Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:42 am GMT

PDB ID	:	2UXM
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 10 in the charge-separated state, 2nd dataset
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-28
Resolution	:	2.70 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:

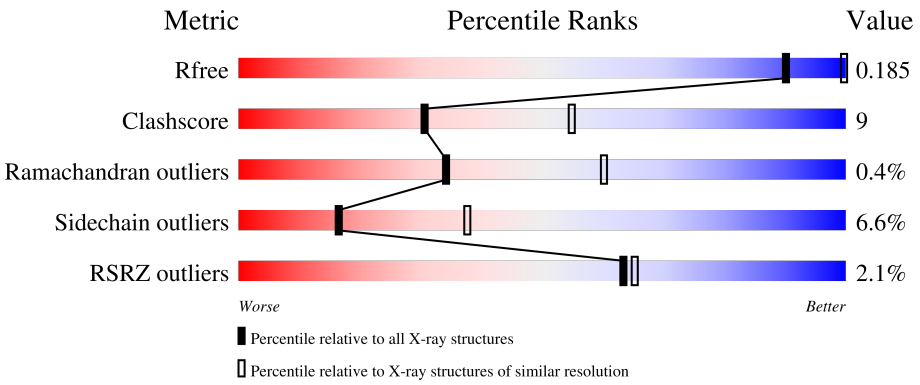
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% 75% 17% • 7%
2	L	281	% 86% 14%
3	M	307	2% 79% 18% ••

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	301	X	-	-	-
5	BCL	L	302	X	-	-	-
5	BCL	M	401	X	-	-	-
5	BCL	M	402	X	-	-	-
6	LDA	L	303	-	-	-	X
6	LDA	L	310	-	-	-	X
6	LDA	L	311	-	-	-	X
6	LDA	L	312	-	-	-	X
6	LDA	M	405	-	-	X	-
6	LDA	M	406	-	-	-	X
9	PO4	L	306	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 7442 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

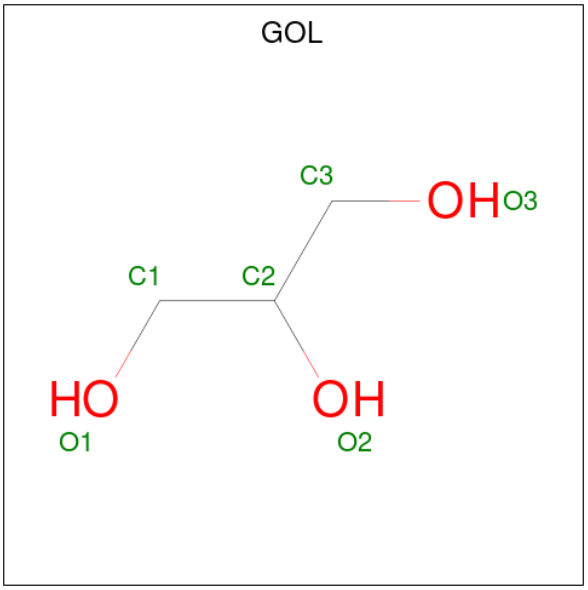
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

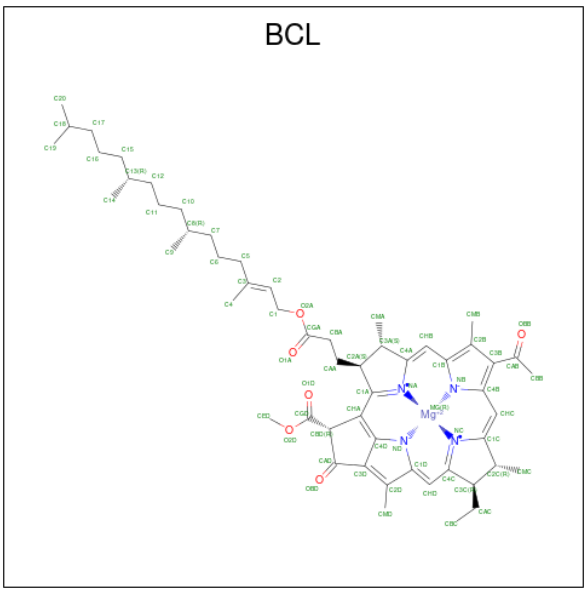
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



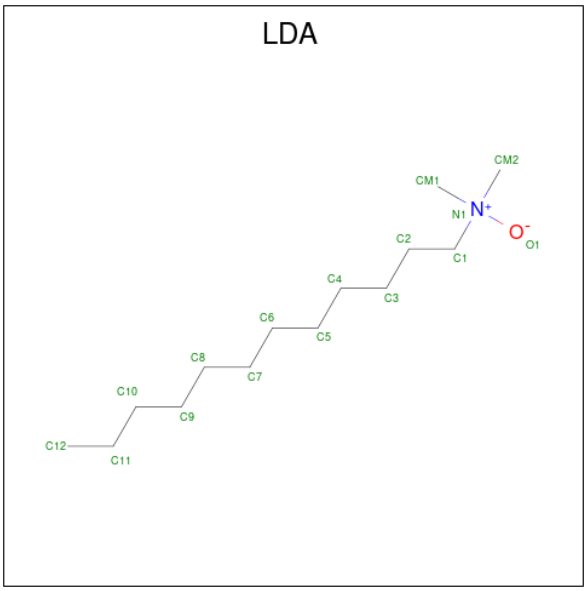
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	H	1	6	3	3		0	0
			Total	C	O			
4	L	1	6	3	3		0	0
			Total	C	O			
4	L	1	6	3	3		0	0
			Total	C	O			
4	L	1	6	3	3		0	0

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



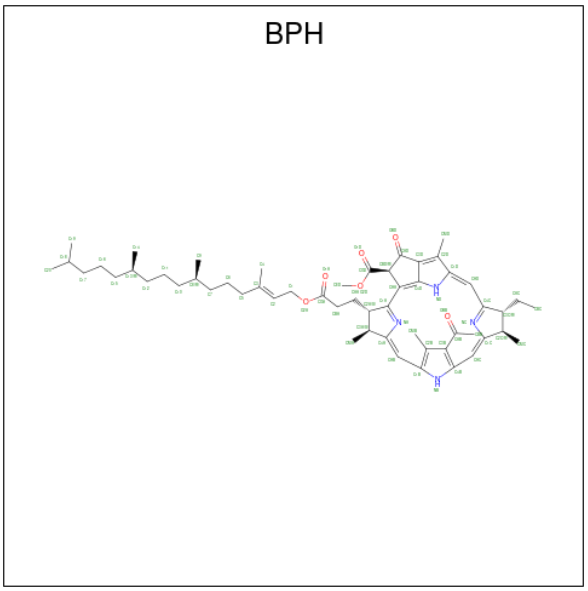
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

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



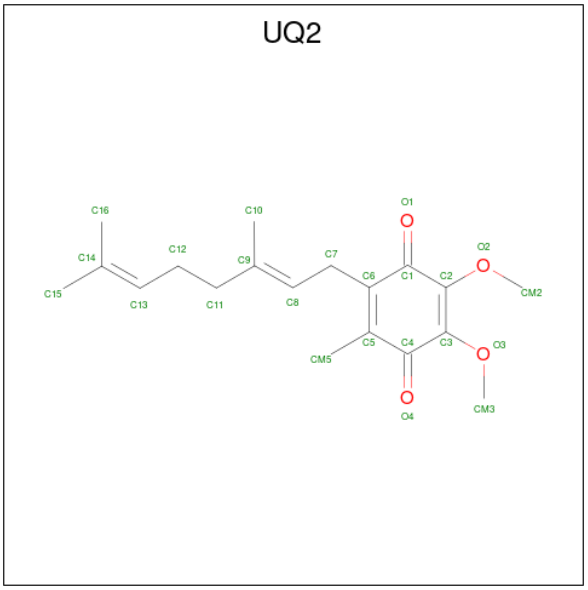
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0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

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



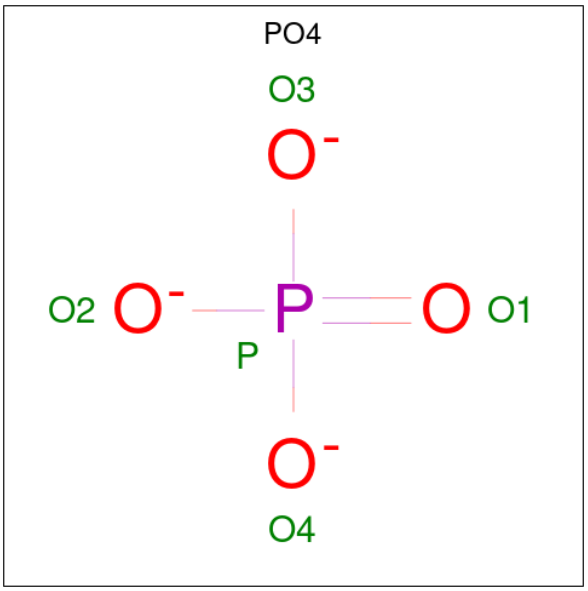
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
			Total	C	N	O		
7	L	1	65	55	4	6	0	0

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



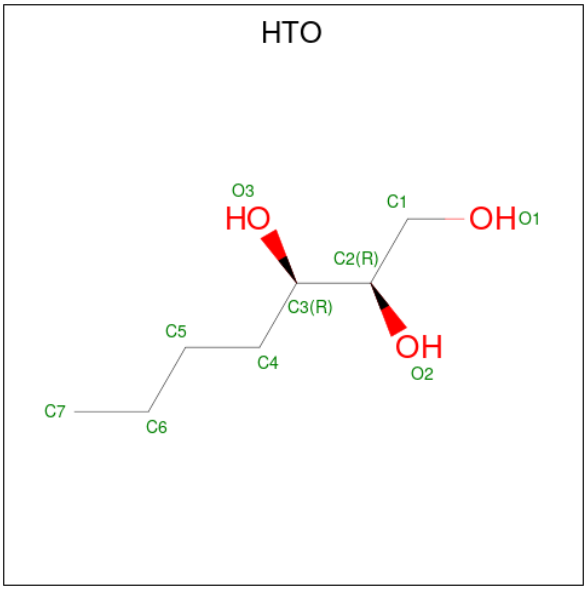
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1

- Molecule 9 is PHOSPHATE ION (three-letter code: 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 (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

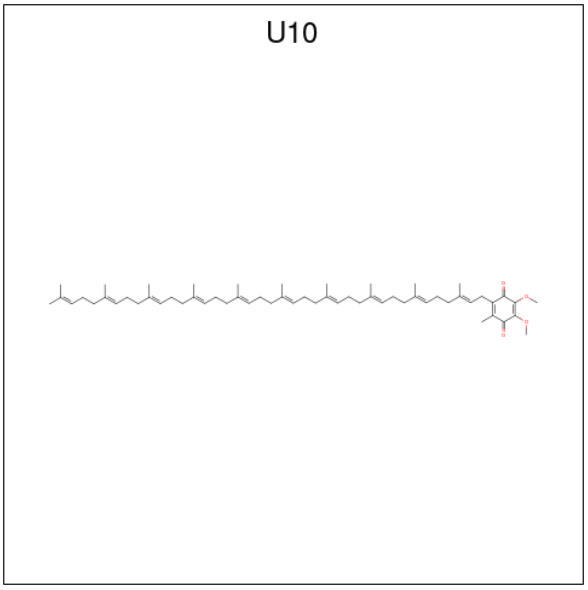


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

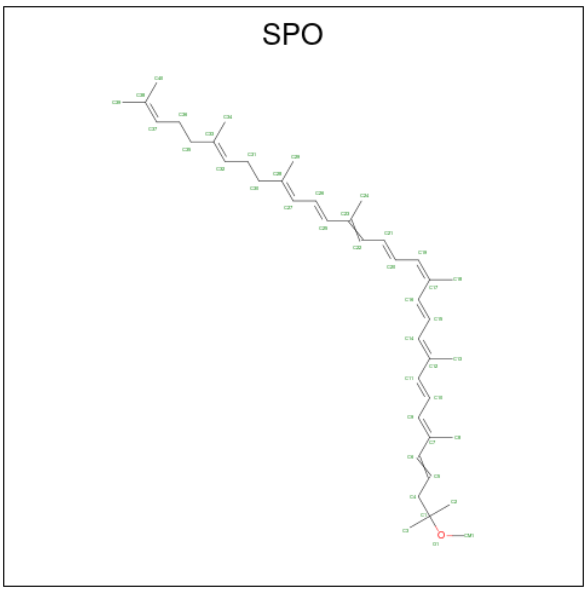
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
11	M	1	1	1	0	0

- Molecule 12 is UBIQUINONE-10 (three-letter code: 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 (three-letter code: 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 water.

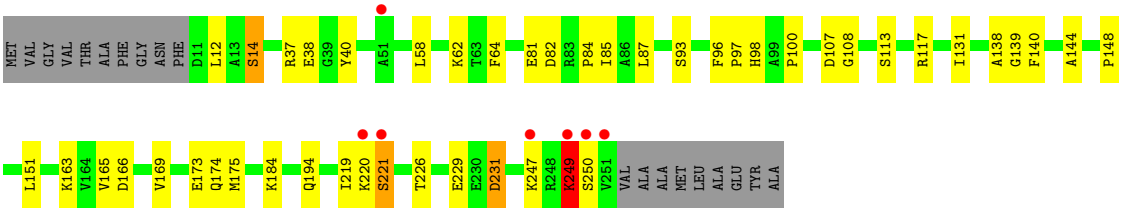
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	H	79	79	79	0	0
			Total	O		
14	L	91	91	91	0	0
			Total	O		
14	M	71	71	71	0	0

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.

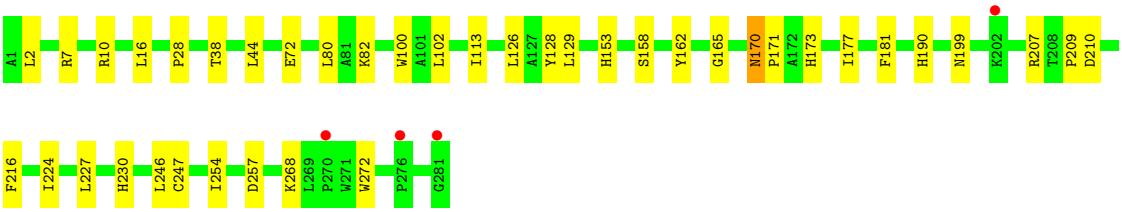
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



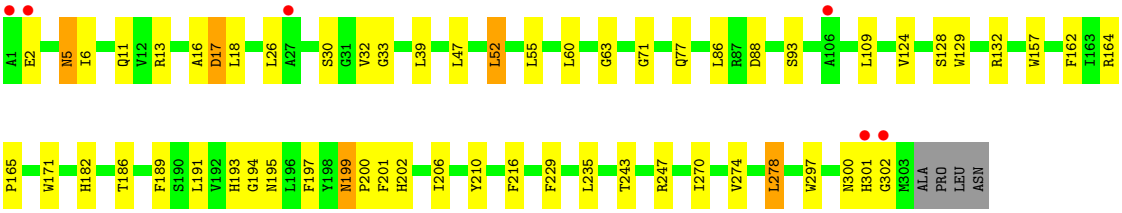
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

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	139.45Å 139.45Å 185.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.70 29.89 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.4 (119.52-2.70) 85.5 (29.89-2.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.186 , 0.221 0.182 , 0.185	Depositor DCC
R_{free} test set	3339 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, UQ2, LDA, U10, FE, HTO, SPO, BPH, BCL, GOL

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	0.70	0/1906	0.81	5/2591 (0.2%)
2	L	0.73	0/2320	0.72	1/3175 (0.0%)
3	M	0.68	0/2501	0.75	3/3415 (0.1%)
All	All	0.70	0/6727	0.76	9/9181 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	231	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	82	ASP	CB-CG-OD2	5.32	123.09	118.30
2	L	257	ASP	CB-CG-OD2	5.32	123.08	118.30
1	H	107	ASP	CB-CG-OD2	5.24	123.02	118.30
3	M	17	ASP	CB-CG-OD2	5.19	122.97	118.30
3	M	88	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	250	SER	O-C-N	-5.09	114.55	122.70
1	H	166	ASP	CB-CG-OD2	5.07	122.86	118.30
3	M	86	LEU	CA-CB-CG	5.06	126.94	115.30

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	28	0
2	L	2232	0	2187	26	0
3	M	2409	0	2321	47	0
4	H	6	0	8	0	0
4	L	18	0	24	2	0
5	L	132	0	148	9	0
5	M	132	0	148	20	0
6	L	80	0	155	11	0
6	M	64	0	124	11	0
7	L	130	0	152	14	0
8	L	46	0	52	13	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	4	0
13	M	42	0	60	6	0
14	H	79	0	0	1	1
14	L	91	0	0	2	0
14	M	71	0	0	0	0
All	All	7442	0	7319	134	1

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 (134) 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)
8:L:305[A]:UQ2:H152	6:L:311:LDA:H111	1.47	0.97
5:M:402:BCL:HBB3	5:M:402:BCL:HHC	1.50	0.91
8:L:305[B]:UQ2:H162	6:L:313:LDA:H121	1.56	0.87
2:L:72:GLU:HB3	14:L:416:HOH:O	1.74	0.87
1:H:249:LYS:HE3	1:H:249:LYS:HA	1.59	0.84
6:L:310:LDA:H62	6:M:405:LDA:H81	1.59	0.83
3:M:197:PHE:HZ	5:M:402:BCL:HBB2	1.42	0.83
3:M:197:PHE:CZ	5:M:402:BCL:HBB2	2.14	0.82
7:L:304:BPH:HHC	7:L:304:BPH:HBB3	1.61	0.81
1:H:226:THR:OG1	1:H:229:GLU:HG3	1.80	0.81
7:L:304:BPH:HHC	7:L:304:BPH:CBB	2.13	0.78
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.66	0.78
5:M:402:BCL:HHC	5:M:402:BCL:CBB	2.13	0.78
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.65	0.76
3:M:243:THR:O	3:M:247:ARG:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:403:LDA:H92	6:M:405:LDA:H121	1.66	0.75
2:L:28:PRO:HG3	6:L:310:LDA:HM21	1.68	0.75
7:L:314:BPH:HHC	5:M:402:BCL:H2	1.68	0.73
6:L:311:LDA:H11	3:M:33:GLY:HA2	1.69	0.73
7:L:304:BPH:HBB2	3:M:210:TYR:HB3	1.70	0.73
2:L:199:ASN:HA	4:L:308:GOL:H31	1.73	0.70
8:L:305[B]:UQ2:H162	6:L:313:LDA:C12	2.22	0.68
2:L:224:ILE:HG22	8:L:305[B]:UQ2:H8	1.74	0.68
6:M:403:LDA:H92	6:M:405:LDA:C12	2.23	0.68
2:L:190:HIS:HA	8:L:305[B]:UQ2:O4	1.94	0.68
2:L:170:ASN:HD22	2:L:170:ASN:C	1.97	0.67
1:H:194:GLN:HG3	3:M:5:ASN:ND2	2.09	0.67
14:L:460:HOH:O	6:M:405:LDA:H21	1.93	0.67
1:H:194:GLN:CG	3:M:5:ASN:ND2	2.58	0.67
2:L:181:PHE:HB3	7:L:314:BPH:HBB2	1.78	0.65
3:M:199:ASN:HD22	3:M:199:ASN:C	2.00	0.65
7:L:314:BPH:HHC	5:M:402:BCL:C2	2.28	0.64
2:L:181:PHE:CD2	7:L:314:BPH:HBB1	2.33	0.64
3:M:189:PHE:O	3:M:193:HIS:HD2	1.80	0.64
5:L:301:BCL:H41	5:L:302:BCL:HBB3	1.82	0.62
5:L:301:BCL:HMB1	5:L:301:BCL:CBB	2.31	0.61
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.82	0.61
1:H:194:GLN:HG3	3:M:5:ASN:HD21	1.67	0.59
7:L:304:BPH:HBB3	7:L:304:BPH:CHC	2.33	0.58
3:M:194:GLY:O	3:M:195:ASN:HB3	2.04	0.57
8:L:305[A]:UQ2:H153	3:M:47:LEU:HD11	1.86	0.57
4:L:315:GOL:H11	6:M:403:LDA:H11	1.86	0.56
3:M:300:ASN:C	3:M:302:GLY:H	2.09	0.56
5:L:301:BCL:HMB2	5:M:402:BCL:HHB	1.87	0.56
7:L:304:BPH:CBB	3:M:210:TYR:HB3	2.36	0.55
3:M:197:PHE:HZ	5:M:402:BCL:CBB	2.16	0.55
3:M:129:TRP:O	3:M:132:ARG:HB3	2.07	0.55
5:M:402:BCL:CBB	5:M:402:BCL:CHC	2.80	0.55
5:M:401:BCL:HHC	5:M:401:BCL:HBB3	1.88	0.55
7:L:304:BPH:CBB	7:L:304:BPH:CHC	2.86	0.54
2:L:209:PRO:HD3	3:M:235:LEU:HD12	1.90	0.53
3:M:16:ALA:HB1	3:M:32:VAL:CG1	2.36	0.53
5:L:301:BCL:HMB1	5:L:301:BCL:HBB2	1.89	0.53
1:H:194:GLN:HG2	3:M:5:ASN:ND2	2.23	0.53
5:M:401:BCL:HBB2	13:M:409:SPO:H243	1.90	0.53
12:M:408:U10:H3M3	12:M:408:U10:H4M2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ILE:CG2	8:L:305[B]:UQ2:H8	2.38	0.52
3:M:270:ILE:O	3:M:274:VAL:HG13	2.09	0.52
1:H:117:ARG:NH1	14:H:401:HOH:O	2.12	0.52
1:H:219:ILE:HD12	1:H:221:SER:O	2.10	0.52
3:M:189:PHE:O	3:M:193:HIS:CD2	2.63	0.51
2:L:181:PHE:HB3	7:L:314:BPH:CBB	2.39	0.51
5:M:401:BCL:H91	5:M:401:BCL:H151	1.92	0.51
5:M:401:BCL:CBB	13:M:409:SPO:H243	2.41	0.50
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.93	0.50
3:M:77:GLN:HE22	3:M:93:SER:H	1.59	0.50
12:M:408:U10:H312	12:M:408:U10:H352	1.94	0.50
1:H:140:PHE:HA	3:M:13:ARG:O	2.12	0.50
5:M:402:BCL:HAA2	5:M:402:BCL:HBD	1.93	0.49
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.47	0.49
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.42	0.49
7:L:304:BPH:HBB1	3:M:210:TYR:CD2	2.47	0.49
3:M:162:PHE:HB2	13:M:409:SPO:H312	1.94	0.49
1:H:194:GLN:CG	3:M:5:ASN:HD21	2.23	0.49
1:H:37:ARG:O	1:H:38:GLU:HG2	2.13	0.48
2:L:224:ILE:H	8:L:305[A]:UQ2:H2M3	1.78	0.48
5:M:401:BCL:HHC	5:M:401:BCL:CBB	2.45	0.47
3:M:71:GLY:HA3	13:M:409:SPO:H6	1.97	0.46
3:M:186:THR:HG22	5:M:402:BCL:HHD	1.96	0.46
3:M:157:TRP:HB2	5:M:402:BCL:H71	1.96	0.46
8:L:305[B]:UQ2:C16	6:L:313:LDA:C12	2.93	0.46
5:L:301:BCL:CMB	5:M:402:BCL:HHB	2.46	0.46
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.98	0.46
1:H:108:GLY:O	1:H:113:SER:HA	2.16	0.46
6:M:405:LDA:H31	6:M:405:LDA:H61	1.68	0.45
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.98	0.45
1:H:163:LYS:HE2	1:H:165:VAL:HG12	1.99	0.45
5:L:302:BCL:H142	5:L:302:BCL:H161	1.78	0.45
2:L:190:HIS:CE1	2:L:230:HIS:CE1	3.05	0.44
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.99	0.44
2:L:153:HIS:CD2	5:L:302:BCL:NC	2.86	0.44
5:M:401:BCL:H203	13:M:409:SPO:H10	2.00	0.44
1:H:14:SER:OG	3:M:302:GLY:HA3	2.17	0.44
1:H:87:LEU:HD22	1:H:98:HIS:O	2.17	0.44
8:L:305[B]:UQ2:H71	8:L:305[B]:UQ2:H5M1	1.73	0.44
2:L:170:ASN:C	2:L:170:ASN:ND2	2.69	0.44
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.36	0.43
2:L:2:LEU:HD11	2:L:10:ARG:CZ	2.48	0.43
1:H:40:TYR:HB3	1:H:58:LEU:HD21	2.00	0.43
3:M:194:GLY:O	3:M:195:ASN:CB	2.66	0.43
3:M:199:ASN:HD22	3:M:200:PRO:N	2.16	0.43
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.54	0.43
6:L:303:LDA:HM21	6:L:303:LDA:H22	1.82	0.43
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	0.43
2:L:113:ILE:HG22	3:M:229:PHE:HE1	1.82	0.43
2:L:173:HIS:O	2:L:177:ILE:HG13	2.18	0.43
6:L:310:LDA:HM22	6:M:405:LDA:HM22	1.99	0.43
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	2.19	0.42
1:H:131:ILE:HA	1:H:169:VAL:O	2.19	0.42
6:M:405:LDA:H112	12:M:408:U10:H202	2.00	0.42
3:M:26:LEU:H	3:M:26:LEU:HD12	1.84	0.42
3:M:199:ASN:C	3:M:199:ASN:ND2	2.72	0.42
5:L:301:BCL:HHC	5:M:402:BCL:CHC	2.49	0.42
8:L:305[B]:UQ2:C16	6:L:313:LDA:H121	2.37	0.42
6:M:405:LDA:HM11	6:M:405:LDA:H22	1.59	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.85	0.42
1:H:144:ALA:HB3	3:M:11:GLN:HB2	2.01	0.42
2:L:128:TYR:HD1	5:L:302:BCL:HBB1	1.85	0.42
2:L:162:TYR:HA	2:L:165:GLY:O	2.19	0.42
6:M:405:LDA:H81	6:M:405:LDA:H51	1.71	0.42
8:L:305[A]:UQ2:H101	8:L:305[A]:UQ2:H121	1.57	0.42
1:H:173:GLU:O	1:H:174:GLN:C	2.58	0.41
2:L:224:ILE:HD12	8:L:305[A]:UQ2:H102	2.01	0.41
2:L:170:ASN:HD22	2:L:171:PRO:N	2.18	0.41
6:L:310:LDA:H62	6:M:405:LDA:H51	2.03	0.41
3:M:199:ASN:ND2	3:M:201:PHE:H	2.18	0.41
7:L:304:BPH:HBB1	3:M:210:TYR:CG	2.56	0.40
7:L:314:BPH:H5C1	3:M:63:GLY:HA3	2.03	0.40
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.86	0.40
3:M:171:TRP:CZ3	13:M:409:SPO:H343	2.56	0.40
2:L:227:LEU:HD21	3:M:5:ASN:OD1	2.21	0.40
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.57	0.40
12:M:408:U10:H351	12:M:408:U10:H372	1.78	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:457:HOH:O	14:H:457:HOH:O[4_555]	1.99	0.21

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%)	34	60
2	L	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
3	M	301/307 (98%)	282 (94%)	17 (6%)	2 (1%)	22	46
All	All	822/848 (97%)	781 (95%)	38 (5%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	52	LEU
3	M	301	HIS

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%)	21	45
2	L	220/220 (100%)	203 (92%)	17 (8%)	13	30
3	M	236/240 (98%)	220 (93%)	16 (7%)	16	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	654/668 (98%)	610 (93%)	44 (7%)	16 37

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	14	SER
1	H	93	SER
1	H	175	MET
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
2	L	16	LEU
2	L	44	LEU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	158	SER
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	254	ILE
2	L	268	LYS
2	L	272	TRP
3	M	2	GLU
3	M	5	ASN
3	M	6	ILE
3	M	17	ASP
3	M	18	LEU
3	M	30	SER
3	M	39	LEU
3	M	52	LEU
3	M	60	LEU

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Mol	Chain	Res	Type
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	5	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\#\|Z\| > 2$
13	SPO	M	409	-	40,41,41	4.25	12 (30%)	47,50,50	1.95	12 (25%)
6	LDA	M	403	-	12,15,15	2.04	1 (8%)	14,17,17	0.94	1 (7%)
4	GOL	L	309	-	5,5,5	0.29	0	5,5,5	0.41	0
6	LDA	M	406	-	12,15,15	1.98	1 (8%)	14,17,17	0.52	0
8	UQ2	L	305[A]	-	23,23,23	2.80	7 (30%)	28,31,31	1.19	1 (3%)
7	BPH	L	314	-	51,70,70	2.86	8 (15%)	52,101,101	2.07	12 (23%)
6	LDA	M	405	-	12,15,15	2.02	1 (8%)	14,17,17	0.58	0
5	BCL	L	301	-	64,74,74	2.01	11 (17%)	78,115,115	2.54	22 (28%)
6	LDA	L	312	-	12,15,15	2.03	1 (8%)	14,17,17	0.56	0
6	LDA	L	303	-	12,15,15	1.98	1 (8%)	14,17,17	0.73	0
6	LDA	L	310	-	12,15,15	2.09	1 (8%)	14,17,17	0.69	0
5	BCL	M	401	-	64,74,74	2.13	12 (18%)	78,115,115	2.32	23 (29%)
4	GOL	L	315	-	5,5,5	0.36	0	5,5,5	0.47	0
4	GOL	L	308	-	5,5,5	0.35	0	5,5,5	0.57	0
6	LDA	L	311	-	12,15,15	2.11	1 (8%)	14,17,17	0.64	0
7	BPH	L	304	-	51,70,70	2.80	8 (15%)	52,101,101	2.15	12 (23%)
8	UQ2	L	305[B]	-	23,23,23	2.71	8 (34%)	28,31,31	1.64	6 (21%)
12	U10	M	408	-	48,48,63	2.76	12 (25%)	58,61,79	1.60	13 (22%)
5	BCL	L	302	-	64,74,74	2.04	11 (17%)	78,115,115	2.58	24 (30%)
10	HTO	L	307	-	9,9,9	0.56	0	10,10,10	0.69	0
6	LDA	M	404	-	12,15,15	2.05	1 (8%)	14,17,17	0.51	0
6	LDA	L	313	-	12,15,15	2.11	1 (8%)	14,17,17	0.76	0
5	BCL	M	402	-	64,74,74	1.98	9 (14%)	78,115,115	2.48	26 (33%)
9	PO4	L	306	-	4,4,4	0.84	0	6,6,6	0.54	0
4	GOL	H	301	-	5,5,5	0.38	0	5,5,5	0.36	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
13	SPO	M	409	-	-	11/47/47/47	-
6	LDA	M	403	-	-	5/13/13/13	-
4	GOL	L	309	-	-	4/4/4/4	-
6	LDA	M	406	-	-	11/13/13/13	-
8	UQ2	L	305[A]	-	-	6/15/39/39	0/1/1/1
7	BPH	L	314	-	-	19/37/105/105	0/5/6/6
6	LDA	M	405	-	-	4/13/13/13	-
5	BCL	L	301	-	2/2/21/25	10/37/137/137	-
6	LDA	L	312	-	-	9/13/13/13	-
6	LDA	L	303	-	-	10/13/13/13	-
6	LDA	L	310	-	-	5/13/13/13	-
5	BCL	M	401	-	2/2/21/25	15/37/137/137	-
4	GOL	L	315	-	-	2/4/4/4	-
4	GOL	L	308	-	-	2/4/4/4	-
6	LDA	L	311	-	-	6/13/13/13	-
7	BPH	L	304	-	-	9/37/105/105	0/5/6/6
8	UQ2	L	305[B]	-	-	6/15/39/39	0/1/1/1
12	U10	M	408	-	-	11/45/69/87	0/1/1/1
5	BCL	L	302	-	2/2/21/25	10/37/137/137	-
10	HTO	L	307	-	-	9/10/10/10	-
6	LDA	M	404	-	-	5/13/13/13	-
6	LDA	L	313	-	-	4/13/13/13	-
5	BCL	M	402	-	2/2/21/25	4/37/137/137	-
4	GOL	H	301	-	-	2/4/4/4	-

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	409	SPO	C27-C28	13.69	1.48	1.34
7	L	314	BPH	OBD-CAD	13.59	1.41	1.22
7	L	304	BPH	OBD-CAD	12.46	1.39	1.22
5	L	302	BCL	OBD-CAD	10.83	1.41	1.22
5	M	401	BCL	OBD-CAD	10.45	1.40	1.22
5	M	402	BCL	OBD-CAD	10.36	1.40	1.22
5	L	301	BCL	OBD-CAD	9.93	1.39	1.22
13	M	409	SPO	C14-C12	9.47	1.48	1.35
13	M	409	SPO	C9-C7	9.26	1.48	1.35
13	M	409	SPO	C19-C17	9.01	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	409	SPO	C22-C23	8.74	1.47	1.35
7	L	304	BPH	O1D-CGD	8.06	1.41	1.21
7	L	314	BPH	O1D-CGD	7.27	1.39	1.21
6	L	313	LDA	O1-N1	-7.22	1.25	1.42
6	L	311	LDA	O1-N1	-7.14	1.25	1.42
6	L	310	LDA	O1-N1	-7.08	1.25	1.42
8	L	305[A]	UQ2	C8-C9	6.98	1.49	1.33
6	M	404	LDA	O1-N1	-6.97	1.25	1.42
6	L	312	LDA	O1-N1	-6.92	1.26	1.42
12	M	408	U10	C33-C34	6.92	1.49	1.33
6	M	405	LDA	O1-N1	-6.90	1.26	1.42
8	L	305[B]	UQ2	C8-C9	6.80	1.49	1.33
6	L	303	LDA	O1-N1	-6.76	1.26	1.42
6	M	406	LDA	O1-N1	-6.74	1.26	1.42
12	M	408	U10	C13-C14	6.59	1.48	1.33
6	M	403	LDA	O1-N1	-6.57	1.26	1.42
7	L	304	BPH	O1A-CGA	6.52	1.41	1.22
13	M	409	SPO	C32-C33	6.46	1.48	1.33
7	L	304	BPH	OBB-CAB	6.46	1.42	1.22
5	M	401	BCL	O1A-CGA	6.37	1.41	1.22
12	M	408	U10	C23-C24	6.34	1.48	1.33
7	L	314	BPH	O1A-CGA	6.29	1.41	1.22
13	M	409	SPO	C37-C38	6.27	1.50	1.32
5	M	402	BCL	O1A-CGA	6.25	1.41	1.22
12	M	408	U10	C28-C29	6.22	1.47	1.33
12	M	408	U10	C8-C9	6.19	1.47	1.33
12	M	408	U10	C18-C19	6.16	1.47	1.33
7	L	314	BPH	C3D-C2D	6.11	1.50	1.39
8	L	305[B]	UQ2	C13-C14	6.04	1.49	1.32
7	L	314	BPH	C2-C3	6.01	1.47	1.33
7	L	314	BPH	OBB-CAB	5.99	1.41	1.22
7	L	304	BPH	C3D-C2D	5.95	1.50	1.39
5	L	302	BCL	O1A-CGA	5.78	1.39	1.22
7	L	304	BPH	C2-C3	5.71	1.46	1.33
13	M	409	SPO	C6-C5	5.58	1.46	1.32
5	L	301	BCL	O1A-CGA	5.56	1.39	1.22
8	L	305[A]	UQ2	C13-C14	5.50	1.48	1.32
12	M	408	U10	C38-C39	5.43	1.48	1.32
8	L	305[B]	UQ2	O2-C2	-5.19	1.24	1.36
8	L	305[A]	UQ2	O3-C3	-5.12	1.24	1.36
8	L	305[A]	UQ2	O2-C2	-4.96	1.24	1.36
12	M	408	U10	O4-C4	-4.78	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	409	SPO	C10-C11	4.68	1.46	1.34
13	M	409	SPO	C15-C16	4.65	1.46	1.34
13	M	409	SPO	C26-C25	4.58	1.46	1.34
5	M	401	BCL	C1B-NB	4.41	1.39	1.35
5	M	401	BCL	C4D-ND	-4.30	1.31	1.37
12	M	408	U10	O3-C3	-4.28	1.26	1.36
8	L	305[B]	UQ2	O3-C3	-4.16	1.26	1.36
5	M	401	BCL	C3D-C4D	-4.14	1.34	1.44
5	M	402	BCL	C3D-C4D	-4.08	1.35	1.44
5	L	301	BCL	C4D-ND	-4.06	1.32	1.37
5	L	301	BCL	C3D-C4D	-3.99	1.35	1.44
5	L	302	BCL	C4B-NB	3.98	1.38	1.35
5	L	302	BCL	C4D-ND	-3.88	1.32	1.37
12	M	408	U10	C6-C1	3.88	1.42	1.35
5	M	401	BCL	C4B-NB	3.77	1.38	1.35
8	L	305[A]	UQ2	C6-C5	3.77	1.42	1.35
5	L	301	BCL	C1B-NB	3.76	1.38	1.35
5	L	301	BCL	C4B-NB	3.73	1.38	1.35
5	L	302	BCL	C3D-C4D	-3.72	1.35	1.44
5	L	302	BCL	C1B-NB	3.69	1.38	1.35
5	M	402	BCL	C4D-ND	-3.60	1.32	1.37
13	M	409	SPO	C21-C20	3.59	1.45	1.36
5	M	402	BCL	C4B-NB	3.45	1.38	1.35
5	M	401	BCL	C2-C3	3.35	1.41	1.33
5	M	401	BCL	O2D-CGD	-3.28	1.25	1.33
5	L	302	BCL	C2-C3	3.13	1.40	1.33
5	L	301	BCL	C2-C3	3.08	1.40	1.33
5	M	402	BCL	C2-C3	3.05	1.40	1.33
5	L	301	BCL	O2D-CGD	-3.04	1.25	1.33
7	L	314	BPH	O2D-CGD	-3.02	1.25	1.33
5	L	302	BCL	O2A-CGA	-3.02	1.24	1.33
8	L	305[A]	UQ2	C3-C4	-3.01	1.40	1.48
8	L	305[B]	UQ2	C3-C4	-2.91	1.40	1.48
5	M	402	BCL	C1B-NB	2.87	1.37	1.35
5	L	301	BCL	CHD-C4C	2.81	1.47	1.39
8	L	305[B]	UQ2	C6-C5	2.79	1.40	1.35
8	L	305[A]	UQ2	C2-C1	-2.68	1.41	1.48
12	M	408	U10	C4-C5	-2.64	1.41	1.48
7	L	314	BPH	O2A-CGA	-2.63	1.25	1.33
5	M	401	BCL	CHD-C4C	2.61	1.46	1.39
5	M	402	BCL	CHD-C4C	2.54	1.46	1.39
5	L	302	BCL	O2D-CGD	-2.48	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	305[B]	UQ2	C6-C1	-2.47	1.39	1.46
5	M	402	BCL	O2D-CGD	-2.35	1.27	1.33
8	L	305[B]	UQ2	C2-C1	-2.26	1.42	1.48
5	M	401	BCL	C3D-CAD	-2.19	1.37	1.45
5	L	301	BCL	C1D-ND	2.19	1.40	1.37
7	L	304	BPH	O2D-CED	-2.15	1.40	1.45
5	M	401	BCL	C1D-C2D	-2.10	1.41	1.45
5	M	401	BCL	MG-ND	-2.10	2.01	2.05
5	L	302	BCL	C1D-C2D	-2.06	1.41	1.45
12	M	408	U10	C3-C2	-2.04	1.43	1.48
5	L	301	BCL	O2A-CGA	-2.03	1.27	1.33
7	L	304	BPH	O2D-CGD	-2.03	1.28	1.33
5	L	302	BCL	CHD-C4C	2.02	1.44	1.39

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	314	BPH	O2D-CGD-CBD	9.28	122.75	111.00
5	L	301	BCL	C1D-ND-C4D	9.22	112.88	106.33
7	L	304	BPH	O2D-CGD-CBD	9.07	122.49	111.00
5	L	301	BCL	C2D-C1D-ND	-9.06	103.43	110.10
5	L	302	BCL	CMB-C2B-C1B	-7.98	116.19	128.46
5	L	301	BCL	CHD-C1D-ND	-7.96	117.14	124.45
5	M	402	BCL	CMB-C2B-C1B	-7.94	116.26	128.46
5	L	302	BCL	C1C-NC-C4C	-7.57	103.30	106.71
5	M	401	BCL	CMB-C2B-C1B	-7.00	117.70	128.46
5	M	402	BCL	C2D-C1D-ND	-6.80	105.09	110.10
5	L	301	BCL	CMB-C2B-C1B	-6.75	118.08	128.46
5	M	402	BCL	C1D-ND-C4D	6.69	111.09	106.33
5	L	302	BCL	O2D-CGD-CBD	6.65	123.08	111.27
5	M	401	BCL	C1D-ND-C4D	6.56	110.99	106.33
5	M	401	BCL	C4A-NA-C1A	6.52	109.64	106.71
5	L	302	BCL	C1D-ND-C4D	6.36	110.86	106.33
5	M	401	BCL	O2D-CGD-CBD	6.16	122.21	111.27
5	L	302	BCL	C2D-C1D-ND	-5.96	105.71	110.10
5	M	401	BCL	C2D-C1D-ND	-5.68	105.92	110.10
5	M	402	BCL	O2D-CGD-CBD	5.57	121.17	111.27
7	L	314	BPH	OBD-CAD-CBD	-5.53	117.70	125.82
5	M	402	BCL	CHD-C1D-ND	-5.31	119.57	124.45
12	M	408	U10	C30-C29-C31	5.25	124.10	115.27
5	M	402	BCL	CMB-C2B-C3B	5.04	134.11	124.68
5	M	402	BCL	CHD-C4C-NC	-4.96	119.56	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	402	BCL	CMD-C2D-C1D	4.93	133.39	124.71
7	L	304	BPH	O1D-CGD-CBD	-4.78	116.78	124.74
5	L	302	BCL	CMB-C2B-C3B	4.77	133.60	124.68
5	L	302	BCL	C4A-NA-C1A	4.67	108.81	106.71
5	L	301	BCL	CMB-C2B-C3B	4.58	133.24	124.68
5	M	401	BCL	CMD-C2D-C1D	4.53	132.70	124.71
5	L	302	BCL	C4B-CHC-C1C	-4.48	121.25	130.12
5	M	401	BCL	CMB-C2B-C3B	4.44	132.98	124.68
13	M	409	SPO	C20-C19-C17	-4.37	121.07	127.31
5	L	302	BCL	CHB-C4A-NA	-4.33	118.53	124.51
5	M	401	BCL	C1B-CHB-C4A	-4.28	121.64	130.12
5	L	301	BCL	C4A-NA-C1A	4.24	108.61	106.71
7	L	304	BPH	C1C-C2C-C3C	-4.10	98.94	102.84
13	M	409	SPO	C10-C9-C7	-4.06	121.52	127.31
5	L	302	BCL	O2A-CGA-O1A	-4.02	113.44	123.59
12	M	408	U10	C17-C18-C19	-3.94	118.17	127.66
5	M	402	BCL	C1D-CHD-C4C	-3.87	117.29	126.62
8	L	305[B]	UQ2	CM5-C5-C6	-3.86	118.10	124.40
7	L	304	BPH	CED-O2D-CGD	3.85	124.64	115.94
13	M	409	SPO	C5-C6-C7	-3.85	120.08	125.89
5	M	401	BCL	CHC-C1C-NC	-3.85	119.19	124.51
7	L	304	BPH	C1-C2-C3	-3.79	119.49	126.04
5	M	402	BCL	O2D-CGD-O1D	-3.77	116.46	123.84
5	L	301	BCL	O2A-CGA-CBA	3.73	123.62	111.91
5	M	402	BCL	CHC-C1C-NC	-3.65	119.47	124.51
5	L	302	BCL	C4-C3-C5	3.56	121.26	115.27
7	L	314	BPH	C4A-C3A-C2A	-3.54	99.47	102.84
5	M	401	BCL	O2D-CGD-O1D	-3.49	117.01	123.84
5	L	301	BCL	C1C-NC-C4C	-3.48	105.14	106.71
5	M	402	BCL	C1B-CHB-C4A	-3.47	123.24	130.12
5	M	401	BCL	C1-O2A-CGA	3.47	125.54	116.44
13	M	409	SPO	C21-C22-C23	-3.47	122.36	127.31
5	M	402	BCL	O2A-CGA-CBA	3.46	122.76	111.91
5	L	301	BCL	CMD-C2D-C1D	3.44	130.78	124.71
13	M	409	SPO	C29-C28-C30	3.42	121.02	115.27
5	L	301	BCL	O2D-CGD-CBD	3.40	117.31	111.27
5	L	301	BCL	C1D-CHD-C4C	-3.40	118.43	126.62
13	M	409	SPO	C15-C14-C12	-3.38	122.48	127.31
8	L	305[B]	UQ2	O1-C1-C6	-3.37	115.63	121.55
5	M	401	BCL	C4B-CHC-C1C	-3.32	123.53	130.12
5	L	302	BCL	CHD-C4C-NC	-3.29	121.42	125.08
7	L	314	BPH	O2D-CGD-O1D	-3.28	117.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	409	SPO	C24-C23-C25	3.28	123.24	118.08
5	L	302	BCL	C1B-CHB-C4A	-3.25	123.69	130.12
5	M	402	BCL	CMD-C2D-C3D	-3.24	120.16	127.61
5	L	302	BCL	CMD-C2D-C1D	3.16	130.28	124.71
5	L	302	BCL	C1D-CHD-C4C	-3.15	119.02	126.62
5	M	401	BCL	CHB-C4A-NA	-3.14	120.16	124.51
5	M	401	BCL	C1D-CHD-C4C	-3.10	119.14	126.62
5	L	302	BCL	CHA-C1A-NA	-3.04	119.44	126.40
5	L	301	BCL	C1-O2A-CGA	3.03	124.39	116.44
13	M	409	SPO	C20-C21-C22	-3.00	117.34	123.47
7	L	314	BPH	O1D-CGD-CBD	-2.95	119.83	124.74
5	L	302	BCL	O1D-CGD-CBD	-2.95	118.45	124.48
5	L	302	BCL	C2A-C3A-C4A	2.93	106.61	101.87
13	M	409	SPO	C34-C33-C35	2.93	120.20	115.27
5	M	401	BCL	O2A-CGA-CBA	2.92	121.08	111.91
7	L	304	BPH	C1-O2A-CGA	2.91	124.09	116.44
8	L	305[B]	UQ2	CM3-O3-C3	2.87	126.63	116.47
5	L	301	BCL	CMA-C3A-C4A	-2.86	104.07	111.77
5	L	302	BCL	CAA-CBA-CGA	2.83	121.51	113.25
5	L	301	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
5	M	402	BCL	CED-O2D-CGD	2.78	122.22	115.94
7	L	314	BPH	CMD-C2D-C3D	-2.77	119.50	124.68
5	L	302	BCL	O2D-CGD-O1D	-2.76	118.44	123.84
7	L	304	BPH	O2A-CGA-CBA	2.74	120.49	111.91
5	L	302	BCL	O2A-CGA-CBA	2.68	120.33	111.91
5	M	402	BCL	C4-C3-C5	2.66	119.75	115.27
5	M	401	BCL	O2A-C1-C2	2.66	115.62	108.64
12	M	408	U10	C10-C9-C11	2.65	119.73	115.27
5	L	301	BCL	CED-O2D-CGD	2.64	121.91	115.94
7	L	314	BPH	CAC-C3C-C4C	-2.64	107.84	113.73
7	L	304	BPH	C7-C6-C5	-2.62	106.25	113.36
5	L	301	BCL	C2A-C3A-C4A	2.61	106.08	101.87
7	L	304	BPH	OBD-CAD-CBD	-2.61	122.00	125.82
12	M	408	U10	C4M-O4-C4	2.59	125.64	116.47
5	M	401	BCL	C2A-C3A-C4A	2.58	106.04	101.87
12	M	408	U10	C27-C28-C29	-2.57	121.48	127.66
12	M	408	U10	C30-C29-C28	-2.56	117.10	123.68
5	M	402	BCL	OBB-CAB-C3B	2.56	124.53	119.99
5	M	401	BCL	C3C-C4C-CHD	-2.53	117.99	123.39
7	L	304	BPH	CMA-C3A-C4A	-2.52	108.86	114.38
5	L	301	BCL	CHA-C4D-ND	2.52	137.77	132.50
7	L	304	BPH	CMD-C2D-C3D	-2.51	119.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	305[B]	UQ2	C10-C9-C11	2.48	119.45	115.27
5	L	302	BCL	CED-O2D-CGD	2.46	121.50	115.94
5	M	401	BCL	CHA-C1A-NA	-2.45	120.79	126.40
7	L	314	BPH	C4-C3-C5	2.44	119.38	115.27
12	M	408	U10	C20-C19-C21	2.42	119.35	115.27
13	M	409	SPO	C27-C26-C25	-2.40	115.72	123.22
5	L	302	BCL	C5-C3-C2	-2.40	116.26	121.12
8	L	305[B]	UQ2	C6-C5-C4	2.39	121.07	119.18
5	L	301	BCL	CMD-C2D-C3D	-2.39	122.12	127.61
5	M	401	BCL	CMD-C2D-C3D	-2.38	122.15	127.61
7	L	314	BPH	C1-C2-C3	-2.38	121.93	126.04
5	L	302	BCL	C3C-C4C-CHD	-2.34	118.39	123.39
7	L	314	BPH	CMC-C2C-C1C	-2.33	109.28	114.38
5	M	402	BCL	CHA-C1A-NA	-2.28	121.17	126.40
6	M	403	LDA	O1-N1-C1	2.28	114.87	109.27
5	M	402	BCL	C3C-C4C-CHD	-2.26	118.56	123.39
5	L	301	BCL	CHA-C1A-NA	-2.26	121.23	126.40
12	M	408	U10	C15-C14-C16	2.25	119.06	115.27
5	L	301	BCL	C14-C13-C12	2.25	119.45	111.29
5	L	301	BCL	C1B-CHB-C4A	-2.25	125.67	130.12
5	M	402	BCL	C16-C15-C13	-2.25	108.66	115.92
5	M	402	BCL	CHA-C4D-ND	2.24	137.19	132.50
5	M	401	BCL	CAA-C2A-C3A	-2.24	106.66	112.78
12	M	408	U10	C12-C13-C14	-2.23	122.28	127.66
8	L	305[B]	UQ2	C2-C3-C4	-2.23	116.30	120.68
13	M	409	SPO	C14-C15-C16	-2.19	116.39	123.22
7	L	314	BPH	CED-O2D-CGD	2.19	120.89	115.94
5	M	402	BCL	CHB-C4A-NA	-2.11	121.59	124.51
7	L	304	BPH	CAC-C3C-C4C	2.11	118.46	113.73
12	M	408	U10	C32-C33-C34	-2.11	122.58	127.66
5	M	401	BCL	CMA-C3A-C4A	-2.10	106.12	111.77
12	M	408	U10	C41-C39-C40	2.10	119.24	114.60
5	M	401	BCL	CHA-C4D-ND	2.09	136.87	132.50
5	M	402	BCL	CGD-CBD-CAD	-2.09	103.97	110.73
7	L	314	BPH	CBC-CAC-C3C	-2.07	109.59	113.77
5	M	402	BCL	C4A-NA-C1A	2.07	107.64	106.71
5	M	402	BCL	O2A-CGA-O1A	-2.05	118.42	123.59
13	M	409	SPO	C13-C12-C11	2.03	121.28	118.08
5	M	402	BCL	C4B-CHC-C1C	-2.02	126.11	130.12
12	M	408	U10	C22-C23-C24	-2.01	122.81	127.66
12	M	408	U10	O5-C5-C6	-2.01	118.02	121.55
5	L	301	BCL	CAA-C2A-C1A	-2.00	105.41	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	305[A]	UQ2	CM2-O2-C2	2.00	123.56	116.47

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	301	BCL	C8
5	L	301	BCL	C13
5	L	302	BCL	C8
5	L	302	BCL	C13
5	M	401	BCL	C8
5	M	401	BCL	C13
5	M	402	BCL	C8
5	M	402	BCL	C13

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	308	GOL	C1-C2-C3-O3
4	L	309	GOL	C1-C2-C3-O3
4	L	315	GOL	C1-C2-C3-O3
5	L	301	BCL	C11-C12-C13-C14
5	M	401	BCL	C1-C2-C3-C4
5	M	401	BCL	C1-C2-C3-C5
5	M	401	BCL	C14-C13-C15-C16
6	L	303	LDA	C2-C1-N1-O1
6	L	303	LDA	C2-C1-N1-CM2
6	L	303	LDA	N1-C1-C2-C3
6	L	312	LDA	C2-C1-N1-O1
6	L	312	LDA	C2-C1-N1-CM1
6	L	312	LDA	C2-C1-N1-CM2
6	M	406	LDA	C2-C1-N1-CM2
7	L	304	BPH	O2A-C1-C2-C3
7	L	314	BPH	O2A-C1-C2-C3
8	L	305[B]	UQ2	C7-C8-C9-C10
8	L	305[B]	UQ2	C7-C8-C9-C11
10	L	307	HTO	C1-C2-C3-O3
10	L	307	HTO	O2-C2-C3-O3
10	L	307	HTO	O2-C2-C3-C4
10	L	307	HTO	O3-C3-C4-C5
12	M	408	U10	C27-C28-C29-C30
12	M	408	U10	C27-C28-C29-C31
12	M	408	U10	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
12	M	408	U10	C30-C29-C31-C32
13	M	409	SPO	C5-C6-C7-C8
13	M	409	SPO	C5-C6-C7-C9
13	M	409	SPO	C15-C16-C17-C18
13	M	409	SPO	C15-C16-C17-C19
13	M	409	SPO	C19-C20-C21-C22
13	M	409	SPO	C36-C37-C38-C39
5	M	401	BCL	C10-C11-C12-C13
13	M	409	SPO	C36-C37-C38-C40
5	L	302	BCL	C3-C5-C6-C7
8	L	305[A]	UQ2	C12-C13-C14-C15
6	M	405	LDA	C3-C4-C5-C6
8	L	305[A]	UQ2	C12-C13-C14-C16
8	L	305[B]	UQ2	C12-C13-C14-C16
8	L	305[A]	UQ2	C12-C11-C9-C10
8	L	305[A]	UQ2	C12-C11-C9-C8
8	L	305[A]	UQ2	C9-C11-C12-C13
8	L	305[B]	UQ2	C9-C11-C12-C13
13	M	409	SPO	C33-C35-C36-C37
6	M	405	LDA	C5-C6-C7-C8
12	M	408	U10	C31-C32-C33-C34
5	M	401	BCL	C8-C10-C11-C12
5	L	301	BCL	C13-C15-C16-C17
8	L	305[B]	UQ2	C12-C13-C14-C15
5	L	302	BCL	C13-C15-C16-C17
4	L	308	GOL	O2-C2-C3-O3
4	L	309	GOL	O2-C2-C3-O3
5	M	402	BCL	C15-C16-C17-C18
12	M	408	U10	C29-C31-C32-C33
12	M	408	U10	C34-C36-C37-C38
7	L	304	BPH	C8-C10-C11-C12
5	L	301	BCL	C15-C16-C17-C18
13	M	409	SPO	C18-C17-C19-C20
6	L	303	LDA	C5-C6-C7-C8
6	L	303	LDA	C6-C7-C8-C9
6	L	303	LDA	C11-C10-C9-C8
6	L	310	LDA	C11-C10-C9-C8
6	L	313	LDA	C5-C6-C7-C8
6	M	405	LDA	C6-C7-C8-C9
6	M	406	LDA	C2-C3-C4-C5
5	L	301	BCL	C8-C10-C11-C12
6	M	403	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
6	L	303	LDA	C4-C5-C6-C7
13	M	409	SPO	C16-C17-C19-C20
10	L	307	HTO	O1-C1-C2-O2
6	M	406	LDA	C11-C10-C9-C8
6	L	310	LDA	C5-C6-C7-C8
10	L	307	HTO	C2-C3-C4-C5
4	L	309	GOL	O1-C1-C2-C3
6	L	303	LDA	C2-C3-C4-C5
6	L	310	LDA	C4-C5-C6-C7
6	L	311	LDA	C6-C7-C8-C9
6	M	403	LDA	C11-C10-C9-C8
5	M	402	BCL	C3-C5-C6-C7
7	L	314	BPH	C4-C3-C5-C6
7	L	314	BPH	C2-C3-C5-C6
4	L	309	GOL	O1-C1-C2-O2
6	L	313	LDA	C11-C10-C9-C8
6	M	406	LDA	C3-C4-C5-C6
5	M	401	BCL	C2-C1-O2A-CGA
6	L	312	LDA	C6-C7-C8-C9
6	L	312	LDA	C4-C5-C6-C7
6	L	312	LDA	C1-C2-C3-C4
6	L	313	LDA	C2-C3-C4-C5
5	M	401	BCL	C2-C3-C5-C6
5	M	401	BCL	C11-C12-C13-C15
7	L	304	BPH	C2-C3-C5-C6
7	L	314	BPH	C13-C15-C16-C17
6	L	311	LDA	C7-C8-C9-C10
6	L	310	LDA	C1-C2-C3-C4
6	L	312	LDA	C5-C6-C7-C8
7	L	304	BPH	C4-C3-C5-C6
6	L	310	LDA	C7-C8-C9-C10
5	M	401	BCL	C11-C12-C13-C14
6	L	303	LDA	C1-C2-C3-C4
5	L	301	BCL	C10-C11-C12-C13
4	L	315	GOL	O2-C2-C3-O3
5	M	401	BCL	C4-C3-C5-C6
6	M	405	LDA	C7-C8-C9-C10
6	M	406	LDA	C7-C8-C9-C10
6	M	403	LDA	C4-C5-C6-C7
13	M	409	SPO	C2-C1-C4-C5
12	M	408	U10	C25-C24-C26-C27
6	L	312	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	L	301	BCL	C11-C10-C8-C7
7	L	314	BPH	C11-C10-C8-C7
7	L	314	BPH	C12-C13-C15-C16
6	L	312	LDA	C9-C10-C11-C12
6	L	311	LDA	N1-C1-C2-C3
7	L	314	BPH	C5-C6-C7-C8
12	M	408	U10	C23-C24-C26-C27
6	L	311	LDA	C5-C6-C7-C8
6	L	311	LDA	C2-C3-C4-C5
6	L	313	LDA	C9-C10-C11-C12
10	L	307	HTO	C1-C2-C3-C4
7	L	314	BPH	C15-C16-C17-C18
7	L	314	BPH	C6-C7-C8-C9
7	L	304	BPH	CBD-CGD-O2D-CED
5	L	301	BCL	C11-C12-C13-C15
5	L	302	BCL	C1-C2-C3-C4
6	M	406	LDA	C9-C10-C11-C12
5	L	302	BCL	C5-C6-C7-C8
7	L	314	BPH	CAD-CBD-CGD-O2D
6	L	311	LDA	C1-C2-C3-C4
8	L	305[B]	UQ2	C4-C3-O3-CM3
12	M	408	U10	C5-C4-O4-C4M
5	L	302	BCL	CHA-CBD-CGD-O1D
6	M	406	LDA	C2-C1-N1-CM1
4	H	301	GOL	O2-C2-C3-O3
5	M	401	BCL	C11-C10-C8-C9
6	M	406	LDA	C5-C6-C7-C8
4	H	301	GOL	C1-C2-C3-O3
5	L	302	BCL	C16-C17-C18-C19
7	L	314	BPH	C16-C17-C18-C19
6	M	406	LDA	C2-C1-N1-O1
6	L	303	LDA	C7-C8-C9-C10
5	M	401	BCL	C11-C10-C8-C7
5	M	402	BCL	C13-C15-C16-C17
7	L	304	BPH	C4C-C3C-CAC-CBC
8	L	305[A]	UQ2	C1-C2-O2-CM2
5	L	301	BCL	C2A-CAA-CBA-CGA
5	M	401	BCL	C3-C5-C6-C7
6	M	404	LDA	C7-C8-C9-C10
7	L	314	BPH	C10-C11-C12-C13
7	L	304	BPH	O1D-CGD-O2D-CED
7	L	314	BPH	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
5	L	301	BCL	C6-C7-C8-C9
5	L	302	BCL	C14-C13-C15-C16
7	L	314	BPH	C14-C13-C15-C16
5	L	302	BCL	C16-C17-C18-C20
6	M	403	LDA	C7-C8-C9-C10
6	M	406	LDA	C1-C2-C3-C4
10	L	307	HTO	C3-C4-C5-C6
6	M	406	LDA	C6-C7-C8-C9
7	L	314	BPH	C16-C17-C18-C20
5	L	302	BCL	C6-C7-C8-C9
12	M	408	U10	C35-C34-C36-C37
7	L	314	BPH	C6-C7-C8-C10
7	L	314	BPH	C1-C2-C3-C4
5	L	301	BCL	CAD-CBD-CGD-O2D
5	M	401	BCL	CAD-CBD-CGD-O2D
5	M	402	BCL	CAD-CBD-CGD-O2D
6	M	404	LDA	C9-C10-C11-C12
5	L	302	BCL	CHA-CBD-CGD-O2D
6	M	404	LDA	C2-C1-N1-CM1
7	L	304	BPH	CHA-CBD-CGD-O1D
7	L	314	BPH	CHA-CBD-CGD-O1D
7	L	314	BPH	C11-C12-C13-C14
10	L	307	HTO	C4-C5-C6-C7
6	M	404	LDA	C2-C3-C4-C5
6	M	404	LDA	C6-C7-C8-C9
6	M	403	LDA	C6-C7-C8-C9
7	L	304	BPH	C11-C12-C13-C14
5	M	401	BCL	C12-C13-C15-C16

There are no ring outliers.

18 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	409	SPO	6	0
6	M	403	LDA	3	0
8	L	305[A]	UQ2	5	0
7	L	314	BPH	6	0
6	M	405	LDA	10	0
5	L	301	BCL	6	0
6	L	303	LDA	1	0
6	L	310	LDA	4	0
5	M	401	BCL	6	0

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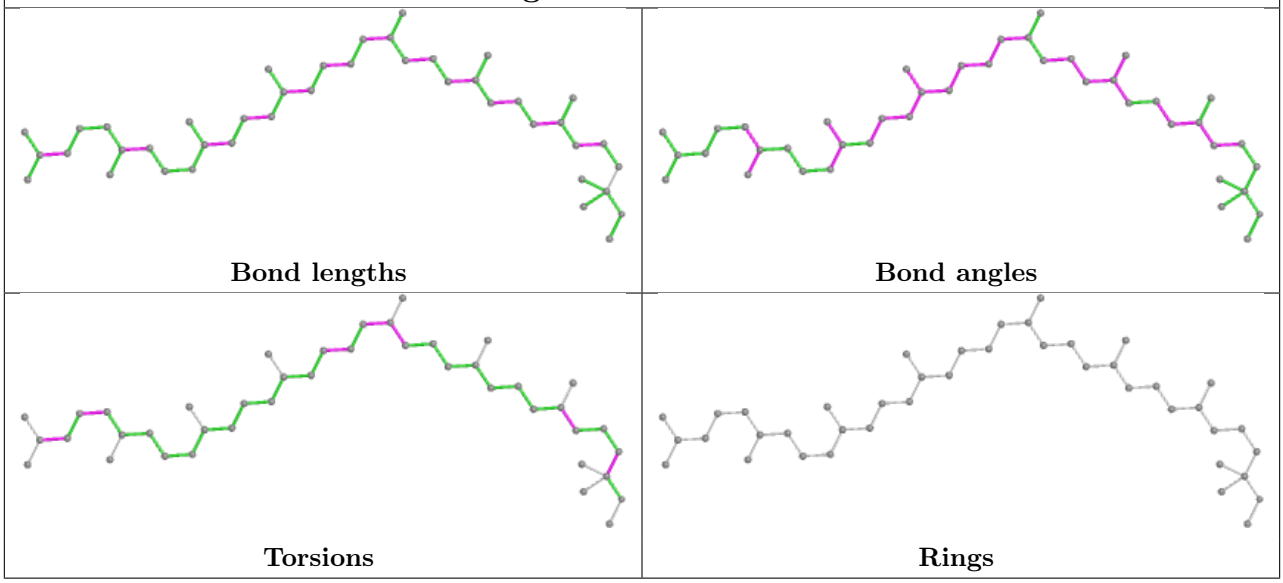
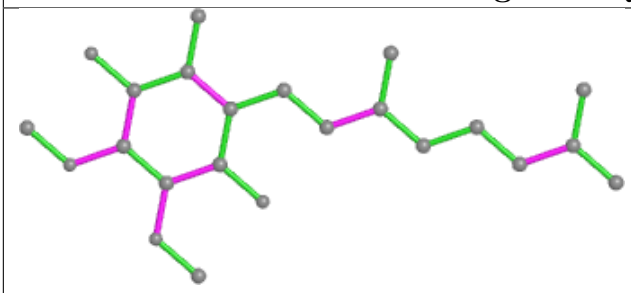
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	315	GOL	1	0
4	L	308	GOL	1	0
6	L	311	LDA	2	0
7	L	304	BPH	8	0
8	L	305[B]	UQ2	8	0
12	M	408	U10	4	0
5	L	302	BCL	4	0
6	L	313	LDA	4	0
5	M	402	BCL	14	0

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.

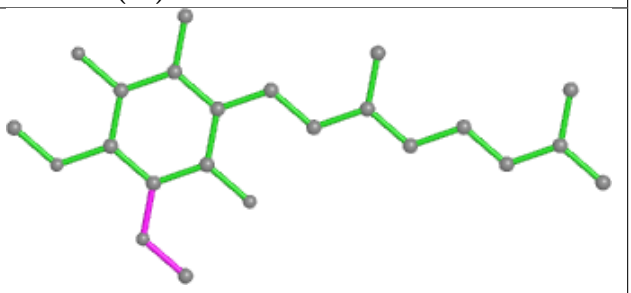
Ligand SPO M 409



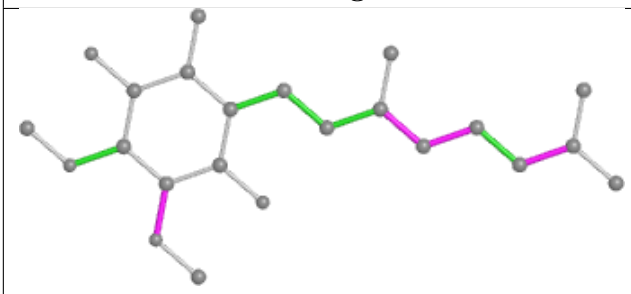
Ligand UQ2 L 305 (A)



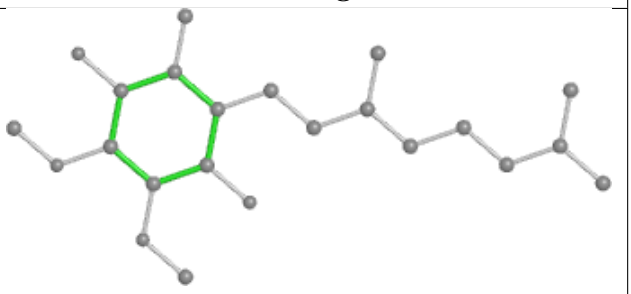
Bond lengths



Bond angles

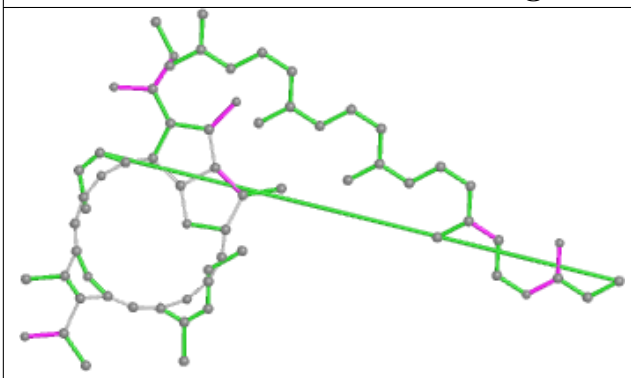


Torsions

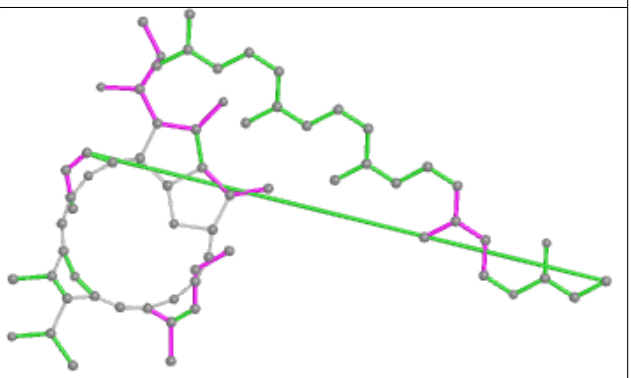


Rings

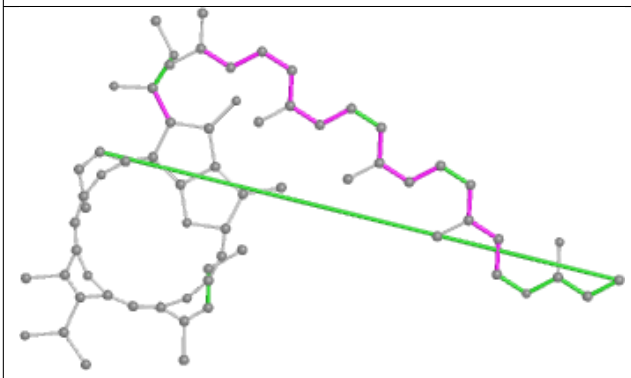
Ligand BPH L 314



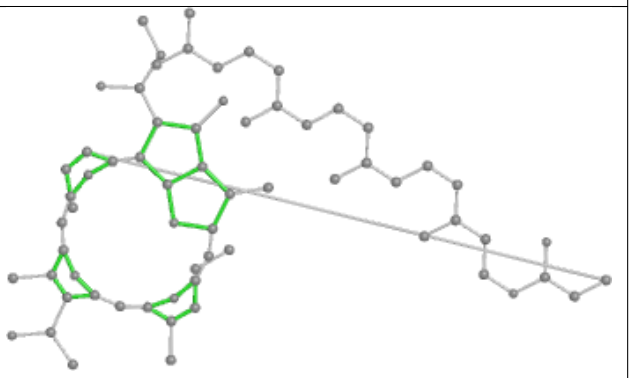
Bond lengths



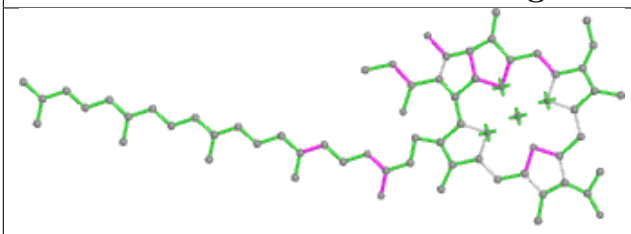
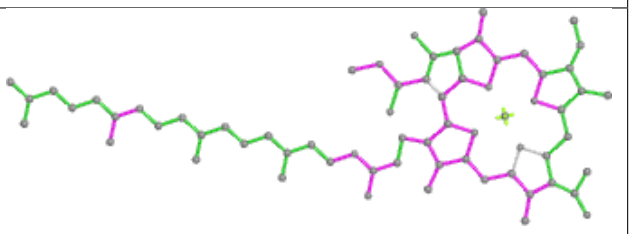
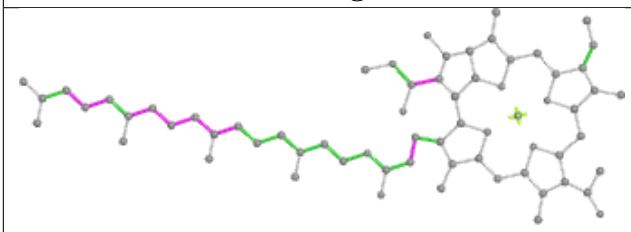
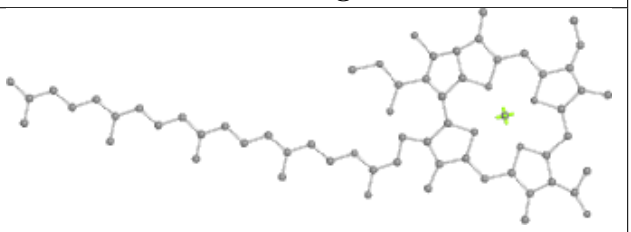
Bond angles

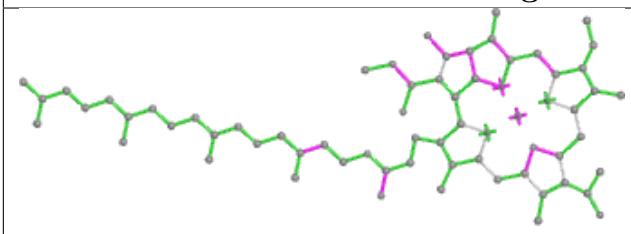
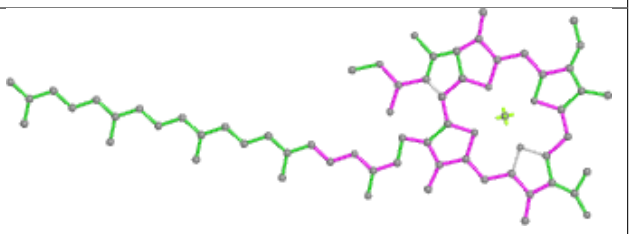
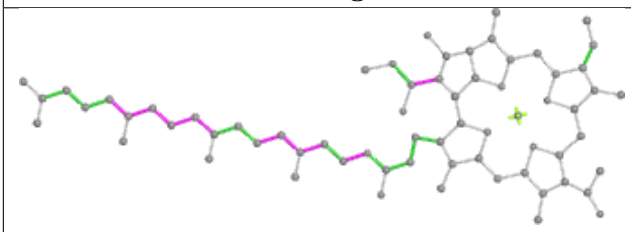
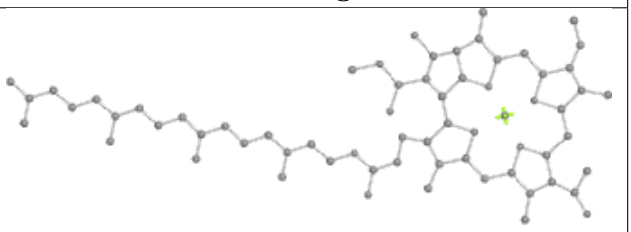


Torsions

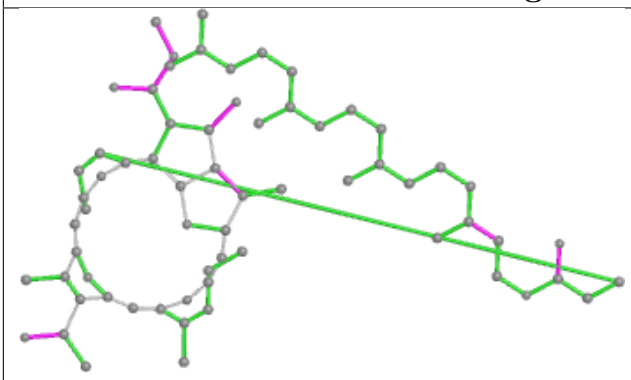


Rings

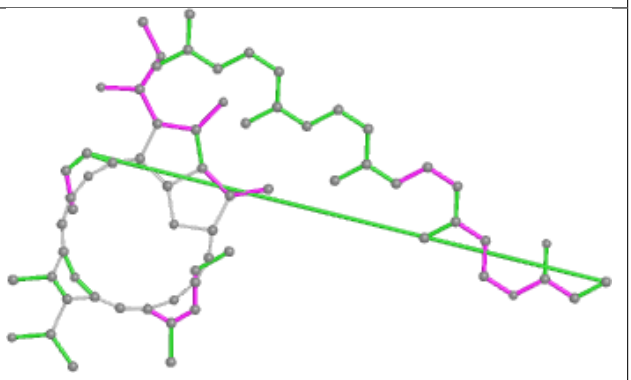
Ligand BCL L 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

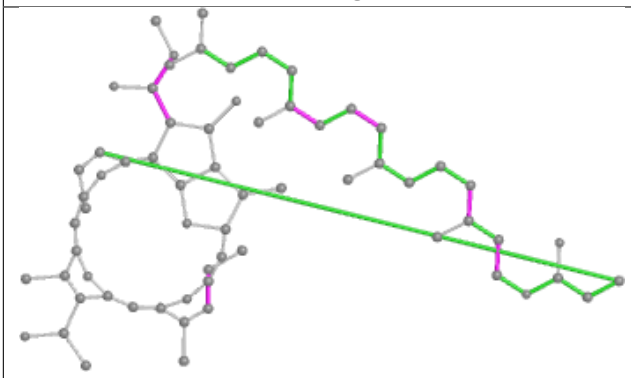
Ligand BPH L 304



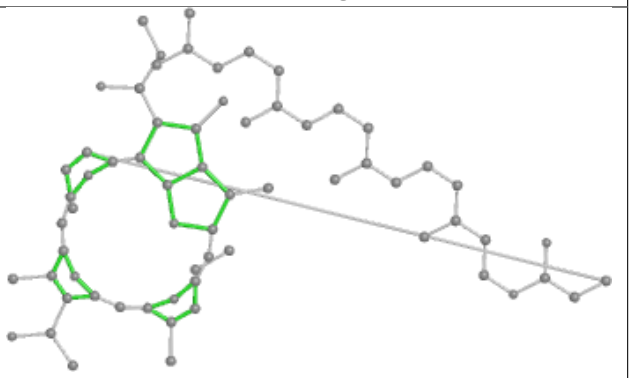
Bond lengths



Bond angles

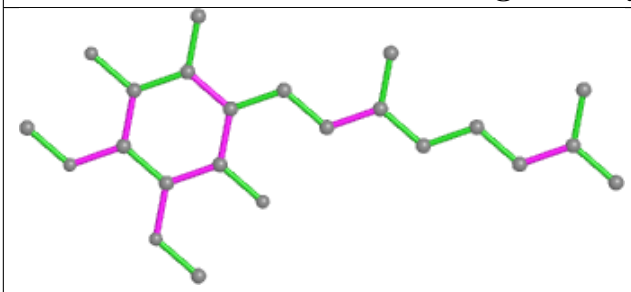


Torsions

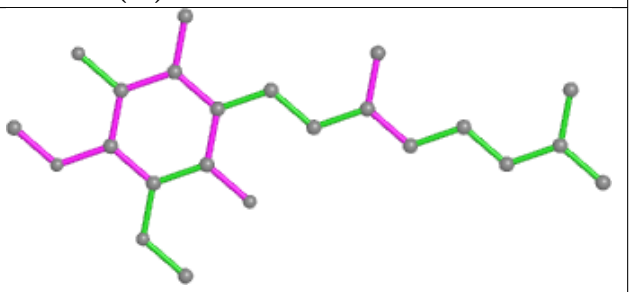


Rings

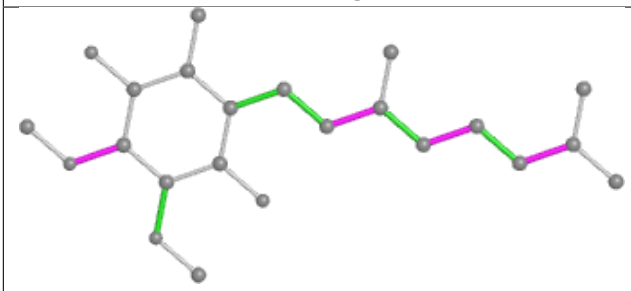
Ligand UQ2 L 305 (B)



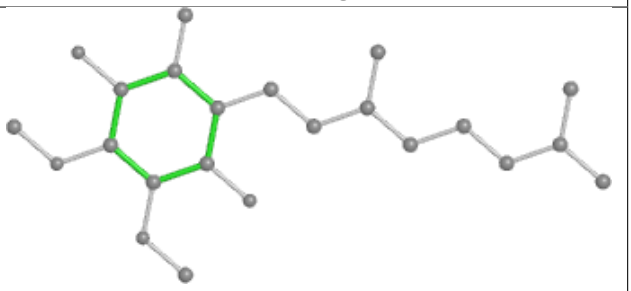
Bond lengths



Bond angles

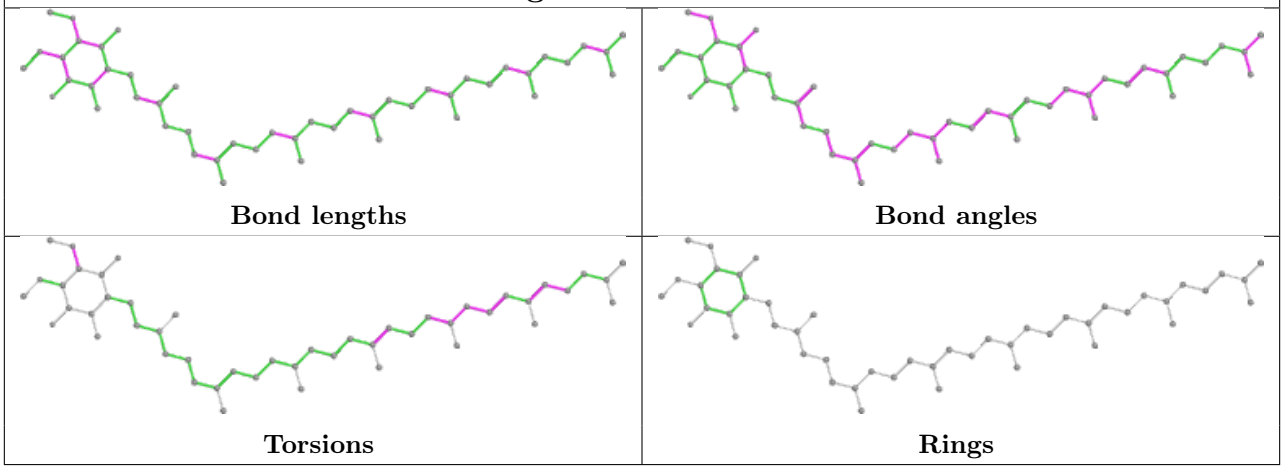


Torsions

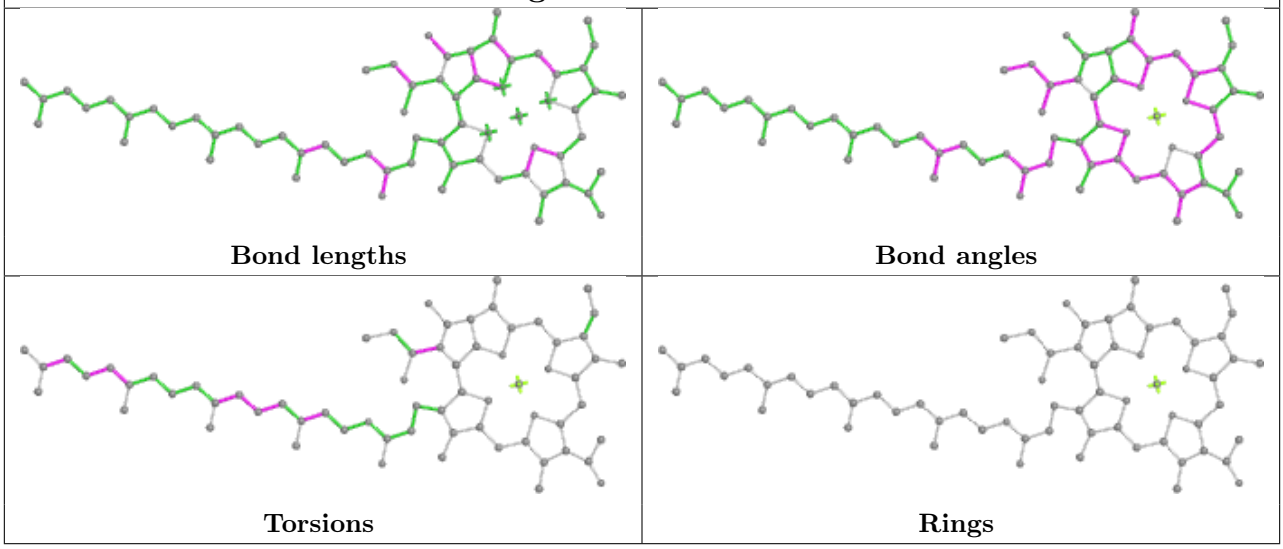


Rings

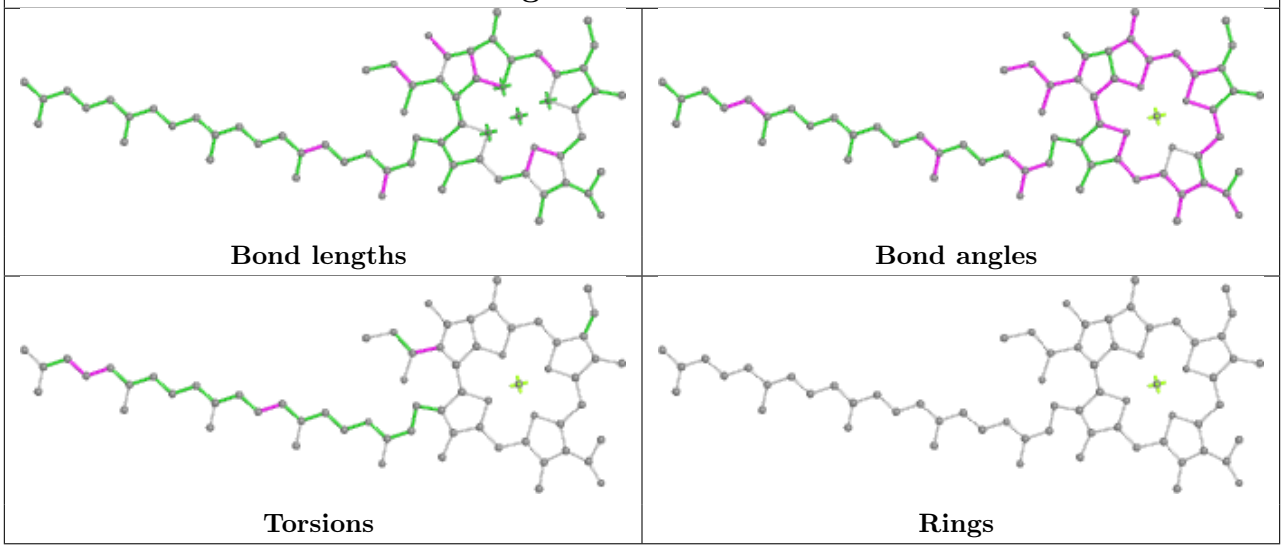
Ligand U10 M 408



Ligand BCL L 302



Ligand BCL M 402



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%)	-0.42	7 (2%)	51	52	38, 50, 63, 104	0
2	L	281/281 (100%)	-0.78	4 (1%)	75	77	32, 43, 69, 77	0
3	M	303/307 (98%)	-0.57	6 (1%)	65	67	31, 50, 75, 96	0
All	All	825/848 (97%)	-0.60	17 (2%)	63	65	31, 48, 71, 104	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	8.9
3	M	1	ALA	8.1
1	H	250	SER	7.8
3	M	302	GLY	4.6
1	H	220[A]	LYS	3.8
1	H	249	LYS	3.7
2	L	281	GLY	3.6
3	M	27	ALA	3.5
3	M	301	HIS	3.3
3	M	2	GLU	3.3
1	H	221	SER	2.7
3	M	106	ALA	2.4
2	L	270	PRO	2.3
2	L	276	PRO	2.2
2	L	202	LYS	2.2
1	H	51	ALA	2.2
1	H	247	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

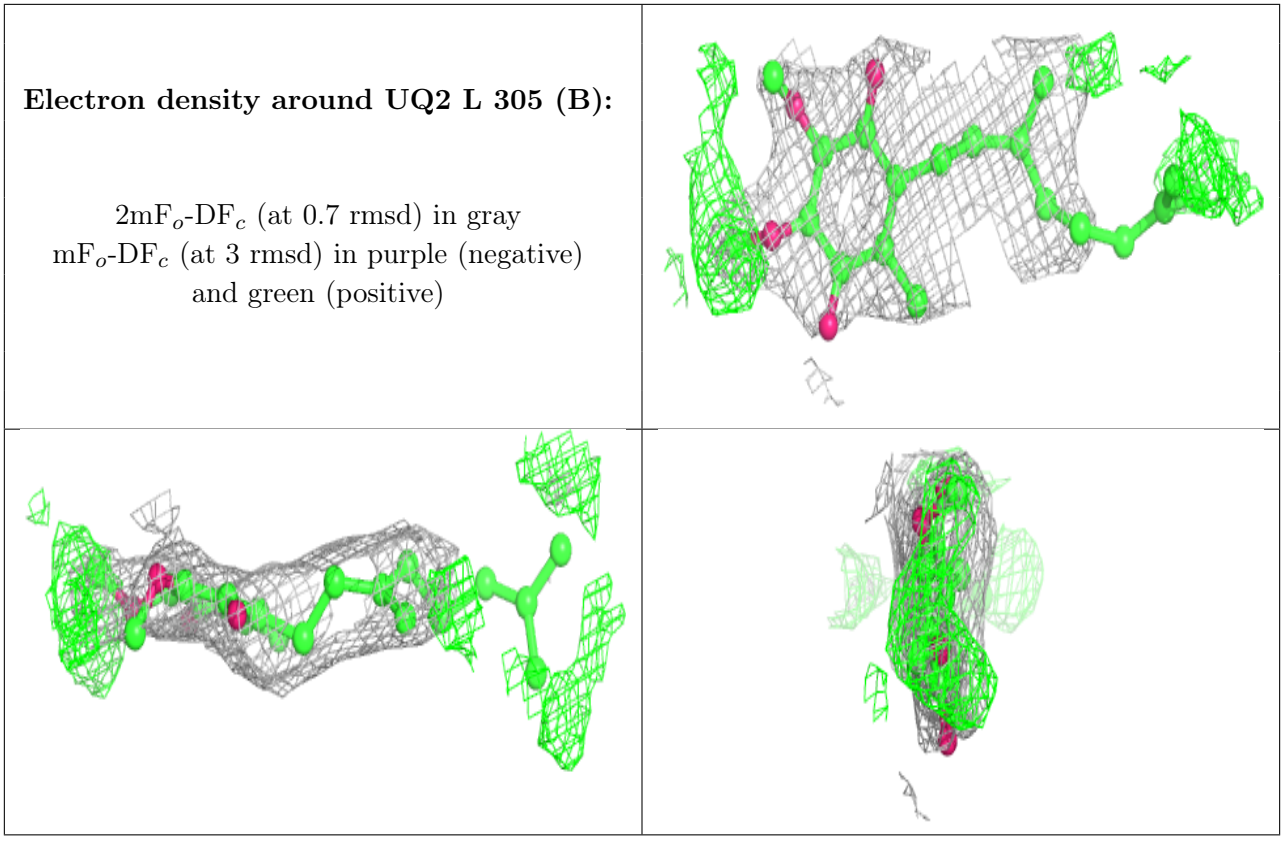
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	406	16/16	0.26	0.59	100,116,126,126	0
6	LDA	L	312	16/16	0.28	0.50	87,101,112,113	0
6	LDA	L	311	16/16	0.37	0.47	111,117,128,129	0
6	LDA	L	303	16/16	0.45	0.52	61,96,114,115	0
6	LDA	L	310	16/16	0.50	0.44	91,99,110,110	0
6	LDA	L	313	16/16	0.54	0.34	101,109,116,116	0
4	GOL	L	315	6/6	0.67	0.26	98,101,101,103	0
9	PO4	L	306	5/5	0.68	0.61	156,156,157,157	0
10	HTO	L	307	10/10	0.74	0.28	77,81,82,82	0
6	LDA	M	403	16/16	0.80	0.26	45,71,82,82	0
8	UQ2	L	305[B]	23/23	0.84	0.30	43,49,55,55	23
6	LDA	M	404	16/16	0.84	0.34	76,79,86,86	0
8	UQ2	L	305[A]	23/23	0.84	0.30	51,53,54,55	23
4	GOL	L	308	6/6	0.85	0.30	71,74,74,76	0
4	GOL	H	301	6/6	0.86	0.31	96,97,98,98	0
4	GOL	L	309	6/6	0.88	0.26	81,81,82,82	0
6	LDA	M	405	16/16	0.89	0.21	65,67,78,79	0
13	SPO	M	409	42/42	0.89	0.19	44,60,78,81	0
7	BPH	L	314	65/65	0.91	0.17	42,50,111,113	0
12	U10	M	408	48/63	0.93	0.18	37,48,78,80	0
5	BCL	M	401	66/66	0.96	0.13	30,34,81,82	0
5	BCL	L	301	66/66	0.97	0.14	30,36,47,52	0
5	BCL	M	402	66/66	0.97	0.15	29,39,60,70	0
5	BCL	L	302	66/66	0.97	0.12	30,37,58,62	0
7	BPH	L	304	65/65	0.98	0.13	26,32,41,43	0
11	FE	M	407	1/1	0.99	0.04	37,37,37,37	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.

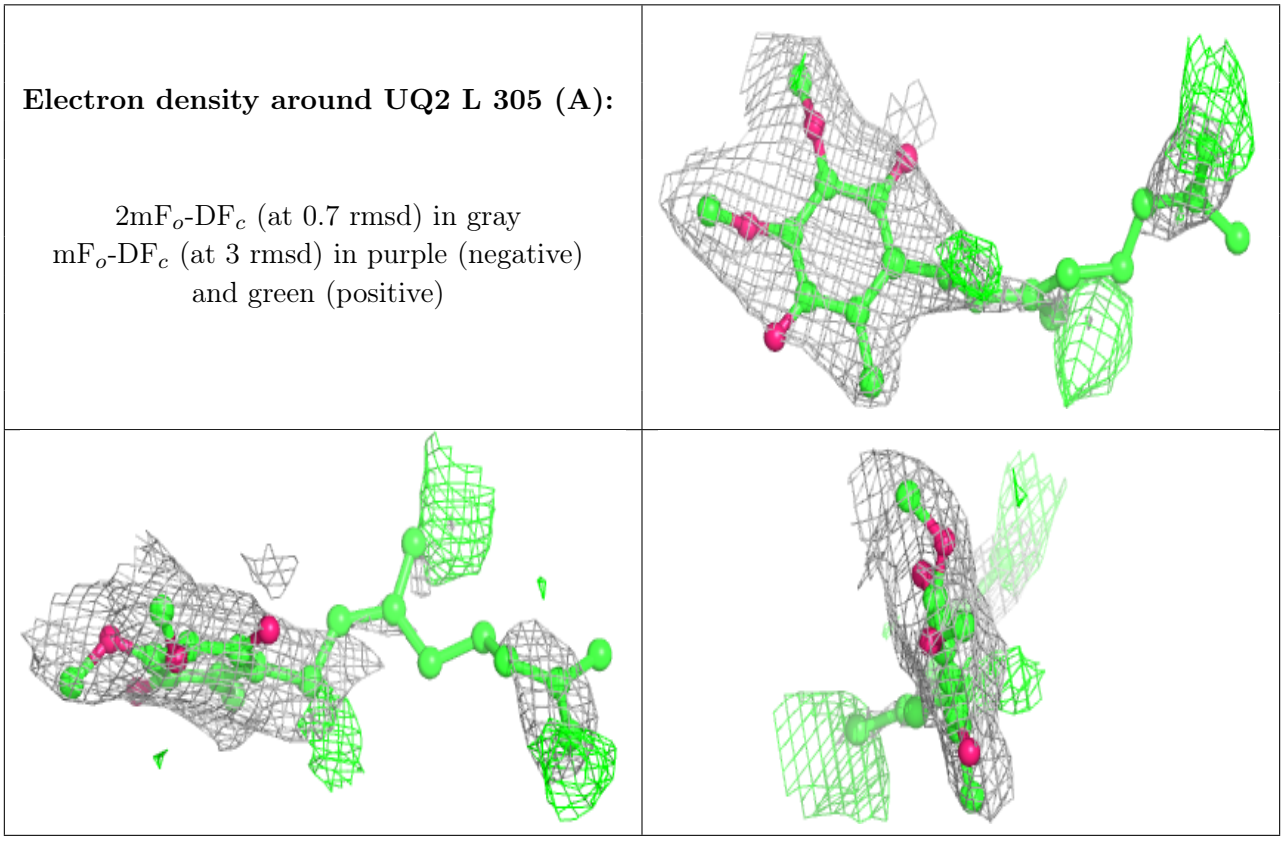
Electron density around UQ2 L 305 (B):

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



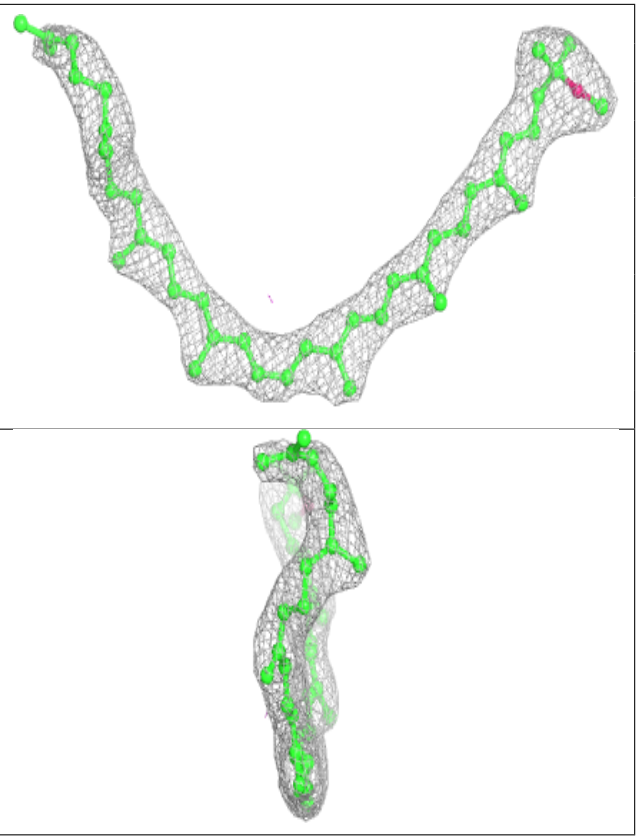
Electron density around UQ2 L 305 (A):

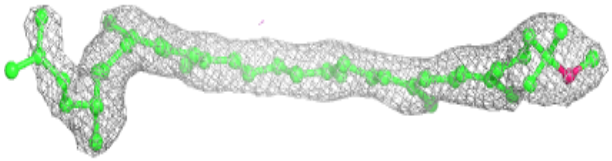
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SPO M 409:

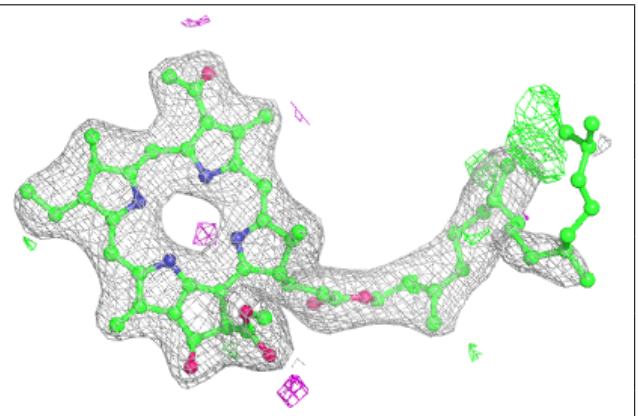
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

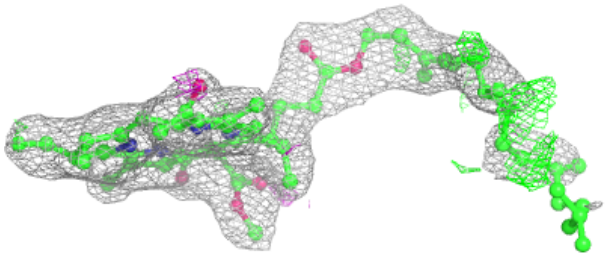


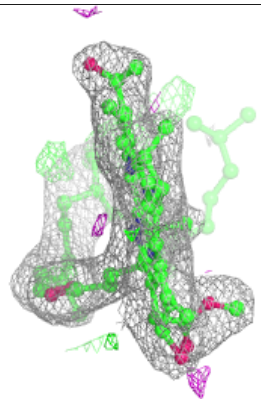


Electron density around BPH L 314:

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

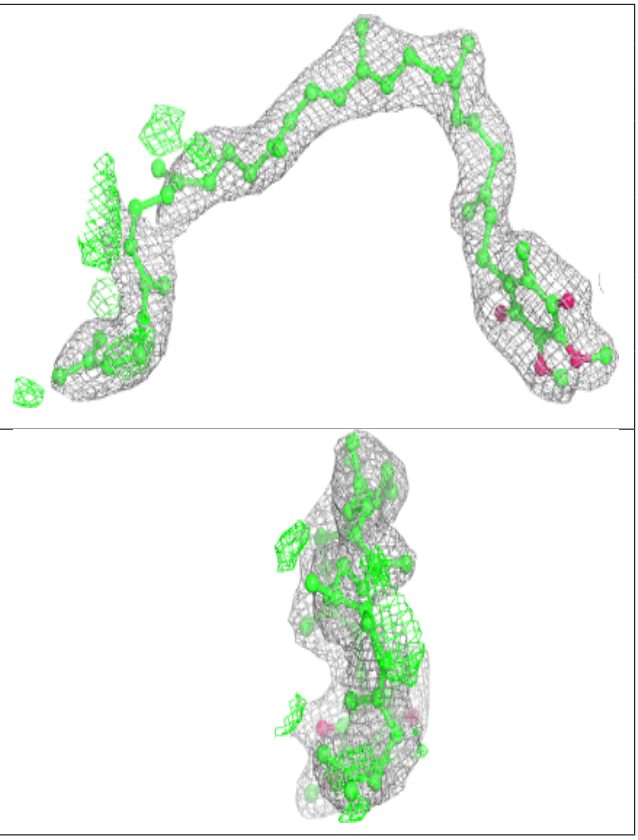






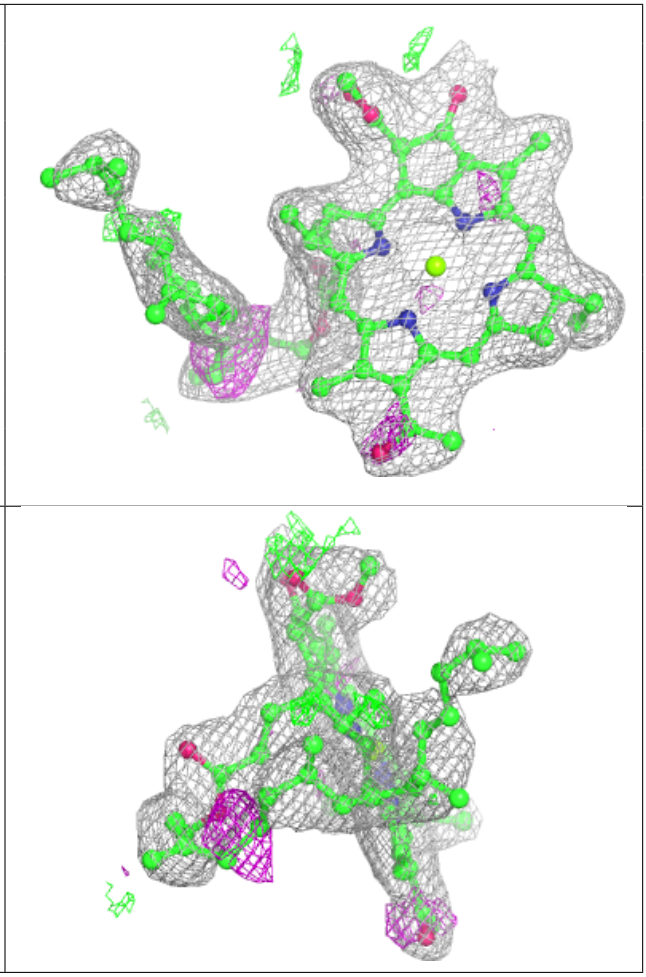
Electron density around U10 M 408:

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



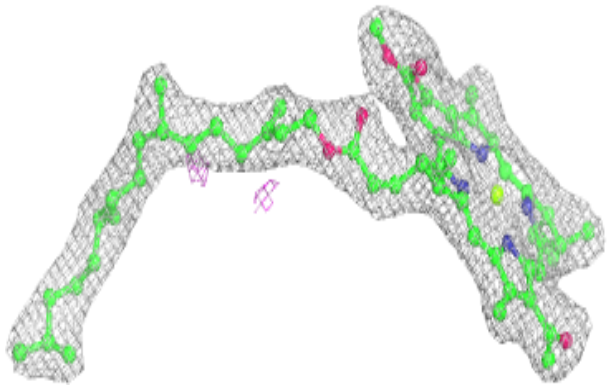
Electron density around BCL M 401:

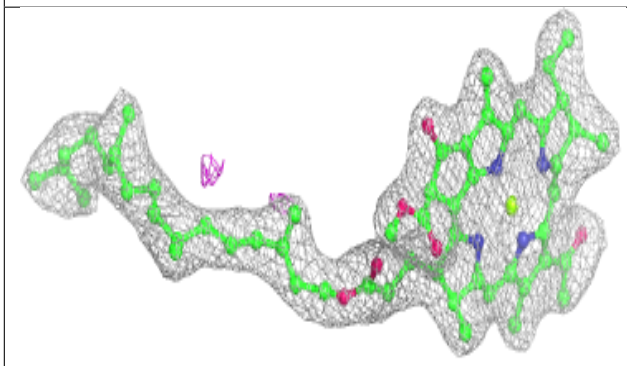
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL L 301:

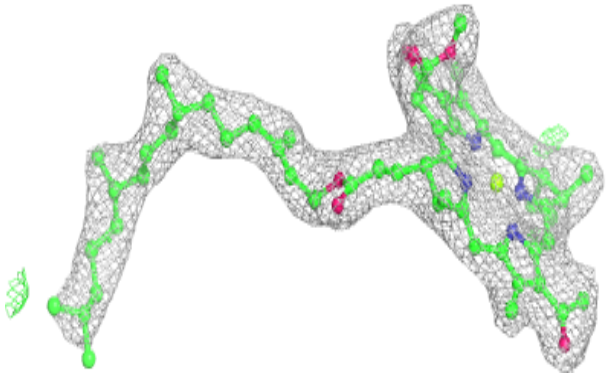
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

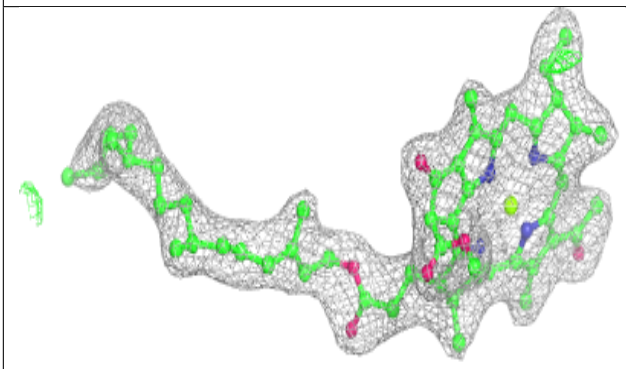


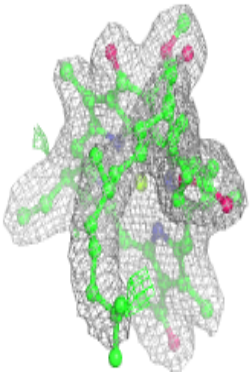


Electron density around BCL M 402:

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

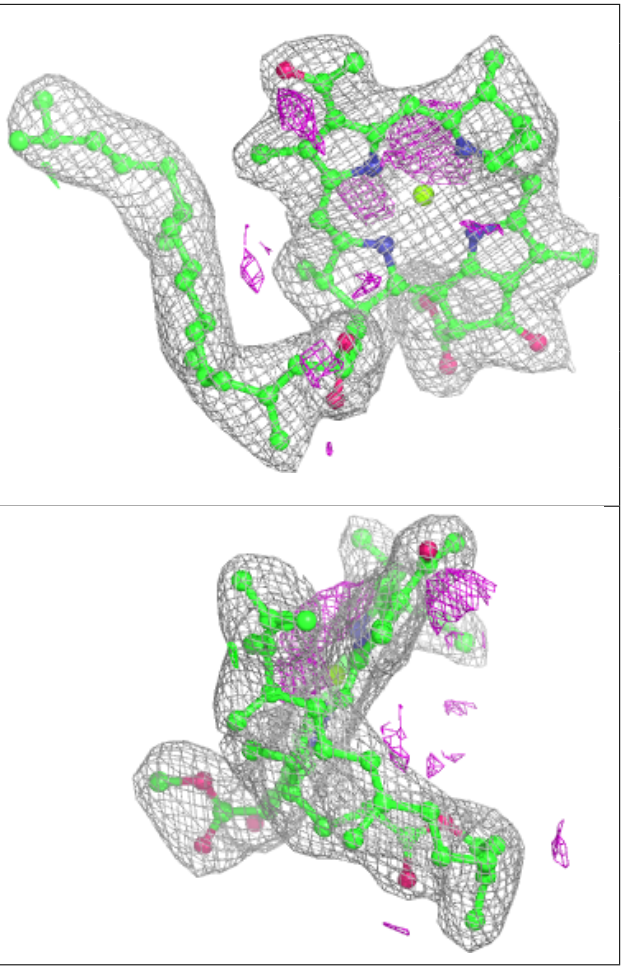






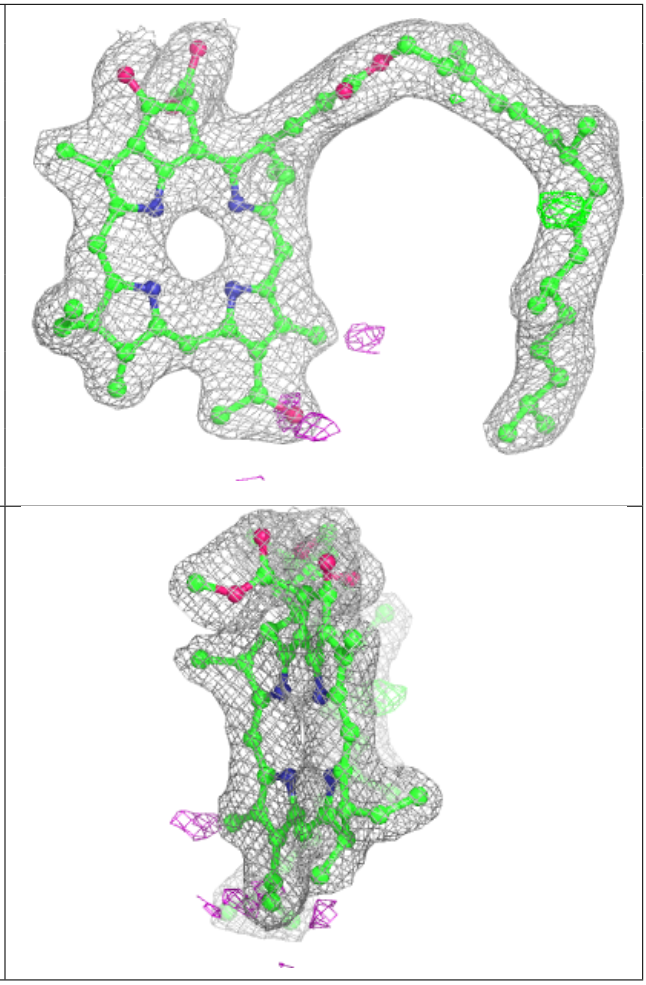
Electron density around BCL L 302:

$2mF_o$-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 304:

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.