Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 05:50 am GMT

PDB ID	:	2UWS
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 6.5 in the charge-separated state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-23
Resolution	:	2.90 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:

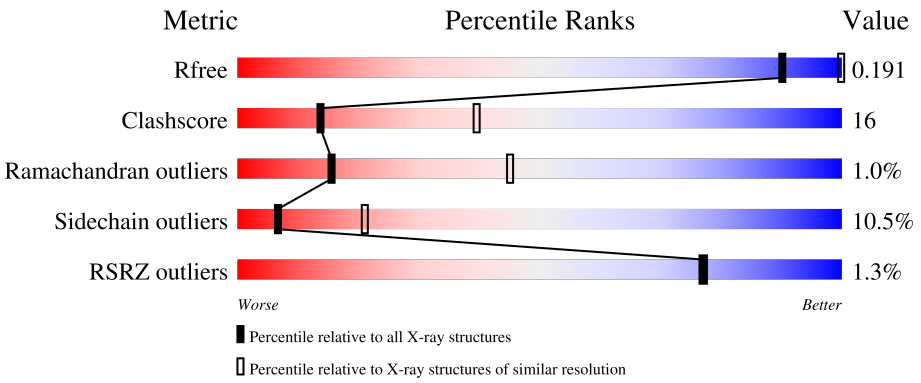
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	2% 64% 24% • 7%
2	L	281	% 69% 27% •
3	M	307	% 68% 26% • •

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	LDA	L	1281	-	-	-	X
5	LDA	L	1283	-	-	-	X
5	LDA	M	1310	-	-	-	X
6	BCL	L	1282	X	-	-	-
6	BCL	L	1286	X	-	-	-
6	BCL	M	1303	X	-	-	-
6	BCL	M	1304	X	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7325 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	1830	1169	315	337	9	0	0	1

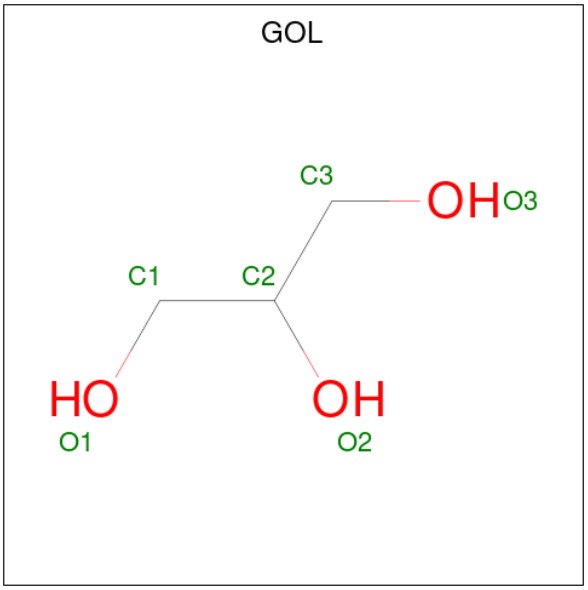
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	280	2222	1501	352	361	8	0	0	0

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

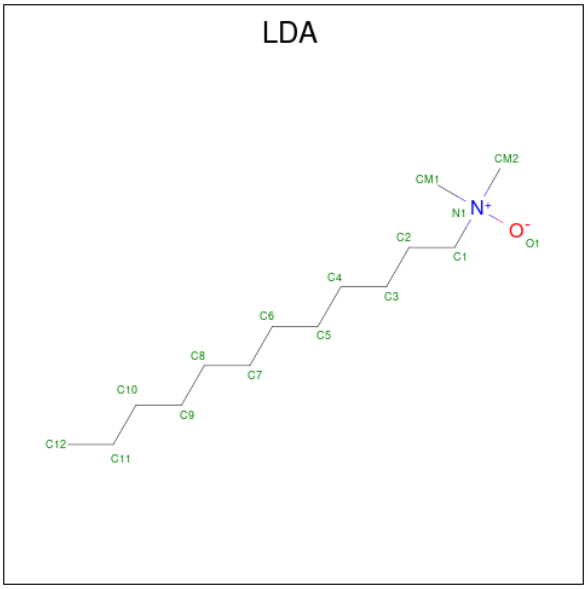
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

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



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

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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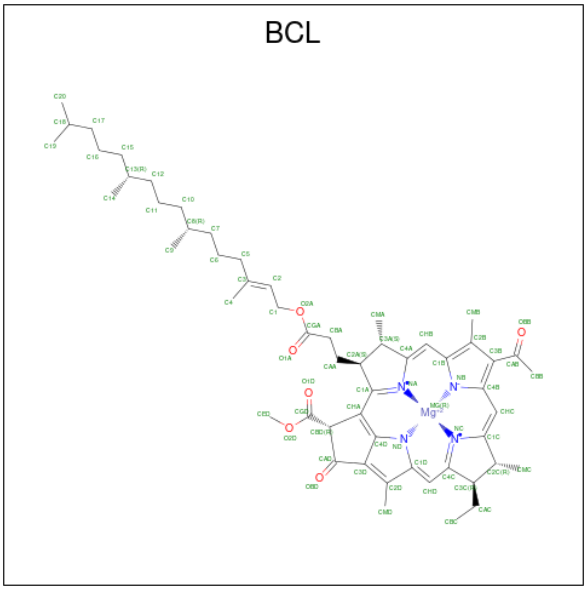
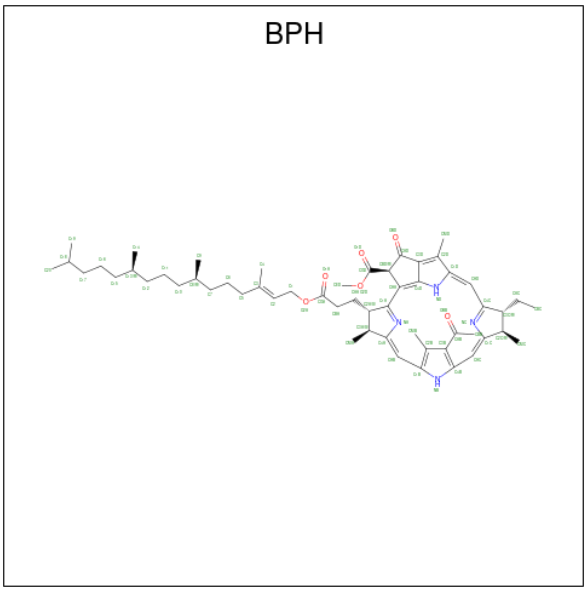
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	16	14	1	1	0	0
			Total	C	N	O		
5	M	1	16	14	1	1	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



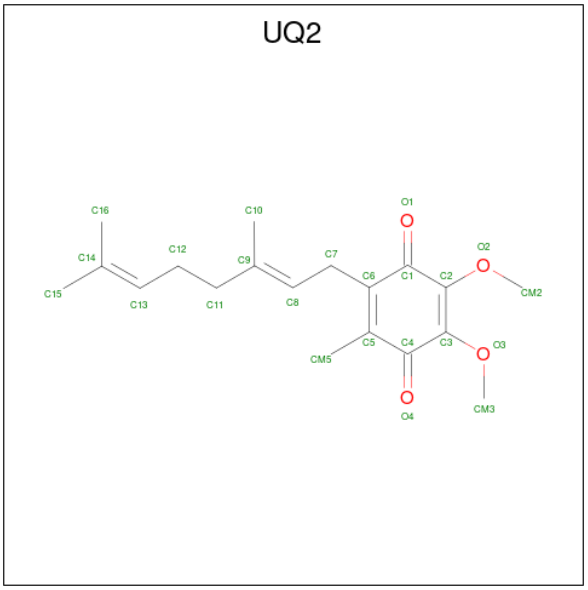
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0

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



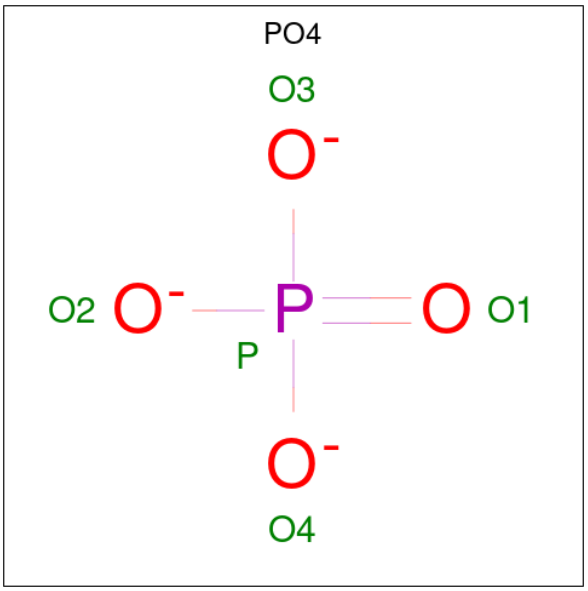
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	65	55	4	6	0	0

- 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).

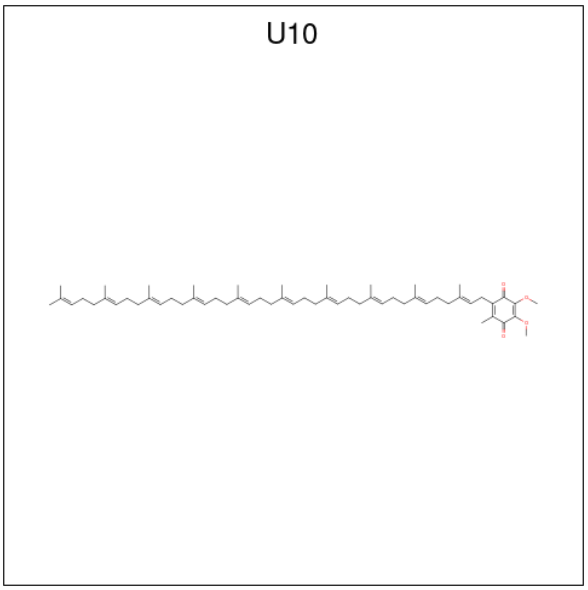


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total O P 5 4 1	0	0

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

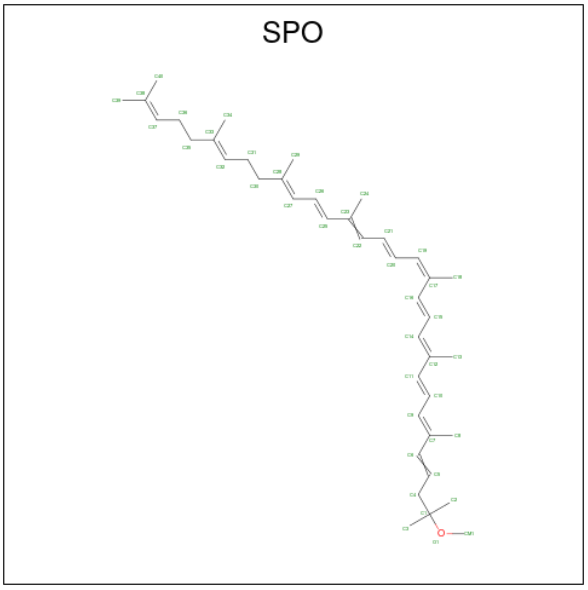
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is water.

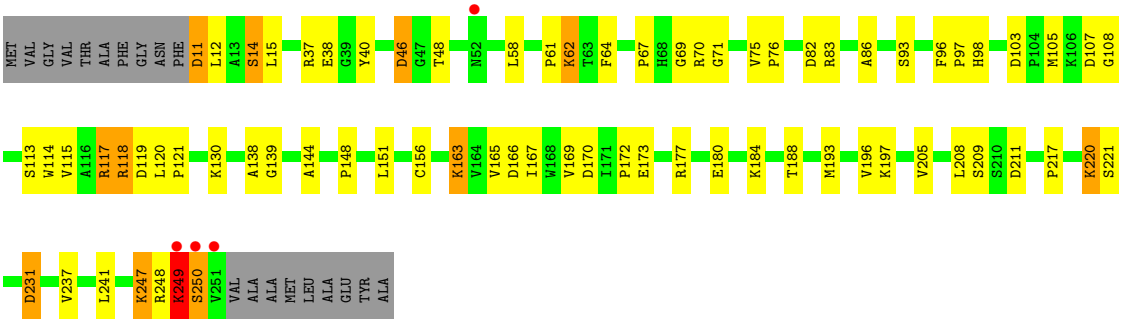
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	H	70	70	70	0	0
			Total	O		
13	L	59	59	59	0	0
			Total	O		
13	M	41	41	41	0	0

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.

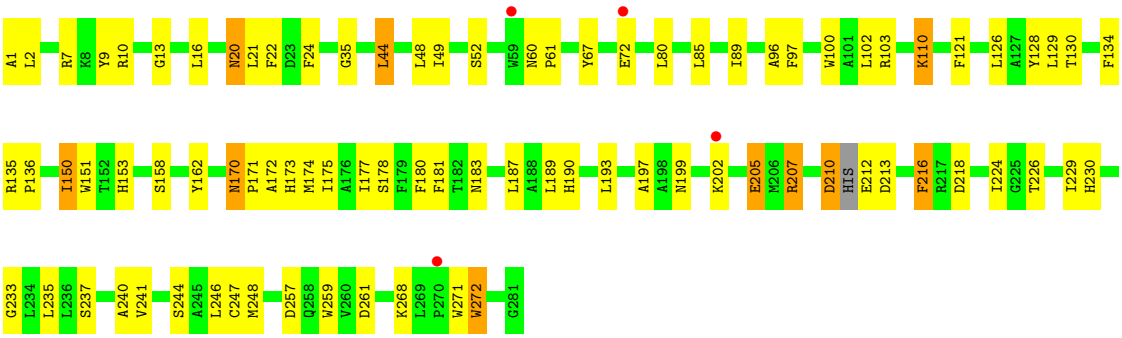
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



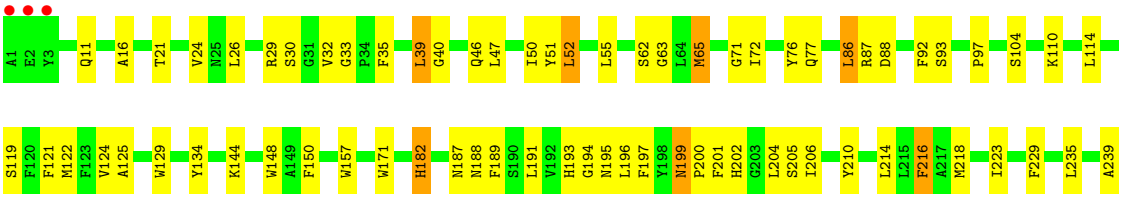
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



D240
R241
G242
T243
A244
A245
E246
R247
L250
F251
W252
R253
F258
N259
A260
E263
G264
I265
W268
A269
T270
D292
N293
V296
M300
H301
G302
M303
ALA
PRO
LEU
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.31Å 139.31Å 184.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.90 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (119.52-2.90) 83.5 (19.99-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.248 0.191 , 0.191	Depositor DCC
R_{free} test set	3032 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7325	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: FE, LDA, PO4, BCL, U10, BPH, SPO, GOL, UQ2

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	0.84	0/1878	0.96	7/2555 (0.3%)
2	L	0.85	0/2308	0.86	5/3157 (0.2%)
3	M	0.81	0/2501	0.88	7/3415 (0.2%)
All	All	0.83	0/6687	0.90	19/9127 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	261	ASP	CB-CG-OD2	8.36	125.83	118.30
1	H	82	ASP	CB-CG-OD2	7.12	124.70	118.30
3	M	292	ASP	CB-CG-OD2	6.91	124.52	118.30
1	H	107	ASP	CB-CG-OD2	6.89	124.50	118.30
1	H	119	ASP	CB-CG-OD2	6.74	124.36	118.30
3	M	302	GLY	O-C-N	-6.66	112.04	122.70
3	M	86	LEU	CA-CB-CG	6.38	129.97	115.30
1	H	250	SER	O-C-N	-6.14	112.88	122.70
1	H	231	ASP	CB-CG-OD2	5.79	123.51	118.30
2	L	213	ASP	CB-CG-OD2	5.55	123.30	118.30
3	M	240	ASP	CB-CG-OD1	5.53	123.27	118.30
2	L	257	ASP	CB-CG-OD2	5.47	123.22	118.30
3	M	241	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	L	218	ASP	CB-CG-OD2	5.37	123.13	118.30
1	H	211	ASP	CB-CG-OD2	5.33	123.10	118.30
2	L	207	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	H	46	ASP	CB-CG-OD2	5.29	123.06	118.30
3	M	182	HIS	CB-CA-C	5.26	120.92	110.40
3	M	88	ASP	CB-CG-OD2	5.19	122.97	118.30

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	1830	0	1836	50	0
2	L	2222	0	2179	65	0
3	M	2409	0	2321	75	0
4	H	12	0	16	1	0
4	L	12	0	16	2	0
4	M	6	0	8	0	0
5	L	32	0	62	2	0
5	M	96	0	186	10	0
6	L	132	0	148	20	0
6	M	132	0	148	28	0
7	L	65	0	76	18	0
7	M	65	0	76	11	0
8	L	46	0	52	12	0
9	L	5	0	0	0	0
10	M	1	0	0	0	0
11	M	48	0	63	10	0
12	M	42	0	60	6	0
13	H	70	0	0	5	1
13	L	59	0	0	0	0
13	M	41	0	0	1	0
All	All	7325	0	7247	229	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 16.

All (229) 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)
6:M:1303:BCL:H71	6:M:1304:BCL:H202	1.36	1.04
7:L:1284:BPH:CBB	7:L:1284:BPH:HHC	1.95	0.96
11:M:1313:U10:H352	11:M:1313:U10:H312	1.49	0.95
3:M:197:PHE:CZ	6:M:1304:BCL:HBB2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:1313:U10:H312	11:M:1313:U10:C35	2.06	0.86
2:L:199:ASN:HA	4:L:1288:GOL:H31	1.58	0.86
3:M:243:THR:O	3:M:247:ARG:HG3	1.75	0.85
3:M:197:PHE:HZ	6:M:1304:BCL:HBB2	1.43	0.83
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.63	0.80
7:L:1284:BPH:HHC	7:L:1284:BPH:HBB3	1.64	0.79
1:H:62:LYS:HE3	1:H:64:PHE:CZ	2.19	0.77
2:L:229:ILE:HD13	8:L:1285[A]:UQ2:O3	1.86	0.75
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.68	0.75
3:M:300:ASN:C	3:M:302:GLY:H	1.90	0.73
2:L:224:ILE:H	8:L:1285[A]:UQ2:H2M3	1.52	0.73
7:L:1284:BPH:HHC	7:L:1284:BPH:HBB2	1.70	0.72
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.72	0.72
7:L:1284:BPH:CBB	7:L:1284:BPH:CHC	2.68	0.72
2:L:170:ASN:C	2:L:170:ASN:HD22	1.91	0.72
5:M:1307:LDA:H112	11:M:1313:U10:H202	1.72	0.71
2:L:181:PHE:CD2	7:M:1312:BPH:HBB1	2.26	0.71
1:H:220:LYS:NZ	13:H:2064:HOH:O	2.24	0.71
6:M:1303:BCL:CBB	12:M:1314:SPO:H243	2.21	0.70
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.74	0.70
7:L:1284:BPH:CBB	3:M:210:TYR:HB3	2.22	0.70
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.74	0.69
2:L:244:SER:OG	6:L:1286:BCL:HMA2	1.92	0.69
8:L:1285[B]:UQ2:H153	5:M:1309:LDA:H121	1.74	0.69
2:L:96:ALA:HB1	7:L:1284:BPH:H2	1.74	0.68
6:M:1303:BCL:HBB2	12:M:1314:SPO:H243	1.76	0.68
1:H:70:ARG:HH12	1:H:121:PRO:HD2	1.59	0.68
8:L:1285[A]:UQ2:C15	5:M:1309:LDA:H91	2.25	0.67
3:M:77:GLN:HE22	3:M:93:SER:H	1.41	0.67
3:M:194:GLY:O	3:M:195:ASN:HB3	1.94	0.66
5:M:1305:LDA:H101	5:M:1307:LDA:H121	1.77	0.65
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.32	0.65
3:M:197:PHE:HZ	6:M:1304:BCL:CBB	2.08	0.65
2:L:181:PHE:HB3	7:M:1312:BPH:HBB2	1.77	0.65
6:M:1304:BCL:HHC	6:M:1304:BCL:HBB3	1.79	0.65
2:L:49:ILE:HG13	2:L:89:ILE:HD13	1.79	0.65
7:L:1284:BPH:HBB3	7:L:1284:BPH:CHC	2.27	0.65
3:M:199:ASN:C	3:M:199:ASN:HD22	2.01	0.64
3:M:196:LEU:HD12	6:M:1304:BCL:HHD	1.77	0.64
3:M:300:ASN:O	3:M:302:GLY:N	2.29	0.64
6:L:1286:BCL:CBB	6:L:1286:BCL:HMB1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1303:BCL:HBB3	6:M:1304:BCL:H41	1.78	0.64
1:H:130:LYS:HE3	1:H:170:ASP:OD2	1.98	0.63
1:H:118:ARG:HH11	1:H:118:ARG:CG	2.11	0.63
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.79	0.63
8:L:1285[A]:UQ2:H152	5:M:1309:LDA:H91	1.81	0.62
3:M:197:PHE:CE1	6:M:1304:BCL:HMC2	2.34	0.62
5:M:1307:LDA:H51	5:M:1308:LDA:H41	1.80	0.62
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.35	0.61
2:L:241:VAL:HG21	7:L:1284:BPH:HAC1	1.81	0.61
3:M:196:LEU:HD12	6:M:1304:BCL:CHD	2.31	0.61
3:M:253:ARG:NE	13:M:2036:HOH:O	2.26	0.61
2:L:100:TRP:CH2	11:M:1313:U10:H251	2.36	0.60
2:L:128:TYR:HD1	6:L:1282:BCL:HBB1	1.67	0.60
3:M:125:ALA:HB1	7:M:1312:BPH:H2	1.84	0.59
2:L:193:LEU:HG	2:L:212:GLU:HG2	1.85	0.59
3:M:62:SER:OG	3:M:124:VAL:HG22	2.03	0.59
2:L:175:ILE:O	2:L:178:SER:HB2	2.03	0.58
6:M:1304:BCL:H121	7:M:1312:BPH:HHB	1.86	0.58
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.34	0.58
3:M:119:SER:HB3	12:M:1314:SPO:H311	1.84	0.58
6:L:1286:BCL:H2C	6:M:1304:BCL:HBC2	1.86	0.57
3:M:189:PHE:O	3:M:193:HIS:HD2	1.87	0.57
3:M:197:PHE:CE1	6:M:1304:BCL:HBB2	2.40	0.56
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.41	0.56
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.86	0.56
6:M:1303:BCL:H101	6:M:1304:BCL:H202	1.88	0.56
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.40	0.56
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.70	0.55
3:M:150:PHE:CD1	7:M:1312:BPH:C3D	2.89	0.55
3:M:241:ARG:HG3	3:M:245:ALA:HB3	1.88	0.55
1:H:40:TYR:HB3	1:H:58:LEU:HD21	1.89	0.55
7:L:1284:BPH:HBB1	3:M:210:TYR:CG	2.43	0.54
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.89	0.54
6:M:1303:BCL:H71	6:M:1304:BCL:C20	2.25	0.54
1:H:108:GLY:O	1:H:113:SER:HA	2.07	0.54
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.23	0.54
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.26	0.53
3:M:33:GLY:HA2	5:M:1309:LDA:HM13	1.90	0.53
2:L:2:LEU:HD11	2:L:10:ARG:CZ	2.38	0.53
3:M:194:GLY:O	3:M:195:ASN:CB	2.57	0.53
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1305:LDA:H101	5:M:1307:LDA:C12	2.40	0.53
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.44	0.52
6:M:1304:BCL:HBB3	6:M:1304:BCL:CHC	2.39	0.52
1:H:144:ALA:HB3	3:M:11:GLN:HG3	1.90	0.52
6:L:1282:BCL:HHC	6:L:1282:BCL:CBB	2.39	0.52
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.45	0.52
2:L:20:ASN:H	2:L:20:ASN:HD22	1.58	0.52
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.43	0.51
3:M:157:TRP:CE2	12:M:1314:SPO:H293	2.45	0.51
3:M:63:GLY:HA3	7:M:1312:BPH:H5C2	1.92	0.51
1:H:37:ARG:O	1:H:38:GLU:HG2	2.10	0.51
1:H:208:LEU:HD21	1:H:237:VAL:HA	1.92	0.51
1:H:209:SER:OG	1:H:247:LYS:HD2	2.10	0.51
2:L:174:MET:HB3	6:M:1303:BCL:O1D	2.10	0.51
6:M:1303:BCL:HBB1	12:M:1314:SPO:H243	1.91	0.51
5:M:1307:LDA:H21	5:M:1308:LDA:H12	1.93	0.51
3:M:239:ALA:O	3:M:240:ASP:HB2	2.09	0.51
6:L:1286:BCL:HMB1	6:L:1286:BCL:HBB3	1.92	0.51
3:M:150:PHE:CD1	7:M:1312:BPH:C4D	2.94	0.51
2:L:226:THR:HG22	8:L:1285[B]:UQ2:H3M3	1.93	0.51
3:M:199:ASN:HD22	3:M:200:PRO:N	2.09	0.51
1:H:180:GLU:OE2	1:H:188:THR:HG21	2.12	0.50
3:M:71:GLY:HA3	12:M:1314:SPO:H6	1.94	0.50
1:H:248:ARG:HA	1:H:249:LYS:CB	2.41	0.50
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.94	0.50
6:L:1282:BCL:H192	7:L:1284:BPH:H7C2	1.92	0.50
1:H:120:LEU:HB3	1:H:121:PRO:CD	2.42	0.49
6:M:1304:BCL:CBB	6:M:1304:BCL:CHC	2.90	0.49
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.41	0.49
6:L:1286:BCL:CMC	6:M:1304:BCL:HBC2	2.42	0.49
2:L:187:LEU:HD13	3:M:216:PHE:CD2	2.48	0.49
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.27	0.49
2:L:171:PRO:HD2	2:L:259:TRP:CZ3	2.47	0.49
2:L:97:PHE:CE1	6:L:1286:BCL:H121	2.47	0.49
6:M:1303:BCL:HBC1	6:M:1304:BCL:HAA1	1.95	0.49
2:L:135:ARG:HD2	2:L:248:MET:O	2.13	0.48
7:L:1284:BPH:ND	3:M:214:LEU:HD13	2.28	0.48
2:L:170:ASN:C	2:L:170:ASN:ND2	2.65	0.48
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.49	0.48
6:L:1282:BCL:HMB1	6:L:1286:BCL:H142	1.95	0.47
2:L:61:PRO:HG2	5:L:1283:LDA:HM11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ILE:HB	8:L:1285[A]:UQ2:O1	2.14	0.47
2:L:181:PHE:HB3	7:M:1312:BPH:CBB	2.45	0.47
1:H:114:TRP:HE3	1:H:115:VAL:O	1.97	0.47
3:M:76:TYR:C	3:M:76:TYR:CD2	2.88	0.47
2:L:229:ILE:HD13	8:L:1285[A]:UQ2:C3	2.43	0.47
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.45	0.47
1:H:103:ASP:OD1	1:H:105:MET:HB2	2.14	0.47
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.55	0.47
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.50	0.47
3:M:199:ASN:ND2	3:M:201:PHE:H	2.14	0.46
11:M:1313:U10:C35	11:M:1313:U10:C31	2.86	0.46
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.51	0.46
1:H:118:ARG:HH11	1:H:118:ARG:HG2	1.81	0.46
3:M:35:PHE:CE2	3:M:46:GLN:HB2	2.51	0.46
3:M:24:VAL:HG21	3:M:29:ARG:NH1	2.31	0.46
3:M:50:ILE:HG13	3:M:51:TYR:H	1.80	0.46
2:L:216:PHE:HE2	8:L:1285[B]:UQ2:H112	1.80	0.46
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.84	0.46
8:L:1285[A]:UQ2:H13	3:M:39:LEU:HD21	1.98	0.46
6:L:1282:BCL:CBB	6:L:1282:BCL:CHC	2.94	0.45
3:M:300:ASN:OD1	3:M:300:ASN:N	2.49	0.45
1:H:11:ASP:OD1	1:H:14:SER:HB2	2.16	0.45
1:H:71:GLY:HA3	13:H:2021:HOH:O	2.16	0.45
3:M:218:MET:HG2	3:M:252:TRP:CH2	2.51	0.45
2:L:229:ILE:HG13	2:L:229:ILE:O	2.16	0.45
6:L:1282:BCL:HBC1	6:L:1286:BCL:CGA	2.47	0.45
3:M:189:PHE:O	3:M:193:HIS:CD2	2.69	0.45
6:M:1304:BCL:H121	7:M:1312:BPH:CHB	2.45	0.45
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.51	0.45
2:L:241:VAL:CG2	7:L:1284:BPH:HAC1	2.47	0.45
3:M:195:ASN:C	3:M:195:ASN:OD1	2.55	0.45
11:M:1313:U10:H3M3	11:M:1313:U10:H4M2	1.99	0.45
2:L:233:GLY:HA3	3:M:216:PHE:CD1	2.52	0.44
6:L:1286:BCL:HMB1	6:L:1286:BCL:HBB2	2.00	0.44
2:L:13:GLY:O	2:L:110:LYS:HG3	2.17	0.44
2:L:35:GLY:CA	2:L:103:ARG:HD2	2.48	0.44
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.00	0.44
2:L:130:THR:HA	2:L:134:PHE:HB2	1.99	0.44
1:H:170:ASP:OD1	1:H:173:GLU:HG3	2.18	0.44
7:L:1284:BPH:HBB1	3:M:210:TYR:HB3	1.95	0.44
1:H:120:LEU:HB3	1:H:121:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1304:BCL:HAA2	6:M:1304:BCL:HBD	2.00	0.43
3:M:260:ALA:C	11:M:1313:U10:H4M3	2.38	0.43
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.52	0.43
5:L:1281:LDA:H112	8:L:1285[A]:UQ2:H103	2.00	0.43
3:M:39:LEU:HD12	3:M:39:LEU:HA	1.79	0.43
1:H:118:ARG:HH11	1:H:118:ARG:HG3	1.82	0.43
1:H:177:ARG:HH21	1:H:177:ARG:HD3	1.67	0.43
6:L:1286:BCL:HBB2	6:M:1304:BCL:C4A	2.48	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.38	0.43
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.99	0.43
6:M:1303:BCL:H62	7:M:1312:BPH:HMB1	2.01	0.43
2:L:190:HIS:CE1	2:L:230:HIS:CE1	3.06	0.43
2:L:197:ALA:HB1	3:M:235:LEU:HD11	2.01	0.43
1:H:62:LYS:HE2	3:M:263:GLU:OE1	2.19	0.43
2:L:170:ASN:HD22	2:L:171:PRO:N	2.15	0.43
6:L:1282:BCL:HBB3	6:L:1286:BCL:H52	1.99	0.43
5:M:1307:LDA:H51	5:M:1307:LDA:H81	1.45	0.43
1:H:130:LYS:HZ1	1:H:172:PRO:HG2	1.83	0.43
2:L:199:ASN:CA	4:L:1288:GOL:H31	2.39	0.42
8:L:1285[B]:UQ2:H121	8:L:1285[B]:UQ2:H101	1.72	0.42
1:H:62:LYS:NZ	4:H:1251:GOL:H11	2.34	0.42
2:L:121:PHE:CD1	7:L:1284:BPH:C3D	3.03	0.42
2:L:210:ASP:OD1	2:L:210:ASP:N	2.39	0.42
11:M:1313:U10:H1M1	11:M:1313:U10:H8	2.00	0.42
1:H:67:PRO:HA	2:L:205:GLU:OE1	2.19	0.42
1:H:148:PRO:HD2	1:H:167:ILE:HD11	2.02	0.42
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.54	0.42
2:L:150:ILE:HG22	2:L:151:TRP:CD1	2.55	0.42
1:H:117:ARG:HD2	3:M:242:GLY:CA	2.43	0.42
1:H:113:SER:HB2	2:L:9:TYR:CE1	2.55	0.42
6:L:1282:BCL:HAC1	6:L:1286:BCL:HBD	2.01	0.42
6:L:1286:BCL:H2C	6:M:1304:BCL:H2C	2.01	0.42
3:M:129:TRP:CD1	7:M:1312:BPH:HBA1	2.54	0.42
13:H:2032:HOH:O	2:L:1:ALA:CB	2.68	0.41
2:L:44:LEU:HD22	2:L:48:LEU:HG	2.01	0.41
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.48	0.41
1:H:196:VAL:HG12	1:H:205:VAL:HG22	2.02	0.41
3:M:199:ASN:C	3:M:199:ASN:ND2	2.72	0.41
1:H:37:ARG:C	1:H:38:GLU:HG2	2.41	0.41
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.74	0.41
3:M:50:ILE:CG1	3:M:51:TYR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.86	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.90	0.41
1:H:241:LEU:HA	1:H:248:ARG:HH12	1.86	0.41
1:H:46:ASP:OD1	1:H:48:THR:HG23	2.21	0.41
3:M:268:TRP:CD1	11:M:1313:U10:H111	2.55	0.41
1:H:165:VAL:O	1:H:166:ASP:HB2	2.19	0.41
6:L:1282:BCL:H142	6:L:1282:BCL:H161	1.93	0.41
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.03	0.41
3:M:293:ASN:HB3	3:M:296:VAL:HB	2.03	0.41
2:L:172:ALA:O	2:L:173:HIS:C	2.59	0.41
2:L:241:VAL:HG21	7:L:1284:BPH:H2C	2.02	0.41
1:H:69:GLY:HA2	13:H:2020:HOH:O	2.20	0.40
2:L:187:LEU:HD12	2:L:187:LEU:HA	1.99	0.40
6:L:1286:BCL:H142	6:L:1286:BCL:H112	1.92	0.40
6:L:1286:BCL:C2C	6:M:1304:BCL:HBC2	2.51	0.40
1:H:163:LYS:HE2	1:H:165:VAL:HG12	2.03	0.40
13:H:2033:HOH:O	2:L:1:ALA:HB3	2.21	0.40
2:L:35:GLY:HA2	2:L:103:ARG:HD2	2.04	0.40
7:L:1284:BPH:CHD	7:L:1284:BPH:HBC2	2.52	0.40
11:M:1313:U10:H1M1	11:M:1313:U10:C8	2.50	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)
13:H:2021:HOH:O	13:H:2021: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	239/260 (92%)	222 (93%)	14 (6%)	3 (1%)	12 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	276/281 (98%)	253 (92%)	23 (8%)	0	100	100
3	M	301/307 (98%)	274 (91%)	22 (7%)	5 (2%)	9	31
All	All	816/848 (96%)	749 (92%)	59 (7%)	8 (1%)	15	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	30	SER
3	M	240	ASP
3	M	301	HIS
1	H	86	ALA
3	M	52	LEU
1	H	250	SER
3	M	40	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	195/208 (94%)	176 (90%)	19 (10%)	8	25
2	L	219/220 (100%)	193 (88%)	26 (12%)	5	15
3	M	236/240 (98%)	213 (90%)	23 (10%)	8	25
All	All	650/668 (97%)	582 (90%)	68 (10%)	7	21

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	14	SER
1	H	15	LEU
1	H	62	LYS
1	H	83	ARG

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Mol	Chain	Res	Type
1	H	93	SER
1	H	117	ARG
1	H	118	ARG
1	H	163	LYS
1	H	184	LYS
1	H	193	MET
1	H	197	LYS
1	H	217	PRO
1	H	220	LYS
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
2	L	16	LEU
2	L	20	ASN
2	L	21	LEU
2	L	44	LEU
2	L	67	TYR
2	L	72	GLU
2	L	80	LEU
2	L	102	LEU
2	L	110	LYS
2	L	126	LEU
2	L	129	LEU
2	L	150	ILE
2	L	153	HIS
2	L	158	SER
2	L	170	ASN
2	L	202	LYS
2	L	205	GLU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	246	LEU
2	L	247	CYS
2	L	268	LYS
2	L	271	TRP
2	L	272	TRP
3	M	39	LEU
3	M	47	LEU
3	M	52	LEU

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Mol	Chain	Res	Type
3	M	55	LEU
3	M	65	MET
3	M	72	ILE
3	M	86	LEU
3	M	104	SER
3	M	110	LYS
3	M	114	LEU
3	M	122	MET
3	M	182	HIS
3	M	188	ASN
3	M	191	LEU
3	M	199	ASN
3	M	204	LEU
3	M	205	SER
3	M	216	PHE
3	M	253	ARG
3	M	258	PHE
3	M	265	ILE
3	M	270	ILE
3	M	300	ASN

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	20	ASN
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 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	$\#\|Z\| > 2$
5	LDA	M	1306	-	12,15,15	1.99	1 (8%)	14,17,17	0.59	0
6	BCL	M	1304	3	64,74,74	2.00	11 (17%)	78,115,115	3.03	29 (37%)
5	LDA	M	1308	-	12,15,15	2.14	1 (8%)	14,17,17	0.61	0
9	PO4	L	1287	-	4,4,4	0.82	0	6,6,6	0.61	0
5	LDA	M	1305	-	12,15,15	1.99	1 (8%)	14,17,17	0.76	0
8	UQ2	L	1285[B]	-	23,23,23	2.80	8 (34%)	28,31,31	1.48	5 (17%)
4	GOL	H	1252	-	5,5,5	0.49	0	5,5,5	0.57	0
4	GOL	H	1251	-	5,5,5	0.50	0	5,5,5	0.35	0
5	LDA	M	1309	-	12,15,15	1.87	1 (8%)	14,17,17	0.61	0
4	GOL	L	1288	-	5,5,5	0.35	0	5,5,5	0.72	0
7	BPH	L	1284	-	51,70,70	2.98	9 (17%)	52,101,101	2.39	15 (28%)
4	GOL	L	1289	-	5,5,5	0.37	0	5,5,5	0.39	0
5	LDA	M	1310	-	12,15,15	2.03	1 (8%)	14,17,17	0.54	0
12	SPO	M	1314	-	40,41,41	4.24	12 (30%)	47,50,50	2.20	14 (29%)
5	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.69	1 (7%)
6	BCL	M	1303	3	64,74,74	2.18	9 (14%)	78,115,115	2.76	23 (29%)
4	GOL	M	1315	-	5,5,5	0.48	0	5,5,5	0.50	0
6	BCL	L	1286	2	64,74,74	2.01	11 (17%)	78,115,115	2.79	25 (32%)
7	BPH	M	1312	-	51,70,70	2.70	10 (19%)	52,101,101	2.52	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	UQ2	L	1285[A]	-	23,23,23	2.83	9 (39%)	28,31,31	1.31	2 (7%)
5	LDA	M	1307	-	12,15,15	1.87	1 (8%)	14,17,17	0.65	0
11	U10	M	1313	-	48,48,63	2.78	11 (22%)	58,61,79	1.92	15 (25%)
5	LDA	L	1281	-	12,15,15	2.08	1 (8%)	14,17,17	0.62	0
6	BCL	L	1282	2	64,74,74	2.08	10 (15%)	78,115,115	2.60	28 (35%)

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
5	LDA	M	1306	-	-	5/13/13/13	-
6	BCL	M	1304	3	2/2/21/25	12/37/137/137	-
5	LDA	M	1308	-	-	8/13/13/13	-
5	LDA	M	1305	-	-	5/13/13/13	-
8	UQ2	L	1285[B]	-	-	8/15/39/39	0/1/1/1
4	GOL	H	1252	-	-	4/4/4/4	-
4	GOL	H	1251	-	-	2/4/4/4	-
5	LDA	M	1309	-	-	5/13/13/13	-
4	GOL	L	1288	-	-	2/4/4/4	-
7	BPH	L	1284	-	-	12/37/105/105	0/5/6/6
4	GOL	L	1289	-	-	4/4/4/4	-
5	LDA	M	1310	-	-	5/13/13/13	-
12	SPO	M	1314	-	-	25/47/47/47	-
5	LDA	L	1283	-	-	8/13/13/13	-
6	BCL	M	1303	3	2/2/21/25	17/37/137/137	-
4	GOL	M	1315	-	-	2/4/4/4	-
6	BCL	L	1286	2	2/2/21/25	10/37/137/137	-
7	BPH	M	1312	-	-	17/37/105/105	0/5/6/6
8	UQ2	L	1285[A]	-	-	8/15/39/39	0/1/1/1
5	LDA	M	1307	-	-	8/13/13/13	-
11	U10	M	1313	-	-	16/45/69/87	0/1/1/1
5	LDA	L	1281	-	-	8/13/13/13	-
6	BCL	L	1282	2	2/2/21/25	14/37/137/137	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1284	BPH	OBD-CAD	14.21	1.42	1.22
12	M	1314	SPO	C27-C28	13.40	1.48	1.34
7	M	1312	BPH	OBD-CAD	11.80	1.38	1.22
6	L	1286	BCL	OBD-CAD	10.82	1.41	1.22
6	M	1303	BCL	OBD-CAD	10.70	1.40	1.22
6	L	1282	BCL	OBD-CAD	10.41	1.40	1.22
6	M	1304	BCL	OBD-CAD	9.85	1.39	1.22
12	M	1314	SPO	C9-C7	9.83	1.48	1.35
12	M	1314	SPO	C19-C17	9.02	1.47	1.35
12	M	1314	SPO	C22-C23	9.02	1.47	1.35
12	M	1314	SPO	C14-C12	8.32	1.46	1.35
7	L	1284	BPH	O1D-CGD	7.71	1.40	1.21
7	M	1312	BPH	O1D-CGD	7.34	1.39	1.21
8	L	1285[A]	UQ2	C8-C9	7.31	1.50	1.33
5	M	1308	LDA	O1-N1	-7.28	1.25	1.42
8	L	1285[B]	UQ2	C8-C9	7.20	1.50	1.33
11	M	1313	U10	C33-C34	7.20	1.50	1.33
7	L	1284	BPH	O1A-CGA	7.16	1.43	1.22
6	M	1303	BCL	O1A-CGA	7.08	1.43	1.22
5	L	1281	LDA	O1-N1	-7.07	1.25	1.42
5	M	1310	LDA	O1-N1	-6.93	1.25	1.42
5	L	1283	LDA	O1-N1	-6.80	1.26	1.42
11	M	1313	U10	C18-C19	6.74	1.49	1.33
11	M	1313	U10	C13-C14	6.71	1.49	1.33
5	M	1306	LDA	O1-N1	-6.65	1.26	1.42
12	M	1314	SPO	C32-C33	6.58	1.48	1.33
12	M	1314	SPO	C37-C38	6.57	1.51	1.32
5	M	1305	LDA	O1-N1	-6.53	1.26	1.42
7	L	1284	BPH	C2-C3	6.49	1.48	1.33
11	M	1313	U10	C28-C29	6.47	1.48	1.33
5	M	1307	LDA	O1-N1	-6.38	1.27	1.42
5	M	1309	LDA	O1-N1	-6.37	1.27	1.42
7	M	1312	BPH	O1A-CGA	6.36	1.41	1.22
8	L	1285[B]	UQ2	C13-C14	6.21	1.50	1.32
7	M	1312	BPH	C2-C3	6.16	1.47	1.33
6	M	1304	BCL	O1A-CGA	6.10	1.40	1.22
6	L	1282	BCL	O1A-CGA	6.00	1.40	1.22
11	M	1313	U10	C8-C9	5.93	1.47	1.33
12	M	1314	SPO	C6-C5	5.81	1.47	1.32
11	M	1313	U10	C23-C24	5.79	1.46	1.33
6	L	1286	BCL	O1A-CGA	5.77	1.39	1.22
11	M	1313	U10	C38-C39	5.69	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1284	BPH	C3D-C2D	5.65	1.49	1.39
7	L	1284	BPH	OBB-CAB	5.61	1.40	1.22
7	M	1312	BPH	OBB-CAB	5.57	1.40	1.22
6	M	1303	BCL	C1B-NB	5.54	1.40	1.35
8	L	1285[A]	UQ2	C13-C14	5.53	1.48	1.32
7	M	1312	BPH	C3D-C2D	5.14	1.48	1.39
6	L	1282	BCL	C4D-ND	-5.08	1.30	1.37
8	L	1285[B]	UQ2	O2-C2	-4.94	1.24	1.36
12	M	1314	SPO	C10-C11	4.87	1.47	1.34
8	L	1285[A]	UQ2	O3-C3	-4.86	1.25	1.36
8	L	1285[A]	UQ2	O2-C2	-4.84	1.25	1.36
6	M	1304	BCL	C4D-ND	-4.81	1.31	1.37
11	M	1313	U10	O4-C4	-4.81	1.25	1.36
12	M	1314	SPO	C26-C25	4.56	1.46	1.34
8	L	1285[B]	UQ2	O3-C3	-4.23	1.26	1.36
6	M	1303	BCL	C4B-NB	4.18	1.38	1.35
11	M	1313	U10	O3-C3	-4.10	1.26	1.36
6	M	1303	BCL	C3D-C4D	-4.06	1.35	1.44
12	M	1314	SPO	C15-C16	4.05	1.45	1.34
6	M	1304	BCL	C3D-C4D	-4.03	1.35	1.44
6	L	1282	BCL	C4B-NB	4.01	1.38	1.35
8	L	1285[A]	UQ2	C6-C5	3.93	1.42	1.35
6	L	1286	BCL	C3D-C4D	-3.86	1.35	1.44
6	L	1282	BCL	C3D-C4D	-3.73	1.35	1.44
12	M	1314	SPO	C21-C20	3.60	1.45	1.36
6	M	1303	BCL	C4D-ND	-3.58	1.32	1.37
6	L	1286	BCL	C2-C3	3.58	1.41	1.33
6	M	1303	BCL	C2-C3	3.56	1.41	1.33
6	L	1282	BCL	C1B-NB	3.55	1.38	1.35
6	M	1304	BCL	C4B-NB	3.44	1.38	1.35
6	L	1282	BCL	C2-C3	3.32	1.41	1.33
11	M	1313	U10	C6-C1	3.29	1.41	1.35
7	L	1284	BPH	O2D-CGD	-3.25	1.25	1.33
7	M	1312	BPH	O2D-CGD	-3.12	1.25	1.33
6	L	1286	BCL	C4D-ND	-3.10	1.33	1.37
6	M	1303	BCL	CHD-C4C	3.06	1.47	1.39
8	L	1285[B]	UQ2	C3-C4	-3.06	1.40	1.48
8	L	1285[B]	UQ2	C6-C5	3.06	1.40	1.35
8	L	1285[A]	UQ2	C3-C4	-3.03	1.40	1.48
6	M	1304	BCL	C1B-NB	3.02	1.37	1.35
6	M	1304	BCL	O2D-CGD	-3.02	1.25	1.33
6	M	1304	BCL	C2-C3	2.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1286	BCL	CHD-C4C	2.79	1.47	1.39
6	L	1286	BCL	C4B-NB	2.65	1.37	1.35
6	L	1282	BCL	CHD-C4C	2.62	1.46	1.39
6	M	1304	BCL	CHD-C4C	2.61	1.46	1.39
6	L	1286	BCL	MG-ND	-2.58	2.00	2.05
6	L	1286	BCL	C1B-NB	2.57	1.37	1.35
11	M	1313	U10	C4-C5	-2.49	1.41	1.48
8	L	1285[A]	UQ2	C2-C1	-2.43	1.41	1.48
8	L	1285[B]	UQ2	C2-C1	-2.38	1.42	1.48
6	M	1303	BCL	O2D-CGD	-2.36	1.27	1.33
7	M	1312	BPH	O2D-CED	-2.33	1.39	1.45
6	L	1286	BCL	O2D-CGD	-2.32	1.27	1.33
8	L	1285[B]	UQ2	C7-C8	2.24	1.53	1.50
8	L	1285[A]	UQ2	C7-C6	2.20	1.55	1.51
6	L	1282	BCL	O1D-CGD	2.19	1.26	1.21
8	L	1285[A]	UQ2	C7-C8	2.18	1.53	1.50
7	L	1284	BPH	O2D-CED	-2.16	1.40	1.45
6	L	1282	BCL	O2D-CGD	-2.14	1.28	1.33
6	M	1304	BCL	O2D-CED	-2.13	1.40	1.45
7	M	1312	BPH	O2A-CGA	-2.13	1.27	1.33
7	M	1312	BPH	CBD-CGD	-2.12	1.49	1.52
7	L	1284	BPH	O2A-CGA	-2.12	1.27	1.33
6	M	1304	BCL	C3D-CAD	-2.10	1.38	1.45
6	L	1286	BCL	O2A-CGA	-2.08	1.27	1.33

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1286	BCL	C2D-C1D-ND	-11.07	101.95	110.10
7	L	1284	BPH	O2D-CGD-CBD	10.67	124.51	111.00
7	M	1312	BPH	OBD-CAD-CBD	-10.28	110.73	125.82
6	L	1286	BCL	C1D-ND-C4D	10.14	113.54	106.33
6	M	1303	BCL	C2D-C1D-ND	-9.22	103.31	110.10
7	M	1312	BPH	O2D-CGD-CBD	8.99	122.39	111.00
6	M	1304	BCL	C1C-NC-C4C	8.82	110.67	106.71
6	M	1304	BCL	CMB-C2B-C1B	-8.51	115.38	128.46
6	M	1303	BCL	CMB-C2B-C1B	-7.71	116.62	128.46
6	M	1303	BCL	C1D-ND-C4D	7.63	111.75	106.33
6	M	1304	BCL	CHD-C1D-ND	-7.54	117.52	124.45
6	L	1286	BCL	CHD-C1D-ND	-7.52	117.54	124.45
6	M	1304	BCL	C1D-ND-C4D	7.45	111.63	106.33
6	M	1304	BCL	C2D-C1D-ND	-7.30	104.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1282	BCL	C2D-C1D-ND	-7.02	104.93	110.10
6	M	1303	BCL	C4A-NA-C1A	6.94	109.83	106.71
6	L	1286	BCL	C4A-NA-C1A	6.85	109.79	106.71
6	L	1282	BCL	C4A-NA-C1A	6.79	109.76	106.71
6	L	1282	BCL	C1D-ND-C4D	6.67	111.07	106.33
12	M	1314	SPO	C15-C14-C12	-6.65	117.82	127.31
6	L	1282	BCL	CMB-C2B-C1B	-6.52	118.44	128.46
6	M	1304	BCL	CHC-C1C-NC	-6.49	115.53	124.51
7	L	1284	BPH	OBD-CAD-CBD	-6.46	116.34	125.82
6	M	1304	BCL	C4A-NA-C1A	6.44	109.60	106.71
6	L	1282	BCL	O2D-CGD-CBD	6.18	122.25	111.27
6	M	1303	BCL	CHD-C1D-ND	-6.00	118.94	124.45
6	M	1303	BCL	O2D-CGD-CBD	5.92	121.78	111.27
6	M	1304	BCL	CMB-C2B-C3B	5.81	135.55	124.68
11	M	1313	U10	C30-C29-C31	5.72	124.89	115.27
12	M	1314	SPO	C20-C19-C17	-5.56	119.37	127.31
6	L	1286	BCL	CMB-C2B-C1B	-5.56	119.92	128.46
7	M	1312	BPH	O1D-CGD-CBD	-5.46	115.64	124.74
6	M	1303	BCL	CHC-C1C-NC	-5.45	116.98	124.51
6	M	1304	BCL	O2D-CGD-CBD	5.32	120.72	111.27
7	L	1284	BPH	O1D-CGD-CBD	-5.30	115.91	124.74
6	M	1304	BCL	CMD-C2D-C1D	5.17	133.83	124.71
11	M	1313	U10	C25-C24-C26	4.99	123.67	115.27
12	M	1314	SPO	C21-C22-C23	-4.92	120.29	127.31
6	M	1304	BCL	C4B-CHC-C1C	-4.90	120.42	130.12
6	M	1304	BCL	CHD-C4C-NC	-4.81	119.74	125.08
6	L	1282	BCL	C1C-NC-C4C	4.81	108.87	106.71
6	M	1303	BCL	CMD-C2D-C1D	4.80	133.17	124.71
6	L	1286	BCL	CMD-C2D-C1D	4.78	133.14	124.71
6	M	1303	BCL	CMB-C2B-C3B	4.71	133.49	124.68
6	L	1286	BCL	O2D-CGD-CBD	4.62	119.48	111.27
6	L	1282	BCL	CHC-C1C-NC	-4.50	118.29	124.51
6	L	1282	BCL	CHD-C1D-ND	-4.48	120.33	124.45
6	M	1304	BCL	O2A-CGA-CBA	4.40	125.71	111.91
6	M	1303	BCL	O1D-CGD-CBD	-4.36	115.57	124.48
6	M	1303	BCL	C4B-CHC-C1C	-4.33	121.54	130.12
6	L	1286	BCL	C4B-CHC-C1C	-4.23	121.73	130.12
6	L	1282	BCL	C1D-CHD-C4C	-4.21	116.47	126.62
6	L	1286	BCL	CMD-C2D-C3D	-4.18	118.00	127.61
6	L	1282	BCL	C4B-CHC-C1C	-4.17	121.86	130.12
6	M	1304	BCL	C1D-CHD-C4C	-4.16	116.59	126.62
6	M	1303	BCL	C1D-CHD-C4C	-4.12	116.69	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	1313	U10	C17-C18-C19	-4.03	117.96	127.66
6	L	1282	BCL	CMB-C2B-C3B	4.01	132.18	124.68
7	L	1284	BPH	C1C-C2C-C3C	-3.99	99.04	102.84
6	L	1282	BCL	O1D-CGD-CBD	-3.99	116.33	124.48
6	M	1303	BCL	CHA-C1A-NA	-3.94	117.38	126.40
7	M	1312	BPH	C4-C3-C5	3.93	121.89	115.27
6	L	1282	BCL	CMD-C2D-C1D	3.84	131.48	124.71
6	M	1303	BCL	CMD-C2D-C3D	-3.81	118.85	127.61
6	L	1282	BCL	C1B-CHB-C4A	-3.79	122.61	130.12
6	L	1282	BCL	CHD-C4C-NC	-3.77	120.88	125.08
12	M	1314	SPO	C13-C12-C11	3.63	123.80	118.08
6	L	1286	BCL	O2A-CGA-CBA	3.57	123.11	111.91
11	M	1313	U10	C27-C28-C29	-3.48	119.29	127.66
12	M	1314	SPO	C10-C9-C7	-3.47	122.35	127.31
6	L	1282	BCL	CHB-C4A-NA	-3.40	119.81	124.51
11	M	1313	U10	C15-C14-C16	3.35	120.91	115.27
6	L	1282	BCL	O2A-CGA-CBA	3.35	122.42	111.91
12	M	1314	SPO	C5-C6-C7	-3.33	120.85	125.89
6	L	1286	BCL	CMB-C2B-C3B	3.32	130.90	124.68
6	M	1304	BCL	CMD-C2D-C3D	-3.28	120.06	127.61
6	M	1304	BCL	CHA-C1A-NA	-3.26	118.92	126.40
6	L	1286	BCL	CHC-C1C-NC	-3.19	120.10	124.51
6	L	1286	BCL	CED-O2D-CGD	3.17	123.10	115.94
7	L	1284	BPH	CMA-C3A-C4A	-3.16	107.47	114.38
6	M	1303	BCL	CHD-C4C-NC	-3.14	121.59	125.08
7	M	1312	BPH	CAC-C3C-C2C	-3.13	106.43	114.26
7	M	1312	BPH	C1-O2A-CGA	3.12	124.64	116.44
11	M	1313	U10	C41-C39-C40	3.10	121.44	114.60
7	M	1312	BPH	C4A-C3A-C2A	-3.08	99.91	102.84
11	M	1313	U10	C22-C23-C24	-3.07	120.26	127.66
8	L	1285[B]	UQ2	CM3-O3-C3	3.01	127.13	116.47
6	L	1286	BCL	CHB-C4A-NA	-3.00	120.36	124.51
12	M	1314	SPO	C2-C1-C4	-3.00	106.25	110.86
7	M	1312	BPH	C1C-C2C-C3C	-3.00	99.99	102.84
6	M	1303	BCL	CHB-C4A-NA	-3.00	120.37	124.51
6	L	1282	BCL	C2A-C3A-C4A	2.99	106.70	101.87
6	M	1303	BCL	C1B-CHB-C4A	-2.99	124.20	130.12
6	M	1303	BCL	O2A-CGA-CBA	2.98	121.26	111.91
7	L	1284	BPH	C1-C2-C3	-2.97	120.91	126.04
6	L	1282	BCL	C4-C3-C5	2.94	120.22	115.27
11	M	1313	U10	C1M-C1-C6	-2.94	119.60	124.40
6	L	1286	BCL	C1-O2A-CGA	2.92	124.11	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1304	BCL	C16-C15-C13	-2.91	106.50	115.92
6	M	1304	BCL	C1B-CHB-C4A	-2.91	124.36	130.12
6	L	1282	BCL	O2A-CGA-O1A	-2.90	116.27	123.59
6	L	1286	BCL	CHA-C1A-NA	-2.90	119.75	126.40
7	M	1312	BPH	CMD-C2D-C3D	-2.89	119.27	124.68
12	M	1314	SPO	C13-C12-C14	-2.88	118.89	122.92
6	M	1303	BCL	C1-O2A-CGA	2.86	123.94	116.44
7	L	1284	BPH	CMD-C2D-C3D	-2.84	119.36	124.68
6	L	1286	BCL	C1B-CHB-C4A	-2.84	124.50	130.12
6	L	1286	BCL	CHA-C4D-ND	2.83	138.43	132.50
12	M	1314	SPO	C29-C28-C30	2.83	120.03	115.27
6	L	1286	BCL	C1D-CHD-C4C	-2.81	119.84	126.62
6	M	1303	BCL	C2A-C3A-C4A	2.80	106.39	101.87
11	M	1313	U10	C32-C31-C29	2.79	122.15	112.98
8	L	1285[A]	UQ2	O2-C2-C3	-2.79	113.13	123.64
6	M	1304	BCL	C7-C6-C5	-2.78	105.82	113.36
6	M	1304	BCL	CED-O2D-CGD	2.75	122.17	115.94
7	M	1312	BPH	CED-O2D-CGD	2.73	122.10	115.94
12	M	1314	SPO	C34-C33-C35	2.70	119.81	115.27
6	L	1286	BCL	O1D-CGD-CBD	-2.68	118.99	124.48
12	M	1314	SPO	C31-C32-C33	-2.66	121.26	127.66
6	L	1282	BCL	CMD-C2D-C3D	-2.63	121.56	127.61
6	L	1286	BCL	C2A-C3A-C4A	2.61	106.09	101.87
8	L	1285[B]	UQ2	CM5-C5-C6	-2.60	120.15	124.40
6	L	1282	BCL	C5-C3-C2	-2.59	115.88	121.12
6	L	1282	BCL	C3C-C4C-CHD	-2.57	117.90	123.39
12	M	1314	SPO	C15-C16-C17	-2.55	119.25	126.42
7	L	1284	BPH	CMC-C2C-C1C	-2.52	108.86	114.38
11	M	1313	U10	C30-C29-C28	-2.51	117.25	123.68
8	L	1285[A]	UQ2	C5-C6-C1	-2.49	117.24	119.58
6	M	1303	BCL	C1C-NC-C4C	2.48	107.82	106.71
6	L	1282	BCL	C6-C5-C3	-2.46	106.99	113.45
6	M	1304	BCL	CAC-C3C-C4C	-2.46	107.11	112.58
7	M	1312	BPH	O2A-CGA-CBA	2.46	119.62	111.91
6	L	1282	BCL	CED-O2D-CGD	2.42	121.42	115.94
6	M	1304	BCL	CHB-C4A-NA	-2.42	121.17	124.51
11	M	1313	U10	C10-C9-C11	2.41	119.32	115.27
6	M	1304	BCL	C1-O2A-CGA	2.41	122.76	116.44
11	M	1313	U10	C32-C33-C34	-2.40	121.88	127.66
8	L	1285[B]	UQ2	O4-C4-C3	-2.38	115.87	120.93
6	L	1282	BCL	CHA-C1A-NA	-2.37	120.96	126.40
6	M	1304	BCL	O2D-CGD-O1D	-2.36	119.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	1284	BPH	C7-C6-C5	-2.36	106.94	113.36
7	L	1284	BPH	C3D-CAD-CBD	-2.34	104.53	107.61
6	M	1304	BCL	C3C-C4C-CHD	-2.33	118.41	123.39
6	L	1282	BCL	CMA-C3A-C4A	-2.33	105.50	111.77
7	L	1284	BPH	O2A-CGA-CBA	2.31	119.16	111.91
8	L	1285[B]	UQ2	C10-C9-C11	2.31	119.15	115.27
11	M	1313	U10	C4M-O4-C4	2.28	124.53	116.47
5	L	1283	LDA	CM2-N1-C1	2.21	114.88	110.23
6	M	1304	BCL	CHA-C4D-ND	2.21	137.12	132.50
8	L	1285[B]	UQ2	C10-C9-C8	-2.20	118.03	123.68
11	M	1313	U10	C25-C24-C23	-2.19	118.05	123.68
7	L	1284	BPH	O2D-CGD-O1D	-2.19	119.56	123.84
6	L	1286	BCL	C3D-C2D-C1D	2.19	108.82	105.83
7	L	1284	BPH	O2A-CGA-O1A	-2.18	118.08	123.59
7	L	1284	BPH	CAC-C3C-C4C	2.17	118.58	113.73
6	M	1304	BCL	O1D-CGD-CBD	-2.16	120.06	124.48
11	M	1313	U10	C41-C39-C38	-2.16	116.39	122.65
6	L	1282	BCL	C11-C12-C13	-2.13	109.02	115.92
6	M	1303	BCL	C7-C6-C5	2.13	119.15	113.36
6	M	1303	BCL	O2A-C1-C2	2.11	114.18	108.64
6	M	1304	BCL	C2A-C3A-C4A	2.11	105.28	101.87
6	M	1304	BCL	O1A-CGA-CBA	-2.10	115.53	123.73
12	M	1314	SPO	C34-C33-C32	-2.10	118.30	123.68
6	L	1286	BCL	CMA-C3A-C4A	-2.08	106.17	111.77
7	M	1312	BPH	CMA-C3A-C4A	-2.07	109.84	114.38
7	L	1284	BPH	C4A-C3A-C2A	-2.05	100.89	102.84
6	L	1286	BCL	C2A-C1A-CHA	-2.03	120.31	123.86
12	M	1314	SPO	C24-C23-C25	2.03	121.28	118.08
6	L	1286	BCL	CAA-C2A-C1A	-2.00	105.42	111.97

All (8) chirality outliers are listed below:

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

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	O1-C1-C2-C3
4	H	1252	GOL	C1-C2-C3-O3
4	L	1288	GOL	C1-C2-C3-O3
4	L	1289	GOL	O1-C1-C2-C3
5	M	1307	LDA	C2-C1-N1-O1
5	M	1307	LDA	C2-C1-N1-CM2
5	M	1309	LDA	C2-C1-N1-CM1
5	M	1309	LDA	C2-C1-N1-CM2
6	L	1282	BCL	C1-C2-C3-C4
6	L	1286	BCL	C6-C7-C8-C9
6	M	1303	BCL	C4C-C3C-CAC-CBC
6	M	1303	BCL	C1-C2-C3-C4
6	M	1303	BCL	C1-C2-C3-C5
6	M	1304	BCL	C2C-C3C-CAC-CBC
6	M	1304	BCL	C4C-C3C-CAC-CBC
7	L	1284	BPH	CBD-CGD-O2D-CED
7	L	1284	BPH	O2A-C1-C2-C3
7	L	1284	BPH	C1-C2-C3-C4
7	L	1284	BPH	C1-C2-C3-C5
7	M	1312	BPH	C1-C2-C3-C4
7	M	1312	BPH	C1-C2-C3-C5
8	L	1285[A]	UQ2	C7-C8-C9-C10
8	L	1285[A]	UQ2	C7-C8-C9-C11
8	L	1285[A]	UQ2	C12-C11-C9-C8
8	L	1285[A]	UQ2	C12-C11-C9-C10
8	L	1285[A]	UQ2	C12-C13-C14-C15
8	L	1285[B]	UQ2	C12-C11-C9-C8
8	L	1285[B]	UQ2	C12-C11-C9-C10
11	M	1313	U10	C27-C28-C29-C30
11	M	1313	U10	C27-C28-C29-C31
11	M	1313	U10	C31-C32-C33-C34
11	M	1313	U10	C34-C36-C37-C38
12	M	1314	SPO	C5-C6-C7-C8
12	M	1314	SPO	C5-C6-C7-C9
12	M	1314	SPO	C19-C20-C21-C22
12	M	1314	SPO	C21-C22-C23-C24
12	M	1314	SPO	C21-C22-C23-C25
12	M	1314	SPO	C31-C32-C33-C34
12	M	1314	SPO	C31-C32-C33-C35
8	L	1285[A]	UQ2	C12-C13-C14-C16
12	M	1314	SPO	C36-C37-C38-C39
12	M	1314	SPO	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
7	L	1284	BPH	O1D-CGD-O2D-CED
6	L	1282	BCL	C3-C5-C6-C7
8	L	1285[B]	UQ2	C12-C13-C14-C15
8	L	1285[B]	UQ2	C7-C8-C9-C10
11	M	1313	U10	C22-C23-C24-C25
8	L	1285[B]	UQ2	C7-C8-C9-C11
11	M	1313	U10	C22-C23-C24-C26
5	M	1307	LDA	C5-C6-C7-C8
11	M	1313	U10	C37-C38-C39-C41
7	M	1312	BPH	C4-C3-C5-C6
11	M	1313	U10	C30-C29-C31-C32
7	M	1312	BPH	C2-C3-C5-C6
11	M	1313	U10	C28-C29-C31-C32
8	L	1285[A]	UQ2	C9-C11-C12-C13
8	L	1285[B]	UQ2	C9-C11-C12-C13
11	M	1313	U10	C29-C31-C32-C33
8	L	1285[B]	UQ2	C12-C13-C14-C16
6	L	1282	BCL	CBD-CGD-O2D-CED
12	M	1314	SPO	C12-C14-C15-C16
6	L	1282	BCL	C6-C7-C8-C9
6	L	1286	BCL	C11-C12-C13-C14
6	M	1304	BCL	C11-C10-C8-C9
12	M	1314	SPO	C15-C16-C17-C18
12	M	1314	SPO	C24-C23-C25-C26
12	M	1314	SPO	C15-C16-C17-C19
12	M	1314	SPO	C22-C23-C25-C26
6	M	1303	BCL	C8-C10-C11-C12
6	M	1303	BCL	C13-C15-C16-C17
11	M	1313	U10	C37-C38-C39-C40
4	H	1252	GOL	O2-C2-C3-O3
4	L	1288	GOL	O2-C2-C3-O3
6	L	1286	BCL	C10-C11-C12-C13
6	L	1282	BCL	C13-C15-C16-C17
11	M	1313	U10	C14-C16-C17-C18
11	M	1313	U10	C19-C21-C22-C23
12	M	1314	SPO	C9-C10-C11-C12
12	M	1314	SPO	C14-C15-C16-C17
12	M	1314	SPO	C23-C25-C26-C27
6	L	1286	BCL	C13-C15-C16-C17
6	L	1286	BCL	C15-C16-C17-C18
6	L	1286	BCL	C8-C10-C11-C12
12	M	1314	SPO	C17-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
12	M	1314	SPO	C8-C7-C9-C10
12	M	1314	SPO	C13-C12-C14-C15
5	M	1308	LDA	C6-C7-C8-C9
12	M	1314	SPO	C6-C7-C9-C10
12	M	1314	SPO	C11-C12-C14-C15
7	M	1312	BPH	CBA-CGA-O2A-C1
7	M	1312	BPH	C16-C17-C18-C20
5	M	1305	LDA	C11-C10-C9-C8
4	H	1251	GOL	O1-C1-C2-C3
4	L	1289	GOL	C1-C2-C3-O3
4	M	1315	GOL	O1-C1-C2-C3
5	M	1305	LDA	C2-C3-C4-C5
5	L	1283	LDA	C3-C4-C5-C6
5	M	1308	LDA	C7-C8-C9-C10
5	L	1281	LDA	C3-C4-C5-C6
5	M	1310	LDA	C7-C8-C9-C10
5	L	1283	LDA	C6-C7-C8-C9
7	M	1312	BPH	O2A-C1-C2-C3
4	H	1252	GOL	O1-C1-C2-O2
4	L	1289	GOL	O1-C1-C2-O2
4	L	1289	GOL	O2-C2-C3-O3
7	M	1312	BPH	O1A-CGA-O2A-C1
5	L	1283	LDA	C1-C2-C3-C4
7	M	1312	BPH	C13-C15-C16-C17
5	L	1281	LDA	C11-C10-C9-C8
5	M	1305	LDA	C6-C7-C8-C9
7	L	1284	BPH	C2-C3-C5-C6
5	M	1305	LDA	C4-C5-C6-C7
5	M	1308	LDA	C2-C3-C4-C5
5	M	1306	LDA	C7-C8-C9-C10
5	M	1308	LDA	C3-C4-C5-C6
5	M	1306	LDA	C1-C2-C3-C4
5	L	1281	LDA	C4-C5-C6-C7
7	L	1284	BPH	C4-C3-C5-C6
6	M	1303	BCL	C6-C7-C8-C9
6	M	1303	BCL	C11-C10-C8-C9
5	M	1310	LDA	C1-C2-C3-C4
7	M	1312	BPH	C16-C17-C18-C19
5	M	1307	LDA	C6-C7-C8-C9
6	L	1282	BCL	C5-C6-C7-C8
5	L	1283	LDA	C5-C6-C7-C8
5	M	1308	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	L	1283	LDA	C11-C10-C9-C8
5	M	1310	LDA	C9-C10-C11-C12
6	M	1304	BCL	C3-C5-C6-C7
5	L	1283	LDA	C4-C5-C6-C7
11	M	1313	U10	C20-C19-C21-C22
5	L	1283	LDA	C9-C10-C11-C12
5	M	1310	LDA	C3-C4-C5-C6
6	L	1286	BCL	C11-C12-C13-C15
6	M	1303	BCL	C6-C7-C8-C10
6	M	1303	BCL	C11-C10-C8-C7
6	M	1304	BCL	C12-C13-C15-C16
11	M	1313	U10	C18-C19-C21-C22
5	L	1281	LDA	C1-C2-C3-C4
6	M	1304	BCL	C14-C13-C15-C16
7	M	1312	BPH	C11-C12-C13-C14
5	M	1310	LDA	C11-C10-C9-C8
5	L	1281	LDA	N1-C1-C2-C3
5	M	1307	LDA	N1-C1-C2-C3
5	M	1308	LDA	N1-C1-C2-C3
7	L	1284	BPH	C8-C10-C11-C12
5	L	1281	LDA	C9-C10-C11-C12
5	L	1281	LDA	C5-C6-C7-C8
6	L	1282	BCL	O1D-CGD-O2D-CED
5	M	1306	LDA	C4-C5-C6-C7
5	M	1307	LDA	C2-C3-C4-C5
5	M	1309	LDA	C9-C10-C11-C12
12	M	1314	SPO	C28-C30-C31-C32
6	L	1282	BCL	C14-C13-C15-C16
6	M	1304	BCL	C11-C12-C13-C14
5	M	1306	LDA	C6-C7-C8-C9
6	L	1282	BCL	C1-C2-C3-C5
6	L	1286	BCL	C6-C7-C8-C10
6	M	1303	BCL	C11-C12-C13-C15
7	M	1312	BPH	C11-C12-C13-C15
7	M	1312	BPH	CAD-CBD-CGD-O2D
5	M	1308	LDA	C11-C10-C9-C8
11	M	1313	U10	C5-C4-O4-C4M
6	M	1303	BCL	C16-C17-C18-C20
6	L	1282	BCL	CHA-CBD-CGD-O1D
6	L	1282	BCL	CHA-CBD-CGD-O2D
6	M	1303	BCL	C4-C3-C5-C6
5	L	1281	LDA	C2-C3-C4-C5

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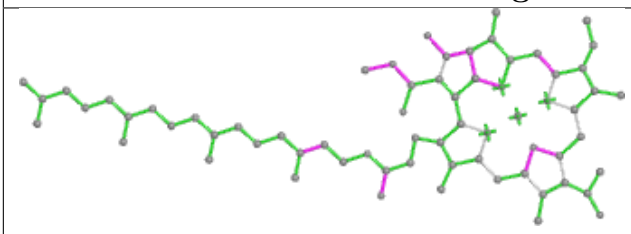
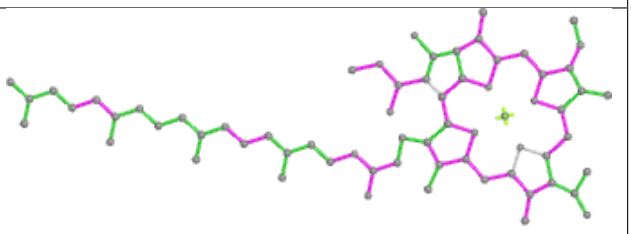
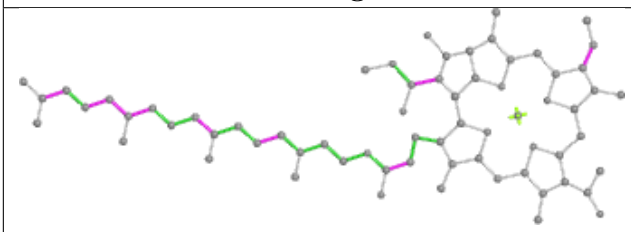
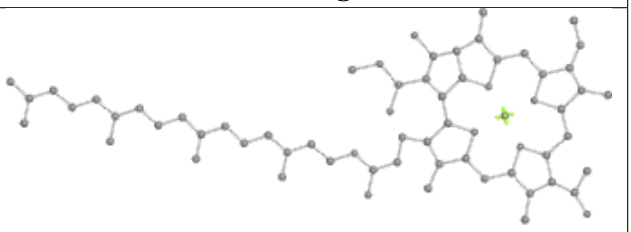
Mol	Chain	Res	Type	Atoms
6	M	1303	BCL	C2-C3-C5-C6
5	M	1309	LDA	C6-C7-C8-C9
7	L	1284	BPH	C2C-C3C-CAC-CBC
6	M	1303	BCL	C15-C16-C17-C18
6	M	1303	BCL	C10-C11-C12-C13
6	M	1304	BCL	CAA-CBA-CGA-O2A
8	L	1285[A]	UQ2	C4-C3-O3-CM3
6	M	1304	BCL	CAD-CBD-CGD-O1D
6	L	1282	BCL	C11-C12-C13-C15
6	M	1304	BCL	C11-C10-C8-C7
7	L	1284	BPH	C4C-C3C-CAC-CBC
6	M	1303	BCL	C11-C12-C13-C14
4	M	1315	GOL	O1-C1-C2-O2
6	M	1303	BCL	C16-C17-C18-C19
8	L	1285[B]	UQ2	C4-C3-O3-CM3
5	M	1307	LDA	C9-C10-C11-C12
5	L	1283	LDA	C2-C3-C4-C5
5	M	1308	LDA	C1-C2-C3-C4
7	L	1284	BPH	C11-C10-C8-C9
5	M	1307	LDA	C1-C2-C3-C4
5	M	1305	LDA	C9-C10-C11-C12
6	M	1304	BCL	C16-C17-C18-C19
5	M	1306	LDA	C9-C10-C11-C12
7	M	1312	BPH	C5-C6-C7-C8
6	L	1286	BCL	C1-C2-C3-C4
12	M	1314	SPO	C18-C17-C19-C20
6	L	1282	BCL	C11-C12-C13-C14
6	L	1286	BCL	CAD-CBD-CGD-O2D
12	M	1314	SPO	C29-C28-C30-C31
6	M	1304	BCL	C13-C15-C16-C17
4	H	1251	GOL	O1-C1-C2-O2
6	L	1282	BCL	C12-C13-C15-C16
7	M	1312	BPH	C8-C10-C11-C12
7	L	1284	BPH	C2-C1-O2A-CGA
5	M	1309	LDA	C2-C1-N1-O1
7	M	1312	BPH	C6-C7-C8-C9
7	M	1312	BPH	C11-C10-C8-C7

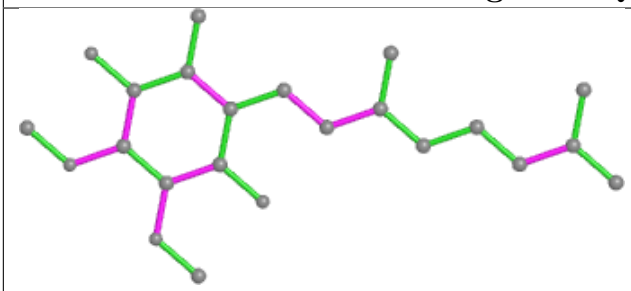
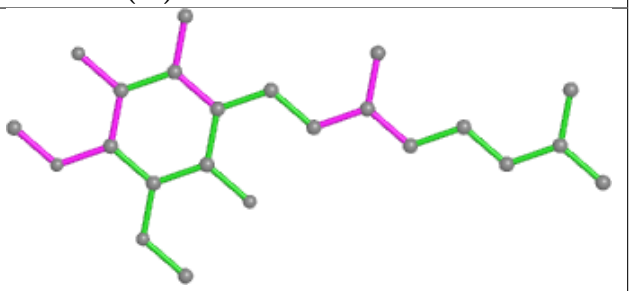
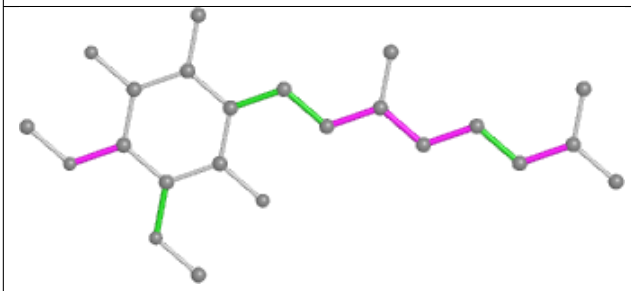
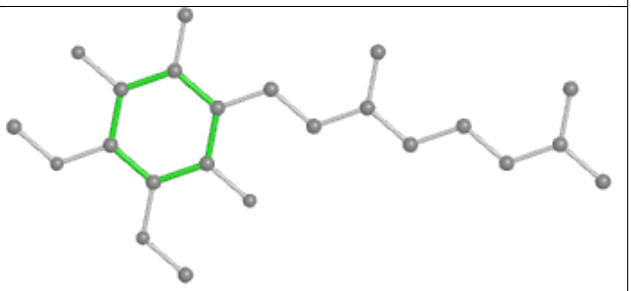
There are no ring outliers.

18 monomers are involved in 103 short contacts:

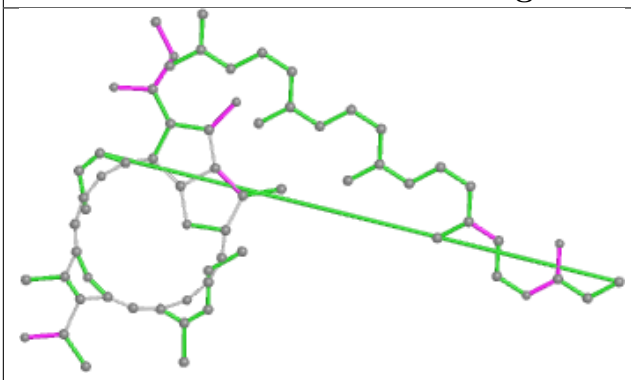
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1304	BCL	23	0
5	M	1308	LDA	2	0
5	M	1305	LDA	2	0
8	L	1285[B]	UQ2	4	0
4	H	1251	GOL	1	0
5	M	1309	LDA	4	0
4	L	1288	GOL	2	0
7	L	1284	BPH	18	0
12	M	1314	SPO	6	0
5	L	1283	LDA	1	0
6	M	1303	BCL	10	0
6	L	1286	BCL	15	0
7	M	1312	BPH	11	0
8	L	1285[A]	UQ2	8	0
5	M	1307	LDA	6	0
11	M	1313	U10	10	0
5	L	1281	LDA	1	0
6	L	1282	BCL	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.

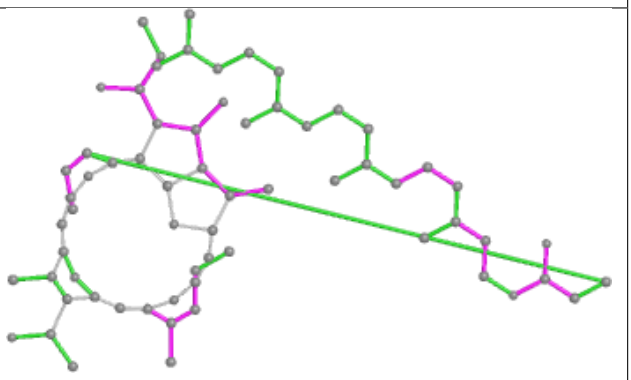
Ligand BCL M 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ2 L 1285 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

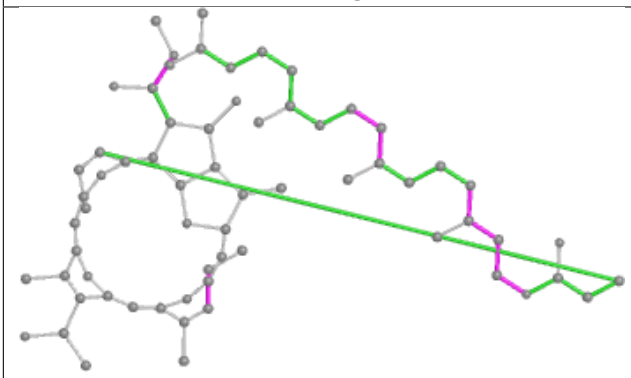
Ligand BPH L 1284



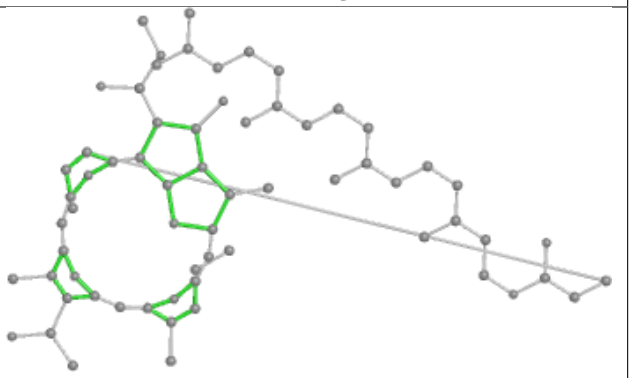
Bond lengths



Bond angles

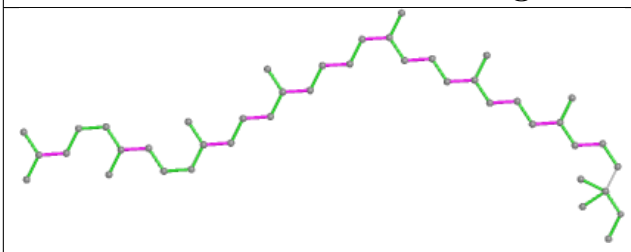


Torsions

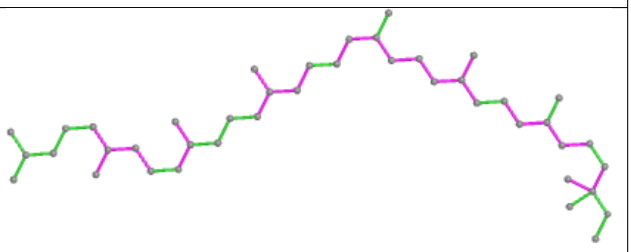


Rings

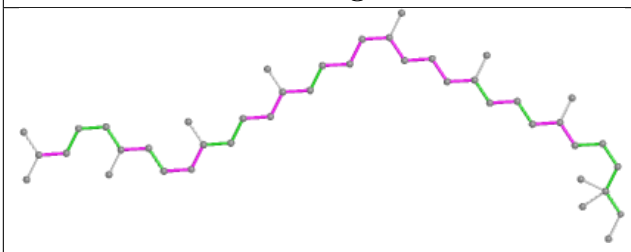
Ligand SPO M 1314



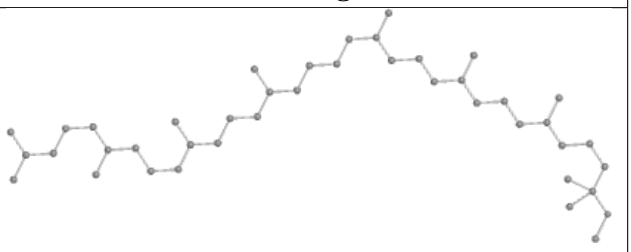
Bond lengths



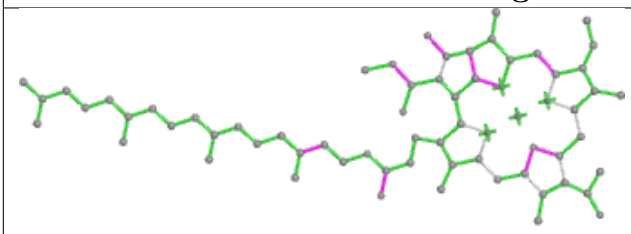
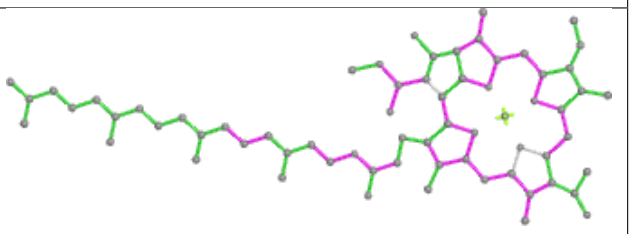
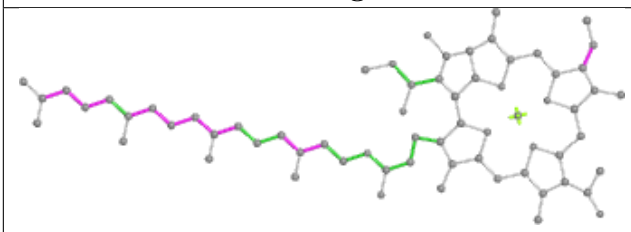
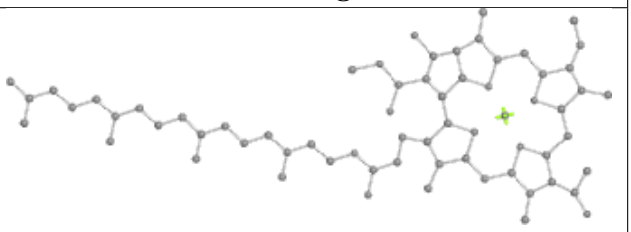
Bond angles

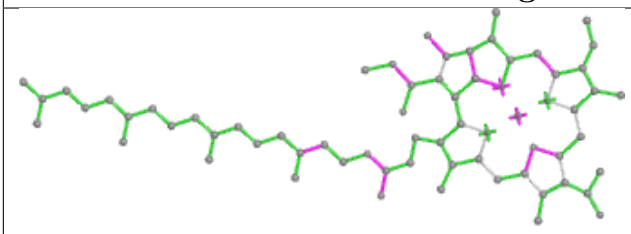
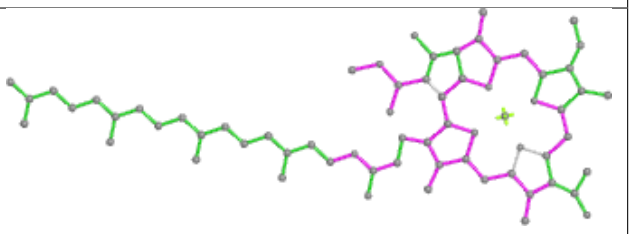
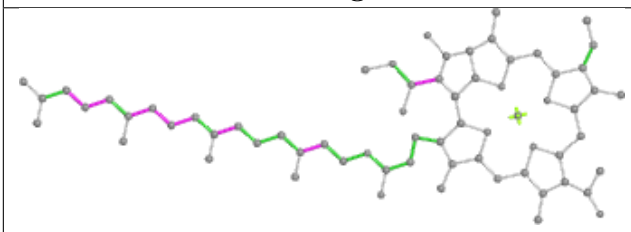
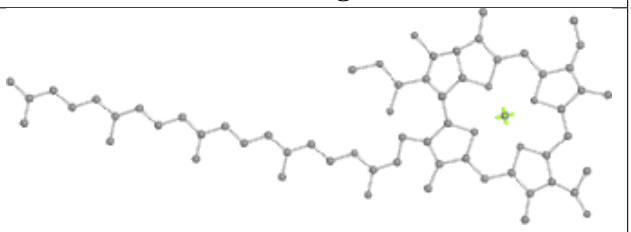


Torsions

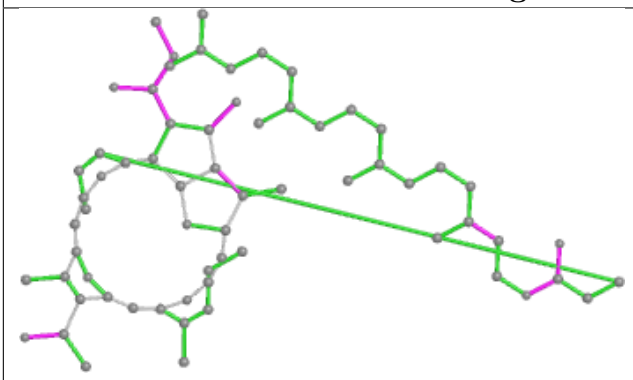


Rings

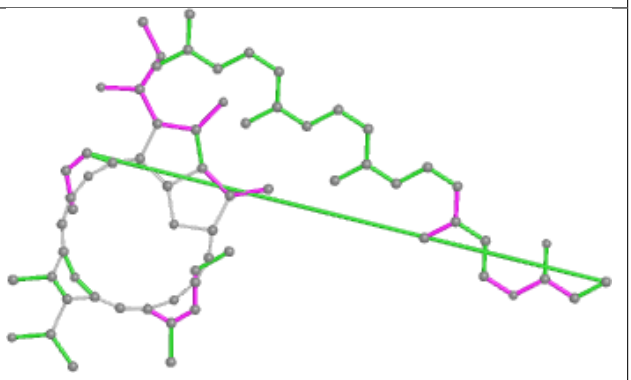
Ligand BCL M 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL L 1286	
 Bond lengths	 Bond angles
 Torsions	 Rings

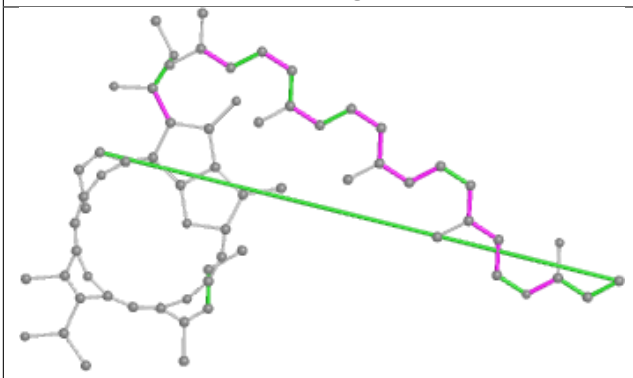
Ligand BPH M 1312



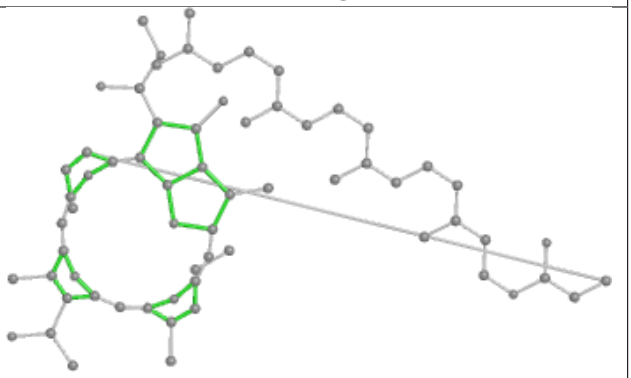
Bond lengths



Bond angles

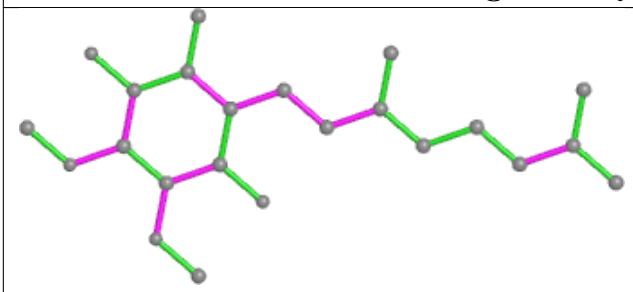


Torsions

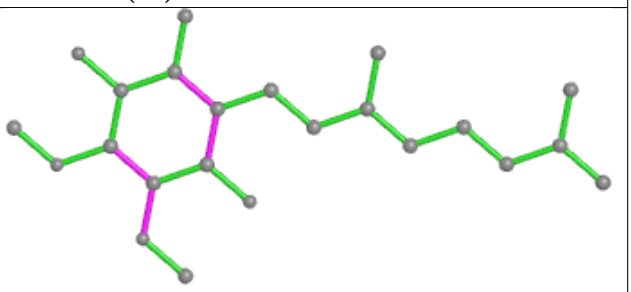


Rings

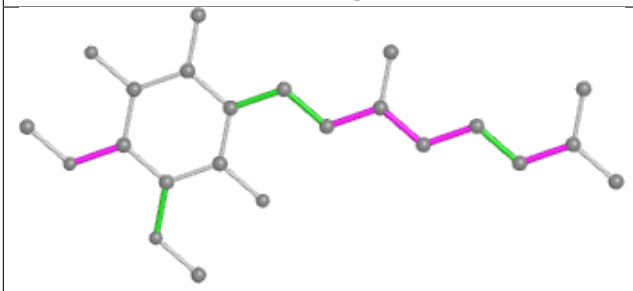
Ligand UQ2 L 1285 (A)



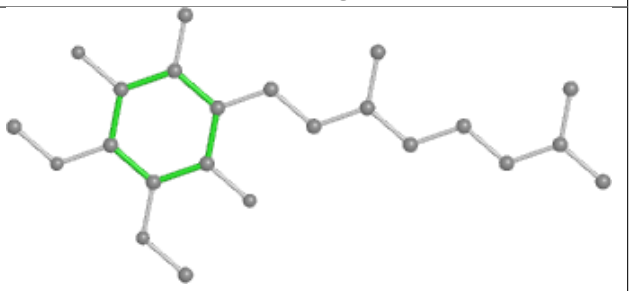
Bond lengths



Bond angles

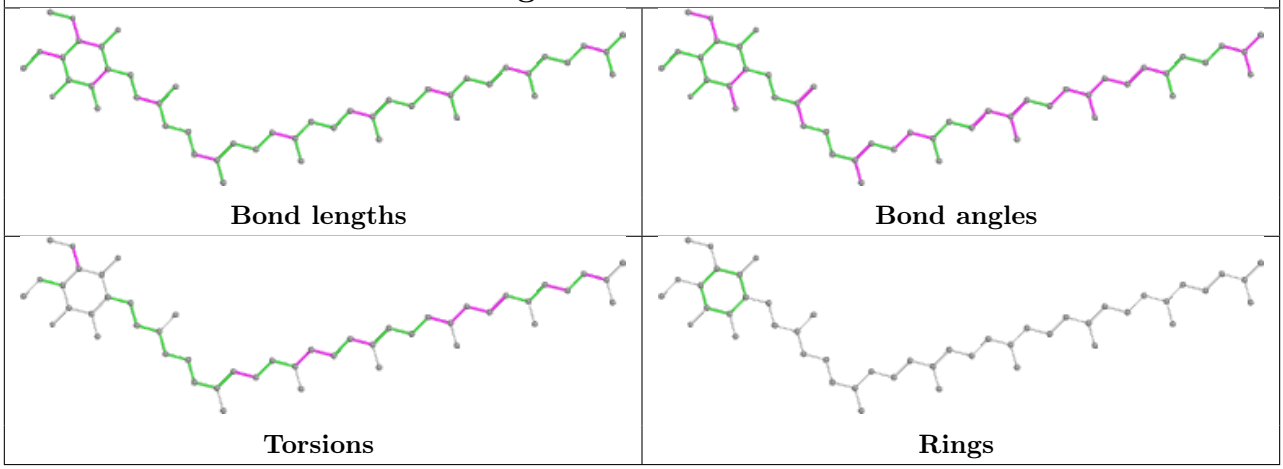


Torsions

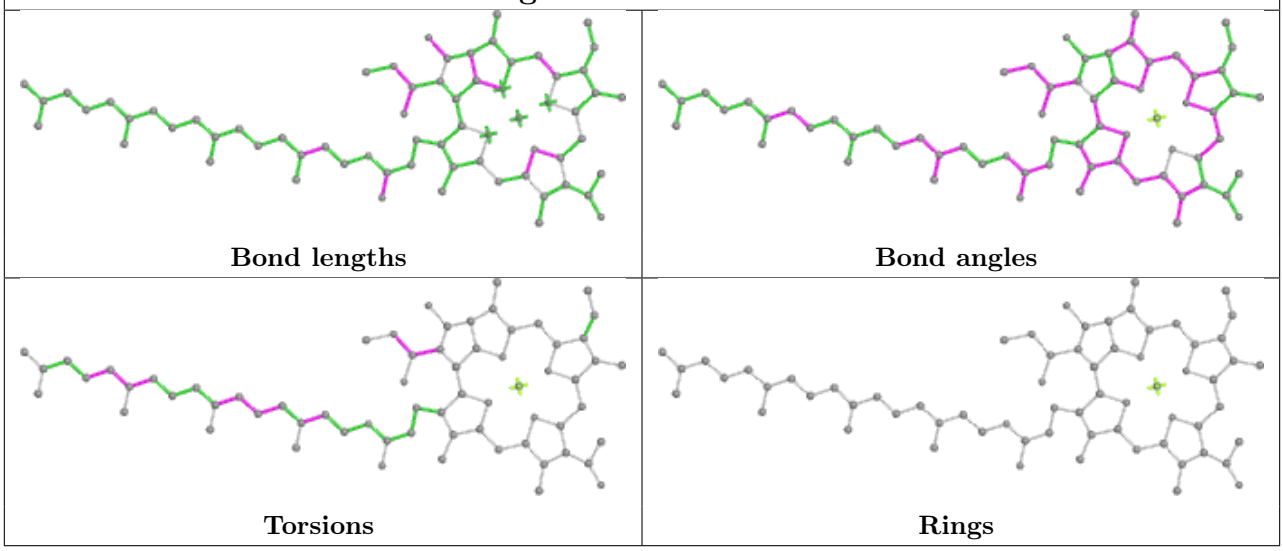


Rings

Ligand U10 M 1313



Ligand BCL L 1282



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%)	-0.63	4 (1%)	70	69	35, 48, 61, 97	0
2	L	280/281 (99%)	-0.73	4 (1%)	75	75	32, 45, 72, 82	0
3	M	303/307 (98%)	-0.73	3 (0%)	82	82	31, 50, 75, 92	0
All	All	824/848 (97%)	-0.70	11 (1%)	77	77	31, 48, 72, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	5.8
1	H	250	SER	5.7
1	H	251	VAL	3.0
2	L	202	LYS	2.8
3	M	2	GLU	2.7
1	H	249	LYS	2.4
1	H	52	ASN	2.4
2	L	59	TRP	2.3
2	L	270	PRO	2.3
2	L	72	GLU	2.2
3	M	3	TYR	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)

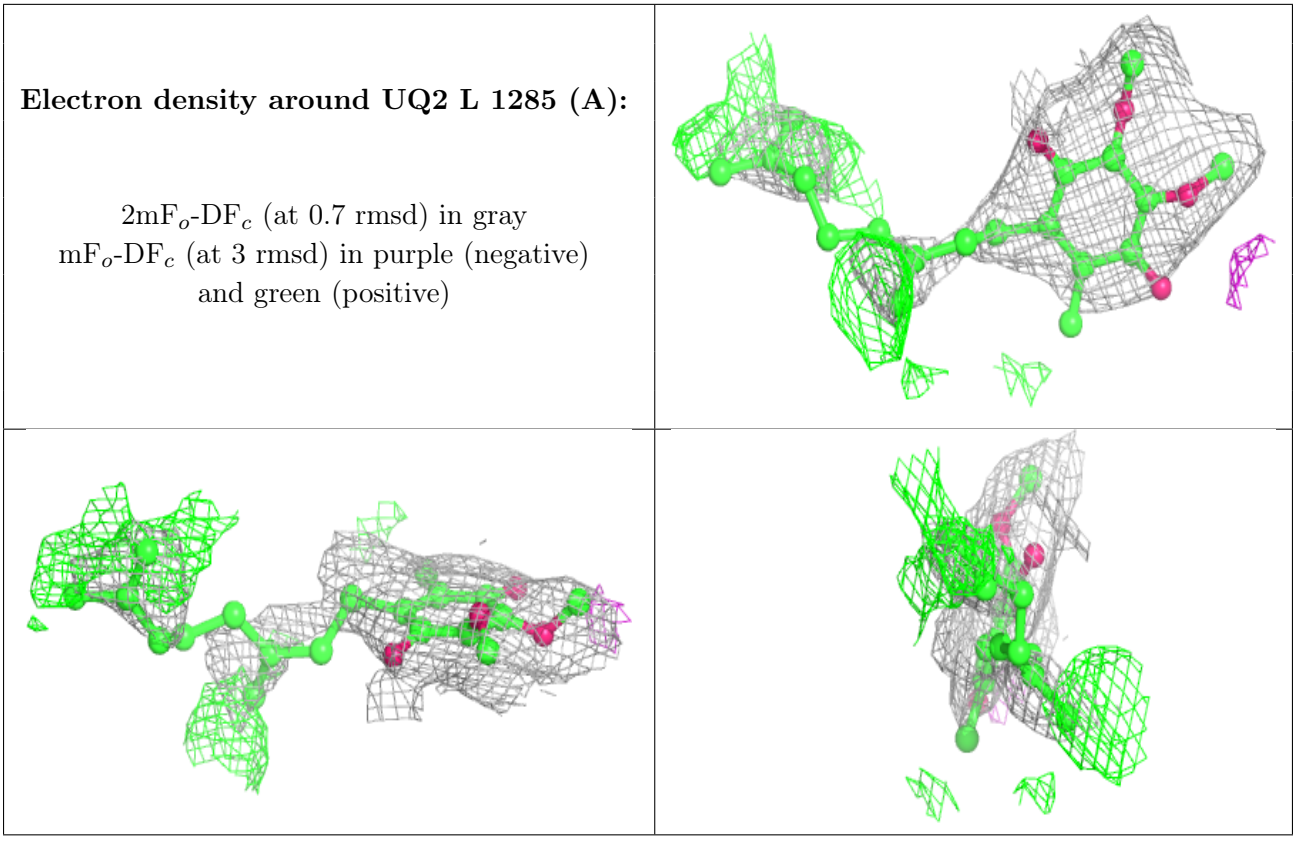
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LDA	L	1283	16/16	0.28	0.53	51,105,127,128	0
5	LDA	M	1310	16/16	0.35	0.47	91,109,117,117	0
4	GOL	M	1315	6/6	0.49	0.31	98,100,101,101	0
5	LDA	M	1309	16/16	0.58	0.31	97,102,115,115	0
5	LDA	M	1308	16/16	0.61	0.36	114,120,127,128	0
5	LDA	L	1281	16/16	0.65	0.42	102,111,115,115	0
4	GOL	H	1252	6/6	0.76	0.38	80,83,83,85	0
4	GOL	H	1251	6/6	0.78	0.36	98,99,100,100	0
5	LDA	M	1306	16/16	0.81	0.34	70,77,91,91	0
4	GOL	L	1289	6/6	0.83	0.32	95,96,97,97	0
5	LDA	M	1305	16/16	0.84	0.22	55,70,79,80	0
5	LDA	M	1307	16/16	0.85	0.19	62,66,80,80	0
4	GOL	L	1288	6/6	0.89	0.30	58,62,63,65	0
8	UQ2	L	1285[A]	23/23	0.89	0.23	40,45,49,49	23
8	UQ2	L	1285[B]	23/23	0.89	0.23	44,46,51,51	23
12	SPO	M	1314	42/42	0.89	0.23	42,60,83,86	0
11	U10	M	1313	48/63	0.91	0.17	44,53,79,81	0
7	BPH	M	1312	65/65	0.92	0.17	30,50,109,112	0
6	BCL	M	1303	66/66	0.96	0.11	26,37,86,87	0
7	BPH	L	1284	65/65	0.97	0.12	29,39,44,50	0
9	PO4	L	1287	5/5	0.97	0.16	91,91,92,92	0
6	BCL	L	1286	66/66	0.97	0.14	29,38,49,51	0
6	BCL	M	1304	66/66	0.97	0.14	32,37,58,66	0
6	BCL	L	1282	66/66	0.98	0.09	28,36,56,59	0
10	FE	M	1311	1/1	0.99	0.03	41,41,41,41	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.

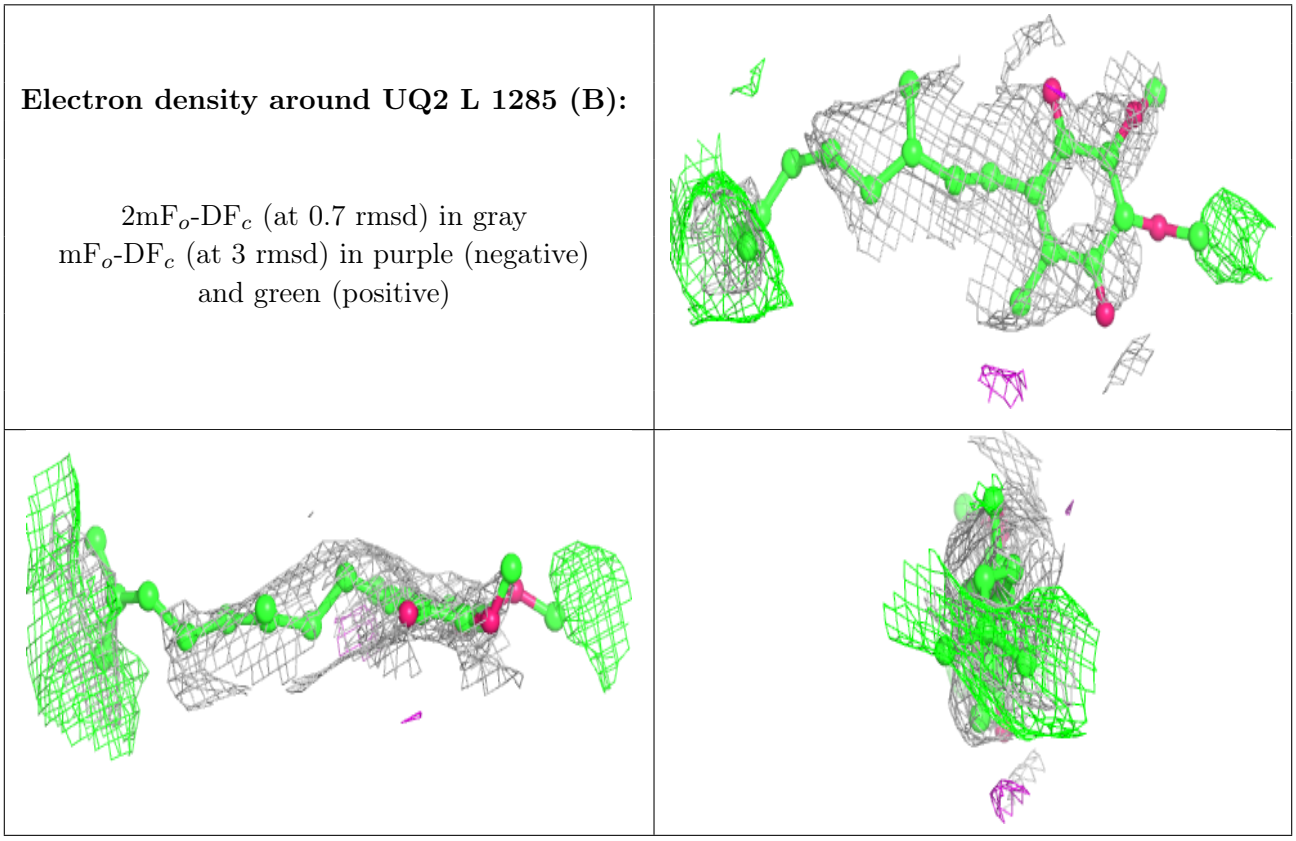
Electron density around UQ2 L 1285 (A):

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



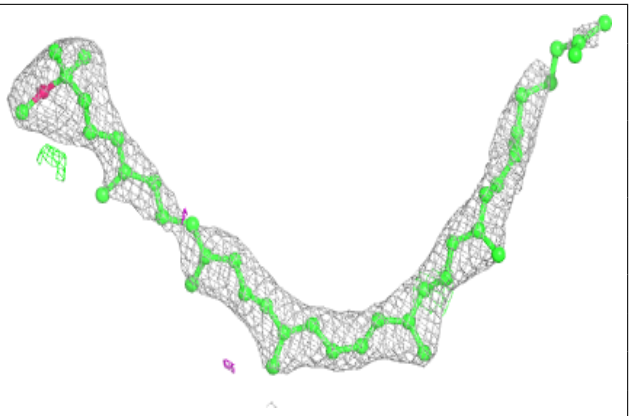
Electron density around UQ2 L 1285 (B):

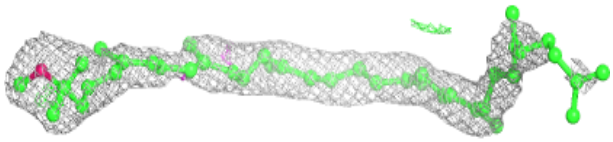
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

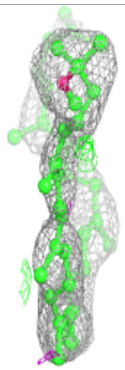


Electron density around SPO M 1314:

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

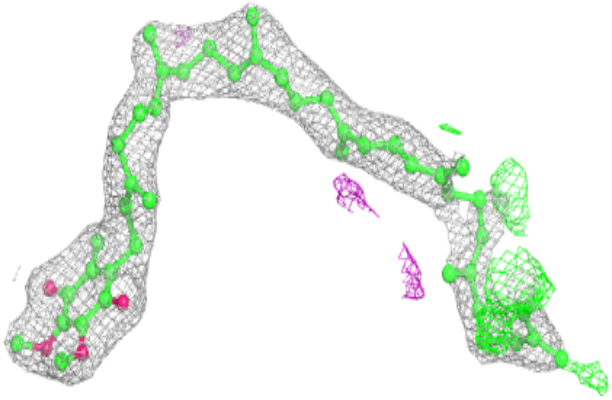


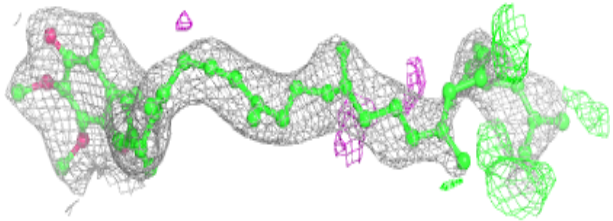


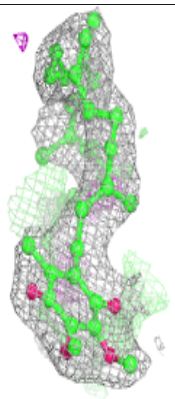


Electron density around U10 M 1313:

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

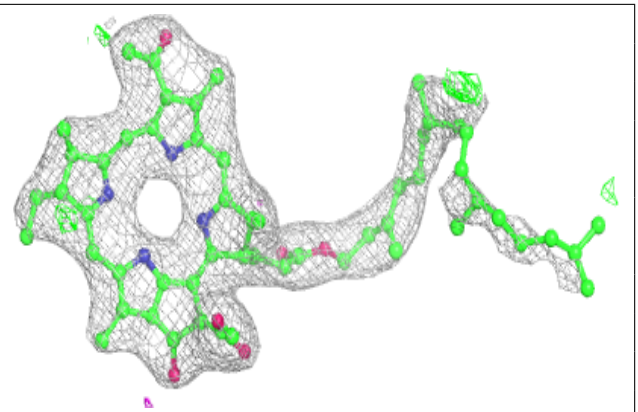


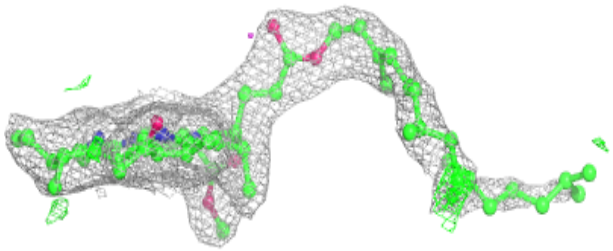


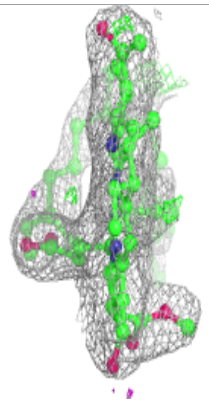


Electron density around BPH M 1312:

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

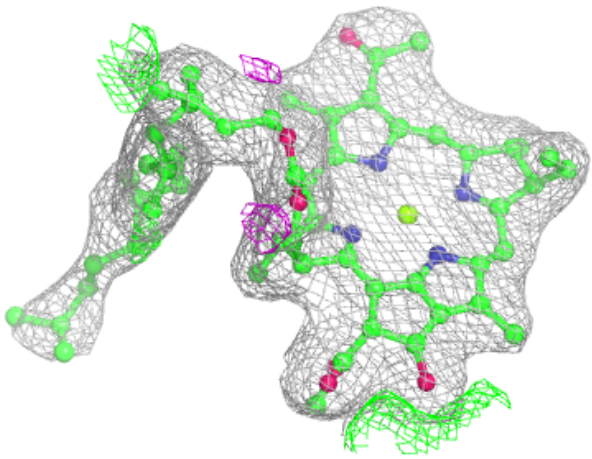


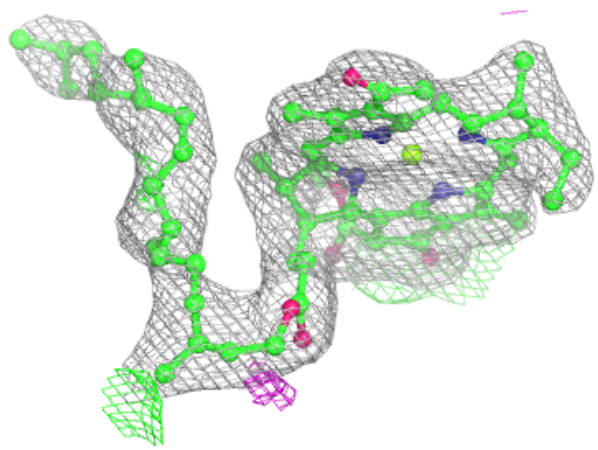


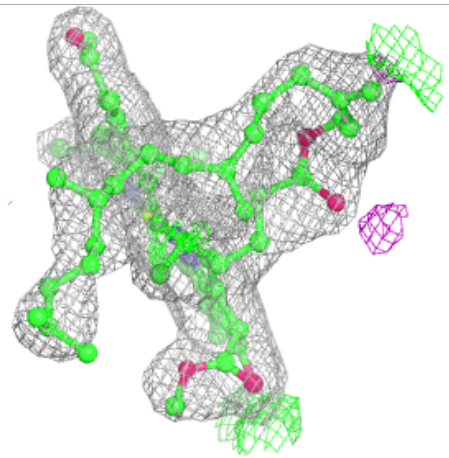


Electron density around BCL M 1303:

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

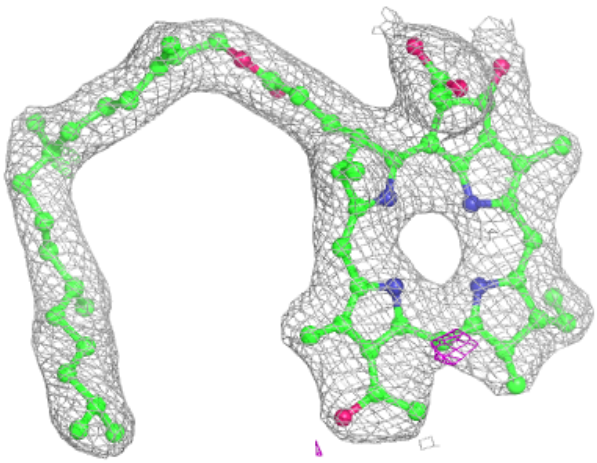


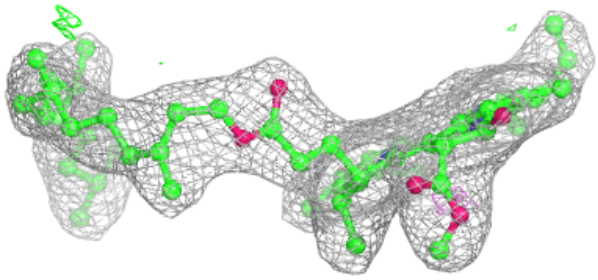


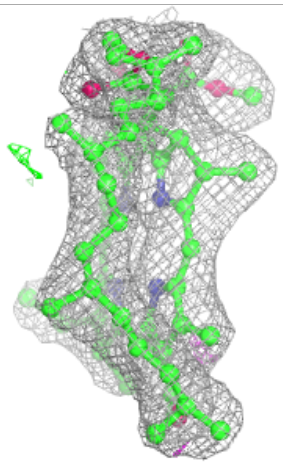


Electron density around BPH L 1284:

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

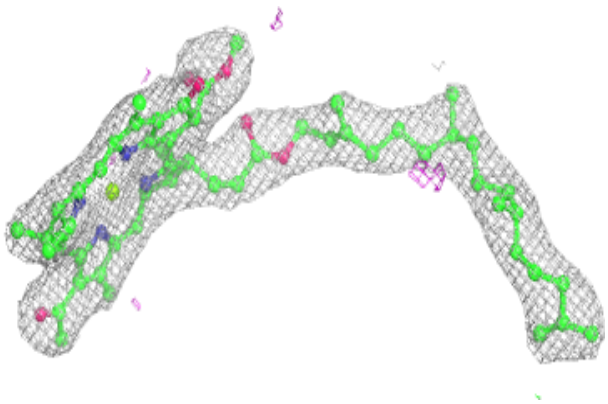


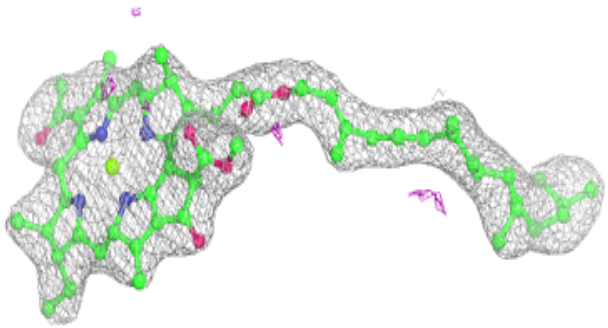


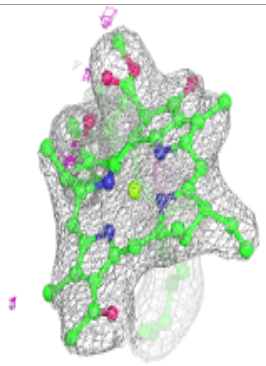


Electron density around BCL L 1286:

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

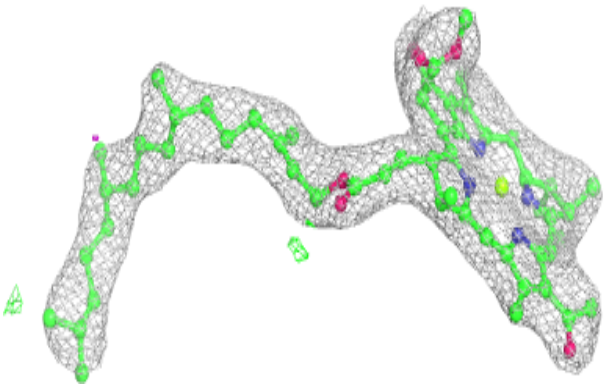


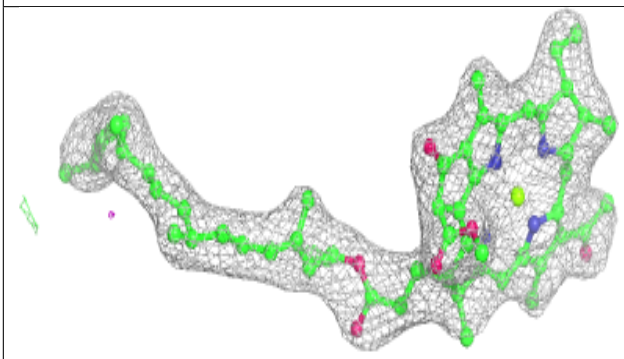


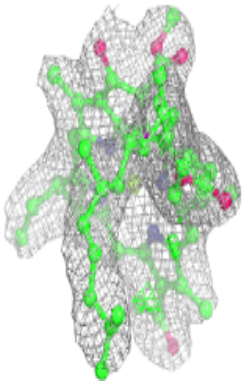


Electron density around BCL M 1304:

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

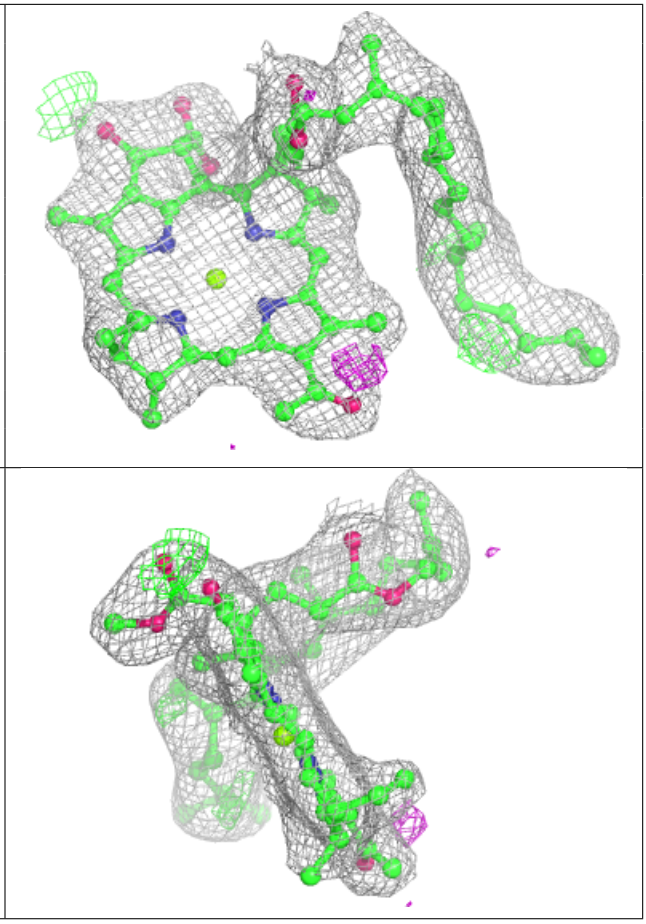






Electron density around BCL L 1282:

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



6.5 Other polymers (i)

There are no such residues in this entry.