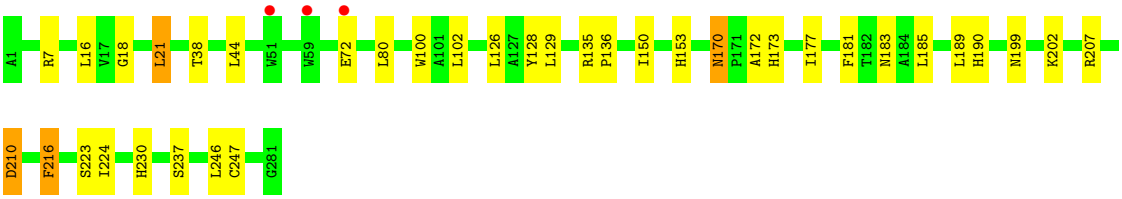
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



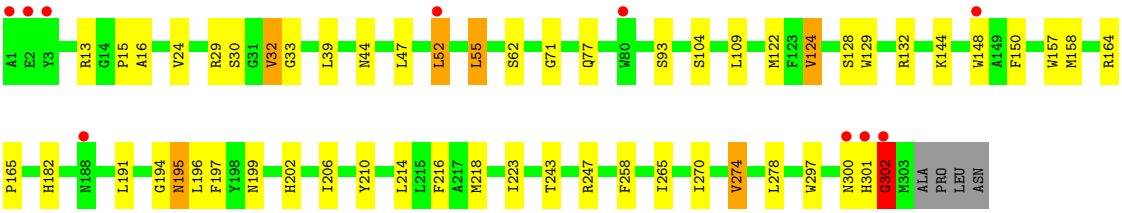
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.58Å 139.58Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.51 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.51) 90.8 (50.00-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.211 0.185 , 0.183	Depositor DCC
R_{free} test set	3493 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FE, GOL, U10, HTO, UQ2, CDL, SPO, LDA, BCL, BPH

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	0.64	1/1906 (0.1%)	0.87	3/2591 (0.1%)
2	L	0.64	0/2320	0.85	0/3175
3	M	0.63	2/2501 (0.1%)	0.88	0/3415
All	All	0.64	3/6727 (0.0%)	0.87	3/9181 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	MET	SD-CE	6.59	1.96	1.79
3	M	302	GLY	C-N	-6.34	1.24	1.33
1	H	250	SER	C-N	-6.30	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	139	GLY	N-CA-C	-5.15	98.37	113.30
1	H	248	ARG	CA-C-N	5.07	130.82	121.70
1	H	248	ARG	C-N-CA	5.07	130.82	121.70

There are no chirality outliers.

There are no planarity outliers.

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	1846	0	1861	16	0
2	L	2232	0	2187	25	0
3	M	2409	0	2321	39	0
4	H	24	0	32	1	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	5	0
5	M	132	0	148	23	0
6	L	48	0	93	7	0
6	M	96	0	186	9	0
7	L	65	0	76	7	0
7	M	65	0	76	11	0
8	L	46	0	52	7	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	0	0
13	M	42	0	60	4	0
14	M	81	0	82	2	0
15	H	149	0	0	3	0
15	L	111	0	0	1	0
15	M	111	0	0	1	0
All	All	7671	0	7425	115	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 8.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.25	1.10
1:H:248:ARG:HA	1:H:249:LYS:CB	1.95	0.96
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.87
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.15	0.80
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.66	0.77
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.21	0.75
7:L:1286:BPH:HHC	7:L:1286:BPH:HBB3	1.67	0.75
2:L:224:ILE:HG22	8:L:1287[A]:UQ2:H8	1.72	0.72
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.73	0.71
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.12	0.70
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.73	0.69
3:M:243:THR:O	3:M:247:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.23	0.67
3:M:300:ASN:C	3:M:302:GLY:H	2.02	0.67
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.79	0.65
5:M:1303:BCL:HHC	5:M:1303:BCL:CBB	2.28	0.64
7:M:1311:BPH:HHC	7:M:1311:BPH:HBB3	1.78	0.63
2:L:170:ASN:HD22	2:L:170:ASN:C	2.06	0.63
5:M:1303:BCL:H203	13:M:1313:SPO:H10	1.81	0.62
1:H:220[B]:LYS:NZ	15:H:2135:HOH:O	2.34	0.61
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.36	0.60
6:M:1305:LDA:H12	4:M:1315:GOL:H12	1.83	0.60
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.19	0.59
3:M:77:GLN:HE22	3:M:93:SER:H	1.49	0.59
6:M:1307:LDA:H52	6:M:1308:LDA:H62	1.84	0.59
5:M:1304:BCL:HHC	5:M:1304:BCL:CBB	2.34	0.58
3:M:199:ASN:HD22	3:M:199:ASN:C	2.11	0.57
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.86	0.57
5:M:1303:BCL:H62	7:M:1311:BPH:HMB3	1.86	0.56
7:L:1286:BPH:HBB1	3:M:210:TYR:CD2	2.41	0.56
5:L:1282:BCL:HBB3	5:L:1288:BCL:H52	1.87	0.56
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.88	0.55
4:H:1251:GOL:H32	15:H:2003:HOH:O	2.06	0.54
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.86	0.54
2:L:199:ASN:HA	4:L:1291:GOL:H31	1.91	0.53
1:H:140:PHE:HA	3:M:13:ARG:O	2.09	0.53
3:M:270:ILE:O	3:M:274:VAL:HG13	2.09	0.53
3:M:24:VAL:HG21	3:M:29:ARG:NH1	2.24	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.91	0.53
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.38	0.53
3:M:62:SER:OG	3:M:124:VAL:HG22	2.09	0.52
1:H:112:ALA:HA	1:H:235:GLY:O	2.10	0.52
1:H:248:ARG:CA	1:H:249:LYS:CB	2.78	0.52
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.45	0.52
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.90	0.52
6:M:1305:LDA:H32	4:M:1315:GOL:H32	1.91	0.52
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.52
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.57	0.52
6:L:1284:LDA:H11	3:M:33:GLY:HA2	1.91	0.51
5:M:1303:BCL:HHC	5:M:1303:BCL:HBB2	1.92	0.51
7:M:1311:BPH:HHC	7:M:1311:BPH:CBB	2.40	0.51
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.40	0.51
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:190:HIS:HA	8:L:1287[A]:UQ2:O4	2.11	0.51
7:L:1286:BPH:HBB3	7:L:1286:BPH:CHC	2.38	0.51
2:L:18:GLY:O	2:L:21:LEU:HB2	2.12	0.50
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.46	0.50
2:L:210:ASP:N	2:L:210:ASP:OD1	2.45	0.49
6:L:1285:LDA:H42	6:M:1309:LDA:H81	1.94	0.49
6:M:1305:LDA:H101	6:M:1307:LDA:H121	1.95	0.49
5:L:1288:BCL:C1C	5:M:1304:BCL:HBB3	2.43	0.49
3:M:300:ASN:C	3:M:302:GLY:N	2.70	0.49
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.95	0.49
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.49	0.48
7:L:1286:BPH:ND	3:M:214:LEU:HD13	2.28	0.48
1:H:14:SER:HA	1:H:17:ILE:HG22	1.97	0.47
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.50	0.47
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.44	0.46
8:L:1287[A]:UQ2:H5M1	8:L:1287[A]:UQ2:H71	1.76	0.46
3:M:150:PHE:CD1	7:M:1311:BPH:C3D	2.98	0.46
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.19	0.46
5:L:1282:BCL:HMD2	3:M:206:ILE:HD13	1.98	0.45
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.81	0.45
6:L:1284:LDA:H62	3:M:47:LEU:HD12	1.99	0.44
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.99	0.44
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.85	0.44
7:L:1286:BPH:CBB	7:L:1286:BPH:CHC	2.94	0.44
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.53	0.44
3:M:197:PHE:CE1	5:M:1304:BCL:HHC	2.52	0.44
6:M:1307:LDA:HM11	6:M:1307:LDA:H22	1.54	0.44
6:M:1307:LDA:H41	6:M:1308:LDA:H42	1.99	0.44
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.81	0.44
5:M:1303:BCL:H101	5:M:1304:BCL:H171	2.00	0.43
3:M:196:LEU:HD12	5:M:1304:BCL:C1D	2.49	0.43
3:M:71:GLY:HA3	13:M:1313:SPO:H42	2.00	0.43
1:H:139:GLY:H	3:M:15:PRO:HD3	1.84	0.43
1:H:130:LYS:HD2	15:L:2087:HOH:O	2.19	0.42
3:M:129:TRP:O	3:M:132:ARG:HB3	2.19	0.42
3:M:194:GLY:O	3:M:195:ASN:CB	2.67	0.42
2:L:224:ILE:HD12	8:L:1287[B]:UQ2:H102	2.01	0.42
6:L:1285:LDA:HM21	6:L:1285:LDA:H21	1.90	0.42
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.55	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.42
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:H161	2.01	0.42
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.72	0.42
2:L:170:ASN:ND2	2:L:172:ALA:H	2.18	0.42
5:M:1303:BCL:HBB2	13:M:1313:SPO:H243	2.02	0.42
7:M:1311:BPH:H141	7:M:1311:BPH:H161	1.90	0.42
1:H:118[A]:ARG:HD3	15:M:2089:HOH:O	2.20	0.41
2:L:224:ILE:CG2	8:L:1287[A]:UQ2:H8	2.46	0.41
5:M:1303:BCL:CBB	13:M:1313:SPO:H243	2.51	0.41
5:M:1303:BCL:HBB3	5:M:1303:BCL:HHC	2.01	0.41
2:L:189:LEU:CD2	7:M:1311:BPH:HMD2	2.50	0.41
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:C16	2.50	0.41
15:H:2003:HOH:O	14:M:1314:CDL:HA32	2.20	0.41
6:L:1283:LDA:HM11	6:L:1283:LDA:H22	1.86	0.41
3:M:122:MET:HE2	5:M:1304:BCL:H142	2.03	0.41
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.36	0.41
7:M:1311:BPH:H2	7:M:1311:BPH:H6C2	1.94	0.41
6:M:1309:LDA:HM11	6:M:1309:LDA:H21	1.75	0.41
2:L:170:ASN:C	2:L:170:ASN:ND2	2.77	0.40
5:M:1303:BCL:CBB	5:M:1303:BCL:CHC	2.99	0.40
3:M:199:ASN:C	3:M:199:ASN:ND2	2.79	0.40
2:L:223:SER:O	3:M:44:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	30 49
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100 100
3	M	301/307 (98%)	287 (95%)	9 (3%)	5 (2%)	7 13
All	All	822/848 (97%)	790 (96%)	26 (3%)	6 (1%)	18 34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS
3	M	52	LEU
3	M	195	ASN
3	M	30	SER
3	M	302	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	198/208 (95%)	187 (94%)	11 (6%)	19 39
2	L	220/220 (100%)	203 (92%)	17 (8%)	12 25
3	M	236/240 (98%)	222 (94%)	14 (6%)	18 37
All	All	654/668 (98%)	612 (94%)	42 (6%)	16 33

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	93	SER
1	H	106	LYS
1	H	171	ILE
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
1	H	250	SER
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU

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Mol	Chain	Res	Type
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	150	ILE
2	L	170	ASN
2	L	185	LEU
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
3	M	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	104	SER
3	M	109	LEU
3	M	124	VAL
3	M	148	TRP
3	M	182	HIS
3	M	191	LEU
3	M	216	PHE
3	M	265	ILE
3	M	274	VAL
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
2	L	258	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BPH	L	1286	-	59,70,70	2.76	10 (16%)	61,101,101	2.25	17 (27%)
8	UQ2	L	1287[B]	-	23,23,23	2.76	7 (30%)	28,31,31	1.18	1 (3%)
6	LDA	M	1306	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
6	LDA	M	1309	-	12,15,15	2.01	1 (8%)	14,17,17	0.45	0
14	CDL	M	1314	-	80,80,99	2.33	18 (22%)	86,92,111	4.01	15 (17%)
4	GOL	L	1291	-	5,5,5	0.32	0	5,5,5	0.51	0
8	UQ2	L	1287[A]	-	23,23,23	2.67	8 (34%)	28,31,31	1.61	5 (17%)
6	LDA	M	1305	-	12,15,15	2.10	1 (8%)	14,17,17	0.49	0
7	BPH	M	1311	-	59,70,70	2.70	11 (18%)	61,101,101	2.12	15 (24%)
5	BCL	M	1304	3	69,74,74	1.92	9 (13%)	83,115,115	2.10	25 (30%)
5	BCL	L	1288	2	69,74,74	1.84	8 (11%)	83,115,115	2.35	22 (26%)
6	LDA	M	1308	-	12,15,15	2.05	1 (8%)	14,17,17	0.46	0
4	GOL	H	1253	-	5,5,5	0.35	0	5,5,5	0.28	0
4	GOL	H	1251	-	5,5,5	0.52	0	5,5,5	0.73	0
9	PO4	L	1289	-	4,4,4	0.84	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	U10	M	1312	-	48,48,63	2.69	12 (25%)	58,61,79	1.65	12 (20%)
4	GOL	M	1315	-	5,5,5	0.33	0	5,5,5	0.31	0
6	LDA	L	1285	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
6	LDA	M	1307	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0
4	GOL	L	1292	-	5,5,5	0.36	0	5,5,5	0.23	0
5	BCL	M	1303	3	69,74,74	1.93	10 (14%)	83,115,115	2.13	19 (22%)
5	BCL	L	1282	2	69,74,74	1.85	9 (13%)	83,115,115	2.33	25 (30%)
6	LDA	L	1284	-	12,15,15	2.04	1 (8%)	14,17,17	0.50	0
10	HTO	L	1290	-	9,9,9	0.43	0	10,10,10	0.57	0
6	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.49	0
13	SPO	M	1313	-	40,41,41	4.16	12 (30%)	47,50,50	1.89	11 (23%)
4	GOL	H	1252	-	5,5,5	0.38	0	5,5,5	0.22	0
6	LDA	M	1709	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	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
7	BPH	L	1286	-	-	9/37/105/105	0/5/6/6
8	UQ2	L	1287[B]	-	-	8/15/39/39	0/1/1/1
6	LDA	M	1306	-	-	7/13/13/13	-
6	LDA	M	1309	-	-	12/13/13/13	-
14	CDL	M	1314	-	-	46/91/91/110	-
4	GOL	L	1291	-	-	2/4/4/4	-
8	UQ2	L	1287[A]	-	-	8/15/39/39	0/1/1/1
6	LDA	M	1305	-	-	5/13/13/13	-
7	BPH	M	1311	-	-	17/37/105/105	0/5/6/6
5	BCL	M	1304	3	2/2/21/25	9/41/137/137	-
5	BCL	L	1288	2	2/2/21/25	9/41/137/137	-
6	LDA	M	1308	-	-	5/13/13/13	-
4	GOL	H	1253	-	-	1/4/4/4	-
4	GOL	H	1251	-	-	4/4/4/4	-
12	U10	M	1312	-	-	13/45/69/87	0/1/1/1
4	GOL	M	1315	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	L	1285	-	-	9/13/13/13	-
6	LDA	M	1307	-	-	8/13/13/13	-
4	GOL	L	1292	-	-	4/4/4/4	-
5	BCL	M	1303	3	2/2/21/25	16/41/137/137	-
5	BCL	L	1282	2	2/2/21/25	10/41/137/137	-
6	LDA	L	1284	-	-	4/13/13/13	-
10	HTO	L	1290	-	-	7/10/10/10	-
6	LDA	L	1283	-	-	6/13/13/13	-
13	SPO	M	1313	-	-	24/47/47/47	-
4	GOL	H	1252	-	-	4/4/4/4	-
6	LDA	M	1709	-	-	8/13/13/13	-
4	GOL	H	1254	-	-	0/4/4/4	-

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1286	BPH	OBD-CAD	12.97	1.40	1.22
7	M	1311	BPH	OBD-CAD	12.82	1.40	1.22
13	M	1313	SPO	C27-C28	12.67	1.47	1.34
5	M	1304	BCL	OBD-CAD	10.78	1.41	1.22
5	M	1303	BCL	OBD-CAD	10.72	1.41	1.22
5	L	1282	BCL	OBD-CAD	10.35	1.40	1.22
5	L	1288	BCL	OBD-CAD	10.27	1.40	1.22
13	M	1313	SPO	C9-C7	9.40	1.48	1.35
13	M	1313	SPO	C22-C23	9.29	1.48	1.35
13	M	1313	SPO	C14-C12	9.25	1.48	1.35
13	M	1313	SPO	C19-C17	8.90	1.47	1.35
7	L	1286	BPH	O1D-CGD	8.05	1.41	1.21
7	M	1311	BPH	O1D-CGD	7.79	1.40	1.21
14	M	1314	CDL	C11-CA5	-7.36	1.29	1.50
6	L	1285	LDA	O1-N1	-7.12	1.25	1.42
6	M	1305	LDA	O1-N1	-7.07	1.25	1.42
6	M	1306	LDA	O1-N1	-7.00	1.25	1.42
6	M	1308	LDA	O1-N1	-7.00	1.25	1.42
6	L	1284	LDA	O1-N1	-7.00	1.25	1.42
6	L	1283	LDA	O1-N1	-6.94	1.25	1.42
6	M	1709	LDA	O1-N1	-6.92	1.26	1.42
6	M	1307	LDA	O1-N1	-6.89	1.26	1.42
14	M	1314	CDL	C32-C31	-6.86	1.26	1.52
6	M	1309	LDA	O1-N1	-6.86	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1287[B]	UQ2	C8-C9	6.80	1.49	1.33
12	M	1312	U10	C33-C34	6.72	1.49	1.33
12	M	1312	U10	C13-C14	6.65	1.48	1.33
7	L	1286	BPH	O1A-CGA	6.41	1.41	1.22
5	M	1303	BCL	O1A-CGA	6.37	1.41	1.22
8	L	1287[A]	UQ2	C8-C9	6.36	1.48	1.33
7	L	1286	BPH	C2-C3	6.34	1.48	1.33
5	M	1304	BCL	O1A-CGA	6.33	1.41	1.22
13	M	1313	SPO	C32-C33	6.31	1.48	1.33
7	M	1311	BPH	C2-C3	6.26	1.48	1.33
7	L	1286	BPH	OBB-CAB	6.18	1.41	1.22
7	M	1311	BPH	O1A-CGA	6.08	1.40	1.22
12	M	1312	U10	C18-C19	6.07	1.47	1.33
12	M	1312	U10	C8-C9	5.98	1.47	1.33
5	L	1288	BCL	O1A-CGA	5.91	1.40	1.22
5	L	1282	BCL	O1A-CGA	5.90	1.40	1.22
14	M	1314	CDL	C12-C11	-5.85	1.30	1.52
12	M	1312	U10	C23-C24	5.84	1.47	1.33
14	M	1314	CDL	C34-C33	-5.81	1.19	1.51
14	M	1314	CDL	C33-C32	-5.76	1.19	1.51
12	M	1312	U10	C28-C29	5.75	1.46	1.33
7	M	1311	BPH	OBB-CAB	5.73	1.40	1.22
13	M	1313	SPO	C37-C38	5.72	1.48	1.32
8	L	1287[A]	UQ2	C13-C14	5.69	1.48	1.32
13	M	1313	SPO	C6-C5	5.52	1.46	1.32
12	M	1312	U10	C38-C39	5.41	1.47	1.32
7	L	1286	BPH	C3D-C2D	5.40	1.49	1.39
8	L	1287[B]	UQ2	C13-C14	5.40	1.47	1.32
7	M	1311	BPH	C3D-C2D	5.25	1.48	1.39
8	L	1287[A]	UQ2	O2-C2	-5.25	1.24	1.36
8	L	1287[B]	UQ2	O2-C2	-5.11	1.24	1.36
8	L	1287[B]	UQ2	O3-C3	-5.06	1.24	1.36
14	M	1314	CDL	OB6-CB5	4.94	1.48	1.34
13	M	1313	SPO	C15-C16	4.76	1.46	1.34
12	M	1312	U10	O4-C4	-4.76	1.25	1.36
8	L	1287[A]	UQ2	O3-C3	-4.73	1.25	1.36
14	M	1314	CDL	OA6-CA5	4.66	1.47	1.34
13	M	1313	SPO	C10-C11	4.59	1.46	1.34
14	M	1314	CDL	OA8-CA7	4.58	1.46	1.33
13	M	1313	SPO	C26-C25	4.52	1.46	1.34
12	M	1312	U10	O3-C3	-4.52	1.25	1.36
14	M	1314	CDL	C17-C16	-4.49	1.26	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1314	CDL	C16-C15	-4.48	1.26	1.51
7	L	1286	BPH	C3D-CAD	-4.47	1.38	1.47
14	M	1314	CDL	C20-C19	-4.42	1.26	1.51
14	M	1314	CDL	C19-C18	-4.36	1.27	1.51
14	M	1314	CDL	OB8-CB7	4.33	1.46	1.33
5	M	1303	BCL	C4D-ND	-4.27	1.31	1.37
5	M	1303	BCL	C3D-C4D	-4.19	1.34	1.44
5	M	1304	BCL	C3D-C4D	-4.11	1.34	1.44
7	M	1311	BPH	C3D-CAD	-4.01	1.39	1.47
5	M	1304	BCL	C4D-ND	-3.99	1.32	1.37
5	L	1282	BCL	C3D-C4D	-3.92	1.35	1.44
5	L	1288	BCL	C3D-C4D	-3.92	1.35	1.44
13	M	1313	SPO	C21-C20	3.89	1.46	1.36
5	L	1282	BCL	C4D-ND	-3.89	1.32	1.37
14	M	1314	CDL	C13-C12	-3.76	1.30	1.51
5	L	1288	BCL	C2-C3	3.68	1.41	1.33
8	L	1287[B]	UQ2	C6-C5	3.57	1.41	1.35
12	M	1312	U10	C6-C1	3.52	1.41	1.35
7	L	1286	BPH	C3D-C4D	-3.32	1.36	1.41
8	L	1287[A]	UQ2	C3-C4	-3.27	1.39	1.48
5	L	1288	BCL	C4D-ND	-3.23	1.33	1.37
5	L	1282	BCL	C2-C3	3.21	1.40	1.33
12	M	1312	U10	C4-C5	-3.18	1.39	1.48
8	L	1287[B]	UQ2	C3-C4	-3.11	1.39	1.48
7	L	1286	BPH	O2D-CGD	-3.10	1.25	1.33
14	M	1314	CDL	C37-C36	-3.09	1.34	1.51
14	M	1314	CDL	C79-C78	-3.09	1.34	1.51
14	M	1314	CDL	C80-C79	-3.05	1.34	1.51
5	M	1303	BCL	C2-C3	3.02	1.40	1.33
14	M	1314	CDL	C22-C21	-3.00	1.34	1.51
7	M	1311	BPH	O2D-CGD	-2.96	1.26	1.33
8	L	1287[B]	UQ2	C2-C1	-2.82	1.40	1.48
5	M	1304	BCL	C2-C3	2.81	1.39	1.33
8	L	1287[A]	UQ2	C6-C5	2.71	1.40	1.35
7	M	1311	BPH	O2A-CGA	-2.70	1.25	1.33
5	L	1288	BCL	CHD-C4C	2.69	1.46	1.39
5	M	1303	BCL	CHD-C4C	2.61	1.46	1.39
7	M	1311	BPH	C3D-C4D	-2.58	1.37	1.41
5	L	1288	BCL	O2D-CGD	-2.56	1.27	1.33
5	M	1304	BCL	CHD-C4C	2.56	1.46	1.39
5	L	1282	BCL	O2D-CGD	-2.55	1.27	1.33
8	L	1287[A]	UQ2	C6-C1	-2.54	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1282	BCL	O2A-CGA	-2.52	1.25	1.33
5	M	1303	BCL	O2D-CGD	-2.49	1.27	1.33
8	L	1287[A]	UQ2	C2-C1	-2.40	1.42	1.48
7	L	1286	BPH	O2A-CGA	-2.39	1.26	1.33
5	M	1304	BCL	O2A-CGA	-2.37	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.32	1.27	1.33
5	L	1282	BCL	CHD-C4C	2.32	1.45	1.39
5	L	1288	BCL	O2A-CGA	-2.28	1.26	1.33
5	M	1303	BCL	O1D-CGD	2.26	1.26	1.21
7	M	1311	BPH	CBD-CGD	-2.25	1.49	1.52
12	M	1312	U10	C3-C2	-2.20	1.42	1.48
5	M	1303	BCL	C1D-C2D	-2.08	1.41	1.45
5	L	1282	BCL	C1D-C2D	-2.04	1.41	1.45
5	M	1304	BCL	C3C-C4C	-2.03	1.49	1.51
5	M	1303	BCL	O2A-CGA	-2.01	1.27	1.33

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1314	CDL	C33-C32-C31	18.27	178.87	113.19
14	M	1314	CDL	C13-C12-C11	12.79	159.15	113.19
14	M	1314	CDL	C17-C16-C15	12.53	178.05	114.42
14	M	1314	CDL	C35-C34-C33	12.51	177.91	114.42
14	M	1314	CDL	C34-C33-C32	12.33	177.02	114.42
14	M	1314	CDL	C20-C19-C18	12.19	176.33	114.42
14	M	1314	CDL	C12-C11-CA5	11.59	155.76	113.62
5	L	1288	BCL	C2D-C1D-ND	-9.16	103.35	110.10
7	M	1311	BPH	O2D-CGD-CBD	8.07	121.22	111.00
7	L	1286	BPH	O2D-CGD-CBD	8.06	121.21	111.00
5	M	1303	BCL	C2D-C1D-ND	-7.35	104.69	110.10
5	L	1288	BCL	C1D-ND-C4D	7.23	111.47	106.33
5	M	1303	BCL	C1D-ND-C4D	7.17	111.43	106.33
7	M	1311	BPH	C2B-C1B-NB	6.73	114.17	109.53
5	L	1282	BCL	C2B-C1B-NB	-6.31	106.00	110.23
5	L	1282	BCL	C1C-NC-C4C	-6.24	103.90	106.71
7	L	1286	BPH	C2B-C1B-NB	6.24	113.83	109.53
5	L	1288	BCL	CHD-C1D-ND	-6.18	118.78	124.45
5	M	1304	BCL	C2D-C1D-ND	-6.15	105.57	110.10
5	L	1282	BCL	C1D-ND-C4D	5.93	110.55	106.33
5	L	1282	BCL	C2D-C1D-ND	-5.91	105.75	110.10
5	L	1288	BCL	C4A-NA-C1A	5.82	109.32	106.71
5	L	1282	BCL	CMB-C2B-C1B	-5.77	116.58	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1282	BCL	O2D-CGD-CBD	5.72	121.43	111.27
5	L	1282	BCL	C4A-NA-C1A	5.64	109.24	106.71
5	M	1304	BCL	C1D-ND-C4D	5.59	110.31	106.33
5	M	1303	BCL	CMB-C2B-C1B	-5.57	116.88	125.37
5	M	1304	BCL	CMB-C2B-C1B	-5.49	117.01	125.37
5	M	1303	BCL	C4A-NA-C1A	5.47	109.17	106.71
5	M	1304	BCL	CMD-C2D-C1D	5.44	134.30	124.71
5	L	1288	BCL	CMB-C2B-C1B	-5.38	117.18	125.37
14	M	1314	CDL	OA6-CA5-C11	5.28	122.88	111.50
5	M	1303	BCL	C2B-C1B-NB	-5.16	106.77	110.23
5	L	1282	BCL	CHC-C4B-NB	-5.13	118.82	124.26
5	M	1304	BCL	C2B-C1B-NB	-5.03	106.86	110.23
5	L	1288	BCL	CMD-C2D-C1D	4.90	133.34	124.71
12	M	1312	U10	C30-C29-C31	4.87	123.47	115.27
7	L	1286	BPH	C2D-C1D-ND	4.87	112.89	109.53
5	M	1303	BCL	O2D-CGD-CBD	4.86	119.91	111.27
13	M	1313	SPO	C10-C9-C7	-4.52	120.86	127.31
7	L	1286	BPH	OBD-CAD-C3D	-4.49	120.52	127.98
5	L	1282	BCL	CMD-C2D-C1D	4.42	132.50	124.71
13	M	1313	SPO	C20-C19-C17	-4.38	121.05	127.31
5	M	1304	BCL	O2D-CGD-CBD	4.36	119.02	111.27
7	M	1311	BPH	OBD-CAD-CBD	-4.26	119.58	125.82
7	L	1286	BPH	C3D-C4D-ND	4.25	113.51	107.72
7	M	1311	BPH	C3D-C4D-ND	4.25	113.51	107.72
7	L	1286	BPH	C4D-ND-C1D	-4.10	104.66	108.83
5	M	1304	BCL	CHD-C1D-ND	-4.09	120.69	124.45
13	M	1313	SPO	C3-C1-C4	-4.08	104.59	110.86
5	L	1288	BCL	C2B-C1B-NB	-4.05	107.52	110.23
7	M	1311	BPH	O1D-CGD-CBD	-4.01	118.07	124.74
5	L	1288	BCL	CMD-C2D-C3D	-3.99	118.44	127.61
5	L	1288	BCL	O2D-CGD-CBD	3.95	118.28	111.27
5	L	1288	BCL	C1C-NC-C4C	-3.92	104.94	106.71
5	M	1303	BCL	C1-O2A-CGA	3.87	126.60	116.44
12	M	1312	U10	C10-C9-C11	3.81	121.67	115.27
5	M	1303	BCL	CMD-C2D-C1D	3.78	131.38	124.71
12	M	1312	U10	C27-C28-C29	-3.70	118.76	127.66
7	M	1311	BPH	OBD-CAD-C3D	-3.68	121.87	127.98
14	M	1314	CDL	OB6-CB5-C51	3.65	119.37	111.50
7	L	1286	BPH	C1B-NB-C4B	-3.57	103.30	108.83
8	L	1287[A]	UQ2	CM5-C5-C6	-3.55	118.61	124.40
5	M	1304	BCL	CMD-C2D-C3D	-3.52	119.51	127.61
13	M	1313	SPO	C29-C28-C30	3.51	121.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	CED-O2D-CGD	3.51	123.87	115.94
8	L	1287[A]	UQ2	C10-C9-C11	3.40	120.99	115.27
5	L	1288	BCL	O2A-CGA-CBA	3.29	122.22	111.91
13	M	1313	SPO	C15-C14-C12	-3.28	122.64	127.31
5	L	1288	BCL	CED-O2D-CGD	3.25	123.28	115.94
7	L	1286	BPH	CED-O2D-CGD	3.21	123.21	115.94
5	M	1304	BCL	C1D-CHD-C4C	-3.21	118.88	126.62
5	L	1282	BCL	C4-C3-C5	3.19	120.64	115.27
7	M	1311	BPH	CBC-CAC-C3C	-3.16	107.41	113.77
7	L	1286	BPH	C4D-CHA-CBD	-3.13	107.10	108.52
7	M	1311	BPH	C2D-C1D-ND	3.13	111.69	109.53
5	M	1304	BCL	CHC-C4B-NB	-3.06	121.02	124.26
7	L	1286	BPH	O1D-CGD-CBD	-3.05	119.65	124.74
5	M	1304	BCL	C3C-C4C-CHD	-3.05	116.87	123.39
12	M	1312	U10	C35-C34-C36	3.03	120.37	115.27
5	L	1288	BCL	CHC-C4B-NB	-3.03	121.05	124.26
7	M	1311	BPH	C4D-ND-C1D	-3.02	105.75	108.83
5	M	1304	BCL	O2A-CGA-CBA	3.01	121.36	111.91
12	M	1312	U10	C17-C18-C19	-2.97	120.51	127.66
5	L	1282	BCL	CHA-C1A-NA	-2.93	119.70	126.40
12	M	1312	U10	C22-C23-C24	-2.92	120.63	127.66
5	L	1288	BCL	CMB-C2B-C3B	2.91	133.80	125.93
5	M	1304	BCL	CMB-C2B-C3B	2.87	133.68	125.93
5	M	1303	BCL	CMB-C2B-C3B	2.85	133.62	125.93
5	L	1282	BCL	CMD-C2D-C3D	-2.84	121.09	127.61
14	M	1314	CDL	OB8-CB7-C71	2.83	120.79	111.91
8	L	1287[A]	UQ2	O1-C1-C6	-2.82	116.60	121.55
7	M	1311	BPH	CMD-C2D-C3D	-2.82	119.40	124.68
7	L	1286	BPH	O2A-CGA-CBA	2.82	120.75	111.91
14	M	1314	CDL	OA8-CA7-C31	2.78	120.64	111.91
5	L	1282	BCL	C1D-CHD-C4C	-2.78	119.92	126.62
5	M	1303	BCL	CHB-C4A-NA	-2.78	120.67	124.51
13	M	1313	SPO	C21-C22-C23	-2.77	123.35	127.31
12	M	1312	U10	C25-C24-C26	2.71	119.83	115.27
5	M	1304	BCL	CHB-C1B-NB	-2.68	121.42	124.26
5	M	1303	BCL	C1D-CHD-C4C	-2.67	120.19	126.62
5	L	1288	BCL	C1-O2A-CGA	2.66	123.41	116.44
5	L	1282	BCL	CMB-C2B-C3B	2.64	133.07	125.93
5	M	1304	BCL	C4-C3-C5	2.64	119.72	115.27
5	M	1304	BCL	O2D-CGD-O1D	-2.64	118.67	123.84
5	L	1282	BCL	O2A-CGA-CBA	2.63	120.16	111.91
7	M	1311	BPH	C1C-C2C-C3C	-2.61	100.35	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1282	BCL	CHB-C4A-NA	-2.60	120.91	124.51
5	L	1282	BCL	C3C-C4C-CHD	-2.58	117.87	123.39
5	M	1303	BCL	O2A-CGA-CBA	2.56	119.94	111.91
14	M	1314	CDL	C32-C31-CA7	2.55	122.89	113.62
8	L	1287[A]	UQ2	CM3-O3-C3	2.55	125.50	116.47
5	M	1303	BCL	O2D-CGD-O1D	-2.54	118.87	123.84
5	M	1303	BCL	CMD-C2D-C3D	-2.54	121.78	127.61
5	M	1303	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
12	M	1312	U10	C20-C19-C21	2.52	119.52	115.27
13	M	1313	SPO	C40-C38-C39	2.52	120.17	114.60
7	L	1286	BPH	C1C-C2C-C3C	-2.52	100.44	102.84
5	M	1304	BCL	C16-C15-C13	-2.52	107.78	115.92
13	M	1313	SPO	C34-C33-C35	2.51	119.50	115.27
5	L	1282	BCL	O1D-CGD-CBD	-2.51	119.35	124.48
12	M	1312	U10	C30-C29-C28	-2.48	117.31	123.68
5	L	1288	BCL	C2A-C3A-C4A	2.47	105.85	101.87
5	M	1304	BCL	C4A-NA-C1A	2.43	107.80	106.71
7	L	1286	BPH	O2D-CGD-O1D	-2.42	119.11	123.84
5	M	1303	BCL	CHA-C1A-NA	-2.40	120.89	126.40
5	L	1282	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
12	M	1312	U10	C15-C14-C16	2.37	119.25	115.27
13	M	1313	SPO	C31-C32-C33	-2.34	122.03	127.66
5	M	1304	BCL	CAC-C3C-C4C	-2.33	107.40	112.58
7	M	1311	BPH	O2A-CGA-CBA	2.32	119.18	111.91
8	L	1287[A]	UQ2	C7-C8-C9	-2.31	122.94	126.79
7	M	1311	BPH	CED-O2D-CGD	2.31	121.15	115.94
5	L	1288	BCL	C2A-C1A-CHA	-2.29	119.85	123.86
7	M	1311	BPH	C1B-NB-C4B	-2.29	105.28	108.83
5	L	1282	BCL	C2A-C3A-C4A	2.26	105.51	101.87
5	L	1288	BCL	CHA-C4D-ND	2.25	137.20	132.50
13	M	1313	SPO	C13-C12-C11	2.25	121.62	118.08
5	M	1304	BCL	CHD-C4C-NC	-2.24	122.59	125.08
5	M	1304	BCL	C1-C2-C3	-2.24	122.18	126.04
5	L	1282	BCL	O2A-CGA-O1A	-2.23	117.95	123.59
7	M	1311	BPH	C1-O2A-CGA	2.23	122.30	116.44
14	M	1314	CDL	OA6-CA5-OA7	-2.23	118.31	123.70
12	M	1312	U10	C4M-O4-C4	2.22	124.33	116.47
14	M	1314	CDL	OA8-CA7-OA9	-2.17	118.11	123.59
5	L	1282	BCL	C1-O2A-CGA	2.16	122.11	116.44
7	L	1286	BPH	O2A-CGA-O1A	-2.14	118.19	123.59
5	M	1303	BCL	CED-O2D-CGD	2.12	120.74	115.94
5	L	1288	BCL	CHB-C4A-NA	-2.12	121.58	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1314	CDL	OB8-CB7-OB9	-2.11	118.26	123.59
12	M	1312	U10	C41-C39-C40	2.10	119.24	114.60
5	M	1304	BCL	CBB-CAB-C3B	-2.08	115.99	120.43
7	L	1286	BPH	CMC-C2C-C1C	-2.08	109.83	114.38
5	L	1282	BCL	C4B-C3B-C2B	-2.07	105.03	108.36
7	L	1286	BPH	CMD-C2D-C3D	-2.07	120.81	124.68
5	M	1303	BCL	CAB-C3B-C2B	-2.07	125.25	128.34
5	M	1304	BCL	C7-C6-C5	-2.05	107.79	113.36
5	L	1282	BCL	C1-C2-C3	-2.05	122.50	126.04
5	M	1303	BCL	CHA-C4D-ND	2.03	136.75	132.50
13	M	1313	SPO	C18-C17-C19	-2.03	120.08	122.92
5	L	1288	BCL	C4-C3-C5	2.02	118.67	115.27
5	L	1282	BCL	CED-O2D-CGD	2.02	120.51	115.94
5	L	1288	BCL	CHA-C1A-NA	-2.02	121.78	126.40
5	L	1288	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
7	L	1286	BPH	C4C-C3C-C2C	-2.01	100.93	102.84
8	L	1287[B]	UQ2	C16-C14-C15	2.01	119.04	114.60
5	M	1304	BCL	CHA-C4D-ND	2.00	136.69	132.50

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1288	BCL	C13
5	L	1288	BCL	C8
5	M	1303	BCL	C13
5	M	1303	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8

All (258) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1251	GOL	O1-C1-C2-O2
4	H	1251	GOL	O1-C1-C2-C3
4	H	1252	GOL	O1-C1-C2-C3
4	L	1291	GOL	C1-C2-C3-O3
4	L	1292	GOL	O1-C1-C2-C3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
6	M	1305	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
6	M	1305	LDA	C2-C1-N1-CM1
6	M	1305	LDA	C2-C1-N1-CM2
6	M	1309	LDA	C2-C1-N1-O1
6	M	1309	LDA	C2-C1-N1-CM1
6	M	1309	LDA	N1-C1-C2-C3
7	L	1286	BPH	O2A-C1-C2-C3
7	M	1311	BPH	O2A-C1-C2-C3
7	M	1311	BPH	C1-C2-C3-C4
8	L	1287[A]	UQ2	C7-C8-C9-C10
8	L	1287[A]	UQ2	C7-C8-C9-C11
8	L	1287[A]	UQ2	C12-C13-C14-C16
8	L	1287[B]	UQ2	C12-C11-C9-C8
8	L	1287[B]	UQ2	C12-C11-C9-C10
10	L	1290	HTO	O3-C3-C4-C5
12	M	1312	U10	C27-C28-C29-C30
12	M	1312	U10	C27-C28-C29-C31
12	M	1312	U10	C34-C36-C37-C38
13	M	1313	SPO	C4-C1-O1-CM1
13	M	1313	SPO	C1-C4-C5-C6
13	M	1313	SPO	C4-C5-C6-C7
13	M	1313	SPO	C6-C7-C9-C10
13	M	1313	SPO	C8-C7-C9-C10
13	M	1313	SPO	C9-C10-C11-C12
13	M	1313	SPO	C15-C16-C17-C18
13	M	1313	SPO	C15-C16-C17-C19
13	M	1313	SPO	C19-C20-C21-C22
13	M	1313	SPO	C36-C37-C38-C39
13	M	1313	SPO	C36-C37-C38-C40
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	CB3-OB5-PB2-OB2
14	M	1314	CDL	CB3-OB5-PB2-OB3
5	L	1282	BCL	C3-C5-C6-C7
14	M	1314	CDL	C20-C21-C22-C23
14	M	1314	CDL	C33-C34-C35-C36
14	M	1314	CDL	C78-C79-C80-C81
10	L	1290	HTO	O1-C1-C2-O2
8	L	1287[A]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	OA9-CA7-OA8-CA6
14	M	1314	CDL	OB9-CB7-OB8-CB6
14	M	1314	CDL	C31-CA7-OA8-CA6
7	L	1286	BPH	CBD-CGD-O2D-CED
14	M	1314	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C10-C11-C12-C13
12	M	1312	U10	C29-C31-C32-C33
13	M	1313	SPO	C33-C35-C36-C37
8	L	1287[B]	UQ2	C7-C8-C9-C10
8	L	1287[B]	UQ2	C7-C8-C9-C11
14	M	1314	CDL	C17-C18-C19-C20
14	M	1314	CDL	CB5-C51-C52-C53
5	L	1282	BCL	C11-C10-C8-C9
5	L	1288	BCL	C11-C12-C13-C14
14	M	1314	CDL	CB7-C71-C72-C73
5	L	1282	BCL	C13-C15-C16-C17
5	M	1303	BCL	C3-C5-C6-C7
5	L	1282	BCL	C5-C6-C7-C8
5	L	1288	BCL	C15-C16-C17-C18
8	L	1287[A]	UQ2	C9-C11-C12-C13
14	M	1314	CDL	CA7-C31-C32-C33
5	L	1288	BCL	C10-C11-C12-C13
14	M	1314	CDL	C11-CA5-OA6-CA4
13	M	1313	SPO	C13-C12-C14-C15
13	M	1313	SPO	C18-C17-C19-C20
13	M	1313	SPO	C21-C22-C23-C24
6	L	1285	LDA	C7-C8-C9-C10
14	M	1314	CDL	C12-C13-C14-C15
14	M	1314	CDL	CA5-C11-C12-C13
6	M	1307	LDA	C7-C8-C9-C10
6	M	1308	LDA	C11-C10-C9-C8
6	L	1283	LDA	C3-C4-C5-C6
13	M	1313	SPO	C16-C17-C19-C20
14	M	1314	CDL	C72-C73-C74-C75
6	L	1284	LDA	C7-C8-C9-C10
6	L	1284	LDA	C6-C7-C8-C9
6	L	1285	LDA	C4-C5-C6-C7
6	M	1305	LDA	C2-C3-C4-C5
14	M	1314	CDL	C15-C16-C17-C18
14	M	1314	CDL	C14-C15-C16-C17
4	H	1251	GOL	C1-C2-C3-O3
4	H	1252	GOL	C1-C2-C3-O3
4	H	1253	GOL	O1-C1-C2-C3
4	L	1292	GOL	C1-C2-C3-O3
14	M	1314	CDL	OA7-CA5-OA6-CA4
6	M	1306	LDA	C3-C4-C5-C6
7	L	1286	BPH	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	M	1307	LDA	C4-C5-C6-C7
14	M	1314	CDL	C71-C72-C73-C74
7	M	1311	BPH	C8-C10-C11-C12
6	L	1283	LDA	C6-C7-C8-C9
8	L	1287[B]	UQ2	C12-C13-C14-C15
6	L	1283	LDA	C5-C6-C7-C8
6	L	1285	LDA	C3-C4-C5-C6
6	L	1285	LDA	C2-C3-C4-C5
10	L	1290	HTO	O1-C1-C2-C3
4	L	1291	GOL	O2-C2-C3-O3
4	L	1292	GOL	O1-C1-C2-O2
4	L	1292	GOL	O2-C2-C3-O3
6	L	1283	LDA	C11-C10-C9-C8
6	M	1306	LDA	C2-C3-C4-C5
6	M	1709	LDA	C1-C2-C3-C4
14	M	1314	CDL	C19-C20-C21-C22
5	L	1288	BCL	C8-C10-C11-C12
5	M	1303	BCL	C8-C10-C11-C12
5	M	1304	BCL	C15-C16-C17-C18
7	M	1311	BPH	C15-C16-C17-C18
6	M	1307	LDA	C1-C2-C3-C4
5	L	1288	BCL	C13-C15-C16-C17
7	M	1311	BPH	C16-C17-C18-C19
6	L	1285	LDA	C5-C6-C7-C8
5	L	1288	BCL	C2A-CAA-CBA-CGA
6	M	1306	LDA	C6-C7-C8-C9
6	M	1309	LDA	C7-C8-C9-C10
6	M	1309	LDA	C6-C7-C8-C9
6	M	1309	LDA	C2-C3-C4-C5
6	M	1309	LDA	C11-C10-C9-C8
5	M	1303	BCL	CBD-CGD-O2D-CED
14	M	1314	CDL	C74-C75-C76-C77
7	L	1286	BPH	C2-C3-C5-C6
6	L	1284	LDA	C1-C2-C3-C4
5	L	1282	BCL	C14-C13-C15-C16
14	M	1314	CDL	C16-C17-C18-C19
7	M	1311	BPH	C5-C6-C7-C8
6	L	1283	LDA	C2-C3-C4-C5
6	M	1308	LDA	C5-C6-C7-C8
7	L	1286	BPH	O1D-CGD-O2D-CED
14	M	1314	CDL	CA3-CA4-CA6-OA8
6	M	1306	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	L	1285	LDA	C9-C10-C11-C12
6	L	1283	LDA	C9-C10-C11-C12
14	M	1314	CDL	C40-C41-C42-C43
8	L	1287[B]	UQ2	C12-C13-C14-C16
4	H	1252	GOL	O2-C2-C3-O3
5	M	1303	BCL	C4-C3-C5-C6
7	L	1286	BPH	C4-C3-C5-C6
7	M	1311	BPH	C4-C3-C5-C6
6	M	1309	LDA	C1-C2-C3-C4
6	M	1305	LDA	C11-C10-C9-C8
6	M	1307	LDA	C3-C4-C5-C6
14	M	1314	CDL	C18-C19-C20-C21
13	M	1313	SPO	C3-C1-O1-CM1
13	M	1313	SPO	C11-C12-C14-C15
13	M	1313	SPO	C21-C22-C23-C25
6	M	1307	LDA	C5-C6-C7-C8
7	M	1311	BPH	C16-C17-C18-C20
13	M	1313	SPO	C3-C1-C4-C5
6	M	1306	LDA	C9-C10-C11-C12
6	L	1285	LDA	C11-C10-C9-C8
5	L	1288	BCL	C11-C12-C13-C15
5	M	1304	BCL	C12-C13-C15-C16
7	M	1311	BPH	C6-C7-C8-C10
7	M	1311	BPH	C11-C12-C13-C15
6	L	1285	LDA	C1-C2-C3-C4
5	M	1304	BCL	C14-C13-C15-C16
7	M	1311	BPH	C6-C7-C8-C9
7	M	1311	BPH	C11-C12-C13-C14
10	L	1290	HTO	C2-C3-C4-C5
6	L	1285	LDA	N1-C1-C2-C3
6	M	1306	LDA	N1-C1-C2-C3
6	M	1709	LDA	N1-C1-C2-C3
7	M	1311	BPH	C13-C15-C16-C17
14	M	1314	CDL	OA5-CA3-CA4-CA6
5	M	1303	BCL	C2-C3-C5-C6
7	M	1311	BPH	C2-C3-C5-C6
14	M	1314	CDL	C80-C81-C82-C83
6	M	1308	LDA	C7-C8-C9-C10
6	M	1307	LDA	C11-C10-C9-C8
10	L	1290	HTO	C1-C2-C3-O3
6	M	1309	LDA	C5-C6-C7-C8
12	M	1312	U10	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	O1D-CGD-O2D-CED
4	H	1251	GOL	O2-C2-C3-O3
14	M	1314	CDL	OA5-CA3-CA4-OA6
14	M	1314	CDL	C37-C38-C39-C40
14	M	1314	CDL	OA6-CA4-CA6-OA8
8	L	1287[B]	UQ2	C9-C11-C12-C13
6	L	1284	LDA	C2-C3-C4-C5
5	M	1303	BCL	C14-C13-C15-C16
5	M	1303	BCL	C4C-C3C-CAC-CBC
14	M	1314	CDL	C21-C22-C23-C24
6	M	1307	LDA	C2-C3-C4-C5
5	L	1282	BCL	C12-C13-C15-C16
13	M	1313	SPO	C12-C14-C15-C16
7	L	1286	BPH	CAD-CBD-CGD-O2D
5	M	1304	BCL	C3-C5-C6-C7
14	M	1314	CDL	OB6-CB4-CB6-OB8
4	M	1315	GOL	O1-C1-C2-O2
7	M	1311	BPH	C2C-C3C-CAC-CBC
6	M	1308	LDA	C4-C5-C6-C7
6	M	1309	LDA	C9-C10-C11-C12
6	M	1709	LDA	C7-C8-C9-C10
5	M	1303	BCL	C11-C10-C8-C7
14	M	1314	CDL	C31-C32-C33-C34
6	M	1709	LDA	C6-C7-C8-C9
6	M	1306	LDA	C7-C8-C9-C10
7	M	1311	BPH	C4C-C3C-CAC-CBC
5	M	1303	BCL	C6-C7-C8-C9
5	M	1304	BCL	C11-C10-C8-C9
4	H	1252	GOL	O1-C1-C2-O2
5	M	1304	BCL	C8-C10-C11-C12
8	L	1287[A]	UQ2	C4-C3-O3-CM3
5	M	1303	BCL	C2-C1-O2A-CGA
6	M	1709	LDA	C3-C4-C5-C6
13	M	1313	SPO	C2-C1-O1-CM1
14	M	1314	CDL	CA3-OA5-PA1-OA2
6	M	1709	LDA	C11-C10-C9-C8
5	M	1303	BCL	C11-C10-C8-C9
6	M	1307	LDA	N1-C1-C2-C3
12	M	1312	U10	C33-C34-C36-C37
14	M	1314	CDL	C81-C82-C83-C84
13	M	1313	SPO	C17-C19-C20-C21
14	M	1314	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	L	1288	BCL	C2-C1-O2A-CGA
10	L	1290	HTO	C4-C5-C6-C7
5	M	1304	BCL	C11-C12-C13-C14
14	M	1314	CDL	C79-C80-C81-C82
14	M	1314	CDL	CB3-CB4-CB6-OB8
6	M	1709	LDA	C5-C6-C7-C8
8	L	1287[B]	UQ2	C1-C2-O2-CM2
12	M	1312	U10	C5-C4-O4-C4M
12	M	1312	U10	C14-C16-C17-C18
6	M	1309	LDA	C3-C4-C5-C6
4	M	1315	GOL	C1-C2-C3-O3
8	L	1287[A]	UQ2	C12-C11-C9-C10
12	M	1312	U10	C25-C24-C26-C27
5	M	1304	BCL	C16-C17-C18-C19
6	M	1308	LDA	C2-C3-C4-C5
5	M	1303	BCL	C6-C7-C8-C10
5	L	1282	BCL	C1-C2-C3-C4
7	L	1286	BPH	C1-C2-C3-C4
5	M	1304	BCL	CAA-CBA-CGA-O2A
12	M	1312	U10	C30-C29-C31-C32
5	L	1288	BCL	CAD-CBD-CGD-O2D
7	M	1311	BPH	CAD-CBD-CGD-O2D
12	M	1312	U10	C23-C24-C26-C27
12	M	1312	U10	C31-C32-C33-C34
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
6	M	1309	LDA	C2-C1-N1-CM2
14	M	1314	CDL	C52-C51-CB5-OB6
8	L	1287[A]	UQ2	C12-C11-C9-C8
6	M	1709	LDA	C2-C3-C4-C5
7	L	1286	BPH	CHA-CBD-CGD-O1D
13	M	1313	SPO	C2-C1-C4-C5
12	M	1312	U10	C3-C4-O4-C4M
10	L	1290	HTO	C3-C4-C5-C6
14	M	1314	CDL	CA3-OA5-PA1-OA4
14	M	1314	CDL	C52-C51-CB5-OB7
4	M	1315	GOL	O2-C2-C3-O3
14	M	1314	CDL	C76-C77-C78-C79
14	M	1314	CDL	C72-C71-CB7-OB8
5	L	1282	BCL	C2B-C3B-CAB-OBB

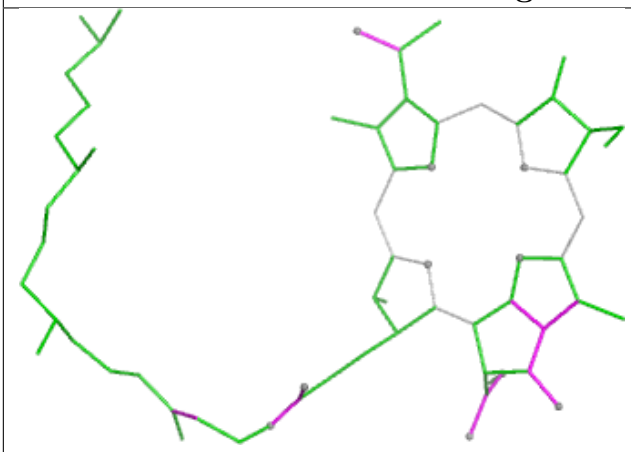
There are no ring outliers.

20 monomers are involved in 69 short contacts:

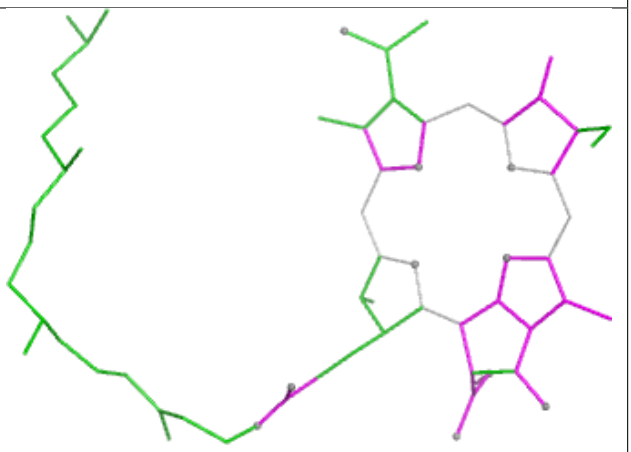
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1286	BPH	7	0
8	L	1287[B]	UQ2	1	0
6	M	1309	LDA	2	0
14	M	1314	CDL	2	0
4	L	1291	GOL	1	0
8	L	1287[A]	UQ2	6	0
6	M	1305	LDA	3	0
7	M	1311	BPH	11	0
5	M	1304	BCL	14	0
5	L	1288	BCL	2	0
6	M	1308	LDA	2	0
4	H	1251	GOL	1	0
4	M	1315	GOL	2	0
6	L	1285	LDA	4	0
6	M	1307	LDA	5	0
5	M	1303	BCL	11	0
5	L	1282	BCL	4	0
6	L	1284	LDA	2	0
6	L	1283	LDA	1	0
13	M	1313	SPO	4	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.

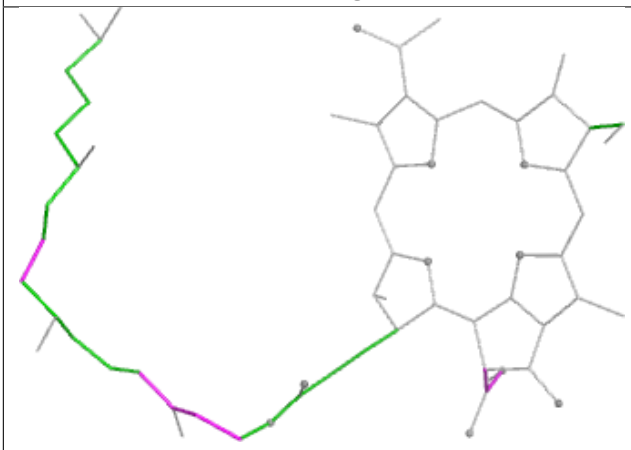
Ligand BPH L 1286



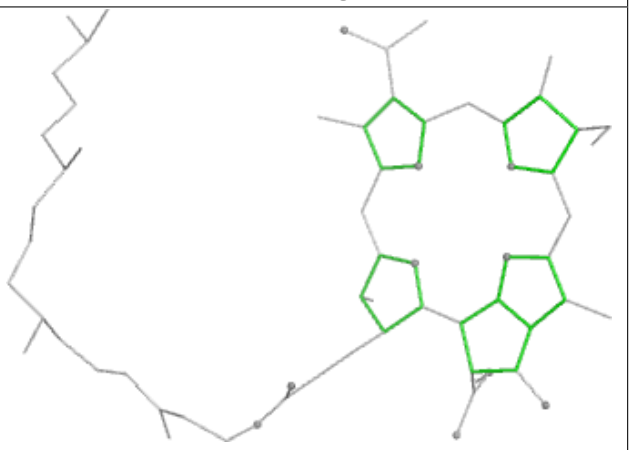
Bond lengths



Bond angles

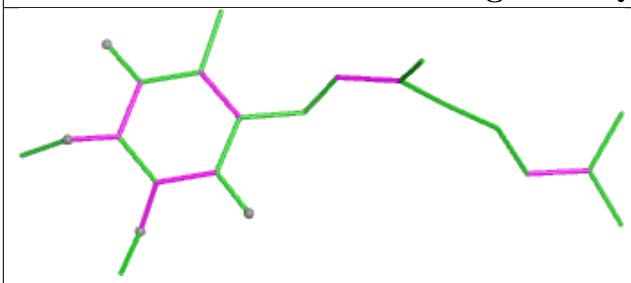


Torsions

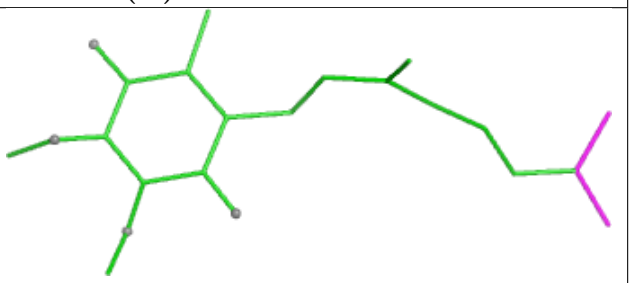


Rings

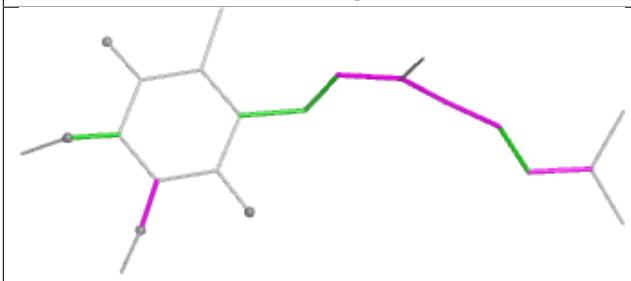
Ligand UQ2 L 1287 (B)



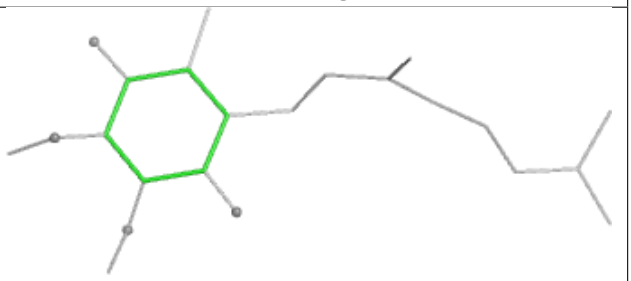
Bond lengths



Bond angles

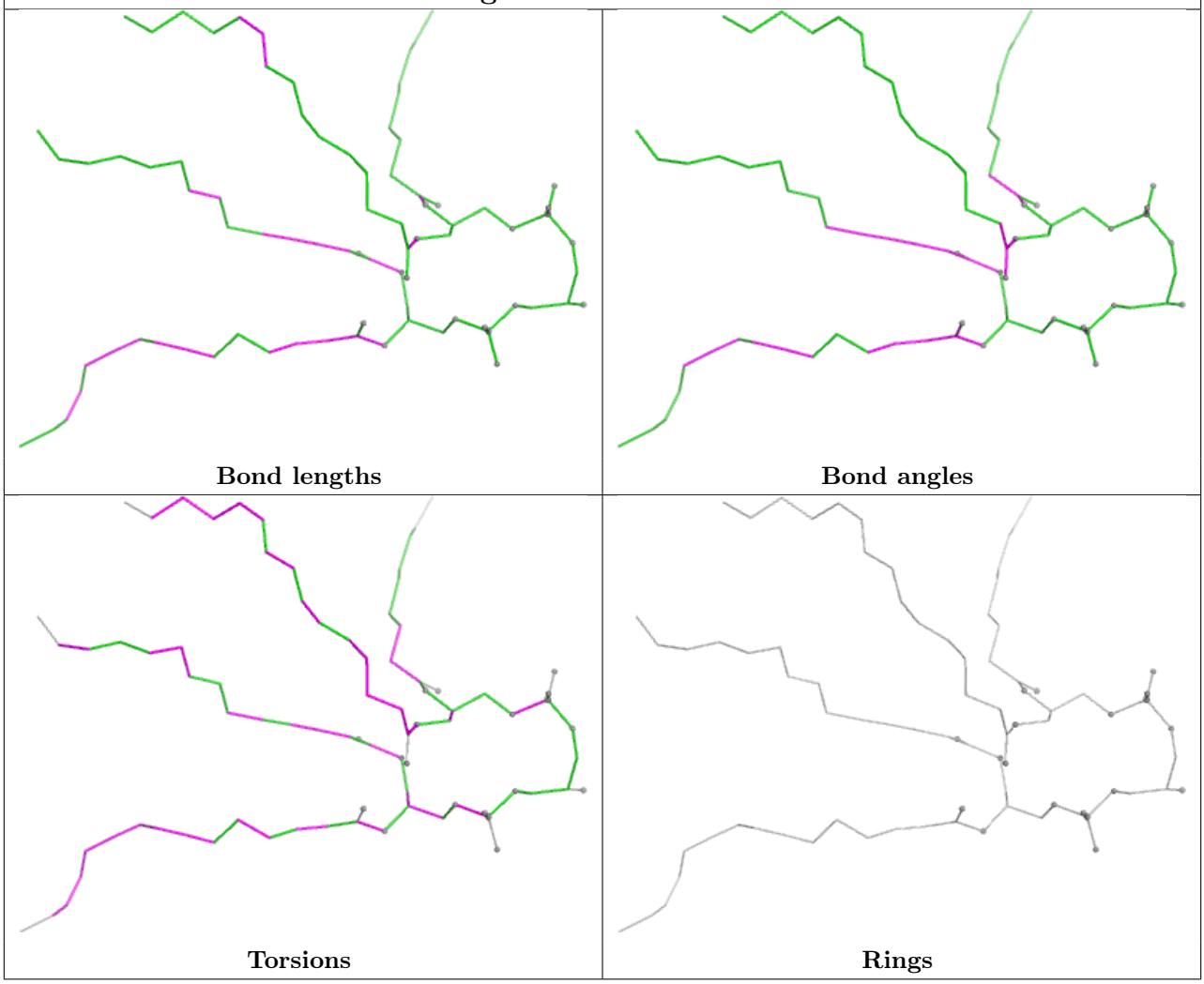


Torsions

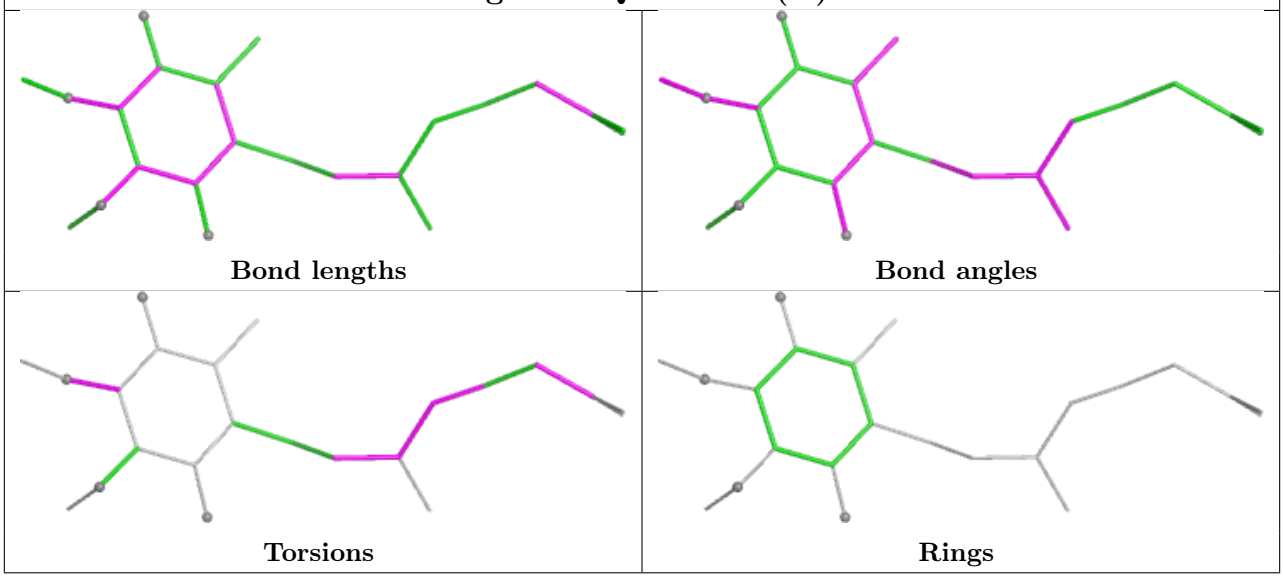


Rings

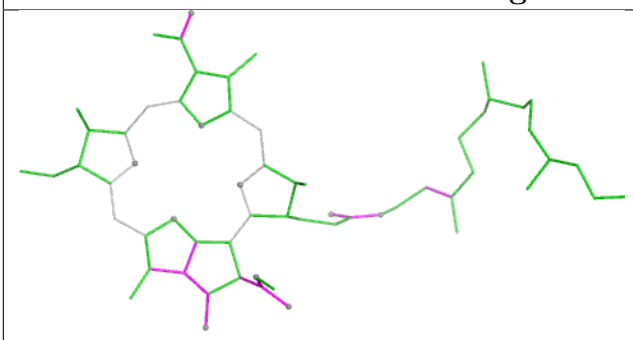
Ligand CDL M 1314



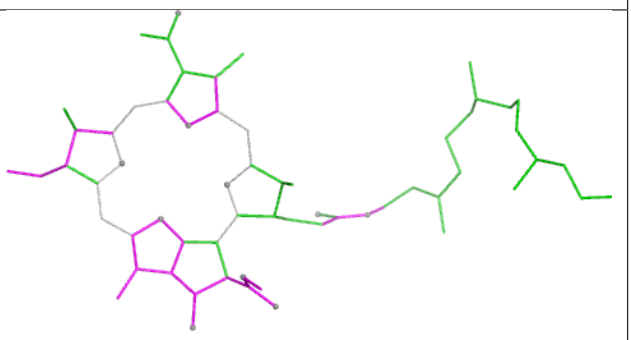
Ligand UQ2 L 1287 (A)



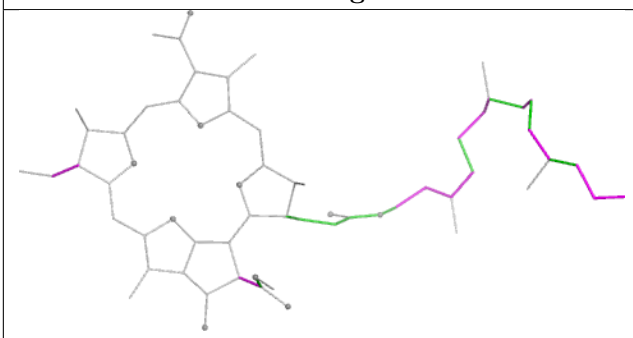
Ligand BPH M 1311



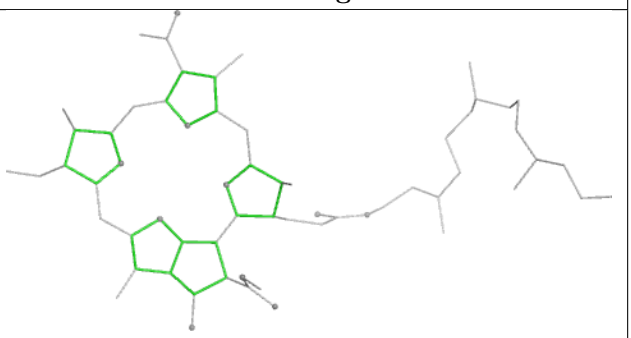
Bond lengths



Bond angles

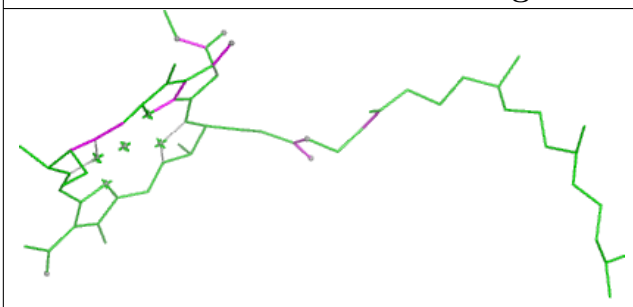


Torsions

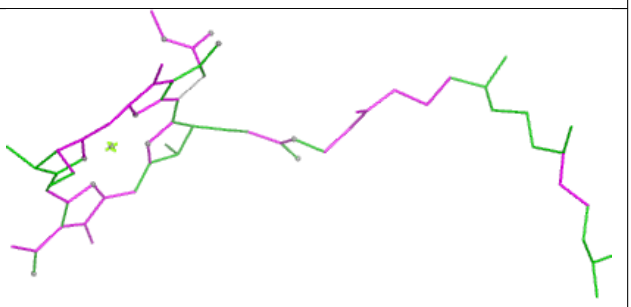


Rings

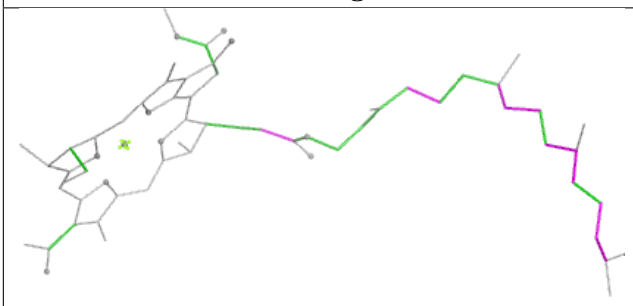
Ligand BCL M 1304



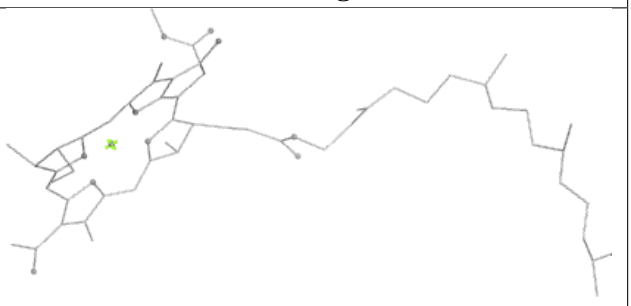
Bond lengths



Bond angles

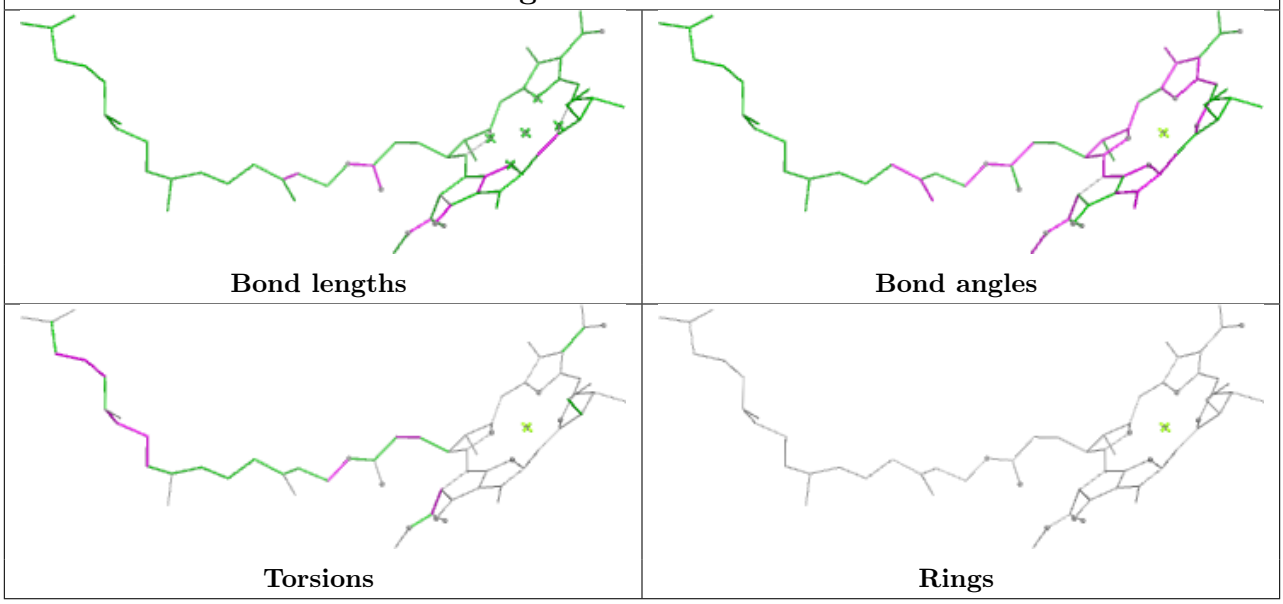


Torsions

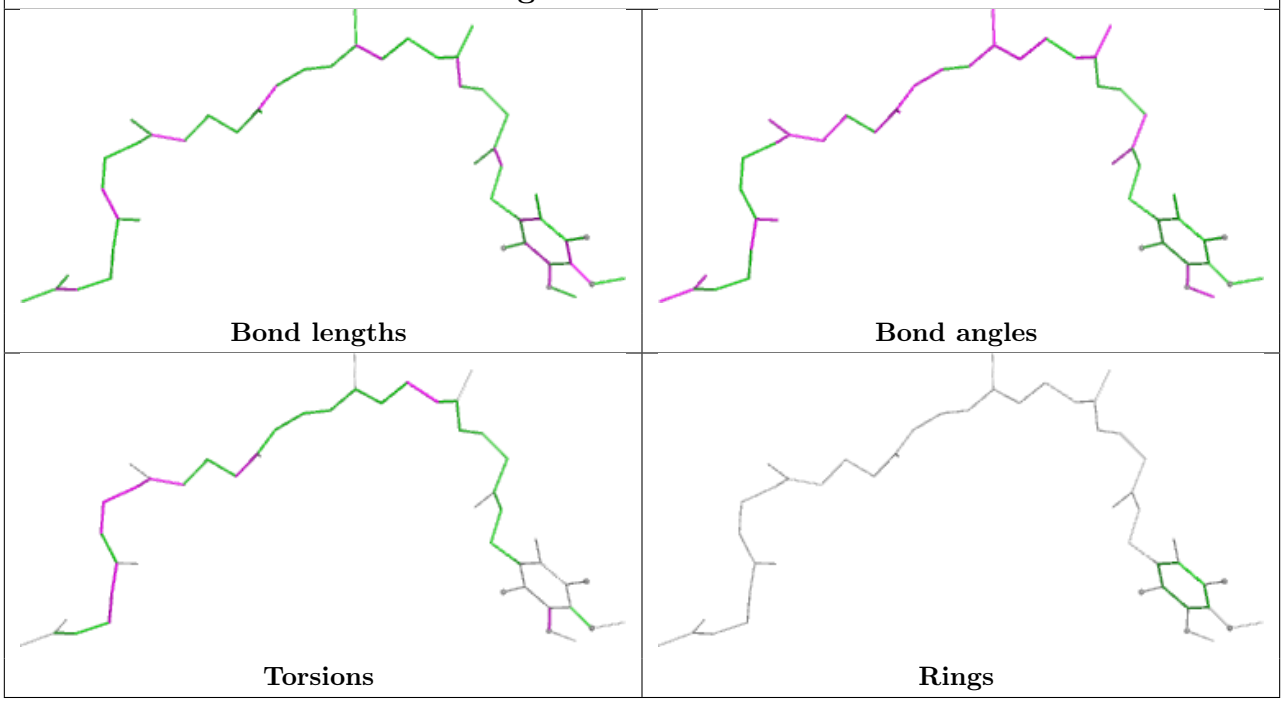


Rings

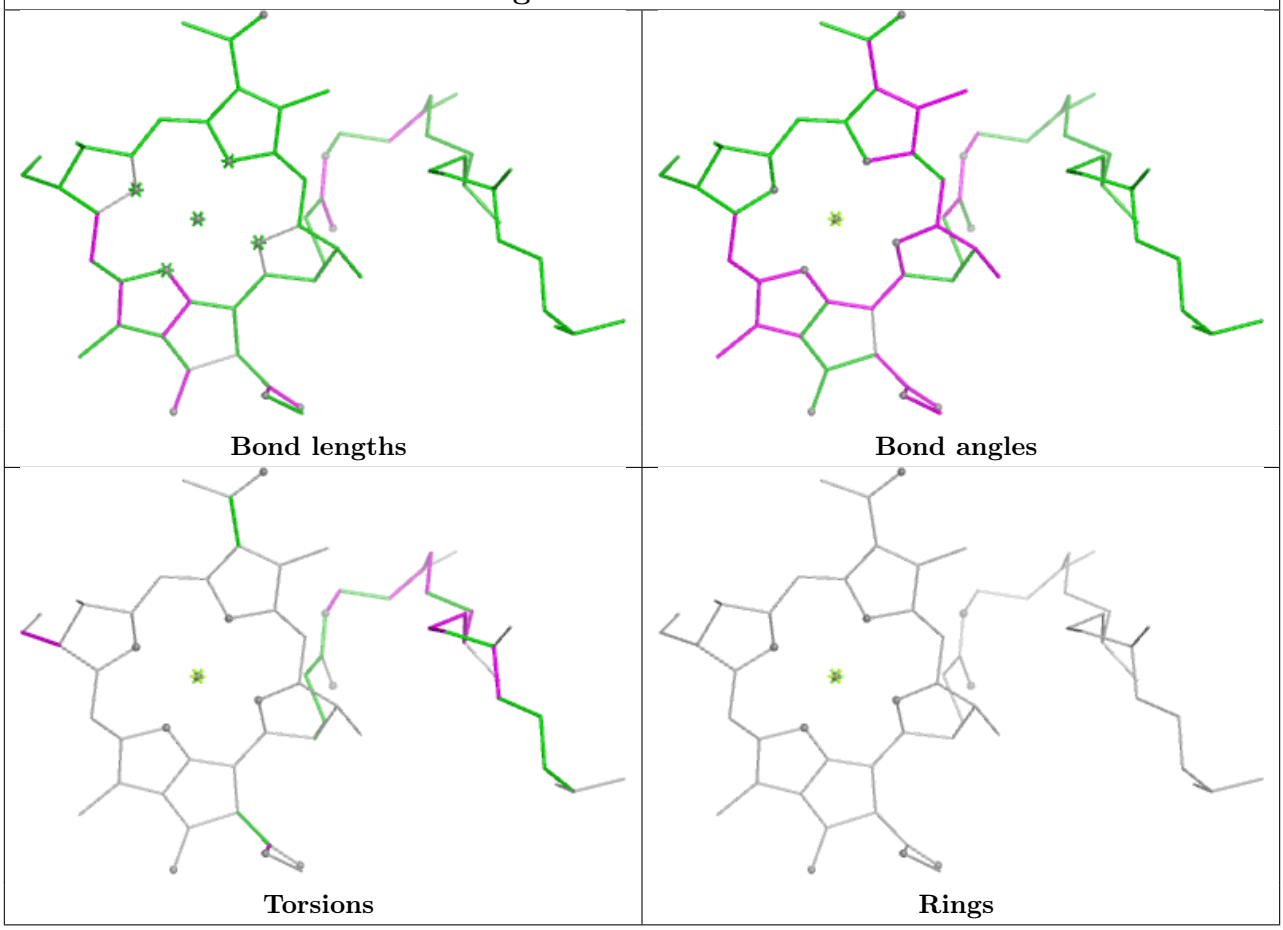
Ligand BCL L 1288



Ligand U10 M 1312

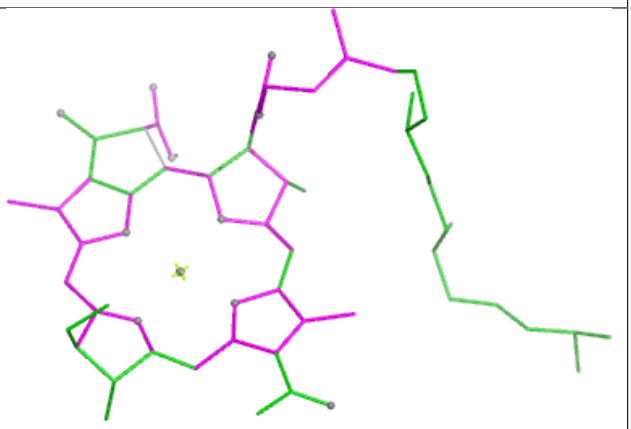


Ligand BCL M 1303

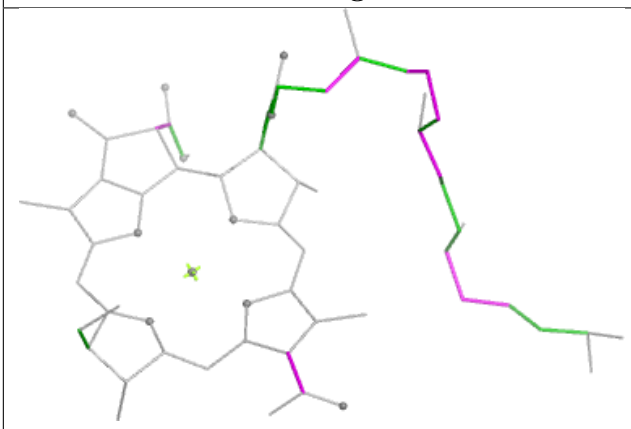


Ligand BCL L 1282

Bond lengths



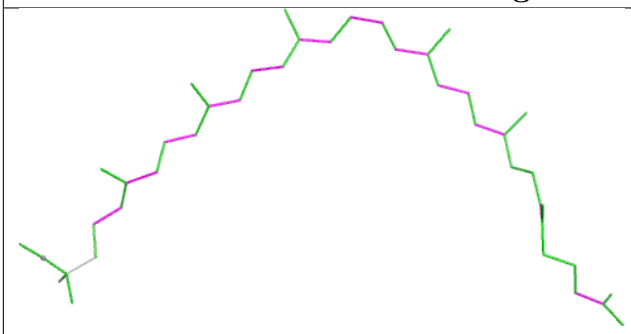
Bond angles



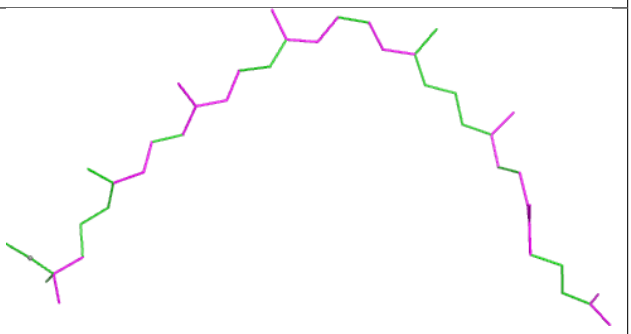
Torsions

Rings

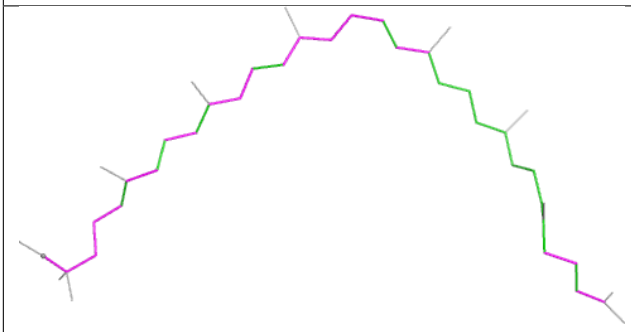
Ligand SPO M 1313



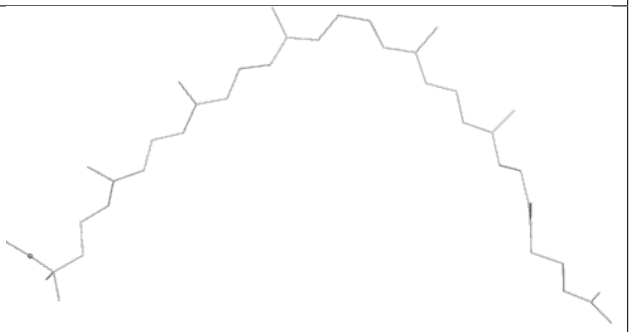
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	241/260 (92%)	-0.21	8 (3%)	49	45	25, 42, 53, 84	3 (1%)
2	L	281/281 (100%)	-0.16	3 (1%)	78	75	30, 39, 61, 68	0
3	M	303/307 (98%)	-0.03	10 (3%)	49	45	29, 44, 69, 76	0
All	All	825/848 (97%)	-0.13	21 (2%)	58	54	25, 42, 63, 84	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	148	TRP	5.4
3	M	1	ALA	5.1
3	M	52	LEU	5.1
3	M	2	GLU	5.0
1	H	249	LYS	4.3
3	M	301	HIS	4.2
3	M	3	TYR	4.0
1	H	251	VAL	3.8
1	H	250	SER	3.5
2	L	72	GLU	2.9
3	M	302	GLY	2.7
3	M	300	ASN	2.6
1	H	247	LYS	2.4
2	L	59	TRP	2.4
3	M	188	ASN	2.3
1	H	138	ALA	2.2
1	H	94	GLU	2.0
2	L	51	TRP	2.0
1	H	18	TYR	2.0
1	H	248	ARG	2.0
3	M	80	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LDA	M	1309	16/16	0.62	0.43	94,102,110,110	0
14	CDL	M	1314	81/100	0.62	0.39	96,107,120,121	0
6	LDA	M	1308	16/16	0.69	0.37	90,97,105,105	0
6	LDA	L	1284	16/16	0.73	0.35	98,102,109,109	0
6	LDA	M	1709	16/16	0.76	0.32	92,100,107,107	0
6	LDA	L	1285	16/16	0.76	0.29	106,109,111,111	0
6	LDA	L	1283	16/16	0.77	0.33	86,103,111,111	0
4	GOL	M	1315	6/6	0.81	0.18	85,86,86,87	0
6	LDA	M	1305	16/16	0.81	0.24	50,63,70,71	0
6	LDA	M	1307	16/16	0.84	0.23	64,68,77,77	0
10	HTO	L	1290	10/10	0.85	0.27	74,77,77,78	0
4	GOL	H	1251	6/6	0.85	0.19	65,68,70,71	0
4	GOL	H	1254	6/6	0.86	0.18	102,102,103,103	0
8	UQ2	L	1287[A]	23/23	0.86	0.21	39,42,51,52	23
8	UQ2	L	1287[B]	23/23	0.86	0.21	40,43,47,48	23
4	GOL	H	1253	6/6	0.86	0.15	102,103,104,104	0
6	LDA	M	1306	16/16	0.86	0.24	72,74,84,84	0
4	GOL	L	1291	6/6	0.89	0.16	47,52,53,54	0
4	GOL	L	1292	6/6	0.91	0.17	85,87,87,87	0
9	PO4	L	1289	5/5	0.91	0.17	103,103,103,103	0
12	U10	M	1312	48/63	0.92	0.13	30,39,68,69	0
4	GOL	H	1252	6/6	0.93	0.15	88,89,89,89	0
5	BCL	M	1303	66/66	0.94	0.11	26,31,80,81	0
13	SPO	M	1313	42/42	0.94	0.13	38,51,68,71	0
7	BPH	M	1311	65/65	0.94	0.12	35,42,94,95	0
7	BPH	L	1286	65/65	0.96	0.07	25,30,39,40	0
5	BCL	M	1304	66/66	0.96	0.08	25,31,53,59	0

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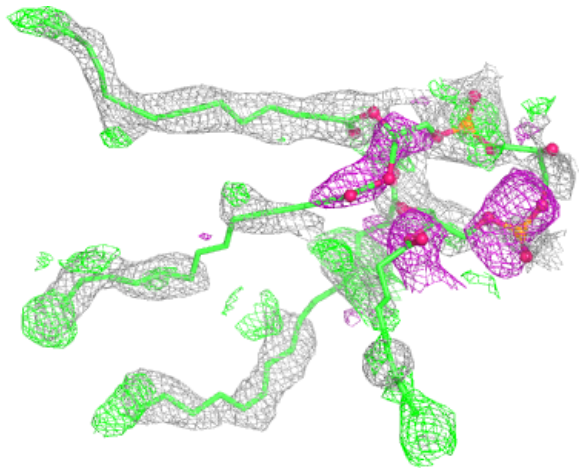
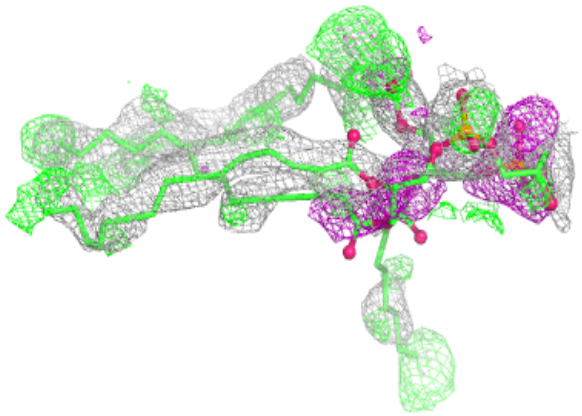
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BCL	L	1282	66/66	0.96	0.08	30,34,51,54	0
5	BCL	L	1288	66/66	0.97	0.07	25,30,48,52	0
11	FE	M	1310	1/1	1.00	0.05	32,32,32,32	0

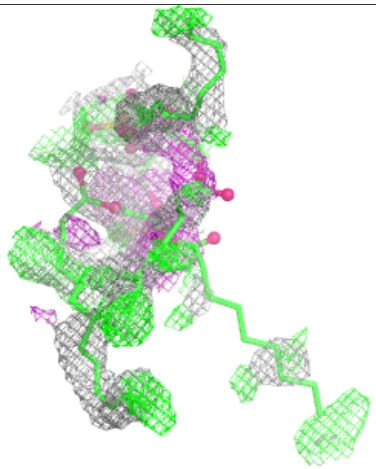
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL M 1314:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

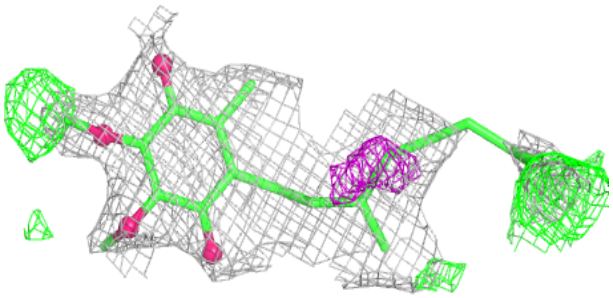


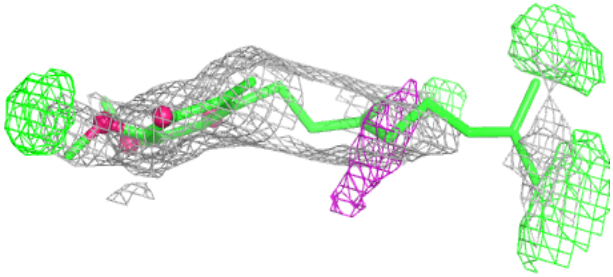


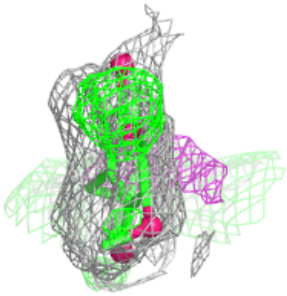


Electron density around UQ2 L 1287 (A):

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

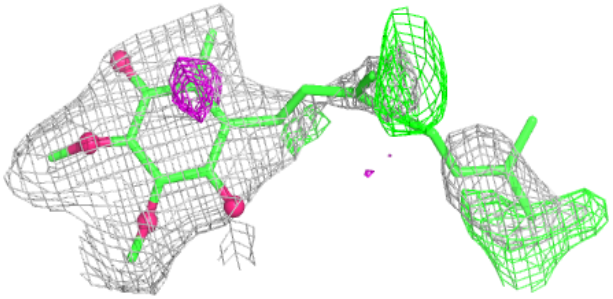


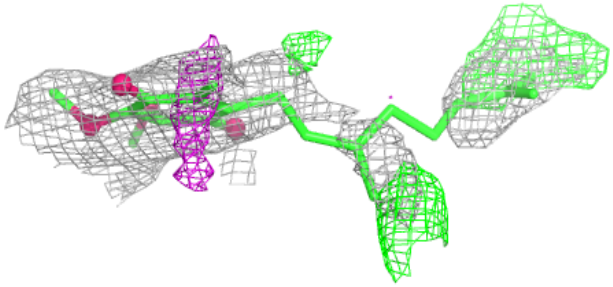


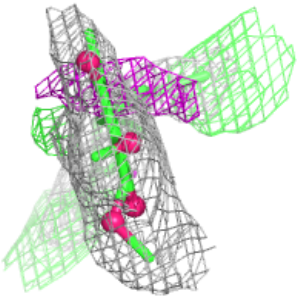


Electron density around UQ2 L 1287 (B):

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

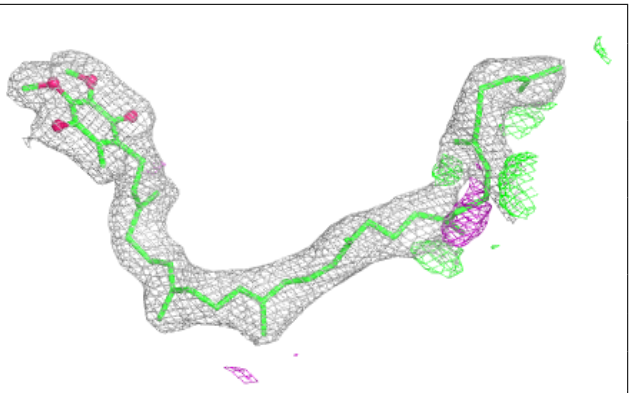


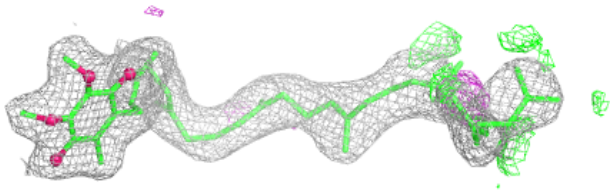


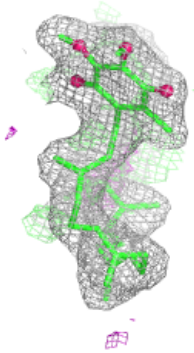


Electron density around U10 M 1312:

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

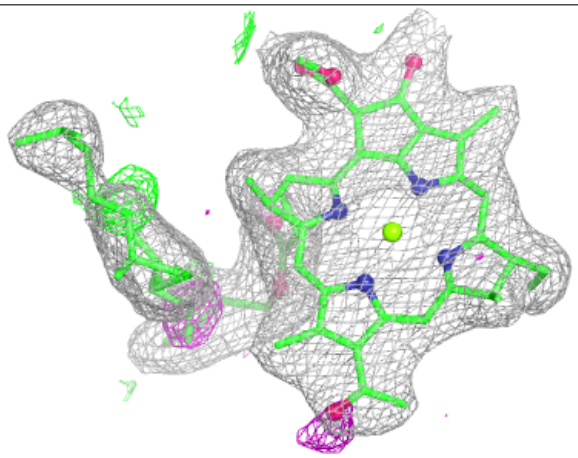


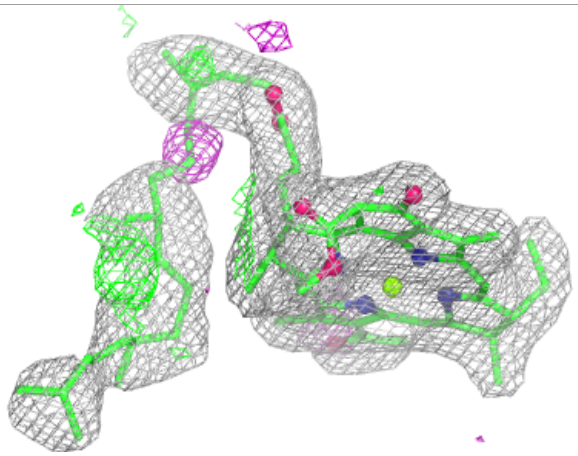




Electron density around BCL M 1303:

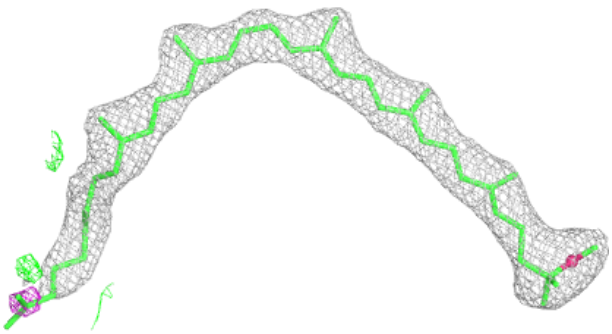
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

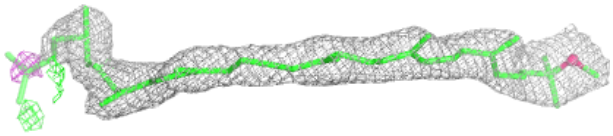


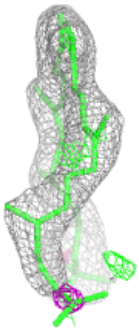


Electron density around SPO M 1313:

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

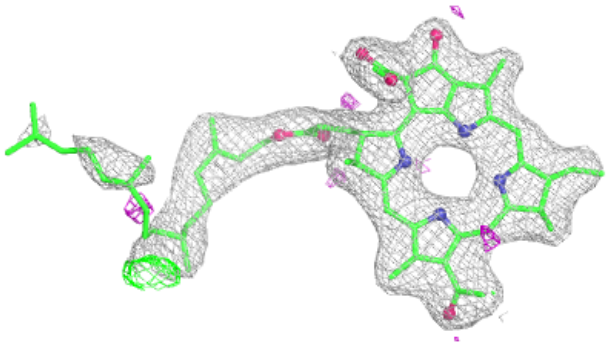


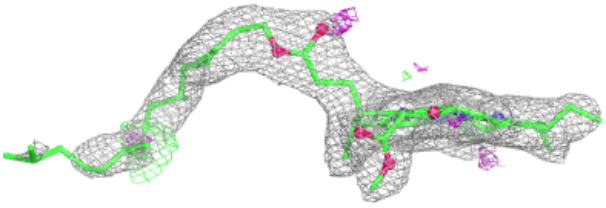




Electron density around BPH M 1311:

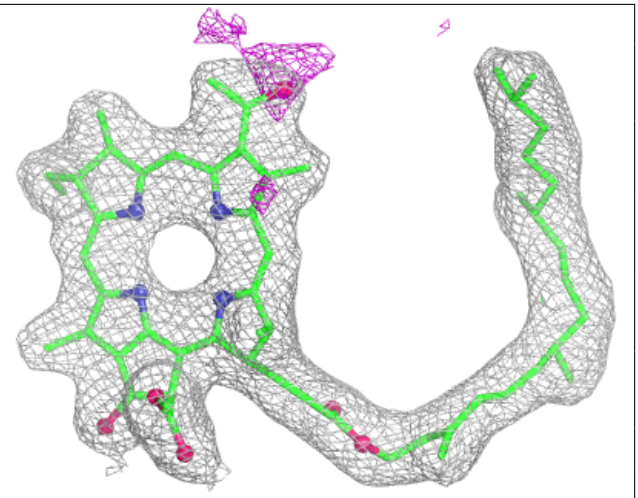
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

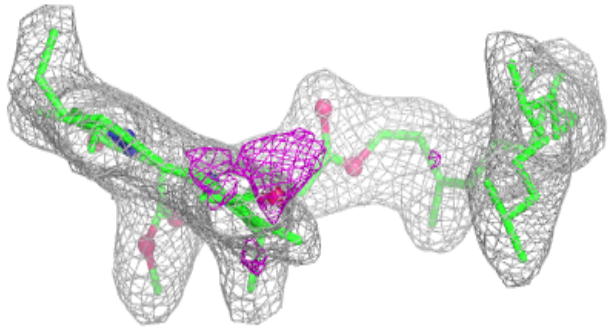


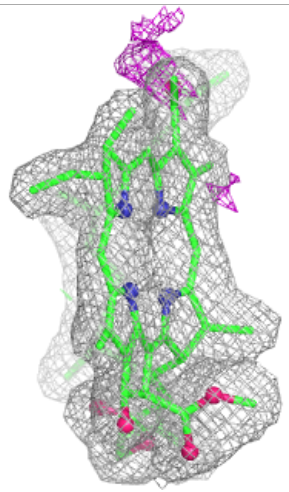


Electron density around BPH L 1286:

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

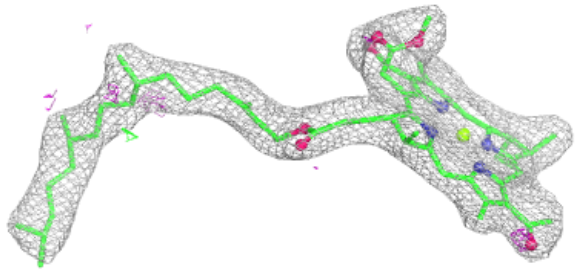


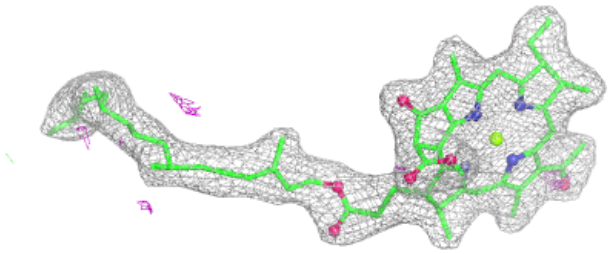


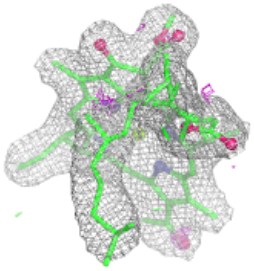


Electron density around BCL M 1304:

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

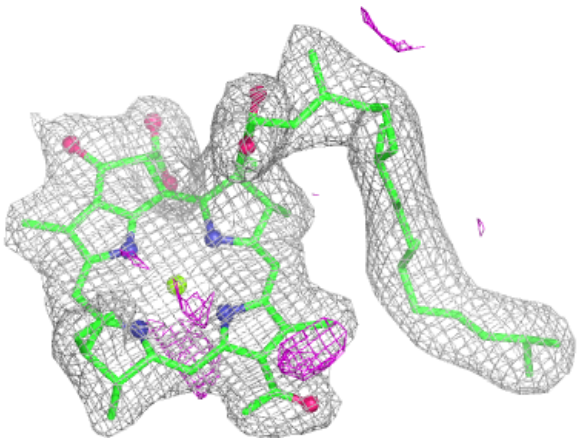


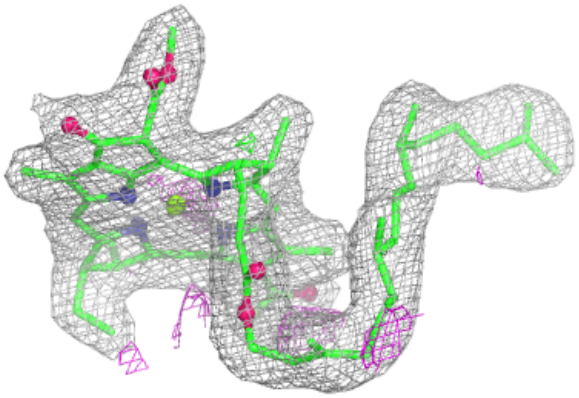


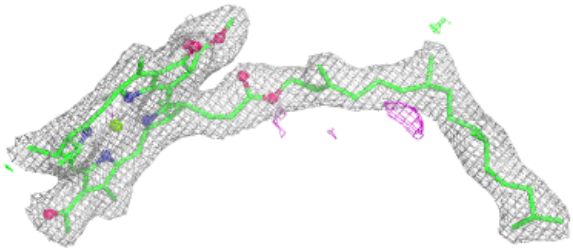
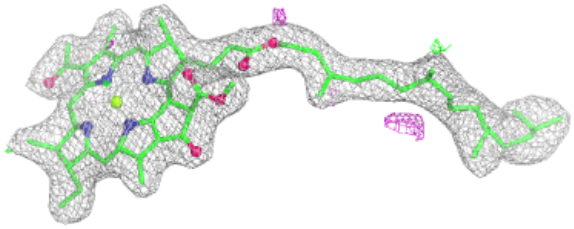
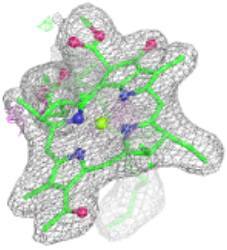


Electron density around BCL L 1282:

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





Electron density around BCL L 1288: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.