Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 07:19 am GMT

PDB ID	:	2UX3
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the neutral state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-26
Resolution	:	2.50 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:

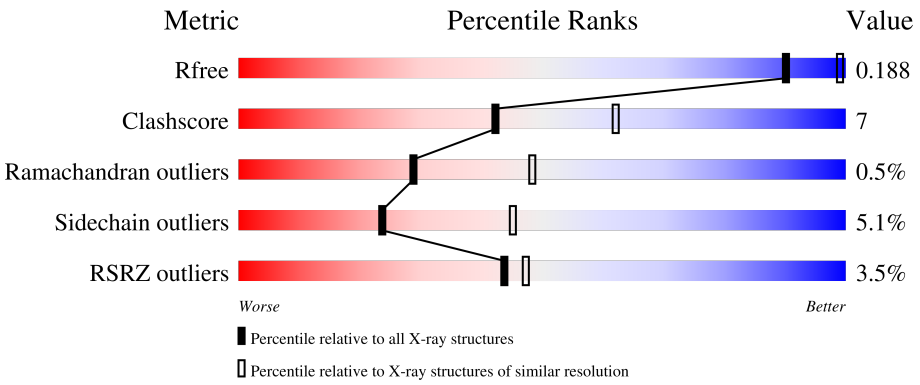
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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% 82% 9% • 7%
2	L	281	3% 84% 15% •
3	M	307	4% 82% 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
10	HTO	L	1288	-	-	-	X
14	CDL	M	1316	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1286	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1711	-	-	-	X
6	LDA	M	1309	-	-	-	X
6	LDA	M	1310	-	-	-	X
6	LDA	M	1311	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7606 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

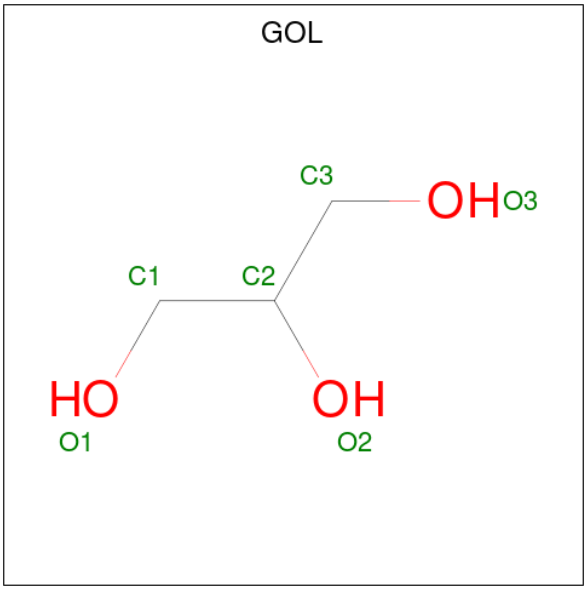
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

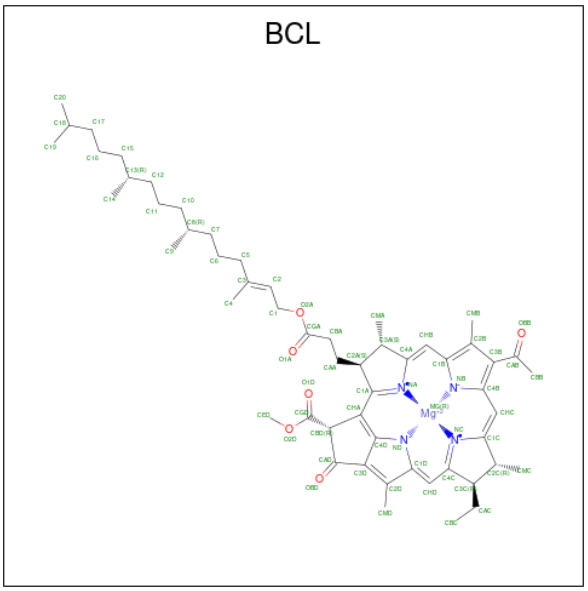
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2419	1616	396	397	10	0	1	1

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



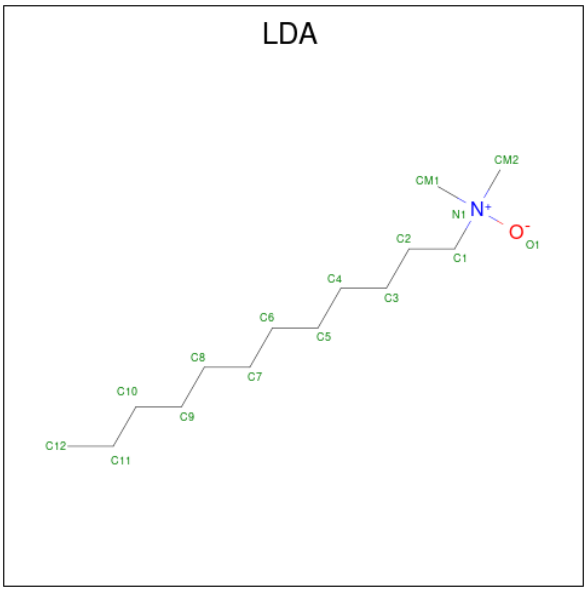
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	H	1	6	3	3	0	0
			Total	C	O		
4	H	1	6	3	3	0	0
			Total	C	O		
4	H	1	6	3	3	0	0
			Total	C	O		
4	H	1	6	3	3	0	0
			Total	C	O		
4	L	1	6	3	3	0	0
			Total	C	O		
4	L	1	6	3	3	0	0

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



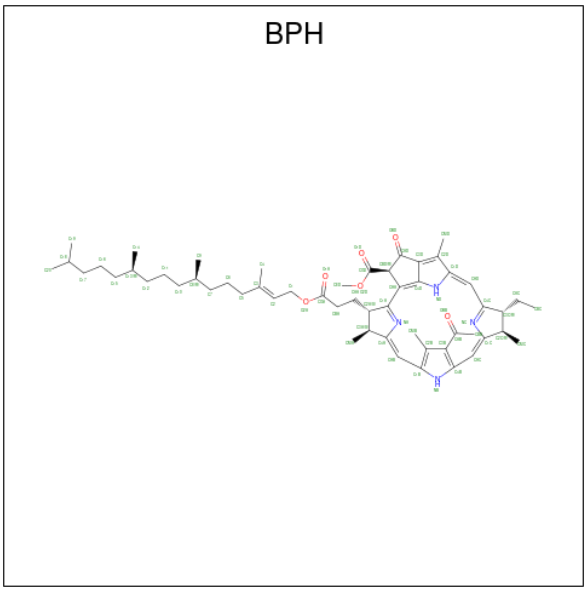
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

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



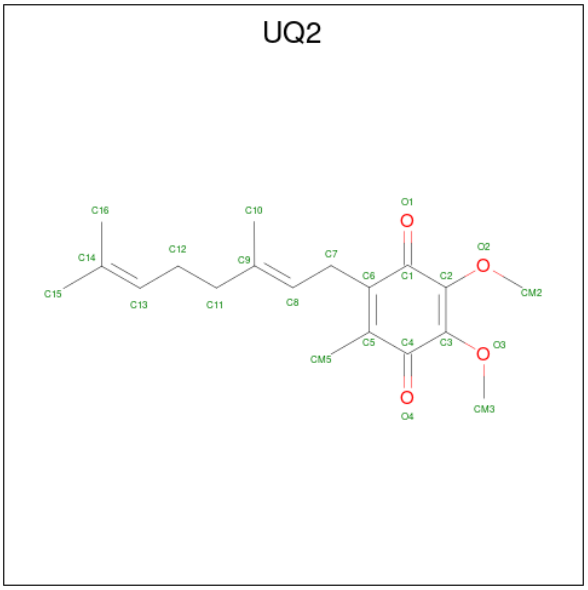
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0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

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



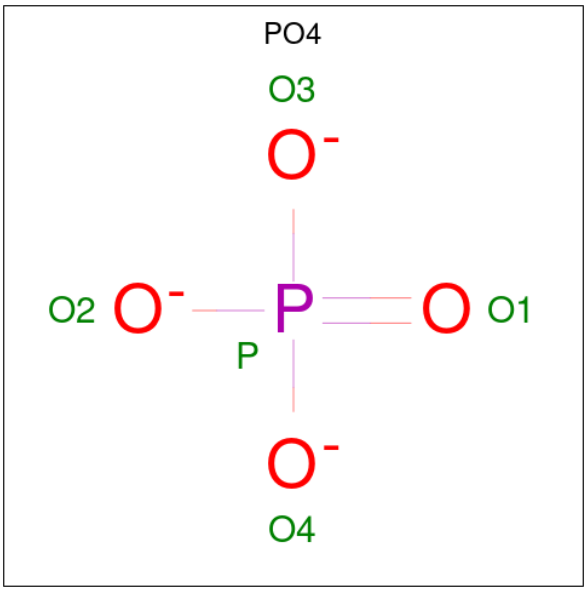
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	65	55	4	6	0	0

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



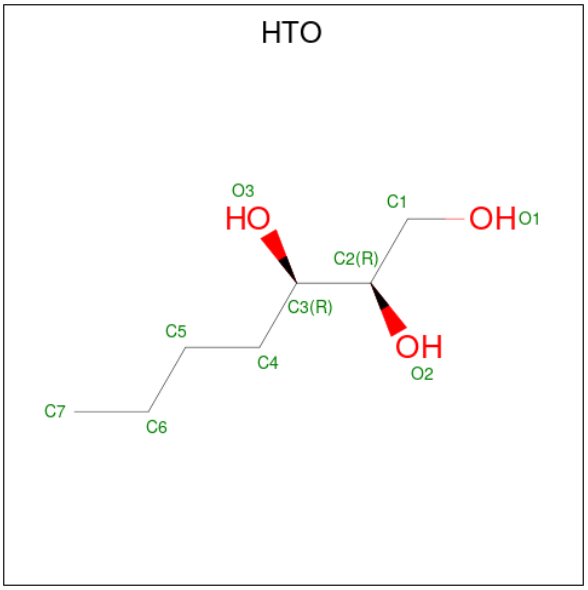
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1

- 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: $C_7H_{16}O_3$).

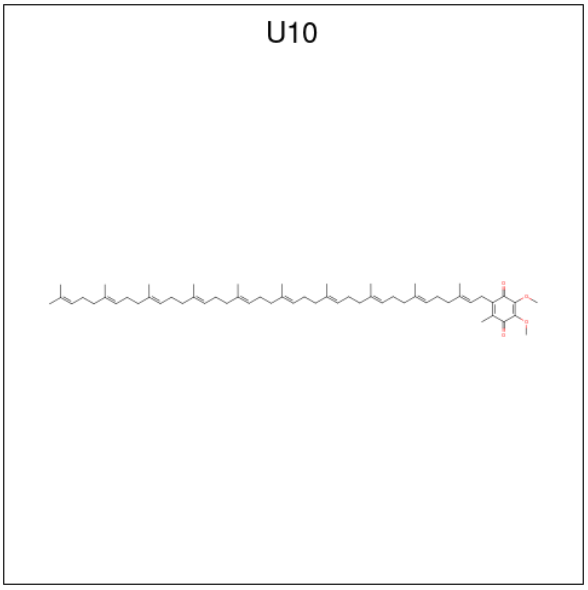


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

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

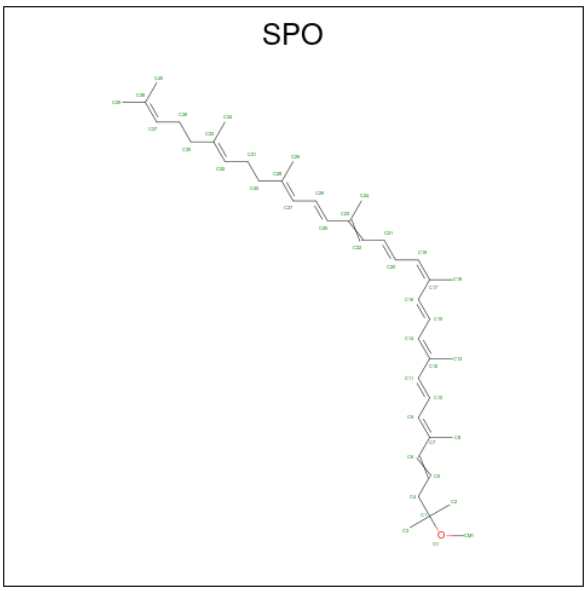
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
11	M	1	1	1	0	0

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



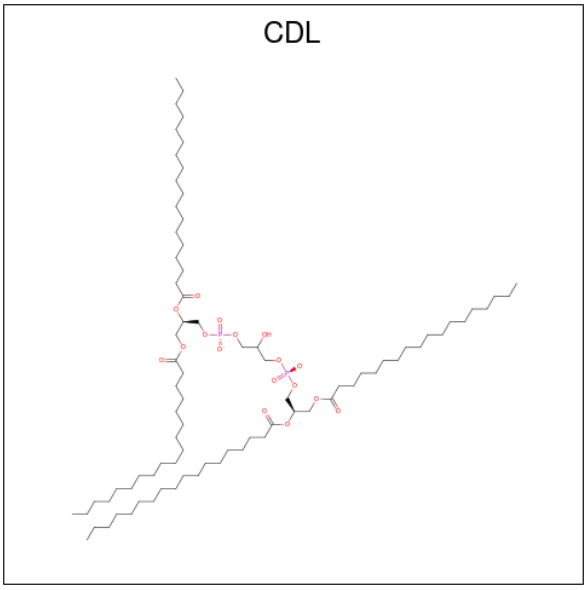
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	M	1	48	44	4	0	0

- 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 CARDIOLIPIN (three-letter code: 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.

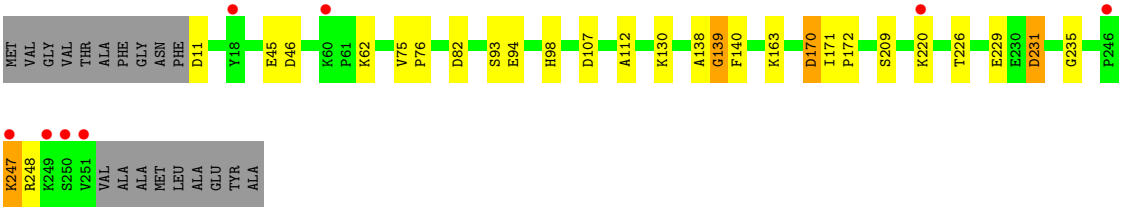
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	H	114	114	114	0	0
			Total	O		
15	L	92	92	92	0	0
			Total	O		
15	M	96	96	96	0	0

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.

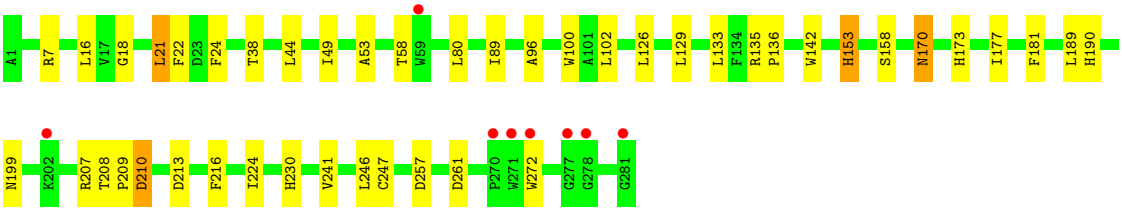
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



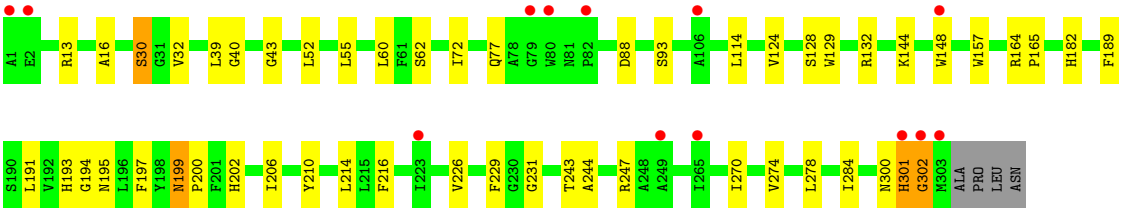
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

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 184.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.50 36.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (119.52-2.50) 86.6 (36.90-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.221 0.182 , 0.188	Depositor DCC
R_{free} test set	2004 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7606	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 2.99% 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: U10, HTO, UQ2, PO4, SPO, LDA, GOL, CDL, BCL, FE, 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	0.63	0/1906	0.78	7/2591 (0.3%)
2	L	0.66	0/2320	0.68	4/3175 (0.1%)
3	M	0.61	0/2517	0.68	2/3438 (0.1%)
All	All	0.63	0/6743	0.71	13/9204 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	82	ASP	CB-CG-OD2	7.62	125.16	118.30
1	H	11	ASP	CB-CG-OD2	7.00	124.60	118.30
2	L	213	ASP	CB-CG-OD2	6.80	124.42	118.30
1	H	139	GLY	N-CA-C	-5.99	98.13	113.10
2	L	210	ASP	CB-CG-OD1	5.96	123.67	118.30
1	H	231	ASP	CB-CG-OD2	5.63	123.36	118.30
3	M	88	ASP	CB-CG-OD2	5.47	123.23	118.30
2	L	257	ASP	CB-CG-OD2	5.43	123.19	118.30
1	H	107	ASP	CB-CG-OD2	5.38	123.14	118.30
2	L	261	ASP	CB-CG-OD2	5.14	122.92	118.30
1	H	170	ASP	CB-CG-OD2	5.13	122.92	118.30
1	H	46	ASP	CB-CG-OD2	5.09	122.88	118.30
3	M	302	GLY	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	13	0
2	L	2232	0	2187	28	0
3	M	2419	0	2327	28	0
4	H	24	0	32	1	0
4	L	12	0	16	1	0
5	L	132	0	148	8	0
5	M	132	0	148	18	0
6	L	32	0	62	2	0
6	M	112	0	217	2	0
7	L	65	0	76	9	0
7	M	65	0	76	14	0
8	L	46	0	52	8	0
9	L	5	0	0	0	0
10	L	10	0	16	2	0
11	M	1	0	0	0	0
12	M	48	0	63	2	0
13	M	42	0	60	3	0
14	M	81	0	82	3	0
15	H	114	0	0	0	1
15	L	92	0	0	0	0
15	M	96	0	0	0	0
All	All	7606	0	7423	101	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 7.

All (101) 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)
2:L:224:ILE:HG22	8:L:1285[A]:UQ2:H8	1.61	0.83
8:L:1285[A]:UQ2:H161	6:L:1711:LDA:H121	1.62	0.81
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.46	0.79
2:L:181:PHE:CD2	7:M:1313:BPH:HBB1	2.18	0.78
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.18	0.78
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.64	0.78
5:M:1303:BCL:H62	7:M:1313:BPH:HMB1	1.66	0.78
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.66	0.75
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.75	0.69
7:L:1284:BPH:HHC	7:L:1284:BPH:CBB	2.22	0.69
2:L:181:PHE:HB3	7:M:1313:BPH:HBB2	1.74	0.69
7:L:1284:BPH:HHC	7:L:1284:BPH:HBB3	1.76	0.66
7:M:1313:BPH:HBB3	7:M:1313:BPH:HHC	1.76	0.65
3:M:144:LYS:N	14:M:1316:CDL:OB3	2.26	0.65
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.78	0.65
2:L:170:ASN:HD22	2:L:170:ASN:C	2.01	0.64
3:M:77:GLN:HE22	3:M:93:SER:H	1.44	0.63
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.79	0.62
7:M:1313:BPH:HHD	7:M:1313:BPH:HBC2	1.80	0.62
2:L:199:ASN:HA	4:L:1289:GOL:H31	1.82	0.61
2:L:199:ASN:O	14:M:1316:CDL:HB22	2.00	0.60
5:M:1303:BCL:H62	7:M:1313:BPH:CMB	2.32	0.59
2:L:181:PHE:HB3	7:M:1313:BPH:CBB	2.33	0.59
1:H:140:PHE:HA	3:M:13:ARG:O	2.03	0.58
2:L:190:HIS:HA	8:L:1285[A]:UQ2:O4	2.04	0.58
5:M:1303:BCL:CBB	13:M:1315:SPO:H243	2.34	0.57
3:M:197:PHE:CE1	5:M:1304:BCL:HHC	2.40	0.57
8:L:1285[A]:UQ2:C16	6:L:1711:LDA:H121	2.34	0.56
6:M:1308:LDA:H71	12:M:1314:U10:H23	1.88	0.56
3:M:199:ASN:HD22	3:M:199:ASN:C	2.09	0.55
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.90	0.54
3:M:62:SER:OG	3:M:124:VAL:HG22	2.07	0.54
3:M:189:PHE:O	3:M:193:HIS:HD2	1.90	0.53
5:M:1303:BCL:HBB2	13:M:1315:SPO:H243	1.90	0.52
5:L:1286:BCL:CBB	5:L:1286:BCL:HMB1	2.40	0.52
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.51
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.46	0.51
7:L:1284:BPH:HBB3	7:L:1284:BPH:CHC	2.40	0.51
7:M:1313:BPH:HHC	7:M:1313:BPH:CBB	2.38	0.51
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.93	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.94	0.49
5:M:1304:BCL:CHC	5:M:1304:BCL:CBB	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.95	0.48
2:L:133:LEU:HD13	10:L:1288:HTO:H62	1.95	0.47
5:L:1282:BCL:HBB3	5:L:1286:BCL:H52	1.95	0.47
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.32	0.47
7:L:1284:BPH:CBB	7:L:1284:BPH:CHC	2.91	0.47
8:L:1285[B]:UQ2:H5M1	8:L:1285[B]:UQ2:H8	1.96	0.47
3:M:243:THR:O	3:M:247:ARG:HG3	2.14	0.47
1:H:75:VAL:HA	1:H:76:PRO:C	2.36	0.47
2:L:224:ILE:CG2	8:L:1285[A]:UQ2:H8	2.40	0.46
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.98	0.46
7:M:1313:BPH:HBC2	7:M:1313:BPH:CHD	2.44	0.46
3:M:284:ILE:HG12	5:M:1304:BCL:HED3	1.97	0.46
1:H:209:SER:OG	1:H:247:LYS:HD3	2.16	0.46
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.98	0.46
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.80	0.45
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.52	0.45
3:M:129:TRP:O	3:M:132:ARG:HB3	2.16	0.45
2:L:49:ILE:HG13	2:L:89:ILE:HD13	1.98	0.45
6:M:1307:LDA:H112	12:M:1314:U10:H202	1.98	0.45
5:M:1304:BCL:HHC	5:M:1304:BCL:CBB	2.47	0.45
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.17	0.45
2:L:189:LEU:CD2	7:M:1313:BPH:HMD2	2.47	0.45
1:H:45:GLU:HG3	1:H:94:GLU:OE1	2.16	0.45
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.98	0.44
8:L:1285[A]:UQ2:H71	8:L:1285[A]:UQ2:H5M1	1.64	0.44
2:L:96:ALA:HB1	7:L:1284:BPH:H2	2.00	0.44
7:M:1313:BPH:HBB3	7:M:1313:BPH:CHC	2.47	0.44
2:L:241:VAL:HG21	7:L:1284:BPH:HBC3	2.00	0.44
5:M:1303:BCL:HBB1	13:M:1315:SPO:H243	2.00	0.43
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.67	0.43
1:H:171:ILE:N	1:H:172:PRO:HD2	2.33	0.43
5:L:1282:BCL:H161	5:L:1282:BCL:H122	1.64	0.43
5:M:1304:BCL:H61	7:M:1313:BPH:C4B	2.49	0.43
7:L:1284:BPH:ND	3:M:214:LEU:HD13	2.34	0.43
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.82	0.43
1:H:112:ALA:HA	1:H:235:GLY:O	2.19	0.42
3:M:189:PHE:O	3:M:193:HIS:CD2	2.71	0.42
2:L:190:HIS:CE1	2:L:230:HIS:CE1	3.07	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.82	0.42
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.55	0.42
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:LEU:HD23	7:M:1313:BPH:HMD2	2.02	0.42
3:M:40:GLY:HA2	3:M:43:GLY:O	2.20	0.42
3:M:199:ASN:HD22	3:M:200:PRO:N	2.18	0.42
7:M:1313:BPH:H142	7:M:1313:BPH:H111	1.95	0.42
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.19	0.42
8:L:1285[B]:UQ2:H5M1	8:L:1285[B]:UQ2:C8	2.50	0.41
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.55	0.41
2:L:53:ALA:HB1	2:L:58:THR:O	2.19	0.41
3:M:148[B]:TRP:CD1	14:M:1316:CDL:HB62	2.56	0.41
5:L:1282:BCL:O1A	5:L:1282:BCL:H43	2.21	0.41
3:M:226:VAL:HG23	3:M:231:GLY:HA3	2.03	0.41
2:L:142:TRP:CZ2	10:L:1288:HTO:H3	2.54	0.41
5:L:1286:BCL:C1C	5:M:1304:BCL:HBB3	2.51	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.21	0.41
2:L:18:GLY:O	2:L:21:LEU:HB2	2.20	0.40
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.89	0.40
2:L:208:THR:HB	2:L:209:PRO:HD2	2.04	0.40
5:L:1286:BCL:HMB1	5:L:1286:BCL:HBB3	2.03	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)
15:H:2033:HOH:O	15:H:2033:HOH:O[4_555]	2.10	0.10

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%)	234 (97%)	7 (3%)	1 (0%)	34 54
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	302/307 (98%)	286 (95%)	13 (4%)	3 (1%)	15	28
All	All	823/848 (97%)	790 (96%)	29 (4%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
1	H	248	ARG
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%)	192 (97%)	6 (3%)	41	68
2	L	220/220 (100%)	204 (93%)	16 (7%)	14	27
3	M	237/240 (99%)	225 (95%)	12 (5%)	24	45
All	All	655/668 (98%)	621 (95%)	34 (5%)	24	44

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	93	SER
1	H	163	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	102	LEU

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Mol	Chain	Res	Type
2	L	126	LEU
2	L	129	LEU
2	L	153	HIS
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	272	TRP
3	M	30	SER
3	M	39	LEU
3	M	52	LEU
3	M	60	LEU
3	M	72	ILE
3	M	114	LEU
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU
3	M	301	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	183	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 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	$\#\|Z\| > 2$
10	HTO	L	1288	-	9,9,9	0.40	0	10,10,10	0.82	0
9	PO4	L	1287	-	4,4,4	0.86	0	6,6,6	0.48	0
4	GOL	L	1289	-	5,5,5	0.35	0	5,5,5	0.30	0
5	BCL	M	1303	3	64,74,74	2.08	12 (18%)	78,115,115	2.17	21 (26%)
5	BCL	M	1304	3	64,74,74	1.95	10 (15%)	78,115,115	2.10	19 (24%)
6	LDA	M	1306	-	12,15,15	2.00	1 (8%)	14,17,17	0.57	0
6	LDA	M	1307	-	12,15,15	2.00	1 (8%)	14,17,17	0.67	0
8	UQ2	L	1285[A]	-	23,23,23	2.64	8 (34%)	28,31,31	1.87	8 (28%)
6	LDA	M	1310	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
8	UQ2	L	1285[B]	-	23,23,23	2.75	7 (30%)	28,31,31	1.22	2 (7%)
5	BCL	L	1282	2	64,74,74	2.02	9 (14%)	78,115,115	2.30	23 (29%)
14	CDL	M	1316	-	80,80,99	2.39	18 (22%)	86,92,111	3.81	16 (18%)
12	U10	M	1314	-	48,48,63	2.71	13 (27%)	58,61,79	1.61	16 (27%)
4	GOL	H	1251	-	5,5,5	0.56	0	5,5,5	0.62	0
6	LDA	M	1311	-	12,15,15	2.02	1 (8%)	14,17,17	0.46	0
4	GOL	H	1253	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	L	1290	-	5,5,5	0.37	0	5,5,5	0.28	0
6	LDA	M	1309	-	12,15,15	2.06	1 (8%)	14,17,17	0.53	0
6	LDA	L	1283	-	12,15,15	2.04	1 (8%)	14,17,17	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BPH	M	1313	-	51,70,70	2.82	9 (17%)	52,101,101	2.04	12 (23%)
6	LDA	M	1305	-	12,15,15	2.03	1 (8%)	14,17,17	0.63	0
13	SPO	M	1315	-	40,41,41	4.16	12 (30%)	47,50,50	1.99	16 (34%)
4	GOL	H	1252	-	5,5,5	0.40	0	5,5,5	0.34	0
6	LDA	L	1711	-	12,15,15	2.11	1 (8%)	14,17,17	0.57	0
6	LDA	M	1308	-	12,15,15	2.04	1 (8%)	14,17,17	0.45	0
4	GOL	H	1254	-	5,5,5	0.34	0	5,5,5	0.33	0
5	BCL	L	1286	2	64,74,74	2.01	10 (15%)	78,115,115	2.41	20 (25%)
7	BPH	L	1284	-	51,70,70	2.81	10 (19%)	52,101,101	1.89	10 (19%)

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
10	HTO	L	1288	-	-	8/10/10/10	-
4	GOL	L	1289	-	-	2/4/4/4	-
5	BCL	M	1303	3	2/2/21/25	17/37/137/137	-
5	BCL	M	1304	3	2/2/21/25	10/37/137/137	-
6	LDA	M	1306	-	-	4/13/13/13	-
6	LDA	M	1307	-	-	4/13/13/13	-
8	UQ2	L	1285[A]	-	-	6/15/39/39	0/1/1/1
6	LDA	M	1310	-	-	6/13/13/13	-
8	UQ2	L	1285[B]	-	-	9/15/39/39	0/1/1/1
5	BCL	L	1282	2	2/2/21/25	12/37/137/137	-
14	CDL	M	1316	-	-	39/91/91/110	-
12	U10	M	1314	-	-	7/45/69/87	0/1/1/1
4	GOL	H	1251	-	-	2/4/4/4	-
6	LDA	M	1311	-	-	7/13/13/13	-
4	GOL	H	1253	-	-	2/4/4/4	-
4	GOL	L	1290	-	-	4/4/4/4	-
6	LDA	M	1309	-	-	9/13/13/13	-
6	LDA	L	1283	-	-	10/13/13/13	-
7	BPH	M	1313	-	-	19/37/105/105	0/5/6/6
6	LDA	M	1305	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SPO	M	1315	-	-	18/47/47/47	-
4	GOL	H	1252	-	-	2/4/4/4	-
6	LDA	L	1711	-	-	7/13/13/13	-
6	LDA	M	1308	-	-	7/13/13/13	-
4	GOL	H	1254	-	-	0/4/4/4	-
5	BCL	L	1286	2	2/2/21/25	9/37/137/137	-
7	BPH	L	1284	-	-	6/37/105/105	0/5/6/6

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1315	SPO	C27-C28	13.22	1.47	1.34
7	M	1313	BPH	OBD-CAD	13.21	1.40	1.22
7	L	1284	BPH	OBD-CAD	12.65	1.40	1.22
5	L	1282	BCL	OBD-CAD	11.02	1.41	1.22
5	L	1286	BCL	OBD-CAD	10.63	1.40	1.22
5	M	1304	BCL	OBD-CAD	10.54	1.40	1.22
5	M	1303	BCL	OBD-CAD	10.36	1.40	1.22
13	M	1315	SPO	C9-C7	9.35	1.48	1.35
13	M	1315	SPO	C22-C23	9.08	1.47	1.35
13	M	1315	SPO	C19-C17	9.02	1.47	1.35
13	M	1315	SPO	C14-C12	8.32	1.46	1.35
14	M	1316	CDL	C11-CA5	-7.97	1.27	1.50
7	L	1284	BPH	O1D-CGD	7.77	1.40	1.21
6	L	1711	LDA	O1-N1	-7.23	1.25	1.42
7	M	1313	BPH	O1D-CGD	7.14	1.39	1.21
6	M	1309	LDA	O1-N1	-7.05	1.25	1.42
6	M	1308	LDA	O1-N1	-6.96	1.25	1.42
6	L	1283	LDA	O1-N1	-6.95	1.25	1.42
6	M	1310	LDA	O1-N1	-6.95	1.25	1.42
14	M	1316	CDL	C12-C11	-6.94	1.26	1.52
14	M	1316	CDL	C32-C31	-6.91	1.26	1.52
6	M	1307	LDA	O1-N1	-6.90	1.26	1.42
6	M	1311	LDA	O1-N1	-6.90	1.26	1.42
6	M	1306	LDA	O1-N1	-6.84	1.26	1.42
6	M	1305	LDA	O1-N1	-6.83	1.26	1.42
12	M	1314	U10	C33-C34	6.81	1.49	1.33
12	M	1314	U10	C13-C14	6.76	1.49	1.33
8	L	1285[B]	UQ2	C8-C9	6.70	1.49	1.33
13	M	1315	SPO	C32-C33	6.56	1.48	1.33
7	L	1284	BPH	OBB-CAB	6.49	1.42	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1285[A]	UQ2	C8-C9	6.37	1.48	1.33
12	M	1314	U10	C8-C9	6.33	1.48	1.33
7	L	1284	BPH	O1A-CGA	6.31	1.41	1.22
7	M	1313	BPH	C2-C3	6.30	1.48	1.33
5	M	1303	BCL	O1A-CGA	6.22	1.41	1.22
12	M	1314	U10	C23-C24	5.95	1.47	1.33
7	M	1313	BPH	OBB-CAB	5.95	1.41	1.22
5	M	1304	BCL	O1A-CGA	5.94	1.40	1.22
7	L	1284	BPH	C2-C3	5.94	1.47	1.33
7	M	1313	BPH	C3D-C2D	5.91	1.50	1.39
5	L	1282	BCL	O1A-CGA	5.90	1.40	1.22
7	M	1313	BPH	O1A-CGA	5.85	1.39	1.22
13	M	1315	SPO	C37-C38	5.84	1.49	1.32
12	M	1314	U10	C28-C29	5.80	1.46	1.33
14	M	1316	CDL	C33-C32	-5.70	1.19	1.51
12	M	1314	U10	C18-C19	5.69	1.46	1.33
5	L	1286	BCL	O1A-CGA	5.58	1.39	1.22
8	L	1285[B]	UQ2	C13-C14	5.50	1.48	1.32
8	L	1285[A]	UQ2	C13-C14	5.46	1.48	1.32
13	M	1315	SPO	C6-C5	5.42	1.46	1.32
12	M	1314	U10	C38-C39	5.41	1.47	1.32
14	M	1316	CDL	C34-C33	-5.41	1.21	1.51
8	L	1285[A]	UQ2	O2-C2	-5.36	1.23	1.36
7	L	1284	BPH	C3D-C2D	5.23	1.48	1.39
8	L	1285[B]	UQ2	O2-C2	-5.03	1.24	1.36
14	M	1316	CDL	OB6-CB5	4.89	1.48	1.34
8	L	1285[B]	UQ2	O3-C3	-4.84	1.25	1.36
14	M	1316	CDL	OA8-CA7	4.80	1.47	1.33
8	L	1285[A]	UQ2	O3-C3	-4.75	1.25	1.36
13	M	1315	SPO	C10-C11	4.74	1.46	1.34
12	M	1314	U10	O4-C4	-4.71	1.25	1.36
13	M	1315	SPO	C15-C16	4.65	1.46	1.34
14	M	1316	CDL	OB8-CB7	4.59	1.46	1.33
14	M	1316	CDL	OA6-CA5	4.55	1.47	1.34
5	L	1286	BCL	C4B-NB	4.49	1.39	1.35
14	M	1316	CDL	C16-C15	-4.47	1.26	1.51
14	M	1316	CDL	C17-C16	-4.41	1.26	1.51
14	M	1316	CDL	C20-C19	-4.39	1.27	1.51
12	M	1314	U10	O3-C3	-4.34	1.26	1.36
14	M	1316	CDL	C19-C18	-4.31	1.27	1.51
13	M	1315	SPO	C26-C25	4.26	1.45	1.34
5	M	1303	BCL	C4D-ND	-4.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1303	BCL	C3D-C4D	-4.12	1.34	1.44
13	M	1315	SPO	C21-C20	3.92	1.46	1.36
5	L	1282	BCL	C4D-ND	-3.84	1.32	1.37
5	L	1286	BCL	C3D-C4D	-3.84	1.35	1.44
5	M	1304	BCL	C3D-C4D	-3.80	1.35	1.44
5	L	1286	BCL	C4D-ND	-3.77	1.32	1.37
5	L	1286	BCL	C2-C3	3.68	1.41	1.33
8	L	1285[B]	UQ2	C6-C5	3.66	1.41	1.35
5	L	1282	BCL	C3D-C4D	-3.61	1.36	1.44
5	M	1303	BCL	C1B-NB	3.58	1.38	1.35
14	M	1316	CDL	C13-C12	-3.56	1.31	1.51
5	M	1303	BCL	C4B-NB	3.54	1.38	1.35
5	M	1304	BCL	C4D-ND	-3.54	1.32	1.37
12	M	1314	U10	C6-C1	3.50	1.41	1.35
5	L	1282	BCL	C4B-NB	3.36	1.38	1.35
5	M	1303	BCL	C2-C3	3.32	1.40	1.33
8	L	1285[A]	UQ2	C3-C4	-3.15	1.39	1.48
14	M	1316	CDL	C37-C36	-3.14	1.34	1.51
12	M	1314	U10	C4-C5	-3.11	1.39	1.48
8	L	1285[B]	UQ2	C3-C4	-3.08	1.40	1.48
5	L	1282	BCL	C2-C3	3.07	1.40	1.33
14	M	1316	CDL	C79-C78	-3.04	1.34	1.51
14	M	1316	CDL	C22-C21	-3.01	1.34	1.51
5	L	1286	BCL	C1B-NB	2.97	1.37	1.35
5	M	1304	BCL	C2-C3	2.97	1.40	1.33
14	M	1316	CDL	C80-C79	-2.95	1.35	1.51
5	L	1282	BCL	C1B-NB	2.91	1.37	1.35
7	L	1284	BPH	O2D-CGD	-2.87	1.26	1.33
5	M	1304	BCL	C4B-NB	2.82	1.37	1.35
7	M	1313	BPH	O2D-CGD	-2.81	1.26	1.33
7	M	1313	BPH	O2A-CGA	-2.81	1.25	1.33
5	M	1303	BCL	C1D-C2D	-2.80	1.39	1.45
5	M	1303	BCL	CHD-C4C	2.78	1.47	1.39
8	L	1285[A]	UQ2	C6-C1	-2.72	1.39	1.46
5	M	1303	BCL	O2D-CGD	-2.71	1.26	1.33
12	M	1314	U10	C3-C2	-2.69	1.41	1.48
8	L	1285[B]	UQ2	C2-C1	-2.63	1.41	1.48
5	L	1282	BCL	O2A-CGA	-2.63	1.25	1.33
8	L	1285[A]	UQ2	C6-C5	2.62	1.40	1.35
5	M	1304	BCL	CHD-C4C	2.50	1.46	1.39
5	M	1304	BCL	C3C-C4C	-2.50	1.48	1.51
5	L	1282	BCL	O2D-CGD	-2.47	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	O2D-CGD	-2.42	1.27	1.33
7	L	1284	BPH	C2C-C3C	-2.40	1.52	1.54
5	L	1286	BCL	CHD-C4C	2.37	1.45	1.39
5	L	1286	BCL	O2D-CGD	-2.28	1.27	1.33
5	M	1304	BCL	C1B-NB	2.24	1.37	1.35
7	M	1313	BPH	C3A-C2A	-2.23	1.52	1.54
12	M	1314	U10	C6-C5	-2.20	1.40	1.46
5	M	1303	BCL	O2A-CGA	-2.15	1.27	1.33
7	L	1284	BPH	O2A-CGA	-2.13	1.27	1.33
7	L	1284	BPH	O2D-CED	-2.07	1.40	1.45
5	M	1303	BCL	MG-ND	-2.06	2.01	2.05
5	L	1286	BCL	O2A-CGA	-2.05	1.27	1.33
8	L	1285[A]	UQ2	C2-C1	-2.00	1.43	1.48

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1316	CDL	C33-C32-C31	17.87	177.43	113.19
14	M	1316	CDL	C12-C11-CA5	13.14	161.41	113.62
14	M	1316	CDL	C17-C16-C15	11.81	174.41	114.42
14	M	1316	CDL	C20-C19-C18	11.54	173.01	114.42
14	M	1316	CDL	C13-C12-C11	10.88	152.29	113.19
14	M	1316	CDL	C34-C33-C32	10.66	168.54	114.42
14	M	1316	CDL	C35-C34-C33	10.59	168.17	114.42
7	M	1313	BPH	O2D-CGD-CBD	9.39	122.89	111.00
5	L	1286	BCL	C2D-C1D-ND	-8.28	104.00	110.10
5	M	1304	BCL	CMB-C2B-C1B	-7.88	116.35	128.46
5	L	1286	BCL	CMB-C2B-C1B	-7.85	116.39	128.46
5	L	1282	BCL	CMB-C2B-C1B	-7.43	117.05	128.46
7	L	1284	BPH	O2D-CGD-CBD	7.37	120.33	111.00
5	L	1286	BCL	C1D-ND-C4D	7.34	111.55	106.33
5	M	1303	BCL	C1D-ND-C4D	7.15	111.41	106.33
5	M	1303	BCL	C2D-C1D-ND	-6.93	105.00	110.10
5	M	1303	BCL	CMB-C2B-C1B	-6.90	117.87	128.46
5	L	1282	BCL	O2D-CGD-CBD	5.98	121.90	111.27
5	L	1282	BCL	C2D-C1D-ND	-5.83	105.81	110.10
5	M	1303	BCL	O2D-CGD-CBD	5.63	121.26	111.27
5	L	1282	BCL	C4A-NA-C1A	5.55	109.20	106.71
5	L	1282	BCL	C1D-ND-C4D	5.23	110.05	106.33
5	M	1304	BCL	C2D-C1D-ND	-5.21	106.27	110.10
5	L	1286	BCL	CHD-C1D-ND	-5.16	119.71	124.45
13	M	1315	SPO	C20-C19-C17	-5.14	119.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	CMB-C2B-C3B	5.09	134.21	124.68
14	M	1316	CDL	OA6-CA5-C11	5.07	122.44	111.50
5	L	1282	BCL	CMD-C2D-C1D	5.04	133.60	124.71
5	L	1286	BCL	CMB-C2B-C3B	4.90	133.84	124.68
5	M	1303	BCL	C4A-NA-C1A	4.83	108.88	106.71
12	M	1314	U10	C30-C29-C31	4.69	123.15	115.27
13	M	1315	SPO	C21-C22-C23	-4.62	120.72	127.31
7	M	1313	BPH	OBD-CAD-CBD	-4.59	119.09	125.82
5	M	1304	BCL	CMD-C2D-C1D	4.59	132.79	124.71
13	M	1315	SPO	C10-C9-C7	-4.57	120.79	127.31
7	L	1284	BPH	OBD-CAD-CBD	-4.57	119.12	125.82
5	L	1282	BCL	CMB-C2B-C3B	4.54	133.18	124.68
5	M	1304	BCL	C1D-ND-C4D	4.53	109.55	106.33
5	M	1303	BCL	CMB-C2B-C3B	4.52	133.14	124.68
5	L	1286	BCL	C4A-NA-C1A	4.48	108.72	106.71
14	M	1316	CDL	OB6-CB5-C51	4.47	121.14	111.50
5	L	1286	BCL	O2D-CGD-CBD	4.42	119.12	111.27
5	M	1304	BCL	O2D-CGD-CBD	4.40	119.08	111.27
5	L	1282	BCL	C1C-NC-C4C	-4.35	104.75	106.71
5	M	1304	BCL	C4B-CHC-C1C	-4.34	121.51	130.12
5	L	1286	BCL	CMD-C2D-C1D	4.20	132.12	124.71
8	L	1285[A]	UQ2	CM5-C5-C6	-4.19	117.57	124.40
7	L	1284	BPH	O1D-CGD-CBD	-3.97	118.13	124.74
5	L	1286	BCL	C4B-CHC-C1C	-3.95	122.29	130.12
13	M	1315	SPO	C15-C14-C12	-3.90	121.75	127.31
8	L	1285[A]	UQ2	O1-C1-C6	-3.85	114.80	121.55
5	M	1304	BCL	C1C-NC-C4C	3.84	108.43	106.71
8	L	1285[A]	UQ2	CM3-O3-C3	3.84	130.06	116.47
5	M	1303	BCL	C1-O2A-CGA	3.64	126.00	116.44
5	L	1282	BCL	CMD-C2D-C3D	-3.60	119.34	127.61
5	L	1282	BCL	C4B-CHC-C1C	-3.59	123.01	130.12
5	M	1303	BCL	C4B-CHC-C1C	-3.58	123.02	130.12
5	L	1282	BCL	O1D-CGD-CBD	-3.58	117.17	124.48
5	L	1286	BCL	O2A-CGA-CBA	3.46	122.77	111.91
5	M	1304	BCL	O2A-CGA-CBA	3.44	122.71	111.91
5	M	1303	BCL	C1B-CHB-C4A	-3.43	123.33	130.12
13	M	1315	SPO	C29-C28-C30	3.39	120.98	115.27
5	M	1303	BCL	CMD-C2D-C1D	3.37	130.65	124.71
5	L	1282	BCL	C4-C3-C5	3.30	120.82	115.27
7	M	1313	BPH	O1D-CGD-CBD	-3.18	119.44	124.74
12	M	1314	U10	C10-C9-C11	3.18	120.62	115.27
7	M	1313	BPH	O2D-CGD-O1D	-3.17	117.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	CED-O2D-CGD	3.16	123.09	115.94
5	L	1286	BCL	CMD-C2D-C3D	-3.15	120.37	127.61
7	M	1313	BPH	CAC-C3C-C4C	3.13	120.73	113.73
12	M	1314	U10	C27-C28-C29	-3.12	120.14	127.66
5	L	1286	BCL	C1-O2A-CGA	3.12	124.62	116.44
5	L	1286	BCL	C2A-C3A-C4A	3.08	106.85	101.87
7	L	1284	BPH	CED-O2D-CGD	3.07	122.87	115.94
5	L	1286	BCL	CED-O2D-CGD	3.06	122.86	115.94
7	M	1313	BPH	C1C-C2C-C3C	-3.03	99.96	102.84
7	L	1284	BPH	C1C-C2C-C3C	-3.01	99.97	102.84
14	M	1316	CDL	OB8-CB7-C71	2.99	121.28	111.91
13	M	1315	SPO	C5-C6-C7	-2.97	121.40	125.89
7	L	1284	BPH	O2A-CGA-CBA	2.96	121.19	111.91
7	M	1313	BPH	CED-O2D-CGD	2.95	122.61	115.94
12	M	1314	U10	C25-C24-C26	2.94	120.22	115.27
7	L	1284	BPH	C1-C2-C3	-2.94	120.95	126.04
5	M	1304	BCL	CMD-C2D-C3D	-2.94	120.85	127.61
5	L	1286	BCL	CMA-C3A-C4A	-2.93	103.91	111.77
12	M	1314	U10	C22-C23-C24	-2.90	120.68	127.66
5	L	1282	BCL	CHA-C1A-NA	-2.89	119.77	126.40
5	M	1304	BCL	O2D-CGD-O1D	-2.76	118.45	123.84
7	M	1313	BPH	O2A-CGA-CBA	2.75	120.53	111.91
5	M	1303	BCL	CMA-C3A-C4A	-2.74	104.40	111.77
5	M	1304	BCL	C4-C3-C5	2.74	119.88	115.27
12	M	1314	U10	C35-C34-C36	2.71	119.84	115.27
5	L	1286	BCL	CHC-C1C-NC	-2.71	120.76	124.51
5	M	1303	BCL	O2A-CGA-CBA	2.69	120.34	111.91
14	M	1316	CDL	OA8-CA7-C31	2.65	120.22	111.91
5	L	1282	BCL	C1-C2-C3	-2.63	121.50	126.04
8	L	1285[B]	UQ2	C10-C9-C11	2.63	119.69	115.27
5	L	1282	BCL	C1B-CHB-C4A	-2.60	124.96	130.12
5	M	1304	BCL	C16-C15-C13	-2.59	107.54	115.92
7	M	1313	BPH	CMD-C2D-C3D	-2.57	119.87	124.68
5	M	1303	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
5	M	1304	BCL	C7-C6-C5	-2.55	106.44	113.36
8	L	1285[A]	UQ2	C16-C14-C15	2.55	120.23	114.60
7	M	1313	BPH	C1-C2-C3	-2.54	121.65	126.04
5	L	1282	BCL	CHB-C4A-NA	-2.54	121.00	124.51
7	L	1284	BPH	CMA-C3A-C4A	-2.53	108.83	114.38
5	M	1304	BCL	CAC-C3C-C4C	-2.52	106.99	112.58
13	M	1315	SPO	C34-C33-C35	2.51	119.49	115.27
12	M	1314	U10	C17-C18-C19	-2.50	121.63	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1316	CDL	C32-C31-CA7	2.50	122.72	113.62
5	M	1303	BCL	CHA-C1A-NA	-2.50	120.67	126.40
5	M	1303	BCL	C1D-CHD-C4C	-2.49	120.61	126.62
5	M	1304	BCL	CHD-C4C-NC	2.48	127.83	125.08
7	M	1313	BPH	C4A-C3A-C2A	-2.46	100.49	102.84
5	M	1304	BCL	C1-C2-C3	-2.44	121.83	126.04
12	M	1314	U10	C15-C14-C16	2.41	119.33	115.27
5	L	1282	BCL	O2A-CGA-CBA	2.40	119.43	111.91
5	L	1282	BCL	C2A-C3A-C4A	2.40	105.74	101.87
8	L	1285[B]	UQ2	C5-C6-C1	-2.39	117.33	119.58
13	M	1315	SPO	C14-C15-C16	-2.38	115.79	123.22
5	L	1282	BCL	O2A-CGA-O1A	-2.37	117.60	123.59
5	L	1286	BCL	CHA-C4D-ND	2.36	137.45	132.50
13	M	1315	SPO	C31-C32-C33	-2.36	121.99	127.66
12	M	1314	U10	C1M-C1-C6	-2.34	120.58	124.40
7	L	1284	BPH	O2A-CGA-O1A	-2.34	117.70	123.59
12	M	1314	U10	C41-C39-C40	2.32	119.72	114.60
13	M	1315	SPO	C40-C38-C39	2.29	119.66	114.60
7	L	1284	BPH	C4A-C3A-C2A	-2.28	100.67	102.84
13	M	1315	SPO	C8-C7-C6	2.28	121.68	118.08
8	L	1285[A]	UQ2	C10-C9-C11	2.26	119.08	115.27
12	M	1314	U10	C20-C19-C21	2.25	119.06	115.27
5	M	1303	BCL	O1D-CGD-CBD	-2.25	119.89	124.48
12	M	1314	U10	C30-C29-C28	-2.24	117.93	123.68
5	L	1286	BCL	C1B-CHB-C4A	-2.21	125.74	130.12
8	L	1285[A]	UQ2	O4-C4-C3	-2.20	116.25	120.93
12	M	1314	U10	C11-C9-C8	-2.18	116.71	121.12
5	L	1286	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
14	M	1316	CDL	OB8-CB7-OB9	-2.16	118.15	123.59
14	M	1316	CDL	C80-C79-C78	2.16	125.37	114.42
12	M	1314	U10	C3M-O3-C3	2.15	124.10	116.47
12	M	1314	U10	C32-C33-C34	-2.15	122.49	127.66
5	M	1303	BCL	CAA-C2A-C3A	-2.13	106.94	112.78
5	M	1303	BCL	CMD-C2D-C3D	-2.13	122.72	127.61
8	L	1285[A]	UQ2	C6-C5-C4	2.13	120.86	119.18
5	L	1282	BCL	CAA-CBA-CGA	2.12	119.46	113.25
5	L	1282	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
13	M	1315	SPO	C27-C26-C25	-2.12	116.59	123.22
5	M	1303	BCL	CHA-C4D-ND	2.10	136.90	132.50
13	M	1315	SPO	C18-C17-C16	2.10	121.39	118.08
13	M	1315	SPO	C8-C7-C9	-2.10	119.98	122.92
14	M	1316	CDL	C81-C80-C79	2.09	125.05	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	1314	U10	C4M-O4-C4	2.09	123.88	116.47
14	M	1316	CDL	OA6-CA5-OA7	-2.09	118.66	123.70
5	M	1303	BCL	C2A-C3A-C4A	2.08	105.23	101.87
5	L	1286	BCL	CHB-C4A-NA	-2.06	121.66	124.51
13	M	1315	SPO	C13-C12-C11	2.06	121.33	118.08
5	L	1282	BCL	C1-O2A-CGA	2.06	121.85	116.44
5	M	1304	BCL	OBB-CAB-C3B	2.04	123.62	119.99
8	L	1285[A]	UQ2	O3-C3-C2	-2.03	115.97	123.64
7	M	1313	BPH	O2A-CGA-O1A	-2.03	118.48	123.59
5	M	1303	BCL	O2A-C1-C2	2.01	113.93	108.64
5	L	1282	BCL	C3C-C4C-CHD	-2.01	119.09	123.39
13	M	1315	SPO	C36-C37-C38	-2.00	120.91	127.75

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1286	BCL	C13
5	L	1286	BCL	C8
5	M	1303	BCL	C13
5	M	1303	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	C1-C2-C3-O3
4	L	1289	GOL	C1-C2-C3-O3
4	L	1290	GOL	O1-C1-C2-C3
4	L	1290	GOL	C1-C2-C3-O3
4	L	1290	GOL	O2-C2-C3-O3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
6	M	1305	LDA	C2-C1-N1-CM2
6	M	1309	LDA	C2-C1-N1-CM1
7	L	1284	BPH	O2A-C1-C2-C3
7	L	1284	BPH	C1-C2-C3-C4
7	M	1313	BPH	C4C-C3C-CAC-CBC
7	M	1313	BPH	C2C-C3C-CAC-CBC
7	M	1313	BPH	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	L	1285[A]	UQ2	C7-C8-C9-C10
8	L	1285[A]	UQ2	C7-C8-C9-C11
8	L	1285[B]	UQ2	C7-C8-C9-C10
8	L	1285[B]	UQ2	C7-C8-C9-C11
8	L	1285[B]	UQ2	C9-C11-C12-C13
10	L	1288	HTO	O1-C1-C2-O2
10	L	1288	HTO	C1-C2-C3-O3
10	L	1288	HTO	C1-C2-C3-C4
10	L	1288	HTO	O2-C2-C3-O3
10	L	1288	HTO	O2-C2-C3-C4
10	L	1288	HTO	O3-C3-C4-C5
12	M	1314	U10	C27-C28-C29-C30
12	M	1314	U10	C27-C28-C29-C31
13	M	1315	SPO	C11-C12-C14-C15
13	M	1315	SPO	C13-C12-C14-C15
13	M	1315	SPO	C15-C16-C17-C18
13	M	1315	SPO	C15-C16-C17-C19
13	M	1315	SPO	C36-C37-C38-C39
14	M	1316	CDL	CB3-OB5-PB2-OB4
14	M	1316	CDL	C51-CB5-OB6-CB4
8	L	1285[A]	UQ2	C12-C13-C14-C15
8	L	1285[A]	UQ2	C12-C13-C14-C16
13	M	1315	SPO	C36-C37-C38-C40
14	M	1316	CDL	OB9-CB7-OB8-CB6
14	M	1316	CDL	OB7-CB5-OB6-CB4
14	M	1316	CDL	C71-CB7-OB8-CB6
14	M	1316	CDL	C20-C21-C22-C23
14	M	1316	CDL	C78-C79-C80-C81
5	M	1303	BCL	C10-C11-C12-C13
5	L	1282	BCL	C3-C5-C6-C7
8	L	1285[B]	UQ2	C12-C11-C9-C10
8	L	1285[B]	UQ2	C12-C11-C9-C8
12	M	1314	U10	C29-C31-C32-C33
13	M	1315	SPO	C33-C35-C36-C37
14	M	1316	CDL	C31-CA7-OA8-CA6
14	M	1316	CDL	OA9-CA7-OA8-CA6
5	L	1282	BCL	C11-C10-C8-C9
5	L	1286	BCL	C11-C12-C13-C14
5	L	1286	BCL	C13-C15-C16-C17
7	M	1313	BPH	C5-C6-C7-C8
4	H	1252	GOL	O2-C2-C3-O3
4	L	1289	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
14	M	1316	CDL	CA7-C31-C32-C33
5	M	1303	BCL	C11-C10-C8-C7
5	L	1282	BCL	C5-C6-C7-C8
5	M	1304	BCL	C15-C16-C17-C18
10	L	1288	HTO	O1-C1-C2-C3
13	M	1315	SPO	C9-C10-C11-C12
5	L	1286	BCL	C15-C16-C17-C18
13	M	1315	SPO	C8-C7-C9-C10
13	M	1315	SPO	C18-C17-C19-C20
13	M	1315	SPO	C21-C22-C23-C24
6	L	1283	LDA	C5-C6-C7-C8
6	L	1283	LDA	C11-C10-C9-C8
6	M	1310	LDA	C7-C8-C9-C10
14	M	1316	CDL	C16-C17-C18-C19
7	M	1313	BPH	C16-C17-C18-C20
6	M	1309	LDA	C6-C7-C8-C9
6	L	1711	LDA	C4-C5-C6-C7
6	M	1311	LDA	C6-C7-C8-C9
14	M	1316	CDL	O1-C1-CB2-OB2
13	M	1315	SPO	C16-C17-C19-C20
13	M	1315	SPO	C21-C22-C23-C25
6	L	1711	LDA	C2-C3-C4-C5
14	M	1316	CDL	C71-C72-C73-C74
5	M	1303	BCL	C11-C10-C8-C9
6	M	1307	LDA	C4-C5-C6-C7
14	M	1316	CDL	C80-C81-C82-C83
4	H	1251	GOL	O1-C1-C2-C3
4	H	1253	GOL	O1-C1-C2-C3
7	M	1313	BPH	C10-C11-C12-C13
6	M	1310	LDA	C3-C4-C5-C6
6	L	1283	LDA	C6-C7-C8-C9
6	M	1309	LDA	C7-C8-C9-C10
6	M	1311	LDA	C4-C5-C6-C7
6	M	1311	LDA	C11-C10-C9-C8
6	M	1305	LDA	C2-C3-C4-C5
6	M	1307	LDA	C6-C7-C8-C9
6	M	1311	LDA	C3-C4-C5-C6
6	M	1308	LDA	C2-C3-C4-C5
7	M	1313	BPH	C16-C17-C18-C19
6	L	1711	LDA	C5-C6-C7-C8
4	H	1253	GOL	O1-C1-C2-O2
4	L	1290	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	M	1307	LDA	C7-C8-C9-C10
14	M	1316	CDL	OA7-CA5-OA6-CA4
7	M	1313	BPH	C13-C15-C16-C17
5	M	1303	BCL	C15-C16-C17-C18
6	M	1309	LDA	C1-C2-C3-C4
7	L	1284	BPH	C4-C3-C5-C6
5	L	1286	BCL	C11-C12-C13-C15
7	L	1284	BPH	C2-C3-C5-C6
5	M	1303	BCL	C8-C10-C11-C12
5	L	1282	BCL	C16-C17-C18-C20
5	M	1304	BCL	C13-C15-C16-C17
6	L	1283	LDA	C2-C3-C4-C5
6	M	1307	LDA	C1-C2-C3-C4
14	M	1316	CDL	C11-CA5-OA6-CA4
6	M	1310	LDA	C11-C10-C9-C8
8	L	1285[B]	UQ2	C12-C13-C14-C15
5	L	1282	BCL	C1A-C2A-CAA-CBA
6	M	1308	LDA	C5-C6-C7-C8
6	L	1283	LDA	C1-C2-C3-C4
6	L	1711	LDA	C11-C10-C9-C8
14	M	1316	CDL	C74-C75-C76-C77
6	M	1308	LDA	C7-C8-C9-C10
14	M	1316	CDL	CA3-CA4-CA6-OA8
6	M	1310	LDA	C9-C10-C11-C12
6	L	1711	LDA	C9-C10-C11-C12
7	L	1284	BPH	C8-C10-C11-C12
6	M	1308	LDA	C11-C10-C9-C8
8	L	1285[B]	UQ2	C1-C6-C7-C8
14	M	1316	CDL	C81-C82-C83-C84
5	M	1303	BCL	C2-C1-O2A-CGA
13	M	1315	SPO	C6-C7-C9-C10
6	L	1283	LDA	C9-C10-C11-C12
7	M	1313	BPH	C15-C16-C17-C18
6	M	1311	LDA	C5-C6-C7-C8
14	M	1316	CDL	C21-C22-C23-C24
5	M	1303	BCL	C6-C7-C8-C10
5	M	1303	BCL	C6-C7-C8-C9
7	M	1313	BPH	C11-C10-C8-C9
5	L	1282	BCL	C16-C17-C18-C19
6	M	1306	LDA	C9-C10-C11-C12
6	L	1283	LDA	N1-C1-C2-C3
6	M	1310	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	L	1288	HTO	C4-C5-C6-C7
12	M	1314	U10	C34-C36-C37-C38
6	M	1306	LDA	C7-C8-C9-C10
5	L	1282	BCL	C15-C16-C17-C18
14	M	1316	CDL	C19-C20-C21-C22
6	L	1283	LDA	C4-C5-C6-C7
6	M	1311	LDA	C9-C10-C11-C12
14	M	1316	CDL	CB3-CB4-CB6-OB8
6	M	1308	LDA	C4-C5-C6-C7
14	M	1316	CDL	OB5-CB3-CB4-OB6
6	M	1305	LDA	C9-C10-C11-C12
14	M	1316	CDL	CA2-C1-CB2-OB2
8	L	1285[B]	UQ2	C12-C13-C14-C16
5	L	1286	BCL	C10-C11-C12-C13
5	L	1286	BCL	C2A-CAA-CBA-CGA
6	M	1305	LDA	C4-C5-C6-C7
5	M	1303	BCL	C11-C12-C13-C15
7	M	1313	BPH	C11-C10-C8-C7
6	M	1309	LDA	C4-C5-C6-C7
5	L	1286	BCL	CAD-CBD-CGD-O2D
5	M	1303	BCL	CAD-CBD-CGD-O2D
5	M	1304	BCL	CAD-CBD-CGD-O2D
6	M	1310	LDA	C1-C2-C3-C4
5	M	1304	BCL	C16-C17-C18-C19
6	M	1305	LDA	C2-C1-N1-CM1
6	M	1309	LDA	C2-C1-N1-CM2
5	M	1303	BCL	C3-C5-C6-C7
14	M	1316	CDL	OA6-CA4-CA6-OA8
6	L	1711	LDA	C6-C7-C8-C9
5	M	1303	BCL	C11-C12-C13-C14
14	M	1316	CDL	CA3-OA5-PA1-OA2
5	M	1303	BCL	C4-C3-C5-C6
14	M	1316	CDL	CB3-OB5-PB2-OB3
14	M	1316	CDL	C40-C41-C42-C43
14	M	1316	CDL	OB5-CB3-CB4-CB6
8	L	1285[B]	UQ2	C1-C2-O2-CM2
6	M	1305	LDA	C2-C1-N1-O1
6	M	1309	LDA	C2-C1-N1-O1
7	M	1313	BPH	C6-C7-C8-C10
7	M	1313	BPH	C12-C13-C15-C16
14	M	1316	CDL	OB6-CB4-CB6-OB8
7	M	1313	BPH	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
6	M	1306	LDA	C6-C7-C8-C9
6	M	1311	LDA	C7-C8-C9-C10
8	L	1285[A]	UQ2	C4-C3-O3-CM3
7	M	1313	BPH	C8-C10-C11-C12
5	L	1286	BCL	C8-C10-C11-C12
5	M	1303	BCL	C2-C3-C5-C6
14	M	1316	CDL	CB3-OB5-PB2-OB2
6	M	1306	LDA	C4-C5-C6-C7
12	M	1314	U10	C31-C32-C33-C34
4	H	1251	GOL	O1-C1-C2-O2
14	M	1316	CDL	C12-C13-C14-C15
6	L	1711	LDA	C1-C2-C3-C4
6	M	1308	LDA	C6-C7-C8-C9
6	M	1309	LDA	C9-C10-C11-C12
5	L	1282	BCL	C11-C10-C8-C7
12	M	1314	U10	C5-C4-O4-C4M
14	M	1316	CDL	CA5-C11-C12-C13
13	M	1315	SPO	C19-C20-C21-C22
13	M	1315	SPO	C12-C14-C15-C16
14	M	1316	CDL	C11-C12-C13-C14
8	L	1285[A]	UQ2	C9-C11-C12-C13
14	M	1316	CDL	C37-C38-C39-C40
14	M	1316	CDL	C17-C18-C19-C20
5	M	1303	BCL	C4C-C3C-CAC-CBC
5	M	1304	BCL	C8-C10-C11-C12
5	M	1304	BCL	CAA-CBA-CGA-O2A
5	L	1286	BCL	C11-C10-C8-C7
6	L	1283	LDA	C3-C4-C5-C6
5	L	1282	BCL	C1-C2-C3-C4
7	M	1313	BPH	C1-C2-C3-C4
6	L	1283	LDA	C7-C8-C9-C10
5	L	1282	BCL	C11-C12-C13-C14
7	M	1313	BPH	C6-C7-C8-C9
7	L	1284	BPH	CAD-CBD-CGD-O2D
7	M	1313	BPH	CAD-CBD-CGD-O2D
12	M	1314	U10	C25-C24-C26-C27
13	M	1315	SPO	C22-C23-C25-C26
5	L	1282	BCL	CHA-CBD-CGD-O1D
6	M	1308	LDA	C2-C1-N1-CM2
5	M	1304	BCL	C3-C5-C6-C7
14	M	1316	CDL	C72-C71-CB7-OB8
7	M	1313	BPH	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	M	1304	BCL	C12-C13-C15-C16
14	M	1316	CDL	C1-CB2-OB2-PB2
5	M	1304	BCL	C14-C13-C15-C16
13	M	1315	SPO	C24-C23-C25-C26
14	M	1316	CDL	C72-C71-CB7-OB9
5	L	1282	BCL	C6-C7-C8-C9
5	M	1304	BCL	C16-C17-C18-C20
6	M	1309	LDA	C11-C10-C9-C8

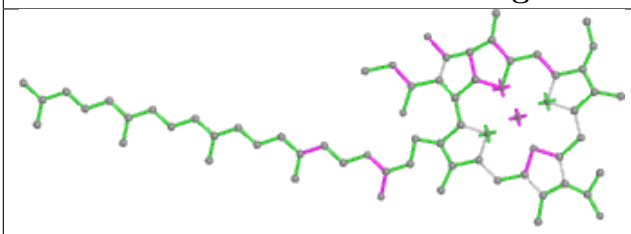
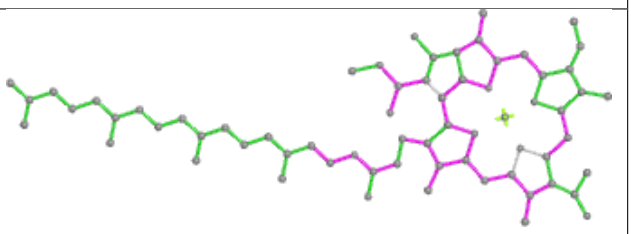
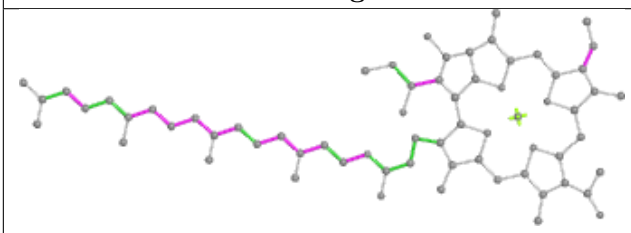
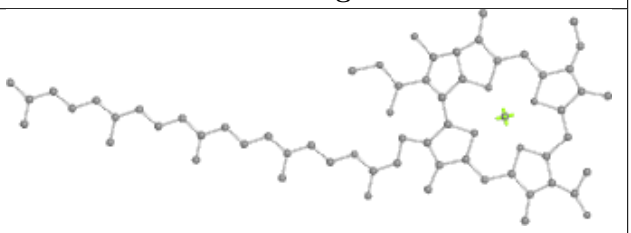
There are no ring outliers.

17 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	1288	HTO	2	0
4	L	1289	GOL	1	0
5	M	1303	BCL	7	0
5	M	1304	BCL	12	0
6	M	1307	LDA	1	0
8	L	1285[A]	UQ2	6	0
8	L	1285[B]	UQ2	2	0
5	L	1282	BCL	5	0
14	M	1316	CDL	3	0
12	M	1314	U10	2	0
4	H	1251	GOL	1	0
7	M	1313	BPH	14	0
13	M	1315	SPO	3	0
6	L	1711	LDA	2	0
6	M	1308	LDA	1	0
5	L	1286	BCL	4	0
7	L	1284	BPH	9	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 BCL M 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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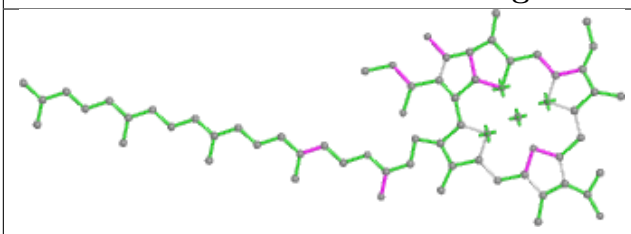
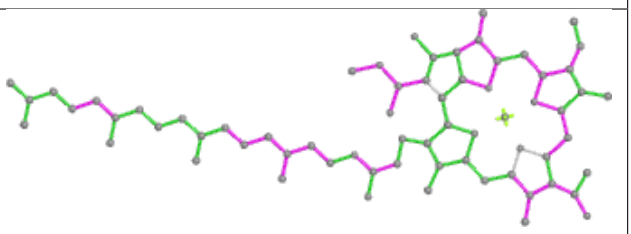
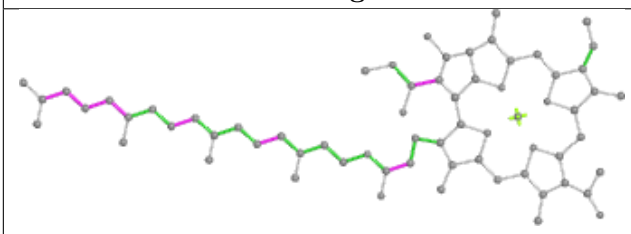
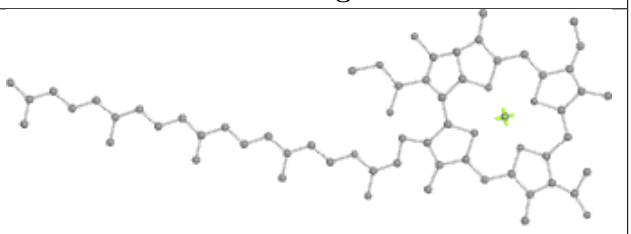
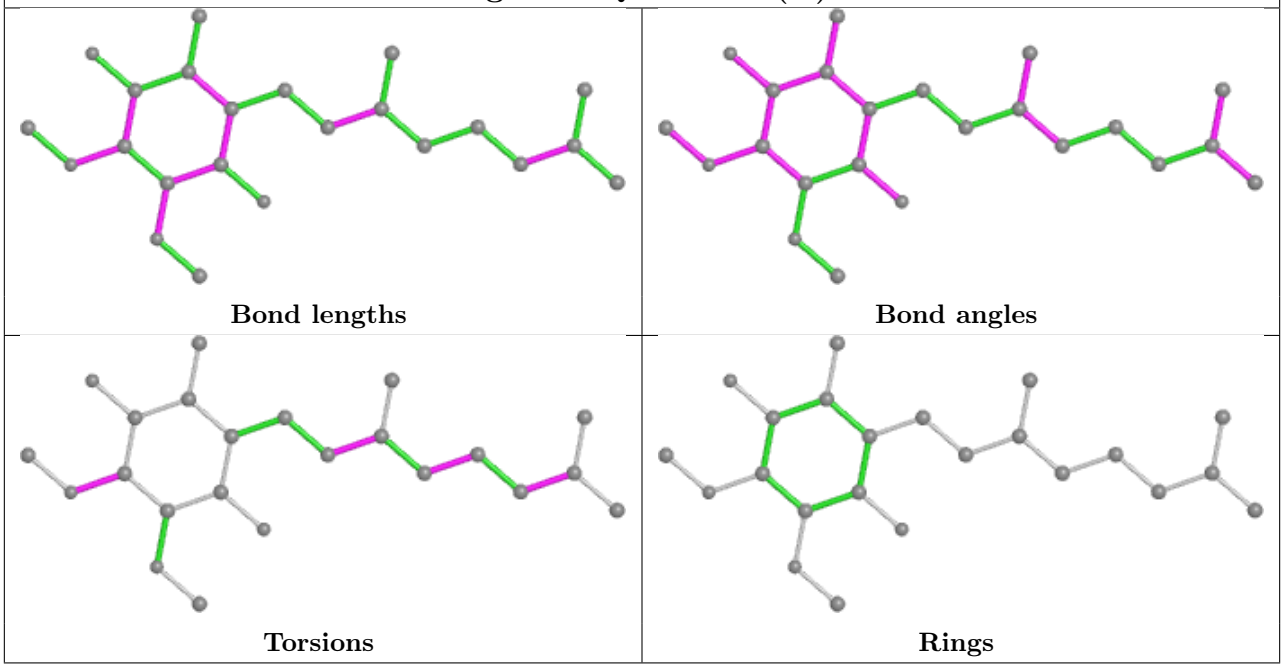
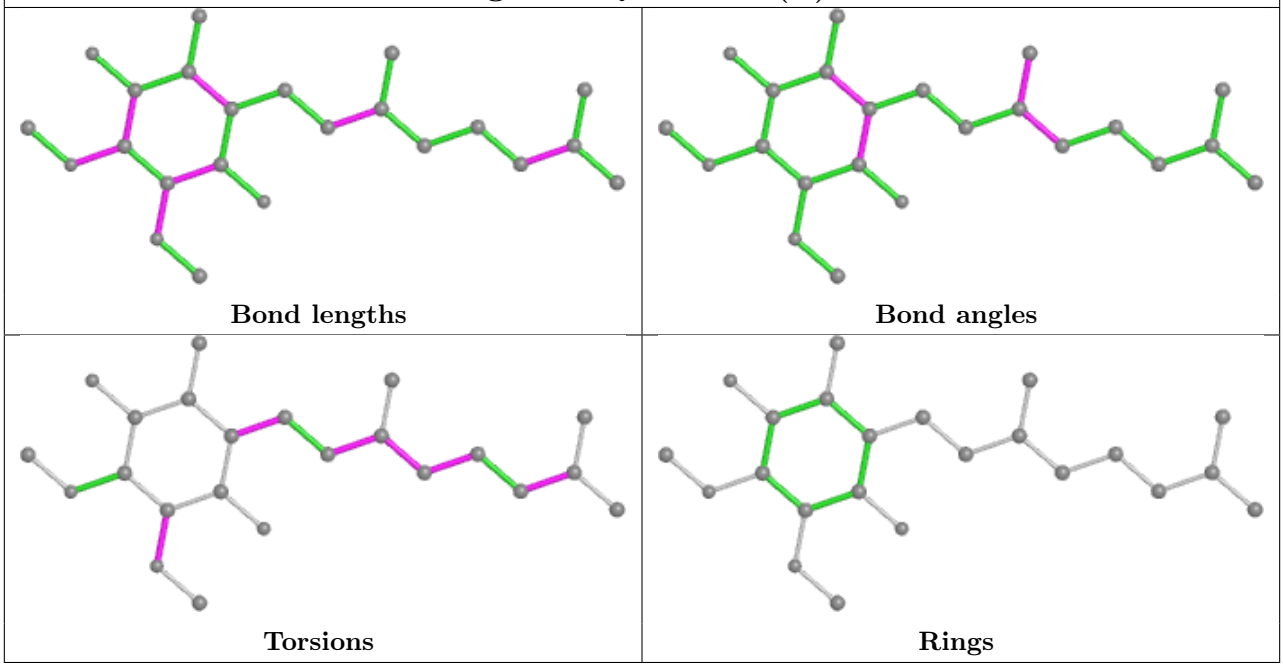
 Bond lengths	 Bond angles
 Torsions	 Rings

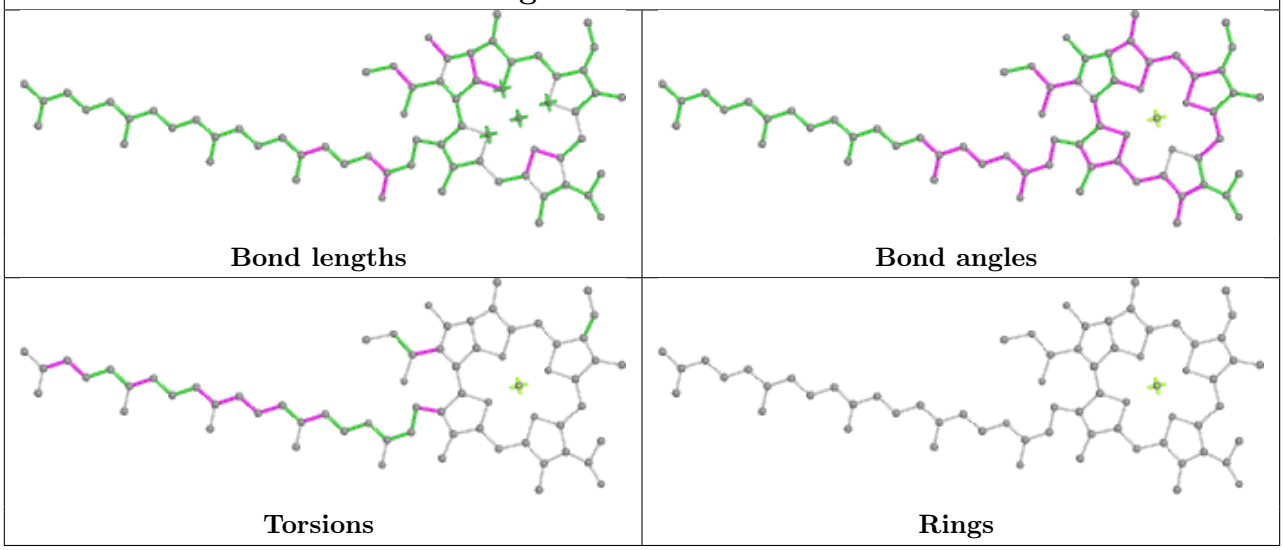
Ligand UQ2 L 1285 (A)



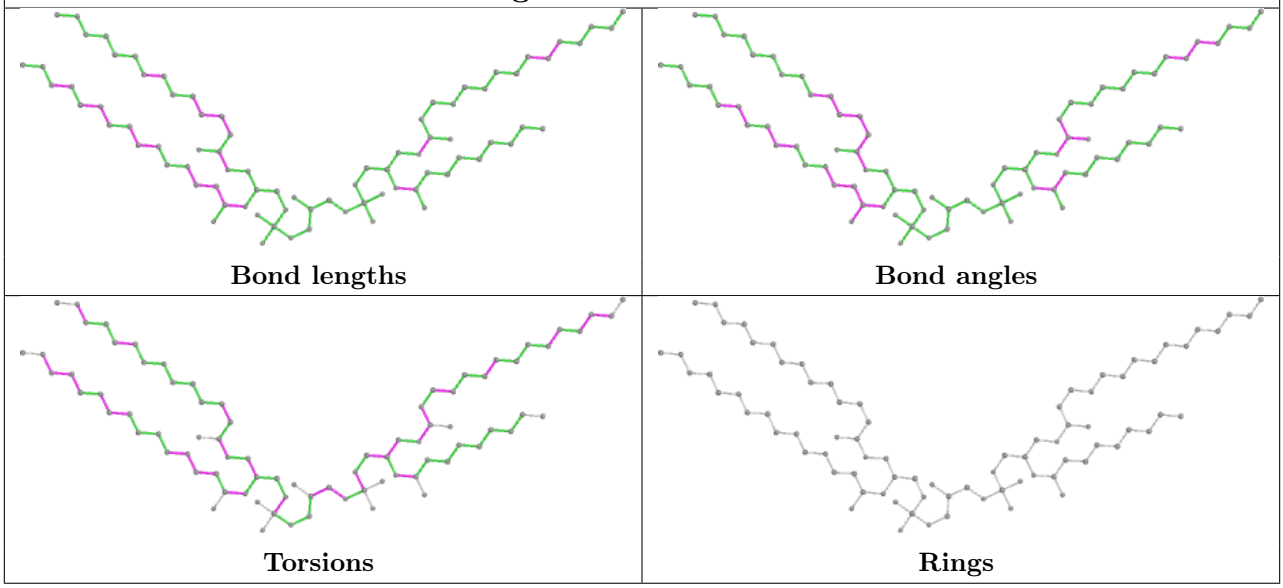
Ligand UQ2 L 1285 (B)



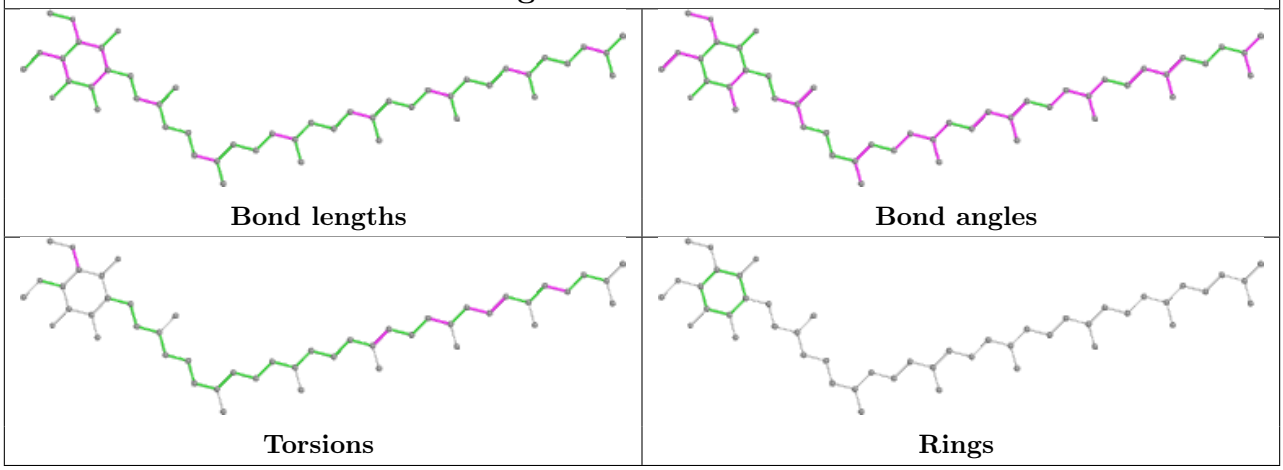
Ligand BCL L 1282



Ligand CDL M 1316



Ligand U10 M 1314



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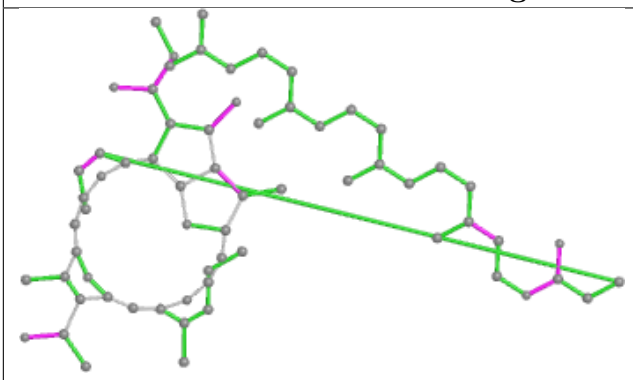
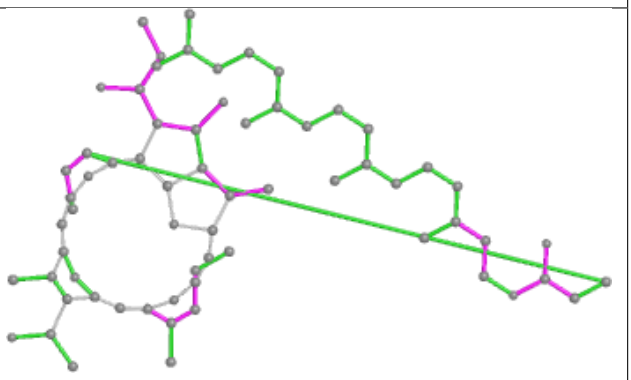
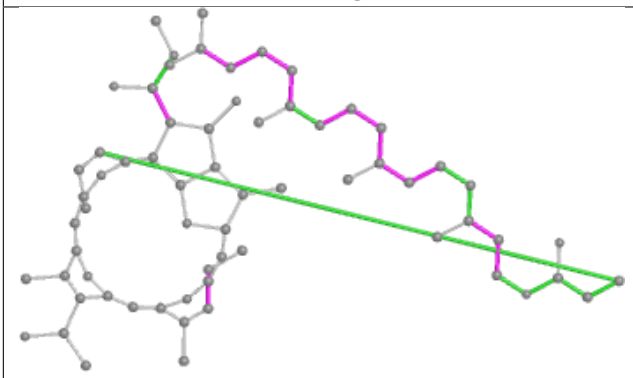


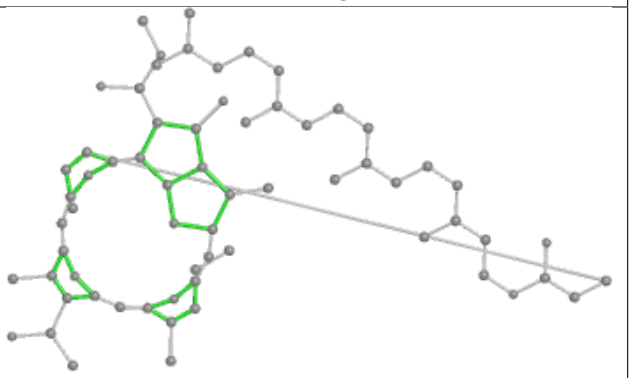
Bond lengths



Bond angles

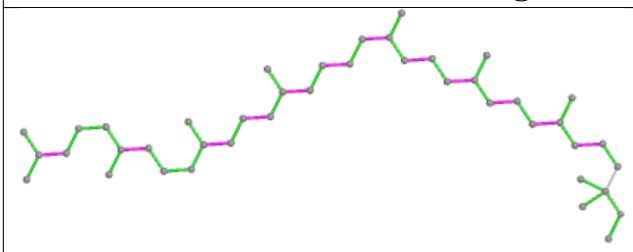


Torsions

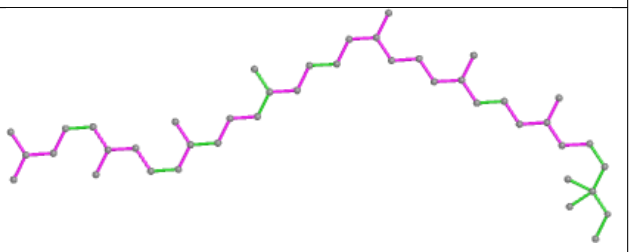


Rings

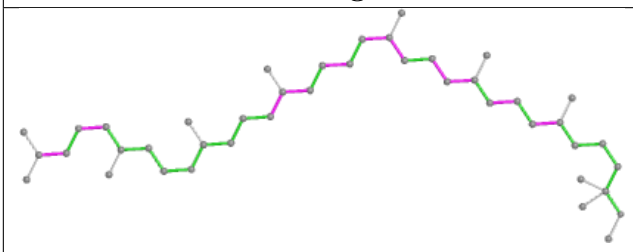
Ligand SPO M 1315



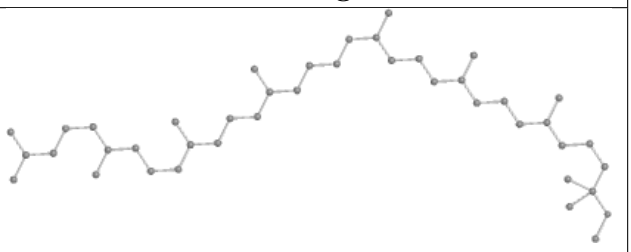
Bond lengths



Bond angles

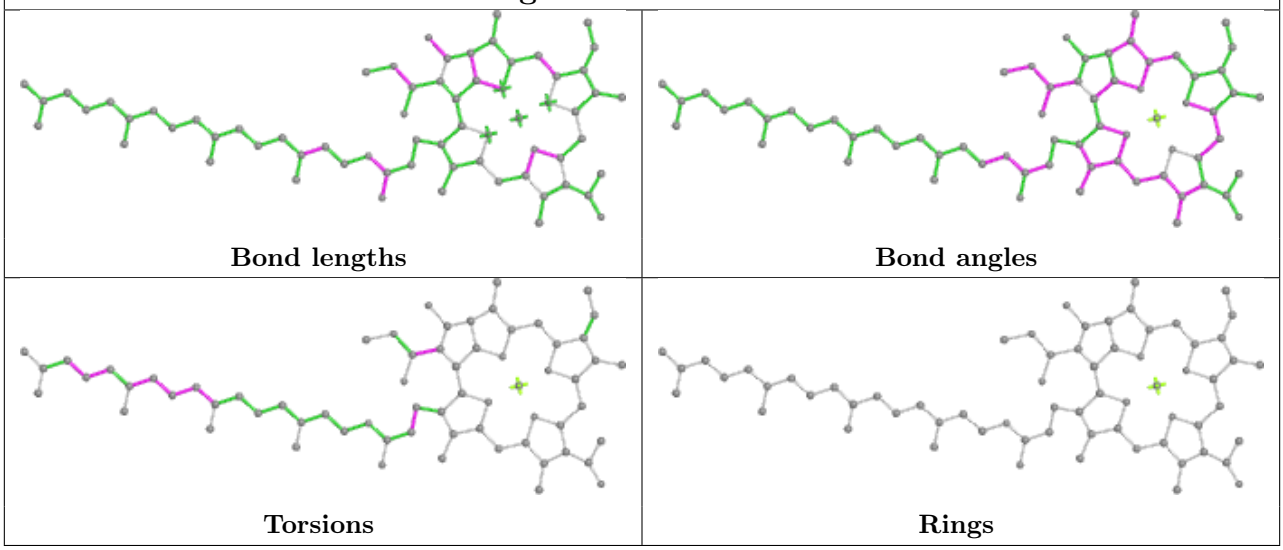


Torsions

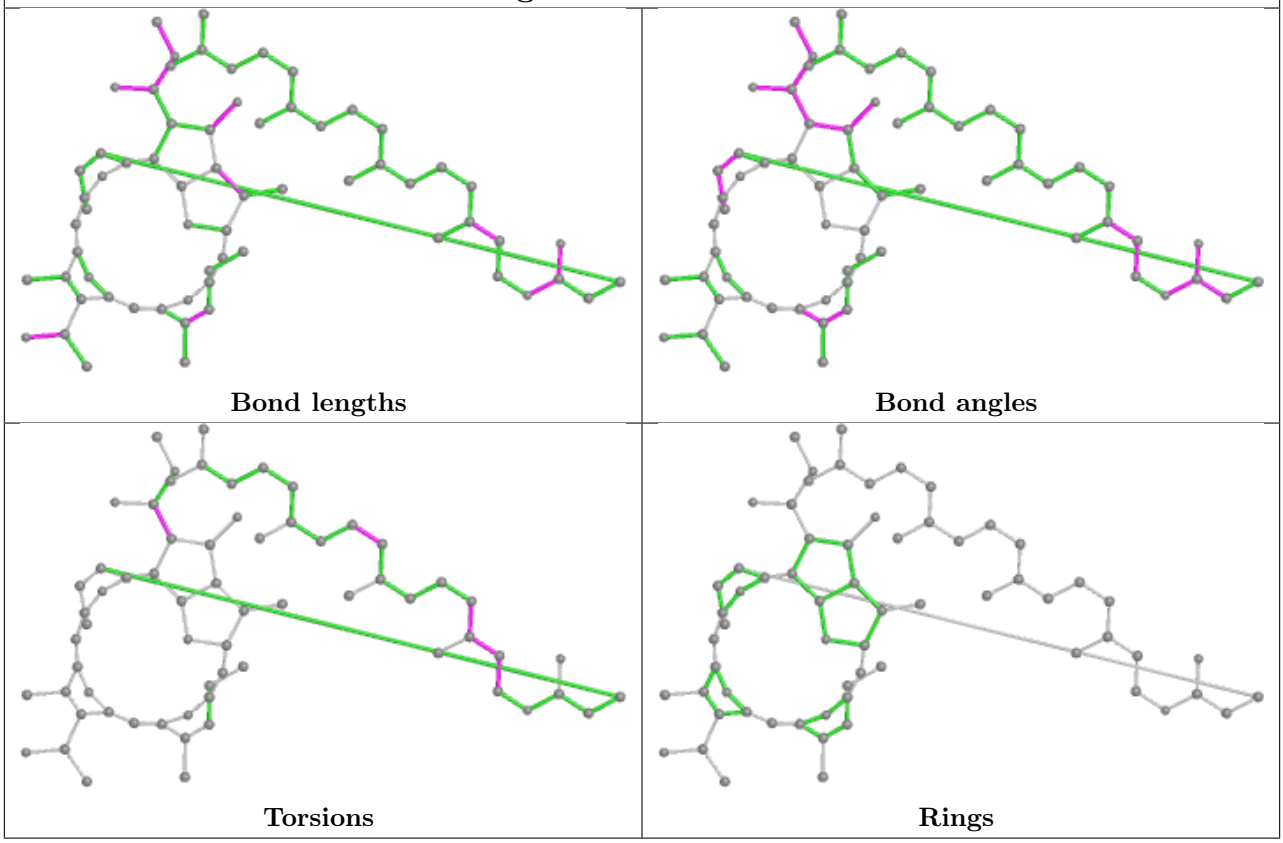


Rings

Ligand BCL L 1286



Ligand BPH L 1284



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%)	-0.26	8 (3%)	46	50	38, 48, 61, 105	0
2	L	281/281 (100%)	-0.31	8 (2%)	53	56	35, 44, 69, 77	0
3	M	303/307 (98%)	-0.02	13 (4%)	35	38	33, 50, 73, 86	0
All	All	825/848 (97%)	-0.19	29 (3%)	44	47	33, 47, 72, 105	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.1
1	H	250	SER	6.2
1	H	249	LYS	5.5
3	M	303	MET	5.1
1	H	246	PRO	4.2
2	L	59	TRP	3.9
1	H	251	VAL	3.4
3	M	2	GLU	3.0
2	L	281	GLY	3.0
2	L	277	GLY	2.9
3	M	80	TRP	2.9
1	H	247	LYS	2.8
3	M	148[A]	TRP	2.8
1	H	220[A]	LYS	2.8
3	M	301	HIS	2.7
1	H	60	LYS	2.7
2	L	270	PRO	2.6
3	M	79	GLY	2.6
3	M	223	ILE	2.6
2	L	271	TRP	2.5
2	L	278	GLY	2.5
2	L	202	LYS	2.4
3	M	106	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	18	TYR	2.3
3	M	82	PRO	2.3
3	M	249	ALA	2.2
2	L	272	TRP	2.2
3	M	265	ILE	2.2
3	M	302	GLY	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	1311	16/16	0.08	0.62	115,118,122,122	0
6	LDA	M	1310	16/16	0.24	0.63	101,111,118,118	0
6	LDA	L	1711	16/16	0.51	0.47	108,112,117,117	0
6	LDA	M	1309	16/16	0.56	0.50	118,120,126,126	0
4	GOL	H	1253	6/6	0.59	0.36	103,104,106,106	0
6	LDA	L	1283	16/16	0.64	0.37	78,103,114,115	0
6	LDA	M	1308	16/16	0.67	0.36	96,99,107,108	0
14	CDL	M	1316	81/100	0.67	0.45	91,107,125,126	0
10	HTO	L	1288	10/10	0.77	0.45	83,85,85,86	0
4	GOL	H	1252	6/6	0.77	0.32	93,94,94,95	0
4	GOL	L	1290	6/6	0.79	0.37	98,99,99,100	0
4	GOL	H	1251	6/6	0.80	0.31	70,75,76,76	0
6	LDA	M	1305	16/16	0.80	0.31	70,80,85,85	0
4	GOL	H	1254	6/6	0.85	0.22	92,93,93,93	0
8	UQ2	L	1285[A]	23/23	0.86	0.32	38,44,54,55	23
8	UQ2	L	1285[B]	23/23	0.86	0.32	42,47,53,54	23
6	LDA	M	1306	16/16	0.87	0.42	70,74,86,87	0

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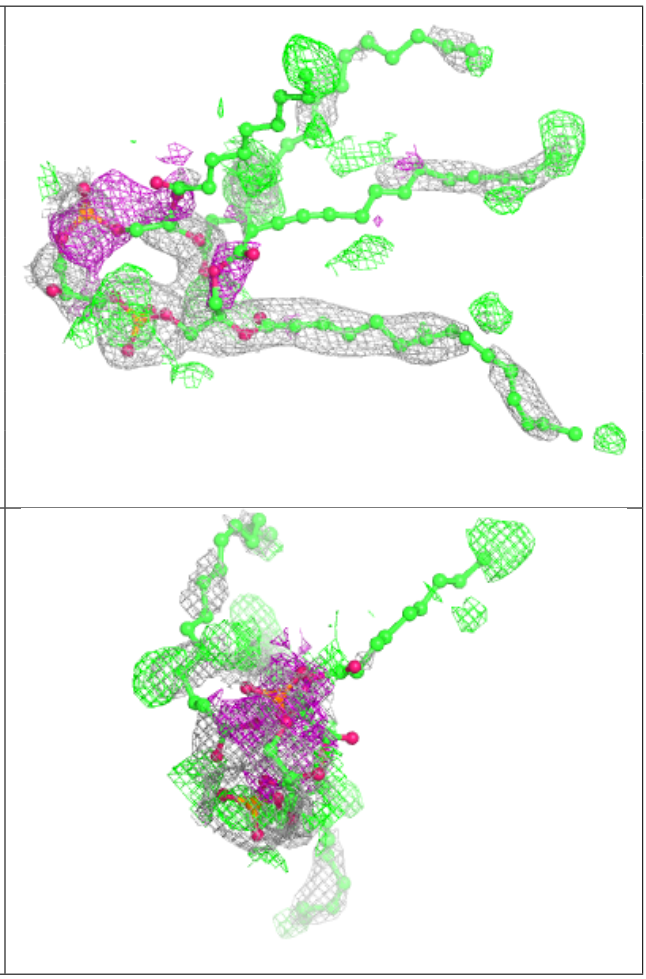
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LDA	M	1307	16/16	0.87	0.21	68,70,76,77	0
4	GOL	L	1289	6/6	0.88	0.25	65,69,70,73	0
13	SPO	M	1315	42/42	0.89	0.21	44,57,77,80	0
12	U10	M	1314	48/63	0.89	0.26	36,47,75,78	0
7	BPH	M	1313	65/65	0.92	0.21	38,45,98,99	0
5	BCL	L	1286	66/66	0.97	0.12	30,38,51,56	0
9	PO4	L	1287	5/5	0.97	0.12	100,100,101,101	0
5	BCL	L	1282	66/66	0.97	0.14	29,35,58,61	0
7	BPH	L	1284	65/65	0.98	0.14	29,36,45,48	0
5	BCL	M	1304	66/66	0.98	0.17	30,36,58,65	0
5	BCL	M	1303	66/66	0.98	0.15	30,36,89,90	0
11	FE	M	1312	1/1	0.99	0.09	34,34,34,34	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.

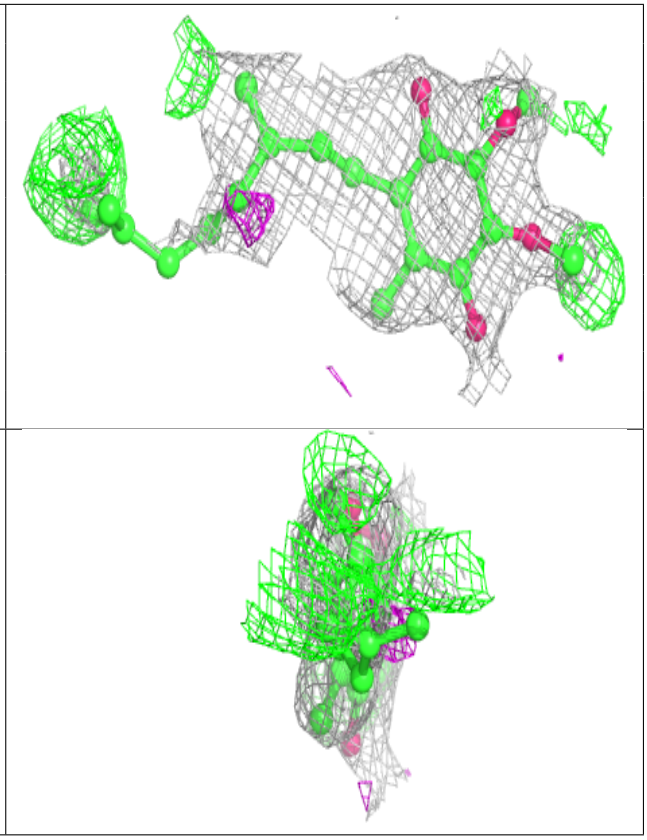
Electron density around CDL M 1316:

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



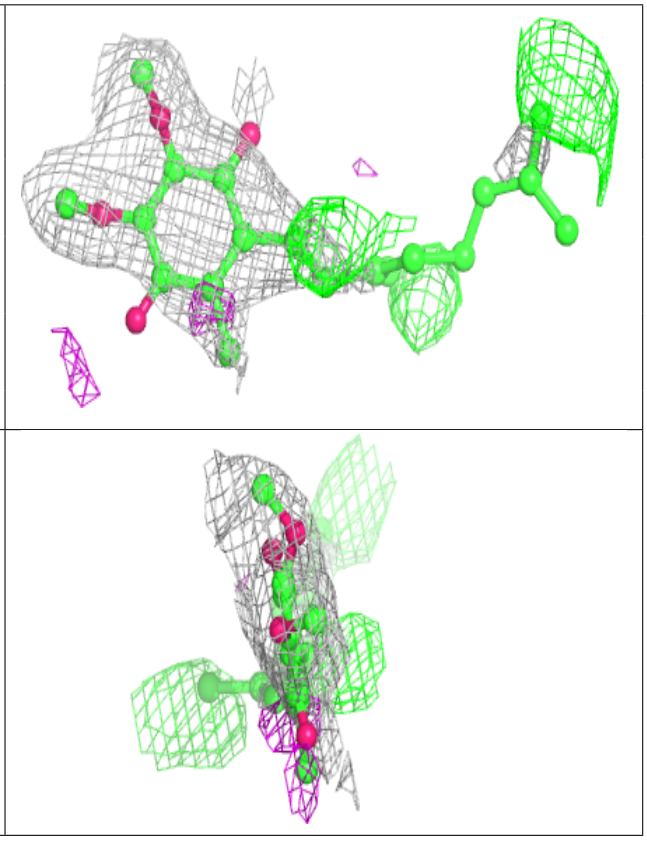
Electron density around UQ2 L 1285 (A):

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



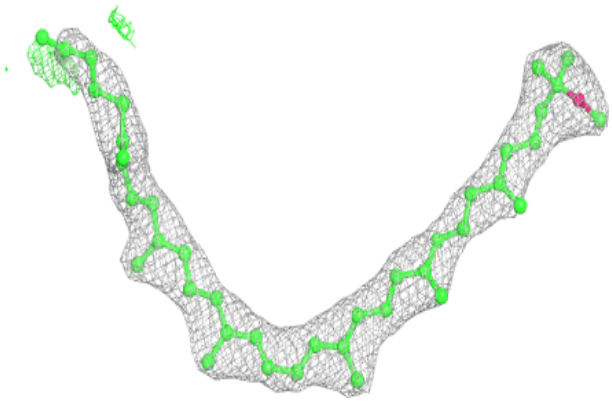
Electron density around UQ2 L 1285 (B):

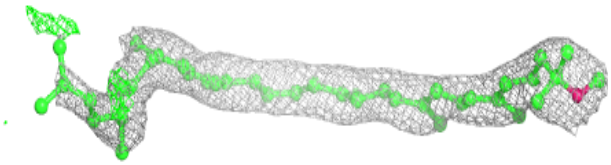
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

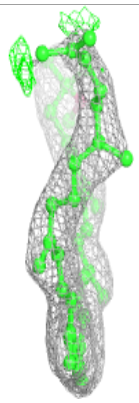


Electron density around SPO M 1315:

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

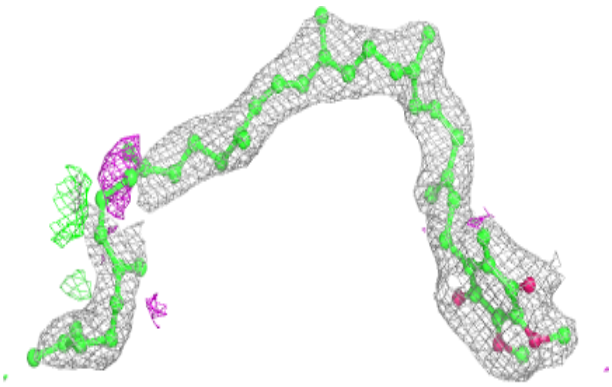


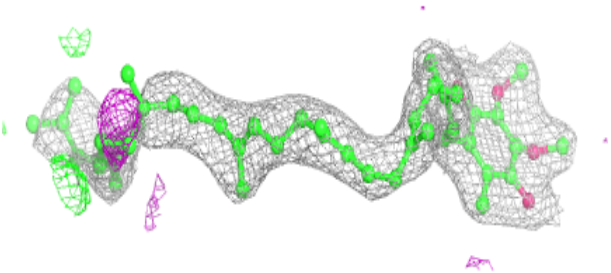


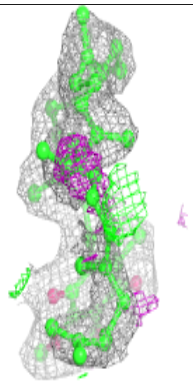


Electron density around U10 M 1314:

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

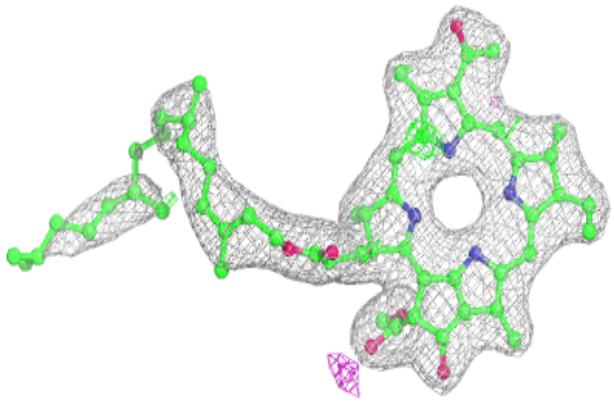


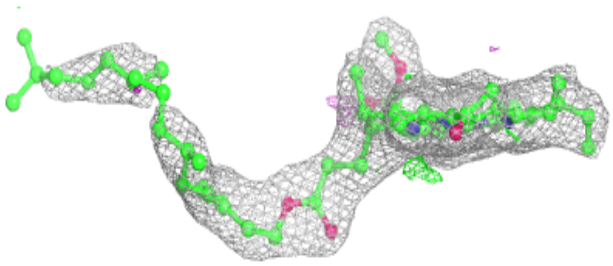


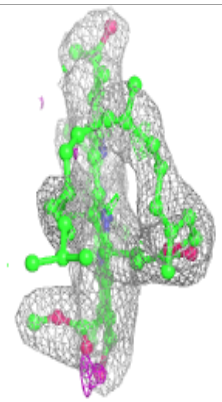


Electron density around BPH M 1313:

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

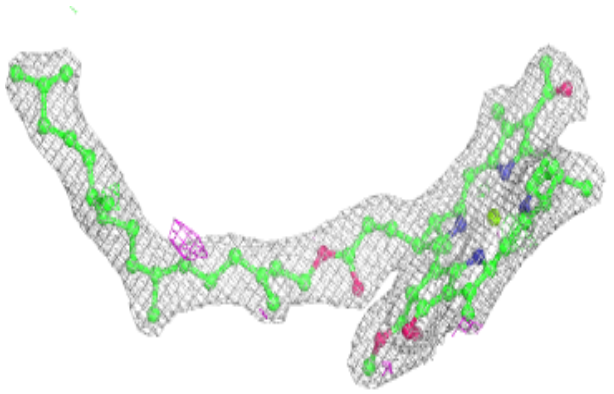


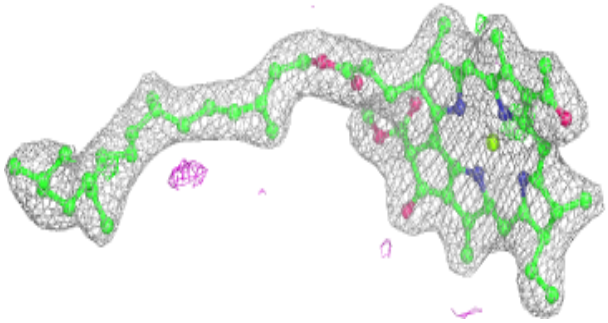


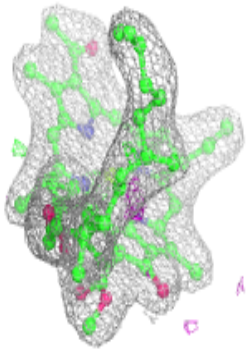


Electron density around BCL L 1286:

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

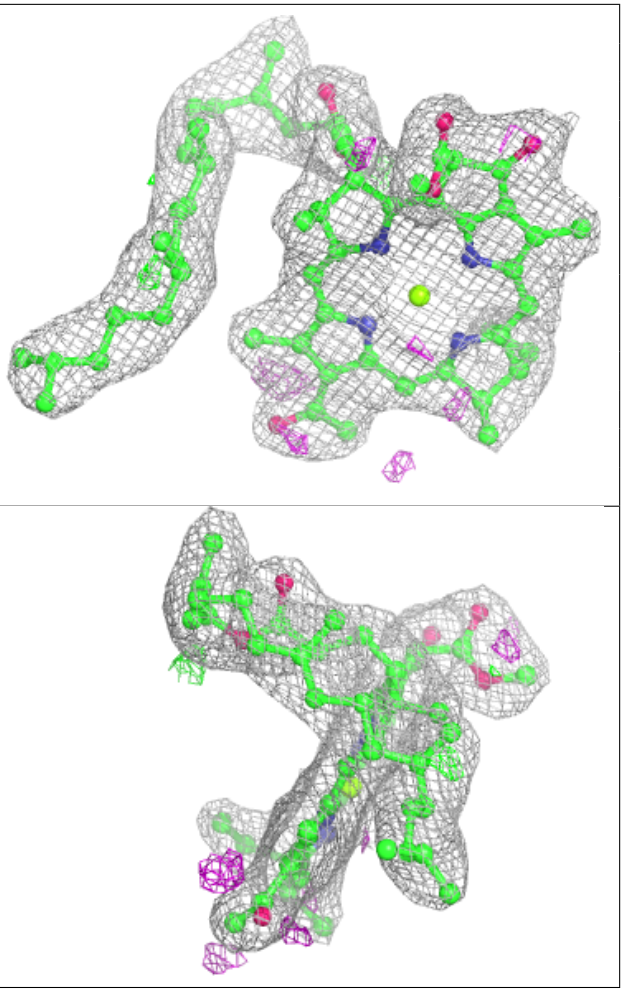






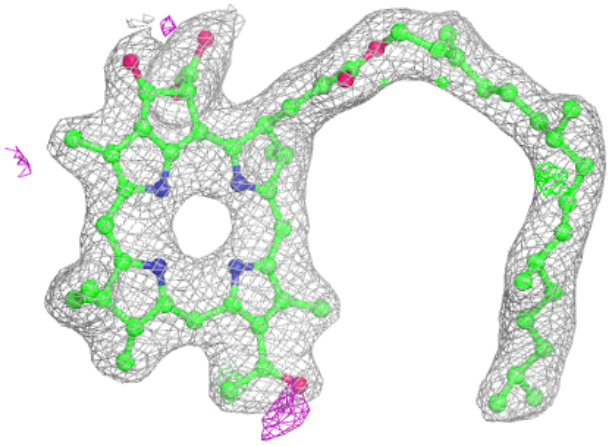
Electron density around BCL L 1282:

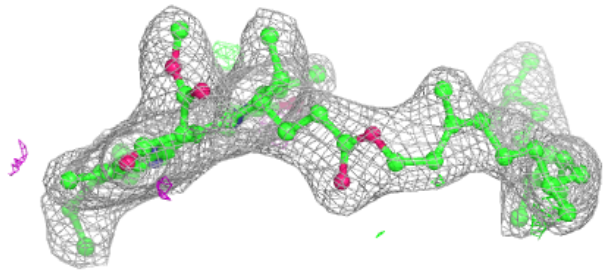
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

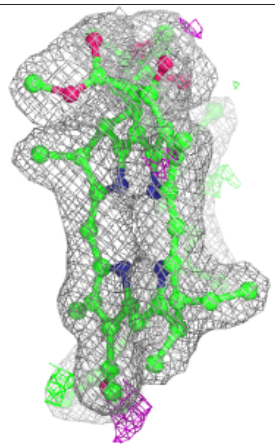


Electron density around BPH L 1284:

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

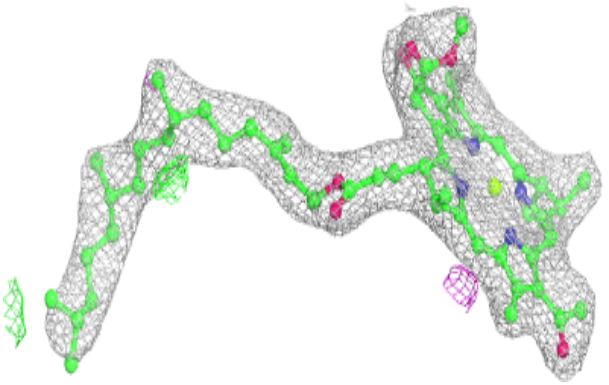


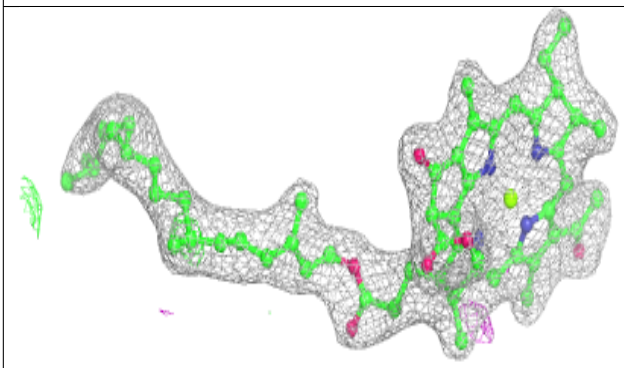


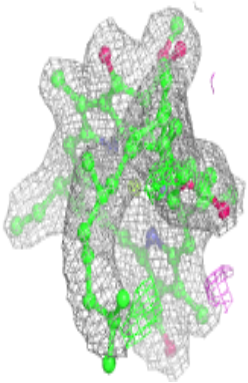


Electron density around BCL M 1304:

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

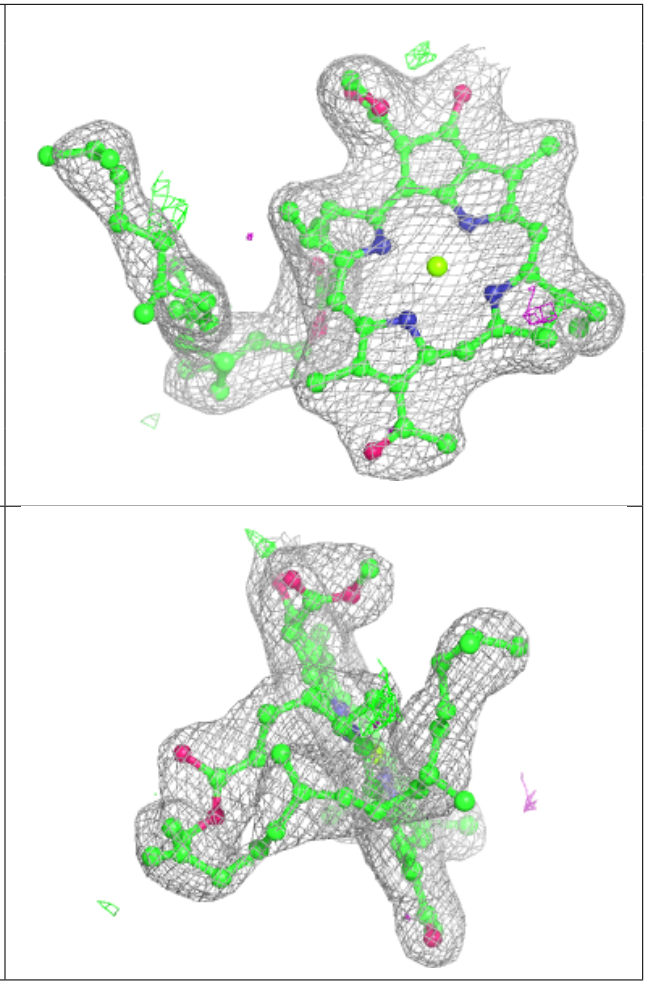






Electron density around BCL M 1303:

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



6.5 Other polymers (i)

There are no such residues in this entry.