Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:34 pm BST

PDB ID	:	2WX5
Title	:	Hexa-coordination of a bacteriochlorophyll cofactor in the Rhodobacter sphaeroides reaction centre
Authors	:	Marsh, M.; Frolov, D.; Crouch, L.I.; Fyfe, P.K.; Robert, B.; van Grondelle, R.; Jones, M.R.; Hadfield, A.T.
Deposited on	:	2009-11-02
Resolution	:	2.63 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

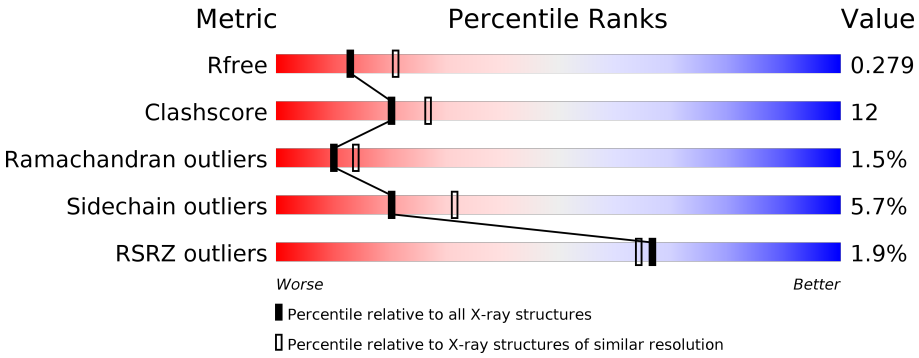
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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% 72% 20% 8%
2	L	281	2% 78% 20%
3	M	307	2% 72% 23%

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
4	LDA	H	1251	-	-	-	X
4	LDA	M	1309	-	-	-	X
4	LDA	M	1310	-	-	-	X
8	HTO	L	1286	X	-	-	-
8	HTO	L	1287	X	-	-	-
8	HTO	M	1313	X	-	X	-
9	BPH	L	1288	X	-	-	-
9	BPH	M	1314	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7468 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
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1504	358	362	8			

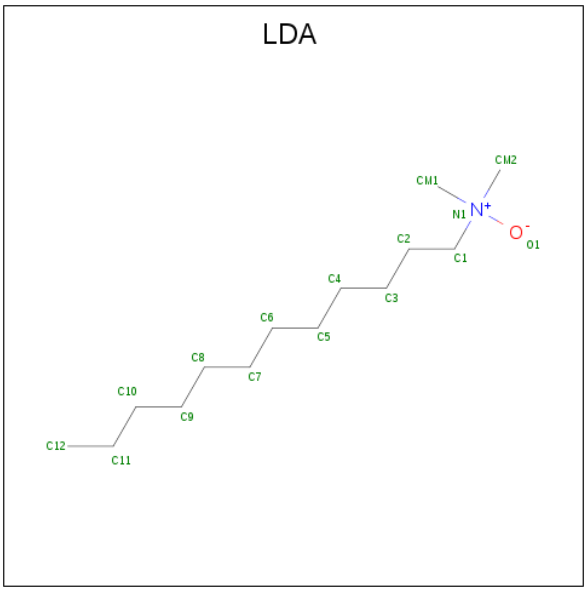
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	181	ARG	PHE	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

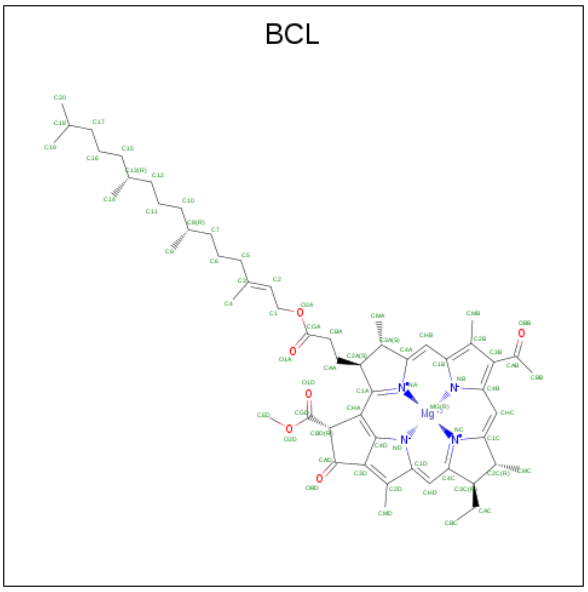


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

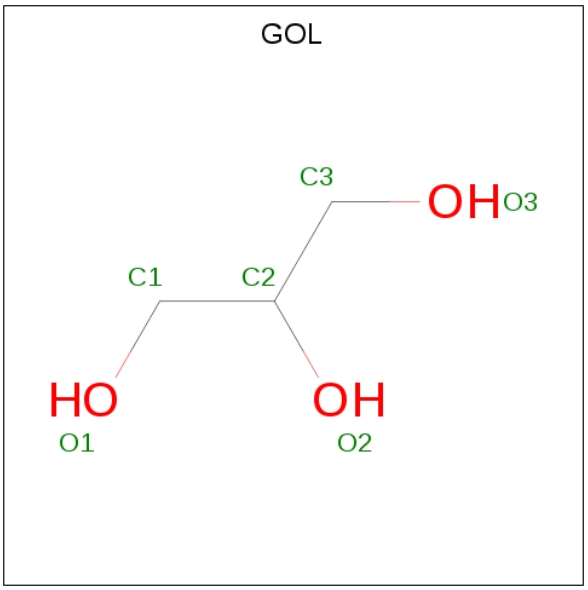
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Na 1 1	0	0
5	M	1	Total Na 1 1	0	0

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



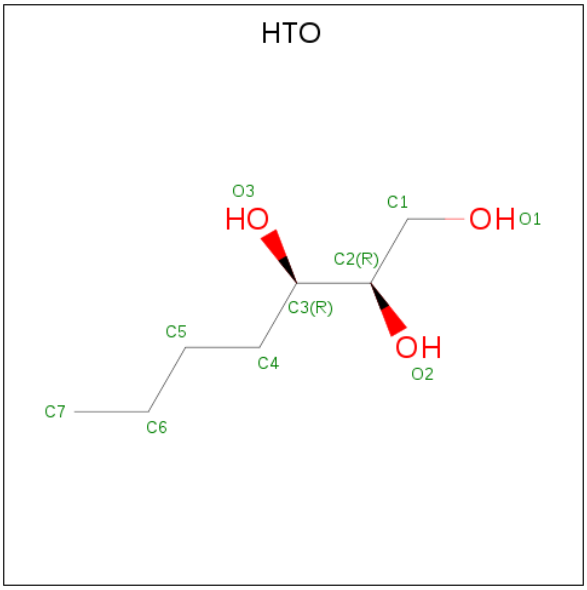
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



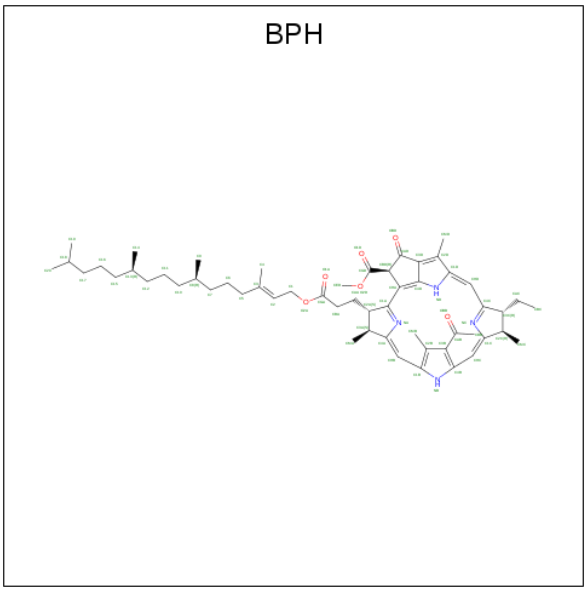
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



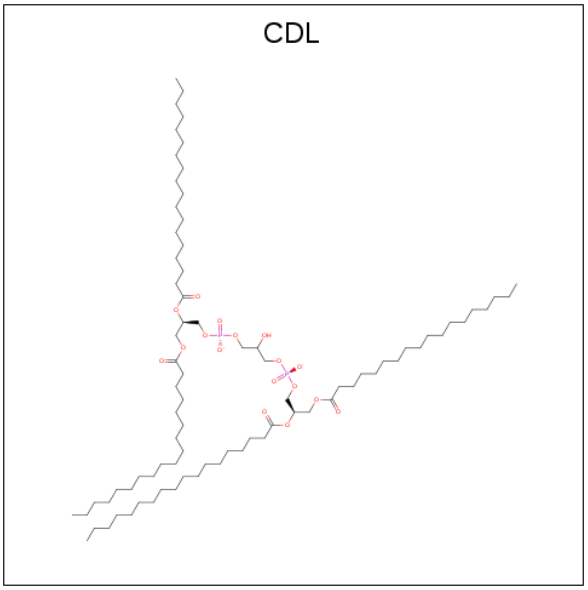
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 10 7 3	0	0
8	L	1	Total C O 10 7 3	0	0
8	M	1	Total C O 10 7 3	0	0

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

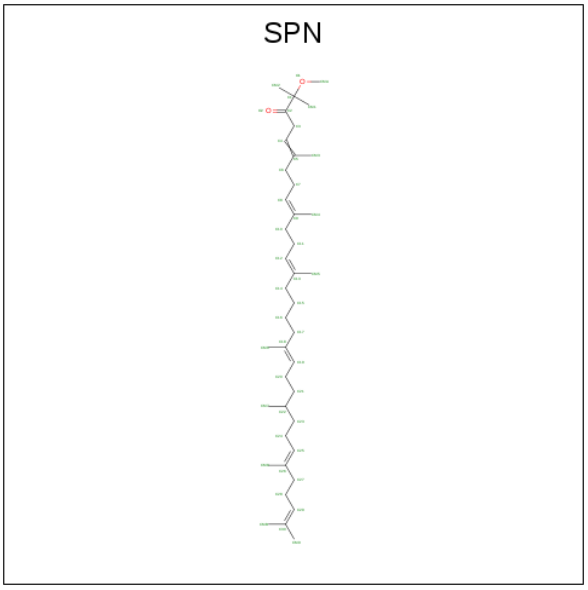


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

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

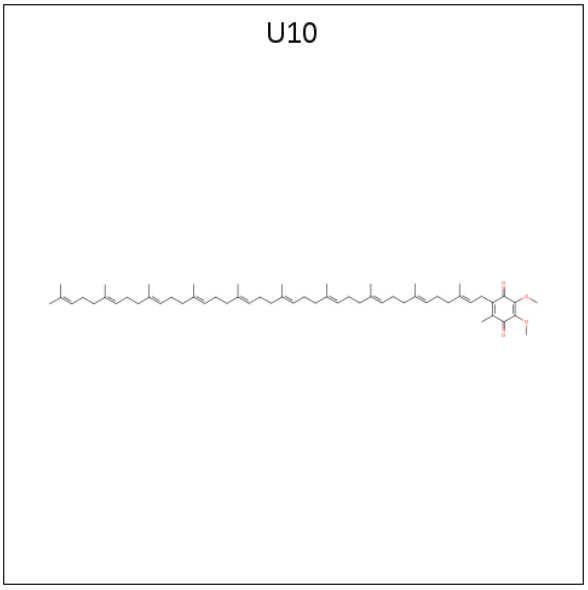
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 43 41 2	0	0

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 14 is water.

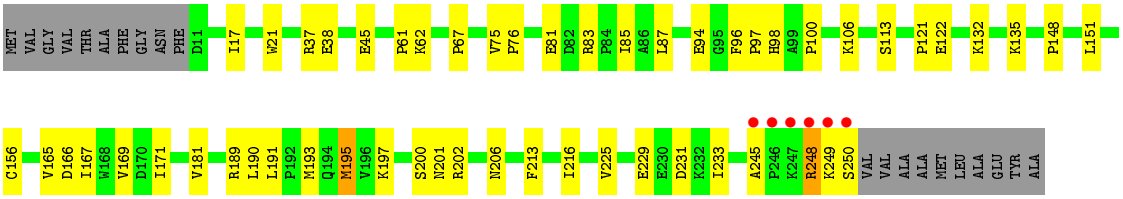
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	111	Total	O	0	0
			111	111		
14	L	99	Total	O	0	0
			99	99		
14	M	82	Total	O	0	0
			82	82		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

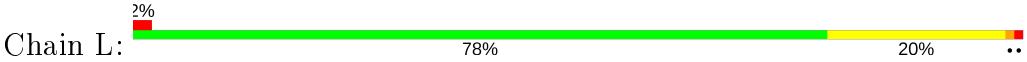
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

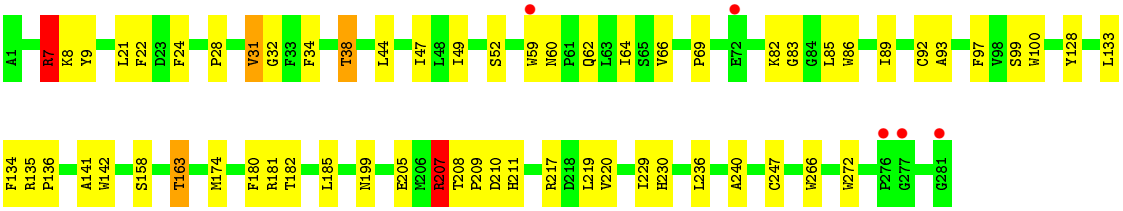
Chain H:



- Molecule 2: REACTION CENTRE PROTEIN L CHAIN

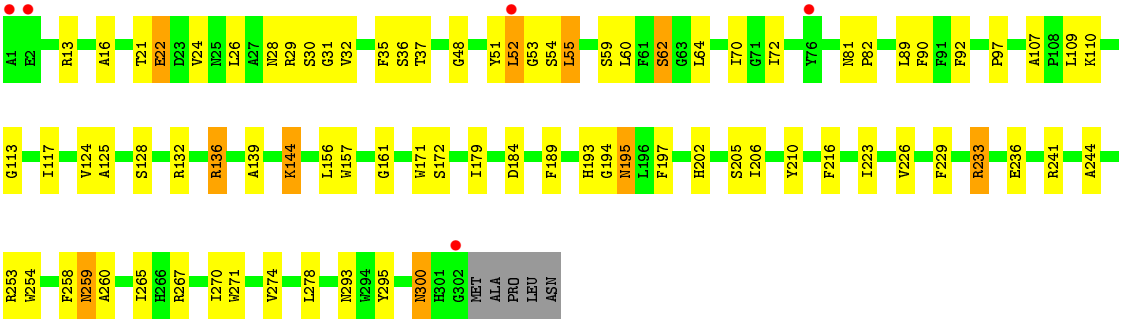
Chain L:





- Molecule 3: REACTION CENTRE 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	140.18Å 140.18Å 185.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.40 – 2.63 20.31 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.40-2.63) 95.6 (20.31-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.63Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.279 0.240 , 0.279	Depositor DCC
R_{free} test set	3047 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 67.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

5.1 Standard geometry

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

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	0.92	1/1877 (0.1%)	0.88	1/2553 (0.0%)
2	L	0.92	0/2319	0.89	3/3173 (0.1%)
3	M	0.87	2/2500 (0.1%)	0.84	3/3413 (0.1%)
All	All	0.90	3/6696 (0.0%)	0.87	7/9139 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	226	VAL	CB-CG2	7.00	1.67	1.52
3	M	236	GLU	CG-CD	6.00	1.60	1.51
1	H	94	GLU	CG-CD	5.13	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	7	ARG	NE-CZ-NH2	-9.86	115.37	120.30
2	L	7	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	H	195	MET	CG-SD-CE	-6.10	90.44	100.20
3	M	233	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	L	207	ARG	NE-CZ-NH2	-5.39	117.61	120.30
3	M	184	ASP	CB-CG-OD1	5.29	123.06	118.30
3	M	29	ARG	NE-CZ-NH2	-5.25	117.68	120.30

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	1829	0	1836	30	0
2	L	2232	0	2191	58	0
3	M	2408	0	2321	65	0
4	H	16	0	31	2	0
4	M	80	0	155	8	0
5	H	1	0	0	0	0
5	M	1	0	0	0	0
6	L	132	0	148	18	0
6	M	132	0	148	19	0
7	L	12	0	16	0	0
8	L	20	0	32	4	0
8	M	10	0	16	7	0
9	L	65	0	76	8	0
9	M	65	0	76	8	0
10	M	81	0	106	3	0
11	M	1	0	0	0	0
12	M	43	0	70	10	0
13	M	48	0	63	4	0
14	H	111	0	0	1	0
14	L	99	0	0	6	0
14	M	82	0	0	5	0
All	All	7468	0	7285	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:HD2	1:H:250:SER:HB2	1.46	0.98
4:M:1306:LDA:H91	4:M:1307:LDA:H121	1.43	0.97
2:L:182:THR:HG22	2:L:236:LEU:HD13	1.50	0.91
2:L:34:PHE:O	2:L:38:THR:HG23	1.71	0.89
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.56	0.86
3:M:271:TRP:CD1	14:M:2075:HOH:O	2.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:THR:HG22	2:L:99:SER:HB3	1.59	0.85
3:M:197:PHE:HZ	6:M:1303:BCL:HBB2	1.42	0.84
2:L:181:ARG:NH2	14:L:2073:HOH:O	2.11	0.83
2:L:219:LEU:O	3:M:132:ARG:NH2	2.13	0.82
1:H:98:HIS:CD2	2:L:7:ARG:HH11	1.98	0.81
3:M:60:LEU:O	3:M:64:LEU:HD12	1.80	0.81
6:L:1283:BCL:HMB1	6:L:1283:BCL:CBB	2.11	0.81
2:L:38:THR:HG22	2:L:99:SER:CB	2.11	0.81
6:M:1303:BCL:CBB	6:M:1303:BCL:HHC	2.12	0.80
3:M:197:PHE:CZ	6:M:1303:BCL:HBB2	2.16	0.79
3:M:300:ASN:N	3:M:300:ASN:HD22	1.81	0.79
2:L:229:ILE:O	2:L:229:ILE:HG13	1.83	0.78
3:M:300:ASN:H	3:M:300:ASN:ND2	1.81	0.78
9:L:1288:BPH:HHC	9:L:1288:BPH:HBB3	1.66	0.76
3:M:267:ARG:O	14:M:2075:HOH:O	2.03	0.76
8:L:1287:HTO:H71	4:M:1310:LDA:H121	1.67	0.75
9:M:1314:BPH:HHC	9:M:1314:BPH:HBB3	1.68	0.75
3:M:300:ASN:N	3:M:300:ASN:ND2	2.33	0.75
6:L:1282:BCL:HHC	6:L:1282:BCL:HBB2	1.68	0.74
1:H:248:ARG:HD2	1:H:250:SER:CB	2.19	0.73
6:L:1283:BCL:HMB1	6:L:1283:BCL:HBB3	1.71	0.73
2:L:229:ILE:HD13	8:L:1286:HTO:H3	1.71	0.72
2:L:49:ILE:HG13	2:L:89:ILE:HD13	1.73	0.71
4:M:1307:LDA:H102	13:M:1316:U10:H202	1.74	0.70
6:L:1282:BCL:CBB	6:L:1282:BCL:HHC	2.22	0.69
2:L:182:THR:HG22	2:L:236:LEU:CD1	2.21	0.69
2:L:82:LYS:NZ	14:L:2044:HOH:O	2.24	0.69
6:M:1303:BCL:HBB3	6:M:1303:BCL:HHC	1.74	0.68
2:L:181:ARG:HG2	9:M:1314:BPH:CBB	2.25	0.67
1:H:121:PRO:HB3	1:H:225:VAL:O	1.95	0.66
2:L:185:LEU:HD13	9:M:1314:BPH:ND	2.10	0.66
3:M:52:LEU:HG	3:M:53:GLY:H	1.61	0.66
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.78	0.66
1:H:165:VAL:O	1:H:166:ASP:HB2	1.95	0.66
1:H:213:PHE:O	1:H:216:ILE:HG13	1.96	0.65
1:H:156:CYS:SG	1:H:248:ARG:HD3	2.36	0.65
2:L:128:TYR:HD1	6:M:1304:BCL:HBB1	1.61	0.64
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.80	0.64
6:L:1282:BCL:HBB2	12:M:1315:SPN:H162	1.79	0.64
9:L:1288:BPH:HBB2	3:M:210:TYR:HB3	1.80	0.63
2:L:93:ALA:HA	9:L:1288:BPH:H9C2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.34	0.62
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.82	0.62
2:L:93:ALA:HA	9:L:1288:BPH:C9	2.29	0.61
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.82	0.61
6:M:1303:BCL:HAA2	6:M:1303:BCL:HBD	1.83	0.61
3:M:194:GLY:O	3:M:195:ASN:HB3	2.02	0.60
3:M:206:ILE:HG12	6:M:1303:BCL:HMB3	1.82	0.59
1:H:62:LYS:NZ	2:L:199:ASN:HD21	2.01	0.59
4:M:1306:LDA:C9	4:M:1307:LDA:H121	2.27	0.59
3:M:161:GLY:HA3	12:M:1315:SPN:H201	1.83	0.59
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.84	0.59
1:H:229:GLU:O	1:H:233:ILE:HD12	2.02	0.59
6:M:1304:BCL:HHC	6:M:1304:BCL:HBB2	1.86	0.58
2:L:174:MET:HG2	6:L:1282:BCL:O1D	2.04	0.58
3:M:157:TRP:CZ2	12:M:1315:SPN:H22	2.38	0.58
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.86	0.57
2:L:207:ARG:HG2	2:L:211:HIS:CG	2.40	0.57
3:M:89:LEU:HB3	8:M:1313:HTO:H52	1.87	0.57
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.87	0.57
2:L:220:VAL:HB	8:L:1287:HTO:H11	1.86	0.56
9:L:1288:BPH:HBB1	3:M:210:TYR:CD2	2.39	0.56
1:H:189:ARG:HA	14:H:2089:HOH:O	2.06	0.56
6:L:1282:BCL:HBB3	6:M:1303:BCL:H41	1.89	0.54
3:M:21:THR:O	3:M:22:GLU:C	2.46	0.54
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.43	0.54
3:M:270:ILE:HG22	14:M:2075:HOH:O	2.07	0.54
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.88	0.54
3:M:89:LEU:HA	3:M:92:PHE:CE2	2.42	0.53
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.44	0.53
10:M:1305:CDL:HA4	10:M:1305:CDL:HB61	1.90	0.52
2:L:185:LEU:HD13	9:M:1314:BPH:C1D	2.39	0.52
8:L:1287:HTO:C7	4:M:1310:LDA:H121	2.38	0.51
3:M:161:GLY:HA3	12:M:1315:SPN:HM72	1.92	0.51
6:M:1303:BCL:HAA2	6:M:1303:BCL:CBD	2.41	0.51
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.93	0.51
1:H:37:ARG:O	1:H:38:GLU:HG2	2.11	0.50
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.37	0.50
2:L:38:THR:HG22	2:L:99:SER:HB2	1.93	0.50
3:M:113:GLY:O	3:M:117:ILE:HG13	2.10	0.50
2:L:31:VAL:HG12	2:L:32:GLY:N	2.27	0.50
3:M:31:GLY:H	4:M:1309:LDA:H92	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:208:THR:HB	2:L:209:PRO:HD2	1.94	0.50
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.47	0.50
3:M:253:ARG:HB2	3:M:259:ASN:OD1	2.12	0.49
2:L:163:THR:HG22	2:L:163:THR:O	2.12	0.49
6:M:1303:BCL:HBB2	6:M:1303:BCL:HHC	1.90	0.49
6:L:1282:BCL:CBB	12:M:1315:SPN:H162	2.42	0.49
6:L:1282:BCL:HBB2	12:M:1315:SPN:HM63	1.95	0.49
1:H:21:TRP:CD2	4:H:1251:LDA:H12	2.48	0.49
3:M:270:ILE:CG2	14:M:2075:HOH:O	2.60	0.49
1:H:122:GLU:OE1	3:M:233:ARG:NH2	2.42	0.48
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.95	0.48
2:L:128:TYR:CD1	6:M:1304:BCL:HBB1	2.44	0.48
2:L:60:ASN:O	2:L:64:ILE:HG13	2.12	0.48
1:H:21:TRP:CE2	4:H:1251:LDA:H12	2.49	0.48
1:H:190:LEU:N	1:H:190:LEU:HD23	2.28	0.47
2:L:207:ARG:HG2	2:L:211:HIS:CD2	2.49	0.47
2:L:133:LEU:HD23	2:L:134:PHE:CE1	2.49	0.47
2:L:207:ARG:CG	2:L:211:HIS:CG	2.98	0.47
3:M:189:PHE:O	3:M:193:HIS:HD2	1.98	0.46
2:L:97:PHE:CE1	6:L:1283:BCL:H121	2.51	0.46
2:L:266:TRP:NE1	8:M:1313:HTO:H62	2.30	0.46
9:L:1288:BPH:H7C1	6:M:1304:BCL:H202	1.97	0.46
2:L:266:TRP:CE2	8:M:1313:HTO:H3	2.51	0.46
4:M:1306:LDA:H91	4:M:1307:LDA:C12	2.28	0.46
3:M:144:LYS:HD3	3:M:144:LYS:HA	1.87	0.46
1:H:67:PRO:HA	2:L:205:GLU:OE2	2.16	0.46
3:M:110:LYS:HE3	3:M:110:LYS:HB2	1.69	0.46
4:M:1309:LDA:H22	4:M:1309:LDA:HM21	1.74	0.46
3:M:271:TRP:HH2	10:M:1305:CDL:H731	1.80	0.45
2:L:266:TRP:CD1	8:M:1313:HTO:H62	2.52	0.45
6:L:1282:BCL:CBB	12:M:1315:SPN:HM63	2.47	0.45
2:L:62:GLN:HG3	14:L:2033:HOH:O	2.17	0.45
6:L:1283:BCL:HMB1	6:L:1283:BCL:HBB2	1.94	0.45
3:M:16:ALA:CB	3:M:32:VAL:HG11	2.47	0.45
3:M:270:ILE:O	3:M:274:VAL:HG13	2.16	0.44
14:L:2022:HOH:O	13:M:1316:U10:H322	2.17	0.44
6:L:1282:BCL:HED1	3:M:179:ILE:HG23	1.98	0.44
9:L:1288:BPH:CBB	9:L:1288:BPH:HHC	2.43	0.44
2:L:207:ARG:CG	2:L:211:HIS:CD2	3.01	0.44
2:L:230:HIS:NE2	3:M:223:ILE:HG13	2.33	0.44
6:L:1283:BCL:H41	6:M:1304:BCL:HBB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.18	0.44
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.52	0.43
2:L:7:ARG:O	2:L:7:ARG:HG3	2.15	0.43
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.00	0.43
3:M:90:PHE:HB2	8:M:1313:HTO:H73	2.01	0.42
2:L:185:LEU:CD1	9:M:1314:BPH:C1D	2.98	0.42
3:M:271:TRP:HD1	14:M:2075:HOH:O	1.85	0.42
1:H:113:SER:HB2	2:L:9:TYR:CE1	2.54	0.42
2:L:266:TRP:CD2	8:M:1313:HTO:H3	2.54	0.42
3:M:97:PRO:O	3:M:172:SER:HB3	2.19	0.42
2:L:85:LEU:O	2:L:89:ILE:HG13	2.19	0.42
2:L:8:LYS:HG2	14:L:2005:HOH:O	2.19	0.42
3:M:136:ARG:HA	3:M:136:ARG:NH1	2.34	0.42
6:L:1283:BCL:H2C	6:M:1303:BCL:HBC2	2.02	0.42
2:L:185:LEU:CD1	9:M:1314:BPH:ND	2.82	0.42
3:M:70:ILE:HD13	12:M:1315:SPN:H102	2.02	0.42
9:L:1288:BPH:H192	6:M:1304:BCL:C2B	2.49	0.42
9:M:1314:BPH:CBB	9:M:1314:BPH:HHC	2.43	0.42
3:M:197:PHE:HZ	6:M:1303:BCL:CBB	2.22	0.42
3:M:202:HIS:CE1	3:M:206:ILE:CD1	3.01	0.42
3:M:31:GLY:O	3:M:32:VAL:C	2.58	0.42
3:M:89:LEU:HA	3:M:92:PHE:CD2	2.55	0.42
3:M:278:LEU:HD11	10:M:1305:CDL:H382	2.02	0.42
3:M:36:SER:O	3:M:37:THR:C	2.58	0.42
1:H:167:ILE:HG22	1:H:169:VAL:CG1	2.49	0.42
1:H:201:ASN:O	1:H:202:ARG:HB3	2.20	0.42
1:H:62:LYS:HZ3	2:L:199:ASN:HD21	1.67	0.42
3:M:13:ARG:NH2	3:M:35:PHE:HB3	2.35	0.42
3:M:52:LEU:CG	3:M:53:GLY:H	2.32	0.42
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.01	0.41
3:M:195:ASN:C	3:M:195:ASN:OD1	2.58	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.01	0.41
6:L:1282:BCL:CAB	12:M:1315:SPN:H162	2.51	0.41
2:L:44:LEU:HD23	2:L:92:CYS:SG	2.60	0.41
3:M:24:VAL:HG22	3:M:139:ALA:HB1	2.02	0.41
1:H:193:MET:C	1:H:195:MET:H	2.24	0.41
2:L:66:VAL:HG12	2:L:86:TRP:HB2	2.02	0.41
2:L:28:PRO:O	3:M:254:TRP:HA	2.20	0.41
3:M:90:PHE:CD2	8:M:1313:HTO:H51	2.56	0.41
3:M:156:LEU:HD23	6:M:1303:BCL:H43	2.02	0.41
6:L:1282:BCL:H51	9:M:1314:BPH:HMB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:157:TRP:CD1	12:M:1315:SPN:H202	2.56	0.41
2:L:100:TRP:CZ2	13:M:1316:U10:H251	2.56	0.41
2:L:141:ALA:HB1	14:L:2040:HOH:O	2.21	0.40
6:L:1282:BCL:H111	6:M:1303:BCL:H192	2.03	0.40
2:L:69:PRO:HD3	2:L:83:GLY:O	2.21	0.40
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.91	0.40
1:H:132:LYS:HB2	1:H:171:ILE:HD11	2.03	0.40
3:M:260:ALA:O	13:M:1316:U10:H4M3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/260 (92%)	221 (93%)	14 (6%)	3 (1%)	12	17
2	L	279/281 (99%)	250 (90%)	26 (9%)	3 (1%)	14	20
3	M	300/307 (98%)	273 (91%)	21 (7%)	6 (2%)	7	10
All	All	817/848 (96%)	744 (91%)	61 (8%)	12 (2%)	10	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	48	GLY
3	M	124	VAL
2	L	163	THR
3	M	22	GLU
3	M	30	SER
1	H	45	GLU
1	H	248	ARG
3	M	195	ASN

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Mol	Chain	Res	Type
3	M	107	ALA
2	L	31	VAL
2	L	47	ILE

5.3.2 Protein sidechains

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%)	185 (95%)	10 (5%)	24	37
2	L	220/220 (100%)	209 (95%)	11 (5%)	24	38
3	M	236/240 (98%)	220 (93%)	16 (7%)	16	24
All	All	651/668 (98%)	614 (94%)	37 (6%)	20	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	ILE
1	H	75	VAL
1	H	83	ARG
1	H	106	LYS
1	H	135	LYS
1	H	197	LYS
1	H	200	SER
1	H	206	ASN
1	H	231	ASP
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	52	SER
2	L	59	TRP
2	L	158	SER
2	L	207	ARG
2	L	210	ASP
2	L	217	ARG

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Mol	Chain	Res	Type
2	L	247	CYS
2	L	272	TRP
3	M	26	LEU
3	M	52	LEU
3	M	54	SER
3	M	55	LEU
3	M	59	SER
3	M	62	SER
3	M	72	ILE
3	M	109	LEU
3	M	136	ARG
3	M	144	LYS
3	M	205	SER
3	M	216	PHE
3	M	258	PHE
3	M	259	ASN
3	M	265	ILE
3	M	300	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	62	GLN
2	L	183	ASN
2	L	199	ASN
3	M	193	HIS
3	M	300	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
9	BPH	L	1288	-	64,70,70	1.39	7 (10%)	76,101,101	1.37	11 (14%)
10	CDL	M	1305	-	80,80,99	1.27	4 (5%)	86,92,111	1.29	10 (11%)
8	HTO	M	1313	-	9,9,9	1.03	1 (11%)	10,10,10	1.26	1 (10%)
7	GOL	L	1284	-	5,5,5	0.39	0	5,5,5	0.28	0
4	LDA	M	1308	-	12,15,15	1.99	1 (8%)	14,17,17	0.69	0
6	BCL	L	1283	2	58,74,74	1.52	4 (6%)	69,115,115	1.69	15 (21%)
6	BCL	M	1303	3	58,74,74	1.42	3 (5%)	69,115,115	1.71	10 (14%)
13	U10	M	1316	-	48,48,63	2.74	14 (29%)	58,61,79	1.96	17 (29%)
12	SPN	M	1315	-	40,42,42	0.66	1 (2%)	50,52,52	1.66	12 (24%)
8	HTO	L	1287	-	9,9,9	0.73	0	10,10,10	1.46	3 (30%)
4	LDA	H	1251	-	12,15,15	2.14	1 (8%)	14,17,17	0.44	0
4	LDA	M	1309	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
6	BCL	M	1304	2	58,74,74	1.86	5 (8%)	69,115,115	2.23	23 (33%)
9	BPH	M	1314	-	64,70,70	1.48	8 (12%)	76,101,101	1.78	19 (25%)
8	HTO	L	1286	-	9,9,9	1.21	1 (11%)	10,10,10	2.14	4 (40%)
4	LDA	M	1310	-	12,15,15	2.07	1 (8%)	14,17,17	0.77	0
4	LDA	M	1306	-	12,15,15	2.13	1 (8%)	14,17,17	1.00	1 (7%)
7	GOL	L	1285	-	5,5,5	0.44	0	5,5,5	0.48	0
4	LDA	M	1307	-	12,15,15	2.05	1 (8%)	14,17,17	0.70	0
6	BCL	L	1282	3,14	58,74,74	1.62	2 (3%)	69,115,115	1.76	15 (21%)

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
9	BPH	L	1288	-	2/2/18/22	16/54/105/105	0/5/6/6
10	CDL	M	1305	-	-	40/91/91/110	-
7	GOL	L	1284	-	-	2/4/4/4	-
4	LDA	M	1308	-	-	5/13/13/13	-
6	BCL	L	1283	2	-	5/37/137/137	-
6	BCL	M	1303	3	-	3/37/137/137	-
13	U10	M	1316	-	-	7/45/69/87	0/1/1/1
9	BPH	M	1314	-	2/2/18/22	16/54/105/105	0/5/6/6
8	HTO	L	1287	-	1/1/2/2	2/10/10/10	-
4	LDA	H	1251	-	-	7/13/13/13	-
4	LDA	M	1309	-	-	11/13/13/13	-
6	BCL	M	1304	2	-	8/37/137/137	-
8	HTO	L	1286	-	1/1/2/2	2/10/10/10	-
4	LDA	M	1310	-	-	6/13/13/13	-
8	HTO	M	1313	-	1/1/2/2	4/10/10/10	-
7	GOL	L	1285	-	-	0/4/4/4	-
4	LDA	M	1306	-	-	7/13/13/13	-
4	LDA	M	1307	-	-	3/13/13/13	-
6	BCL	L	1282	3,14	-	7/37/137/137	-
12	SPN	M	1315	-	-	18/50/51/51	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1304	BCL	C4B-NB	8.84	1.43	1.35
6	M	1304	BCL	C1B-NB	8.54	1.42	1.35
6	L	1282	BCL	C1B-NB	7.65	1.42	1.35
6	L	1282	BCL	C4B-NB	7.49	1.41	1.35
6	M	1303	BCL	C4B-NB	7.36	1.41	1.35
4	H	1251	LDA	O1-N1	-7.24	1.25	1.42
4	M	1309	LDA	O1-N1	-7.04	1.25	1.42
4	M	1307	LDA	O1-N1	-7.00	1.25	1.42
4	M	1306	LDA	O1-N1	-6.99	1.25	1.42
6	L	1283	BCL	C4B-NB	6.96	1.41	1.35
4	M	1310	LDA	O1-N1	-6.94	1.25	1.42
4	M	1308	LDA	O1-N1	-6.76	1.26	1.42
13	M	1316	U10	C33-C34	6.61	1.48	1.33
13	M	1316	U10	C13-C14	6.55	1.48	1.33
13	M	1316	U10	C18-C19	6.54	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BCL	C1B-NB	6.50	1.41	1.35
13	M	1316	U10	C23-C24	6.21	1.47	1.33
13	M	1316	U10	C28-C29	6.11	1.47	1.33
6	M	1303	BCL	C1B-NB	5.83	1.40	1.35
13	M	1316	U10	C38-C39	5.65	1.48	1.32
10	M	1305	CDL	OA6-CA5	5.43	1.49	1.34
13	M	1316	U10	C8-C9	5.42	1.46	1.33
10	M	1305	CDL	OA8-CA7	5.31	1.48	1.33
10	M	1305	CDL	OB8-CB7	4.75	1.47	1.33
13	M	1316	U10	O4-C4	-4.72	1.25	1.36
10	M	1305	CDL	OB6-CB5	4.55	1.47	1.34
9	M	1314	BPH	CHD-C4C	4.54	1.49	1.38
9	M	1314	BPH	CHA-C1A	4.47	1.47	1.38
9	L	1288	BPH	CHD-C4C	4.41	1.49	1.38
13	M	1316	U10	O3-C3	-4.36	1.26	1.36
9	L	1288	BPH	CHA-C1A	4.28	1.47	1.38
9	M	1314	BPH	C1B-C2B	-3.97	1.37	1.45
9	L	1288	BPH	C1A-NA	-3.92	1.29	1.37
9	M	1314	BPH	C4C-NC	-3.82	1.29	1.37
9	L	1288	BPH	C1B-C2B	-3.20	1.38	1.45
9	M	1314	BPH	OBD-CAD	-3.18	1.17	1.22
9	M	1314	BPH	C1A-NA	-3.17	1.31	1.37
6	M	1304	BCL	MG-NC	-2.98	1.99	2.06
9	L	1288	BPH	C4C-NC	-2.85	1.31	1.37
13	M	1316	U10	C6-C5	-2.82	1.38	1.46
9	L	1288	BPH	C3D-C2D	-2.73	1.34	1.39
13	M	1316	U10	C4-C5	-2.66	1.41	1.48
9	M	1314	BPH	C3D-C2D	-2.55	1.34	1.39
6	L	1283	BCL	CHD-C4C	-2.44	1.34	1.41
9	L	1288	BPH	CHB-C1B	2.43	1.43	1.38
13	M	1316	U10	C3-C2	-2.37	1.42	1.48
6	L	1283	BCL	C1D-C2D	-2.33	1.37	1.42
6	M	1304	BCL	MG-NA	-2.30	2.00	2.06
13	M	1316	U10	C6-C1	2.29	1.39	1.35
8	L	1286	HTO	O3-C3	2.27	1.48	1.43
8	M	1313	HTO	C4-C3	2.22	1.56	1.52
13	M	1316	U10	C1-C2	-2.10	1.39	1.47
9	M	1314	BPH	CHB-C1B	2.06	1.42	1.38
6	M	1304	BCL	OBD-CAD	-2.04	1.19	1.22
12	M	1315	SPN	C3-C4	2.01	1.53	1.50
6	M	1303	BCL	C1B-CHB	-2.00	1.35	1.41

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1303	BCL	C1C-NC-C4C	7.36	110.01	106.71
6	M	1304	BCL	CHD-C4C-NC	6.30	132.07	125.08
6	M	1304	BCL	O2D-CGD-CBD	6.13	122.17	111.27
9	M	1314	BPH	C4D-C3D-CAD	-5.75	104.23	107.87
6	M	1304	BCL	C1D-CHD-C4C	-5.68	117.50	125.88
13	M	1316	U10	C30-C29-C31	5.11	123.87	115.27
10	M	1305	CDL	OA6-CA5-C11	5.03	122.34	111.50
6	L	1282	BCL	CHD-C4C-NC	4.80	130.41	125.08
10	M	1305	CDL	OB6-CB5-C51	4.78	121.81	111.50
6	L	1282	BCL	C1C-NC-C4C	4.63	108.79	106.71
13	M	1316	U10	C15-C14-C16	4.41	122.68	115.27
6	M	1304	BCL	C1C-NC-C4C	4.37	108.67	106.71
9	M	1314	BPH	CAC-C3C-C2C	-4.28	103.57	114.26
12	M	1315	SPN	CM4-C9-C10	4.25	122.43	115.27
9	M	1314	BPH	O2D-CGD-CBD	4.21	118.75	111.27
6	M	1303	BCL	CHD-C4C-NC	4.19	129.73	125.08
6	L	1283	BCL	C1-O2A-CGA	4.15	127.34	116.44
12	M	1315	SPN	CM5-C13-C14	4.11	122.19	115.27
6	M	1304	BCL	C16-C15-C13	-4.08	102.72	115.92
6	L	1283	BCL	O2A-CGA-CBA	3.89	124.13	111.91
6	M	1304	BCL	C4A-NA-C1A	3.88	108.45	106.71
9	L	1288	BPH	C4D-CHA-C1A	-3.85	121.02	130.51
6	M	1304	BCL	CHB-C4A-NA	3.83	129.81	124.51
6	L	1282	BCL	O2A-C1-C2	3.83	118.70	108.64
6	M	1303	BCL	O2A-CGA-CBA	3.80	123.82	111.91
6	M	1304	BCL	OBD-CAD-C3D	-3.79	121.68	127.98
9	M	1314	BPH	C4D-CHA-C1A	-3.78	121.18	130.51
9	M	1314	BPH	C6-C5-C3	3.78	123.36	113.45
6	L	1283	BCL	C11-C12-C13	-3.73	103.86	115.92
6	L	1283	BCL	O2D-CGD-CBD	3.73	117.89	111.27
6	M	1304	BCL	C3C-C4C-CHD	-3.60	115.69	123.39
6	L	1282	BCL	O2A-CGA-CBA	3.58	123.15	111.91
8	L	1286	HTO	O3-C3-C2	3.57	117.06	109.72
13	M	1316	U10	C17-C18-C19	-3.55	119.12	127.66
6	M	1304	BCL	C5-C3-C2	-3.53	113.96	121.12
13	M	1316	U10	C22-C23-C24	-3.51	119.20	127.66
9	M	1314	BPH	C1-C2-C3	3.49	132.08	126.04
6	L	1283	BCL	CHD-C4C-NC	3.48	128.94	125.08
13	M	1316	U10	C10-C9-C11	3.47	121.12	115.27
13	M	1316	U10	C6-C1-C2	3.47	121.92	119.18
6	L	1283	BCL	C1C-NC-C4C	3.42	108.24	106.71
13	M	1316	U10	C7-C8-C9	-3.42	121.10	126.79
10	M	1305	CDL	OB6-CB5-OB7	-3.37	115.55	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1303	BCL	O2D-CGD-CBD	3.36	117.23	111.27
6	L	1282	BCL	CAC-C3C-C2C	-3.30	106.02	114.26
13	M	1316	U10	C32-C33-C34	-3.30	119.72	127.66
6	L	1283	BCL	C1D-CHD-C4C	-3.28	121.05	125.88
6	L	1282	BCL	O1D-CGD-CBD	-3.27	117.79	124.48
8	L	1286	HTO	C5-C4-C3	-3.26	108.82	114.18
6	L	1283	BCL	CED-O2D-CGD	3.26	123.30	115.94
12	M	1315	SPN	CM6-C18-C17	3.24	120.72	115.27
9	L	1288	BPH	CAA-CBA-CGA	-3.20	103.91	113.25
6	M	1304	BCL	O1D-CGD-CBD	-3.16	118.01	124.48
8	L	1286	HTO	C1-C2-C3	3.16	119.96	113.11
6	M	1304	BCL	OBD-CAD-CBD	3.11	130.33	125.89
8	M	1313	HTO	O3-C3-C4	3.09	115.88	109.15
9	L	1288	BPH	C1C-NC-C4C	-3.07	107.84	110.54
12	M	1315	SPN	CM3-C5-C6	3.07	120.43	115.27
13	M	1316	U10	C27-C28-C29	-3.06	120.28	127.66
9	L	1288	BPH	CBC-CAC-C3C	3.03	120.21	113.47
10	M	1305	CDL	OA8-CA7-C31	3.02	121.39	111.91
6	L	1282	BCL	C1-C2-C3	3.01	131.25	126.04
6	L	1282	BCL	C2C-C3C-C4C	3.01	105.85	101.34
6	L	1283	BCL	C1-C2-C3	2.95	131.14	126.04
6	L	1282	BCL	O2D-CGD-CBD	2.94	116.50	111.27
13	M	1316	U10	C35-C34-C36	2.94	120.22	115.27
13	M	1316	U10	C1M-C1-C6	-2.93	119.63	124.40
10	M	1305	CDL	OB8-CB7-C71	2.87	120.93	111.91
9	M	1314	BPH	C3D-CAD-CBD	2.85	111.36	107.61
9	M	1314	BPH	CBA-CAA-C2A	-2.81	105.57	113.86
12	M	1315	SPN	C7-C8-C9	-2.81	120.89	127.66
6	M	1303	BCL	CHB-C4A-NA	2.81	128.40	124.51
6	M	1304	BCL	C4-C3-C5	2.79	119.97	115.27
6	M	1304	BCL	C6-C5-C3	-2.76	106.22	113.45
9	M	1314	BPH	C1B-NB-C4B	2.74	111.66	106.51
4	M	1306	LDA	O1-N1-C1	2.73	115.96	109.27
6	M	1304	BCL	C4D-C3D-CAD	-2.72	106.95	108.47
6	L	1282	BCL	CHB-C4A-NA	2.67	128.20	124.51
9	M	1314	BPH	O1D-CGD-CBD	-2.64	119.09	124.48
6	M	1304	BCL	C1B-CHB-C4A	-2.62	124.93	130.12
13	M	1316	U10	C41-C39-C40	2.60	120.33	114.60
10	M	1305	CDL	CB4-OB6-CB5	-2.59	111.41	117.79
6	L	1282	BCL	CMC-C2C-C3C	-2.58	103.41	113.83
12	M	1315	SPN	CMB-C30-CM9	2.58	120.31	114.60
6	M	1303	BCL	O2D-CGD-O1D	-2.58	118.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	1288	BPH	OBB-CAB-C3B	2.57	125.17	120.41
12	M	1315	SPN	C23-C24-C25	-2.57	105.44	112.23
6	L	1282	BCL	C1-O2A-CGA	2.55	123.13	116.44
9	L	1288	BPH	OBB-CAB-CBB	-2.54	114.09	119.73
6	L	1283	BCL	CAC-C3C-C4C	-2.54	106.94	112.58
6	L	1283	BCL	OBD-CAD-CBD	2.54	129.53	125.89
12	M	1315	SPN	C21-C20-C19	-2.54	105.53	112.23
10	M	1305	CDL	OA8-CA6-CA4	2.54	115.82	108.43
9	M	1314	BPH	CAC-C3C-C4C	2.54	119.18	112.67
6	M	1303	BCL	CED-O2D-CGD	2.53	121.65	115.94
6	L	1282	BCL	CMB-C2B-C1B	-2.51	124.61	128.46
13	M	1316	U10	C20-C19-C21	2.48	119.44	115.27
6	M	1304	BCL	CAA-CBA-CGA	2.45	120.43	113.25
9	M	1314	BPH	OBD-CAD-CBD	-2.43	122.42	125.89
10	M	1305	CDL	CB6-CB4-CB3	-2.40	106.11	111.79
6	M	1304	BCL	C16-C17-C18	-2.39	104.73	115.98
9	M	1314	BPH	OBB-CAB-CBB	-2.37	114.47	119.73
9	M	1314	BPH	C2A-C1A-NA	2.36	114.57	111.86
9	L	1288	BPH	C2B-C1B-NB	-2.36	106.23	109.79
6	M	1303	BCL	O2A-CGA-O1A	-2.35	117.65	123.59
9	L	1288	BPH	O2A-C1-C2	-2.34	102.47	108.64
9	L	1288	BPH	C1B-NB-C4B	2.32	110.89	106.51
8	L	1287	HTO	O1-C1-C2	2.31	116.11	111.07
6	L	1283	BCL	C3C-C4C-CHD	-2.30	118.48	123.39
9	M	1314	BPH	CHD-C4C-NC	-2.29	122.48	125.20
6	L	1283	BCL	O1D-CGD-CBD	-2.27	119.83	124.48
12	M	1315	SPN	C16-C17-C18	-2.26	107.53	113.45
6	M	1303	BCL	C4D-C3D-CAD	-2.24	107.22	108.47
6	L	1282	BCL	C1B-CHB-C4A	-2.23	125.69	130.12
8	L	1287	HTO	C1-C2-C3	-2.23	108.28	113.11
13	M	1316	U10	C12-C13-C14	-2.22	122.32	127.66
6	M	1304	BCL	C1-O2A-CGA	2.21	122.24	116.44
6	M	1303	BCL	CMA-C3A-C2A	-2.21	104.93	113.83
9	M	1314	BPH	CMD-C2D-C3D	2.20	128.80	124.68
6	M	1304	BCL	OBB-CAB-CBB	-2.20	115.22	120.17
6	L	1283	BCL	C4A-NA-C1A	-2.18	105.73	106.71
9	M	1314	BPH	OBB-CAB-C3B	2.18	124.43	120.41
10	M	1305	CDL	OB8-CB7-OB9	-2.18	118.10	123.59
10	M	1305	CDL	OA8-CA7-OA9	-2.17	118.12	123.59
6	M	1304	BCL	CHC-C1C-NC	2.17	127.51	124.51
13	M	1316	U10	C40-C39-C38	-2.15	116.44	122.65
9	M	1314	BPH	C2B-C1B-NB	-2.14	106.56	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1282	BCL	C1D-CHD-C4C	-2.12	122.76	125.88
12	M	1315	SPN	CM5-C13-C12	-2.12	118.25	123.68
9	L	1288	BPH	C4-C3-C5	-2.08	111.77	115.27
12	M	1315	SPN	O1-C1-C2	2.07	113.03	108.78
6	M	1304	BCL	O2D-CGD-O1D	-2.06	119.82	123.84
8	L	1287	HTO	O2-C2-C1	2.05	113.97	109.14
6	M	1304	BCL	CBA-CAA-C2A	-2.05	107.81	113.86
8	L	1286	HTO	O2-C2-C1	-2.05	104.34	109.14
12	M	1315	SPN	CM8-C26-C27	2.03	118.69	115.27
9	M	1314	BPH	C11-C10-C8	2.03	122.48	115.92
13	M	1316	U10	O5-C5-C6	-2.03	118.00	121.55
6	L	1283	BCL	OBD-CAD-C3D	-2.02	124.62	127.98
13	M	1316	U10	C15-C14-C13	-2.02	118.50	123.68
9	L	1288	BPH	C4-C3-C2	2.02	128.85	123.68

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	L	1288	BPH	C8
9	L	1288	BPH	C13
8	L	1287	HTO	C2
9	M	1314	BPH	C8
9	M	1314	BPH	C13
8	L	1286	HTO	C2
8	M	1313	HTO	C2

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	1288	BPH	O2A-C1-C2-C3
13	M	1316	U10	C27-C28-C29-C30
13	M	1316	U10	C27-C28-C29-C31
12	M	1315	SPN	C11-C10-C9-CM4
6	L	1282	BCL	C4C-C3C-CAC-CBC
6	L	1282	BCL	O2A-C1-C2-C3
8	L	1287	HTO	C1-C2-C3-O3
4	M	1310	LDA	N1-C1-C2-C3
4	M	1306	LDA	C2-C1-N1-CM1
4	M	1309	LDA	C2-C1-N1-O1
4	M	1309	LDA	C2-C1-N1-CM1
4	M	1309	LDA	C2-C1-N1-CM2
4	M	1309	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	M	1305	CDL	CA2-OA2-PA1-OA3
10	M	1305	CDL	CA2-OA2-PA1-OA4
10	M	1305	CDL	CA2-OA2-PA1-OA5
10	M	1305	CDL	CB2-OB2-PB2-OB3
10	M	1305	CDL	CB2-OB2-PB2-OB4
10	M	1305	CDL	CB2-OB2-PB2-OB5
9	M	1314	BPH	C4C-C3C-CAC-CBC
9	M	1314	BPH	C2C-C3C-CAC-CBC
9	M	1314	BPH	C4B-C3B-CAB-CBB
9	M	1314	BPH	C4B-C3B-CAB-OBB
9	M	1314	BPH	C11-C10-C8-C9
8	M	1313	HTO	O2-C2-C3-C4
8	M	1313	HTO	C2-C3-C4-C5
8	M	1313	HTO	O3-C3-C4-C5
13	M	1316	U10	C37-C38-C39-C40
10	M	1305	CDL	O1-C1-CA2-OA2
9	M	1314	BPH	C3-C5-C6-C7
12	M	1315	SPN	C16-C17-C18-CM6
12	M	1315	SPN	C11-C10-C9-C8
12	M	1315	SPN	C16-C17-C18-C19
13	M	1316	U10	C37-C38-C39-C41
8	L	1286	HTO	O1-C1-C2-C3
12	M	1315	SPN	C14-C15-C16-C17
12	M	1315	SPN	CM7-C22-C23-C24
9	M	1314	BPH	C13-C15-C16-C17
6	L	1282	BCL	C10-C11-C12-C13
6	L	1282	BCL	C15-C16-C17-C18
9	L	1288	BPH	CBD-CGD-O2D-CED
9	M	1314	BPH	C12-C13-C15-C16
13	M	1316	U10	C29-C31-C32-C33
12	M	1315	SPN	C26-C27-C28-C29
6	M	1303	BCL	C5-C6-C7-C8
10	M	1305	CDL	CA3-OA5-PA1-OA2
6	L	1283	BCL	C16-C17-C18-C19
4	M	1308	LDA	C2-C3-C4-C5
10	M	1305	CDL	C73-C74-C75-C76
10	M	1305	CDL	C39-C40-C41-C42
10	M	1305	CDL	C51-C52-C53-C54
9	L	1288	BPH	C14-C13-C15-C16
7	L	1284	GOL	O1-C1-C2-C3
10	M	1305	CDL	C54-C55-C56-C57
10	M	1305	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
10	M	1305	CDL	C56-C57-C58-C59
4	M	1309	LDA	C4-C5-C6-C7
10	M	1305	CDL	CB2-C1-CA2-OA2
4	M	1309	LDA	C1-C2-C3-C4
10	M	1305	CDL	C71-C72-C73-C74
9	L	1288	BPH	C2-C3-C5-C6
9	L	1288	BPH	C11-C10-C8-C7
6	L	1282	BCL	C6-C7-C8-C10
9	M	1314	BPH	C11-C10-C8-C7
6	L	1283	BCL	C16-C17-C18-C20
4	M	1309	LDA	C7-C8-C9-C10
4	M	1310	LDA	C3-C4-C5-C6
10	M	1305	CDL	C79-C80-C81-C82
10	M	1305	CDL	C11-C12-C13-C14
10	M	1305	CDL	CB5-C51-C52-C53
9	M	1314	BPH	C10-C11-C12-C13
4	M	1307	LDA	C5-C6-C7-C8
9	L	1288	BPH	C4-C3-C5-C6
12	M	1315	SPN	C20-C21-C22-CM7
6	L	1282	BCL	C6-C7-C8-C9
6	M	1304	BCL	C13-C15-C16-C17
6	M	1304	BCL	C16-C17-C18-C19
10	M	1305	CDL	OB5-CB3-CB4-CB6
9	L	1288	BPH	O1D-CGD-O2D-CED
4	M	1306	LDA	C1-C2-C3-C4
6	M	1304	BCL	C16-C17-C18-C20
8	M	1313	HTO	C4-C5-C6-C7
4	M	1310	LDA	C1-C2-C3-C4
6	M	1303	BCL	C15-C16-C17-C18
13	M	1316	U10	C14-C16-C17-C18
4	M	1309	LDA	C3-C4-C5-C6
10	M	1305	CDL	C53-C54-C55-C56
9	M	1314	BPH	C8-C10-C11-C12
4	H	1251	LDA	C11-C10-C9-C8
4	M	1307	LDA	C9-C10-C11-C12
12	M	1315	SPN	C21-C22-C23-C24
10	M	1305	CDL	C35-C36-C37-C38
10	M	1305	CDL	C74-C75-C76-C77
6	M	1304	BCL	C14-C13-C15-C16
4	H	1251	LDA	N1-C1-C2-C3
10	M	1305	CDL	C51-CB5-OB6-CB4
10	M	1305	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
10	M	1305	CDL	C80-C81-C82-C83
4	M	1308	LDA	C4-C5-C6-C7
9	L	1288	BPH	C10-C11-C12-C13
10	M	1305	CDL	C36-C37-C38-C39
12	M	1315	SPN	CM1-C1-C2-O2
12	M	1315	SPN	CM1-C1-C2-C3
4	M	1309	LDA	C6-C7-C8-C9
10	M	1305	CDL	C41-C42-C43-C44
7	L	1284	GOL	O1-C1-C2-O2
10	M	1305	CDL	OB5-CB3-CB4-OB6
10	M	1305	CDL	OB7-CB5-OB6-CB4
6	L	1283	BCL	C11-C12-C13-C14
9	M	1314	BPH	C14-C13-C15-C16
10	M	1305	CDL	C59-C60-C61-C62
9	L	1288	BPH	C4C-C3C-CAC-CBC
9	M	1314	BPH	C5-C6-C7-C8
6	L	1283	BCL	C11-C12-C13-C15
6	M	1304	BCL	C12-C13-C15-C16
9	L	1288	BPH	C4B-C3B-CAB-CBB
4	M	1310	LDA	C5-C6-C7-C8
4	H	1251	LDA	C3-C4-C5-C6
9	M	1314	BPH	CAD-CBD-CGD-O2D
12	M	1315	SPN	CM8-C26-C27-C28
4	H	1251	LDA	C9-C10-C11-C12
12	M	1315	SPN	C19-C20-C21-C22
10	M	1305	CDL	CB3-CB4-CB6-OB8
4	M	1306	LDA	C2-C1-N1-CM2
10	M	1305	CDL	OA6-CA4-CA6-OA8
8	L	1286	HTO	O1-C1-C2-O2
4	H	1251	LDA	C2-C3-C4-C5
6	M	1304	BCL	C3-C5-C6-C7
12	M	1315	SPN	O1-C1-C2-O2
6	L	1282	BCL	C8-C10-C11-C12
12	M	1315	SPN	C25-C26-C27-C28
10	M	1305	CDL	CA3-OA5-PA1-OA3
10	M	1305	CDL	CA3-OA5-PA1-OA4
9	L	1288	BPH	C3-C5-C6-C7
4	M	1309	LDA	C9-C10-C11-C12
9	M	1314	BPH	C6-C7-C8-C10
4	M	1307	LDA	C7-C8-C9-C10
4	H	1251	LDA	C1-C2-C3-C4
4	M	1310	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
10	M	1305	CDL	C1-CB2-OB2-PB2
10	M	1305	CDL	C13-C14-C15-C16
12	M	1315	SPN	CM3-C5-C6-C7
8	L	1287	HTO	O2-C2-C3-O3
9	L	1288	BPH	C11-C10-C8-C9
4	M	1309	LDA	C2-C3-C4-C5
4	M	1308	LDA	N1-C1-C2-C3
12	M	1315	SPN	C4-C5-C6-C7
13	M	1316	U10	C5-C4-O4-C4M
4	M	1310	LDA	C6-C7-C8-C9
4	M	1306	LDA	C3-C4-C5-C6
4	M	1306	LDA	C9-C10-C11-C12
4	M	1308	LDA	C9-C10-C11-C12
4	M	1308	LDA	C1-C2-C3-C4
9	L	1288	BPH	C4B-C3B-CAB-OBB
9	L	1288	BPH	C8-C10-C11-C12
9	M	1314	BPH	C6-C7-C8-C9
10	M	1305	CDL	C31-C32-C33-C34
9	L	1288	BPH	CAD-CBD-CGD-O2D
6	L	1283	BCL	CAD-CBD-CGD-O2D
4	M	1306	LDA	C11-C10-C9-C8
6	M	1304	BCL	CHA-CBD-CGD-O1D
6	M	1304	BCL	CHA-CBD-CGD-O2D
4	H	1251	LDA	C2-C1-N1-CM2
10	M	1305	CDL	C72-C71-CB7-OB8
12	M	1315	SPN	C27-C28-C29-C30
10	M	1305	CDL	C72-C71-CB7-OB9
4	M	1306	LDA	C2-C1-N1-O1
9	L	1288	BPH	C11-C12-C13-C15
6	M	1303	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

17 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	1288	BPH	8	0
10	M	1305	CDL	3	0
8	M	1313	HTO	7	0
6	L	1283	BCL	6	0
6	M	1303	BCL	13	0
13	M	1316	U10	4	0
12	M	1315	SPN	10	0

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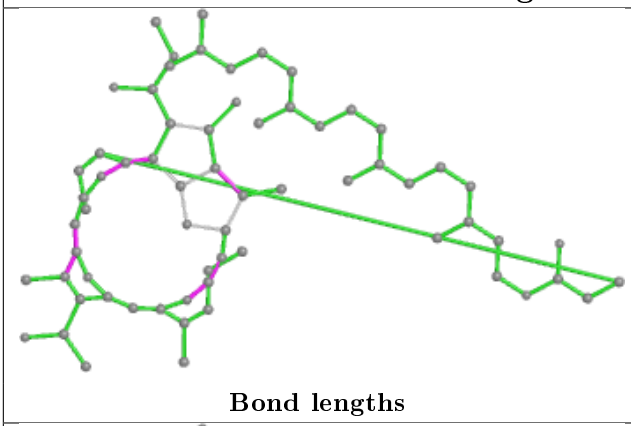
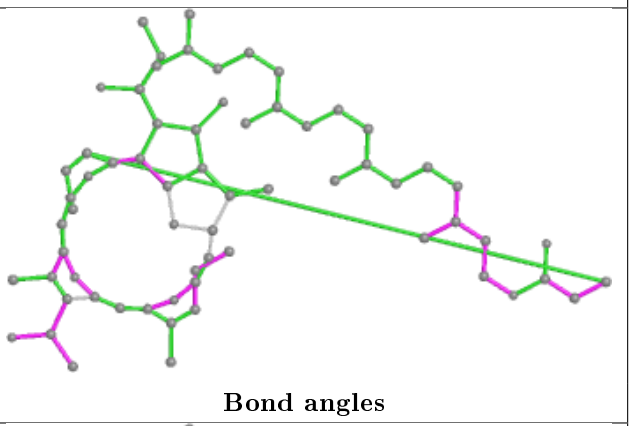
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1287	HTO	3	0
4	H	1251	LDA	2	0
4	M	1309	LDA	2	0
6	M	1304	BCL	6	0
9	M	1314	BPH	8	0
8	L	1286	HTO	1	0
4	M	1310	LDA	2	0
4	M	1306	LDA	3	0
4	M	1307	LDA	4	0
6	L	1282	BCL	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

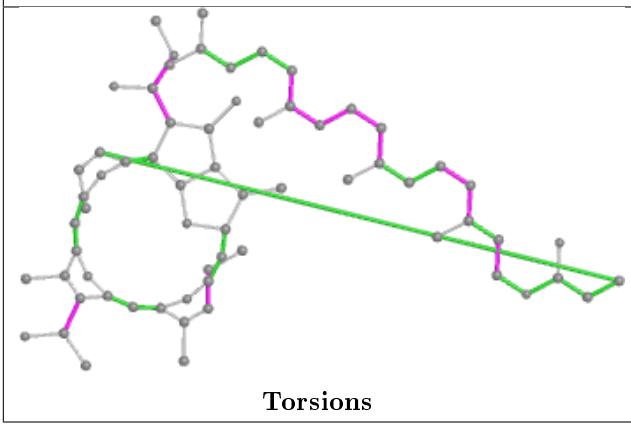
Ligand BPH L 1288



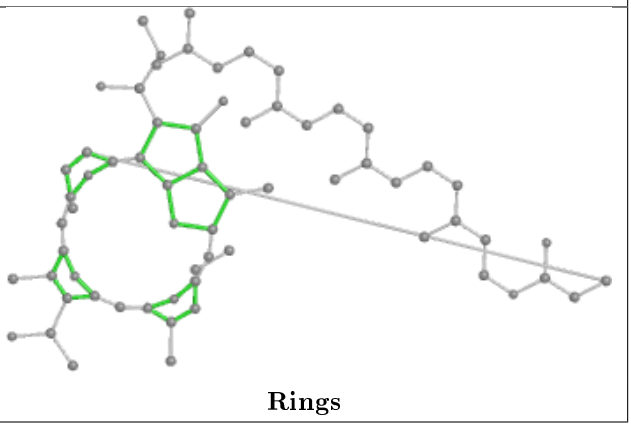
Bond lengths



Bond angles

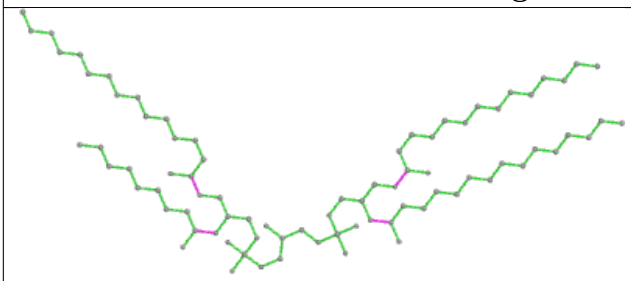


Torsions

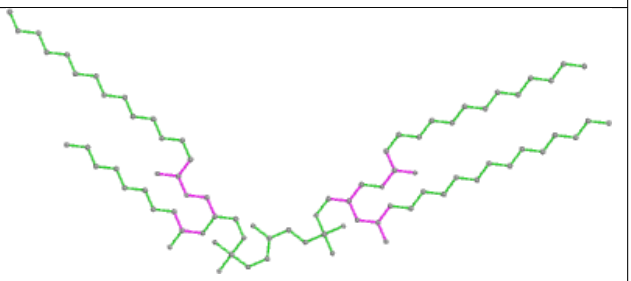


Rings

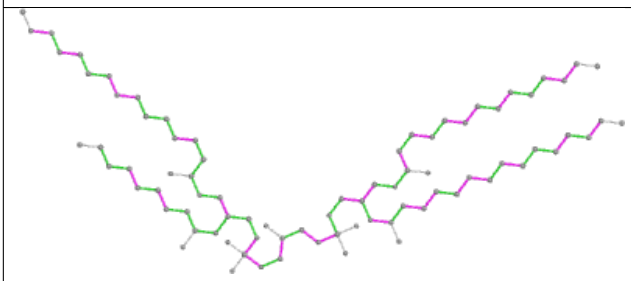
Ligand CDL M 1305



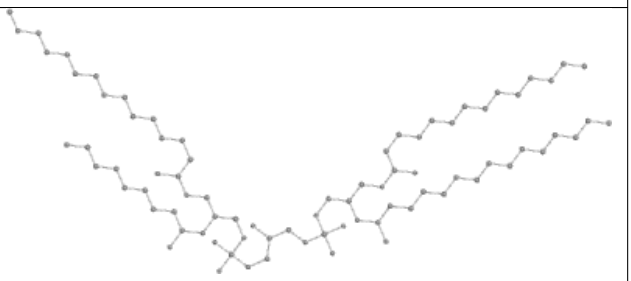
Bond lengths



Bond angles

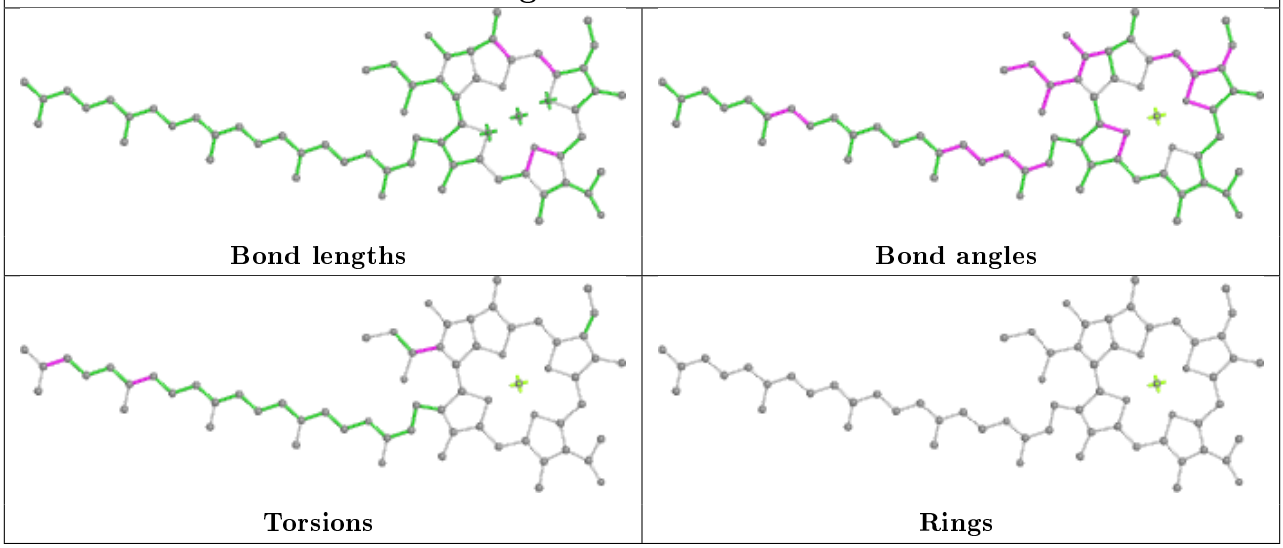


Torsions

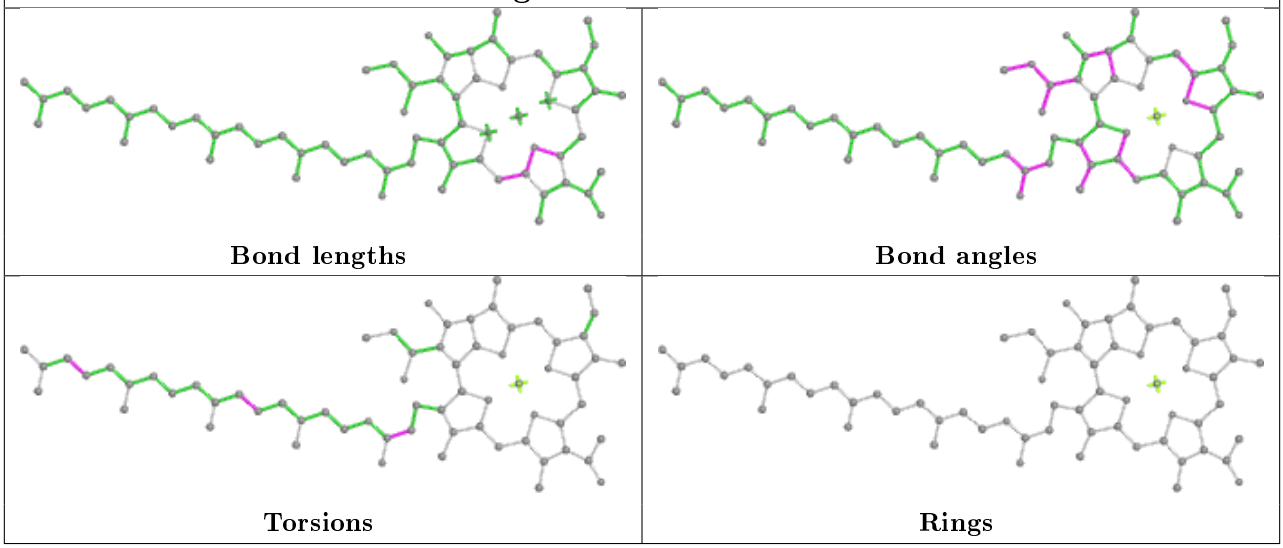


Rings

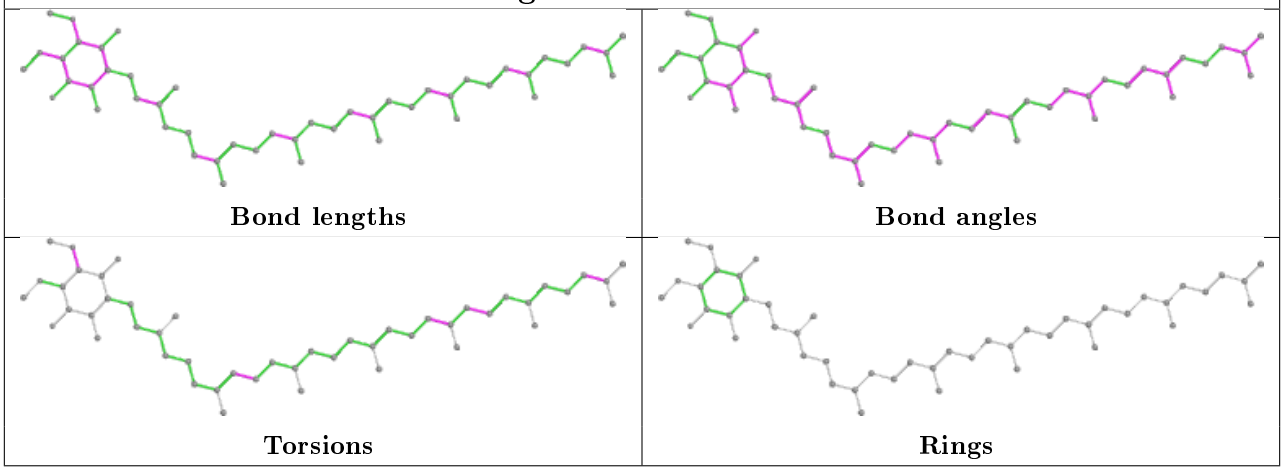
Ligand BCL L 1283



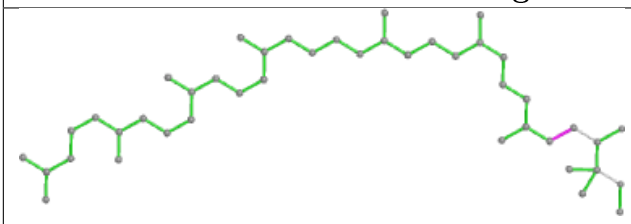
Ligand BCL M 1303



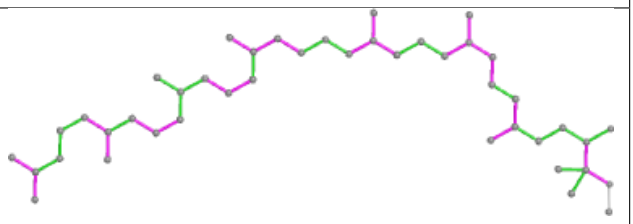
Ligand U10 M 1316



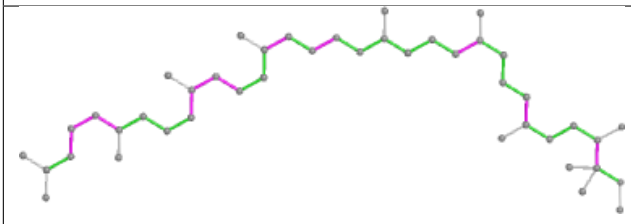
Ligand SPN M 1315



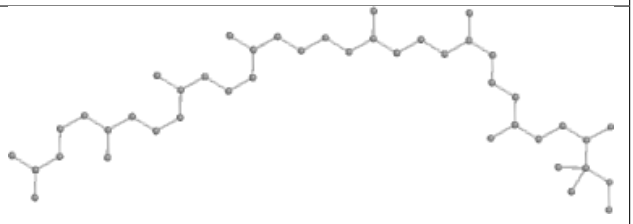
Bond lengths



Bond angles

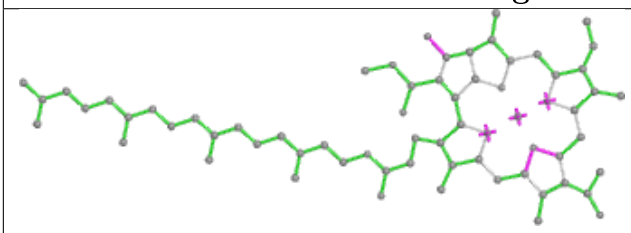


Torsions

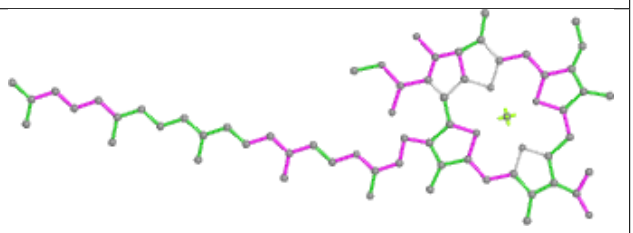


Rings

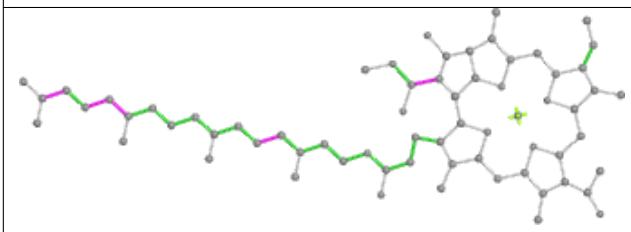
Ligand BCL M 1304



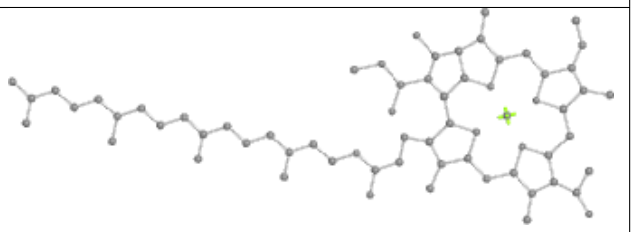
Bond lengths



Bond angles

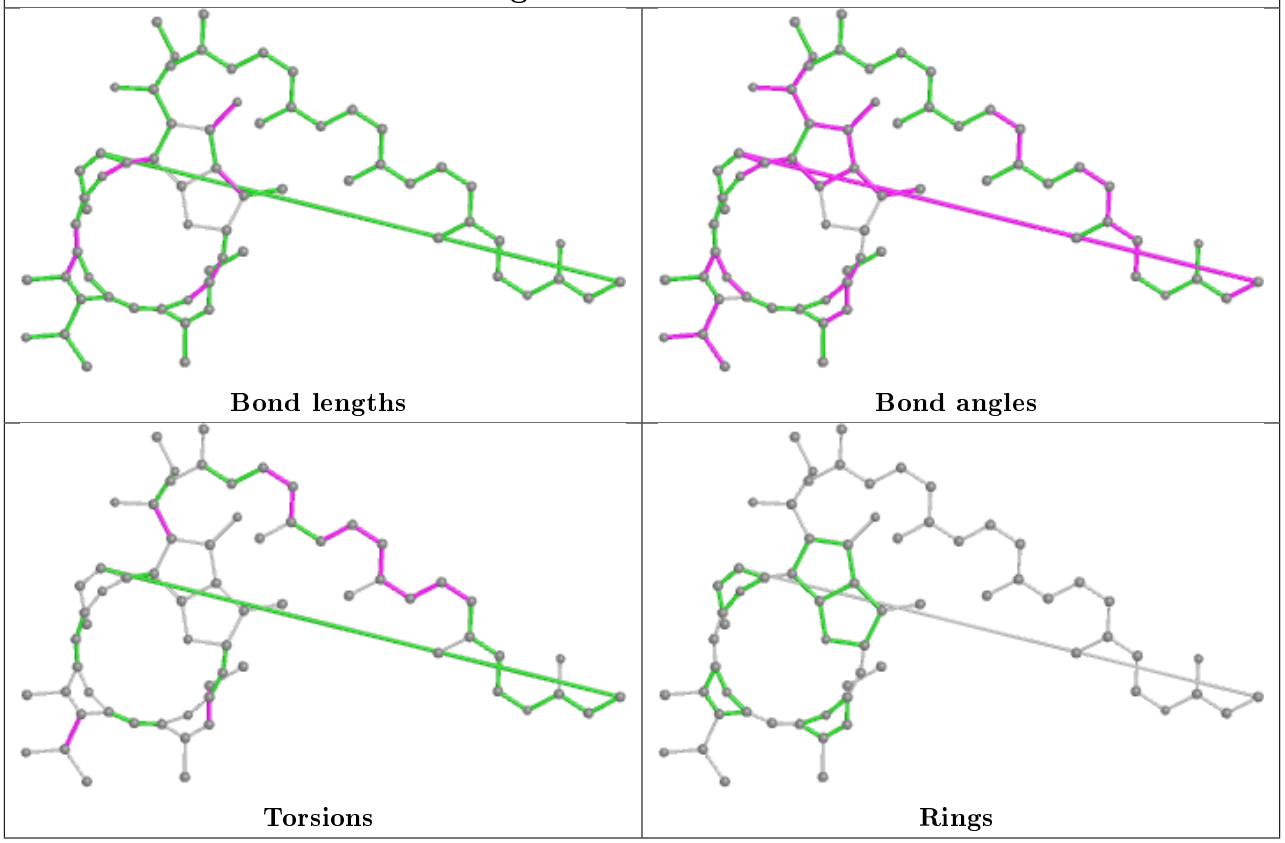


Torsions

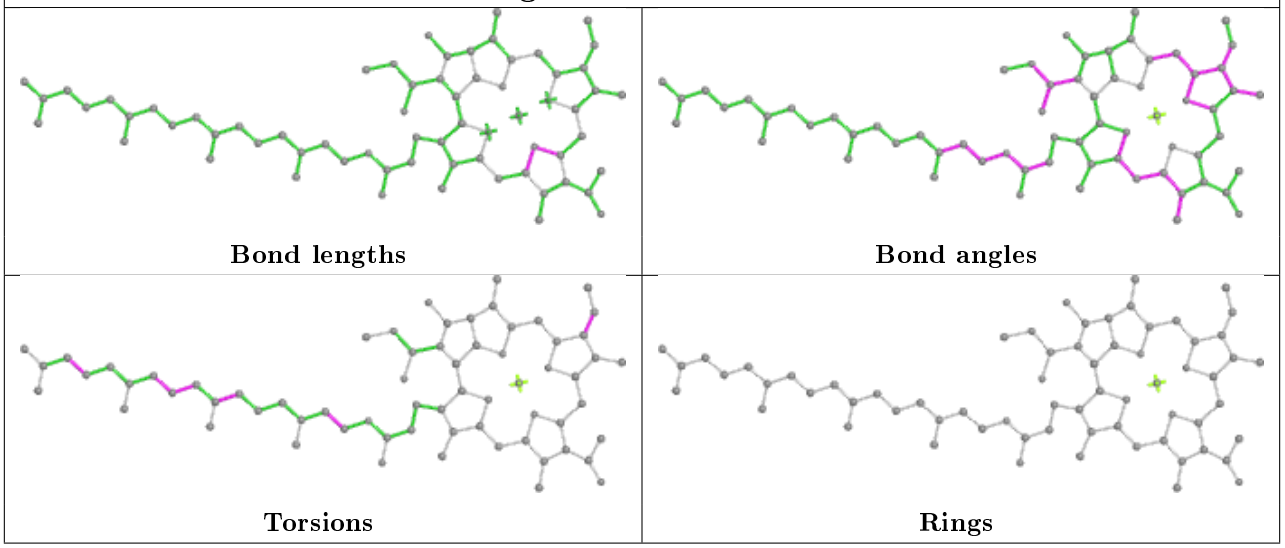


Rings

Ligand BPH M 1314



Ligand BCL L 1282



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	240/260 (92%)	-0.35	6 (2%)	57	53	48, 63, 84, 171	0
2	L	281/281 (100%)	-0.40	5 (1%)	68	66	42, 62, 103, 129	0
3	M	302/307 (98%)	-0.46	5 (1%)	70	67	42, 64, 101, 118	0
All	All	823/848 (97%)	-0.41	16 (1%)	66	64	42, 63, 99, 171	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	249	LYS	8.1
1	H	250	SER	7.1
3	M	1	ALA	6.7
1	H	246	PRO	5.8
1	H	247	LYS	5.0
1	H	248	ARG	4.9
1	H	245	ALA	4.1
3	M	52	LEU	3.6
2	L	59	TRP	3.0
2	L	277	GLY	2.9
2	L	276	PRO	2.5
3	M	302	GLY	2.4
3	M	2	GLU	2.2
2	L	281	GLY	2.2
2	L	72	GLU	2.1
3	M	76	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

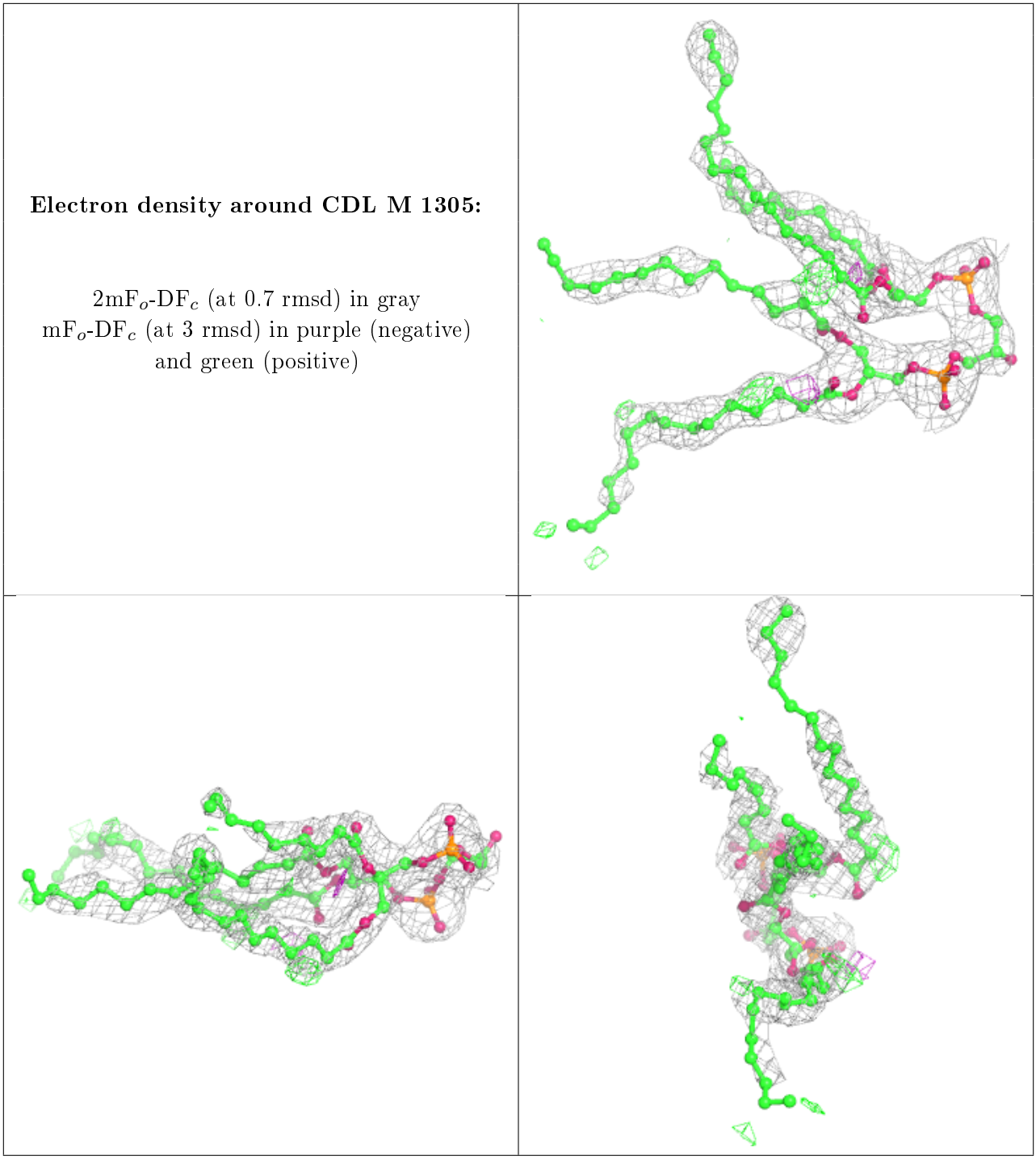
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	LDA	M	1309	16/16	0.60	0.59	115,132,147,148	0
7	GOL	L	1285	6/6	0.67	0.31	86,106,108,109	0
4	LDA	M	1310	16/16	0.70	0.42	74,88,126,127	0
8	HTO	L	1286	10/10	0.75	0.28	71,75,90,97	0
4	LDA	M	1308	16/16	0.79	0.35	74,113,155,156	0
4	LDA	M	1306	16/16	0.80	0.25	52,89,101,102	0
4	LDA	H	1251	16/16	0.80	0.41	98,130,149,151	0
8	HTO	L	1287	10/10	0.85	0.26	92,97,101,102	0
4	LDA	M	1307	16/16	0.85	0.21	88,98,122,123	0
10	CDL	M	1305	81/100	0.85	0.28	52,98,114,118	0
7	GOL	L	1284	6/6	0.87	0.21	84,90,95,95	0
9	BPH	M	1314	65/65	0.89	0.18	44,71,128,133	0
12	SPN	M	1315	43/43	0.89	0.22	47,77,114,118	0
8	HTO	M	1313	10/10	0.91	0.18	77,89,95,97	0
6	BCL	L	1282	66/66	0.91	0.16	42,57,125,132	0
13	U10	M	1316	48/63	0.94	0.15	40,68,98,105	0
5	NA	H	1252	1/1	0.96	0.04	45,45,45,45	0
5	NA	M	1311	1/1	0.96	0.06	71,71,71,71	0
6	BCL	L	1283	66/66	0.96	0.17	39,56,67,83	0
6	BCL	M	1304	66/66	0.97	0.09	14,45,78,88	0
9	BPH	L	1288	65/65	0.97	0.14	30,52,77,81	0
6	BCL	M	1303	66/66	0.97	0.15	39,56,78,103	0
11	FE	M	1312	1/1	1.00	0.05	49,49,49,49	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.

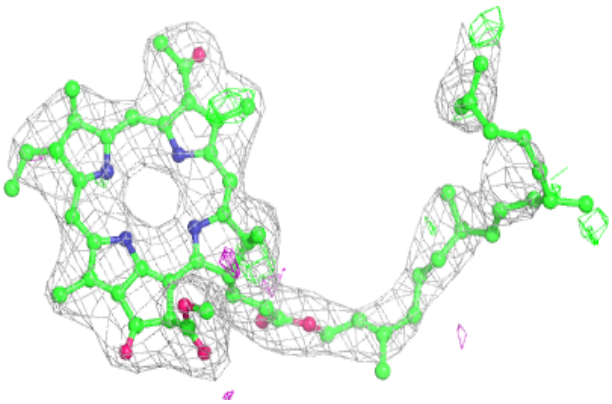
Electron density around CDL M 1305:

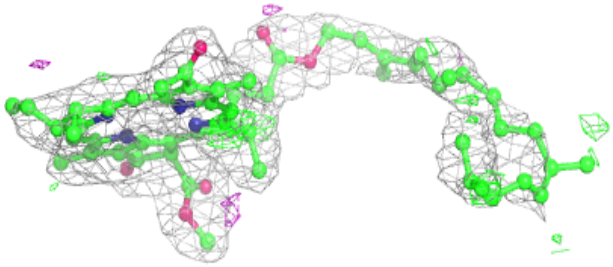
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

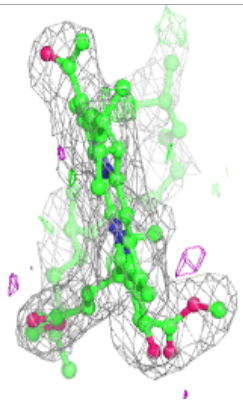


Electron density around BPH M 1314:

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

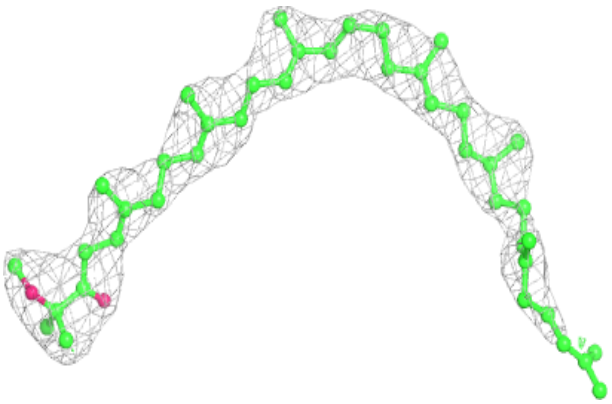


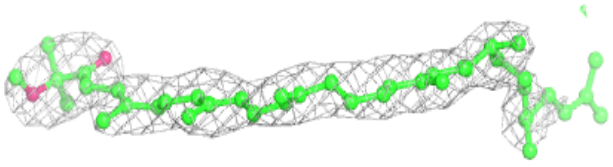


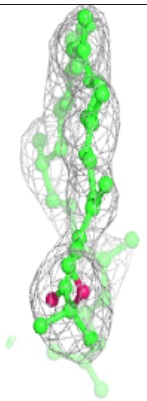


Electron density around SPN M 1315:

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

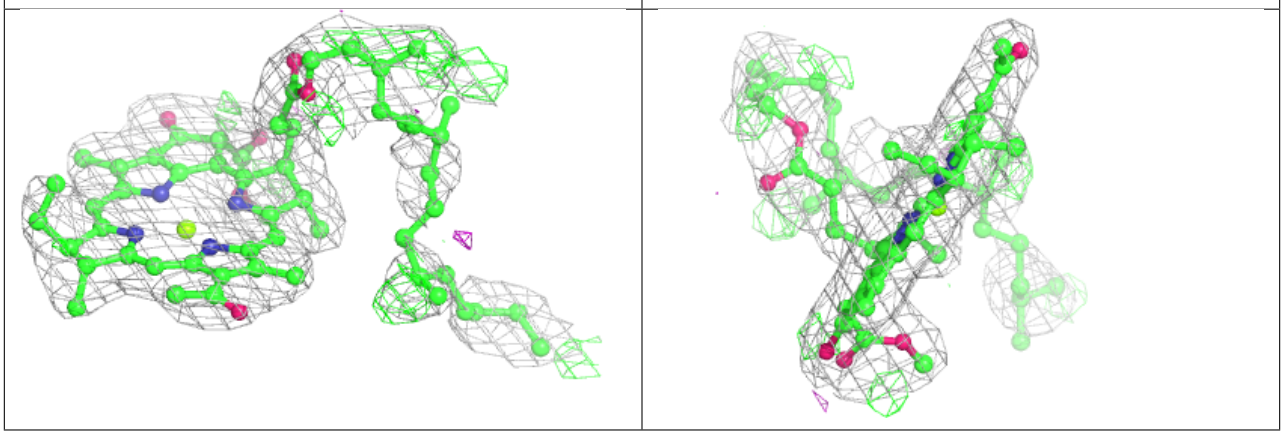






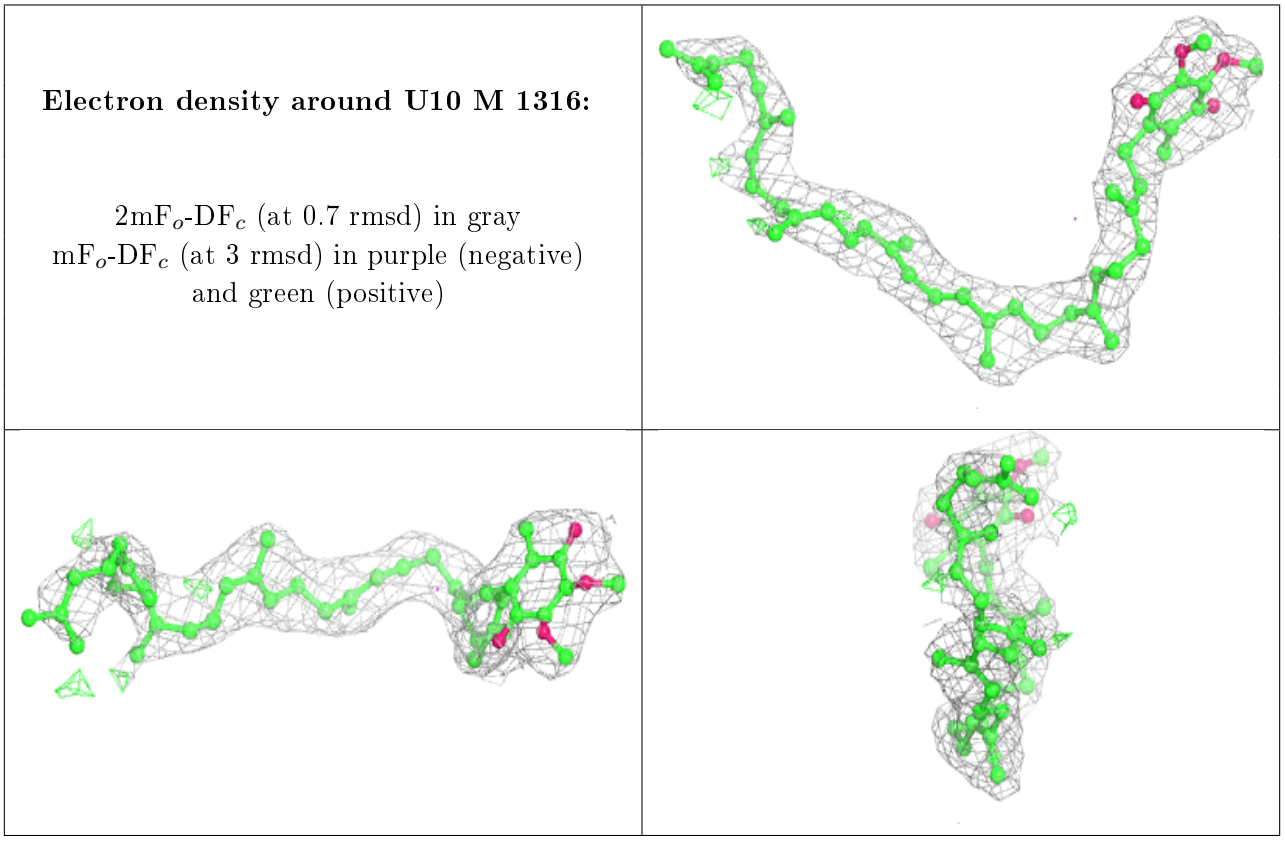
Electron density around BCL L 1282:

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



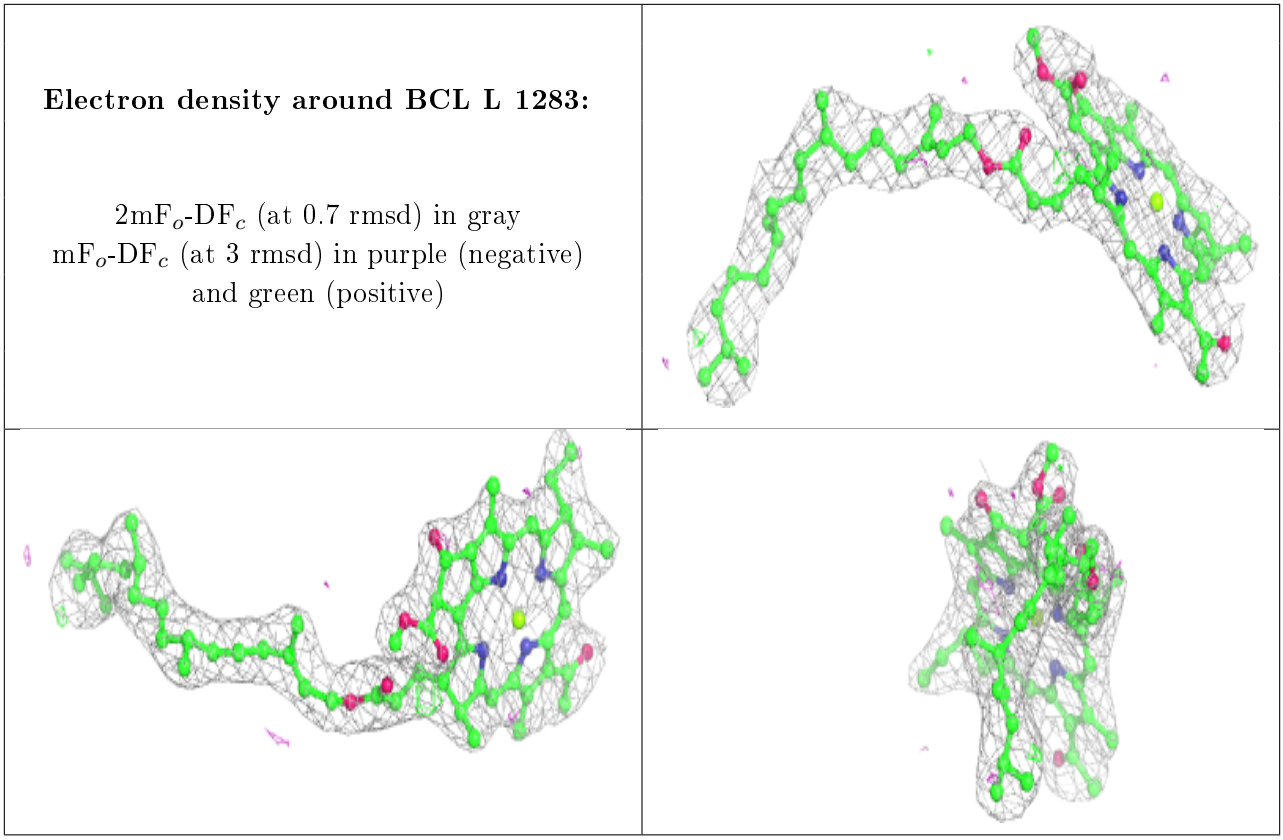
Electron density around U10 M 1316:

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



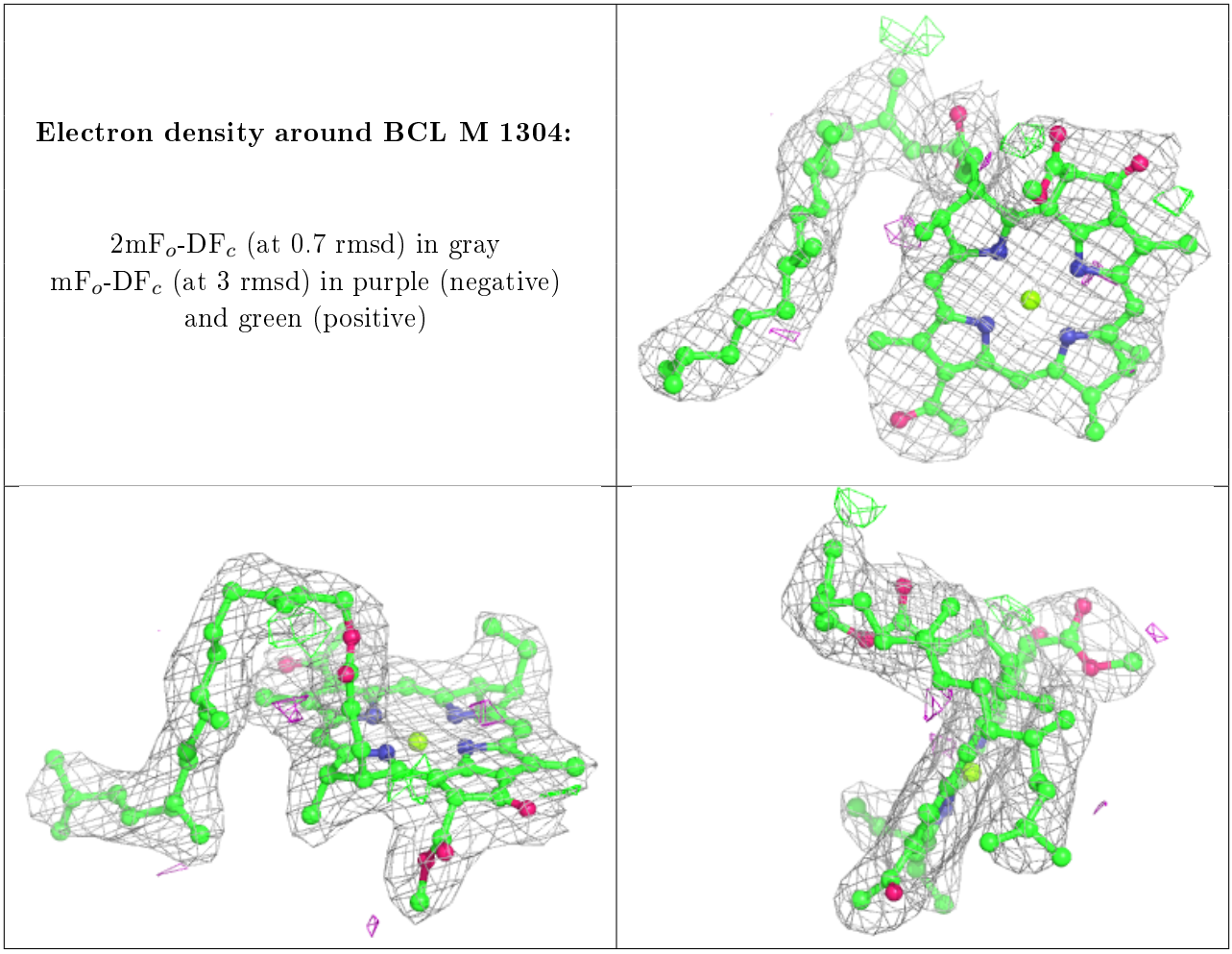
Electron density around BCL L 1283:

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



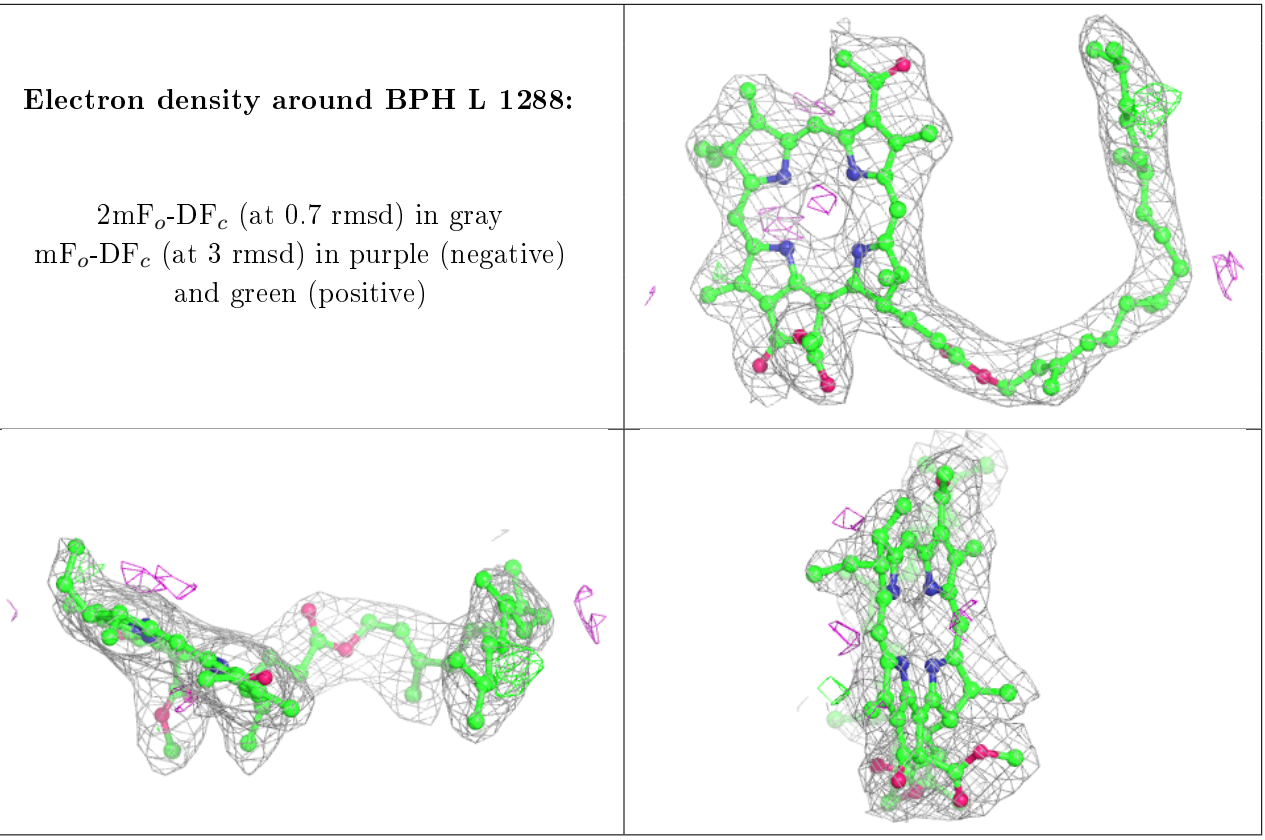
Electron density around BCL M 1304:

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



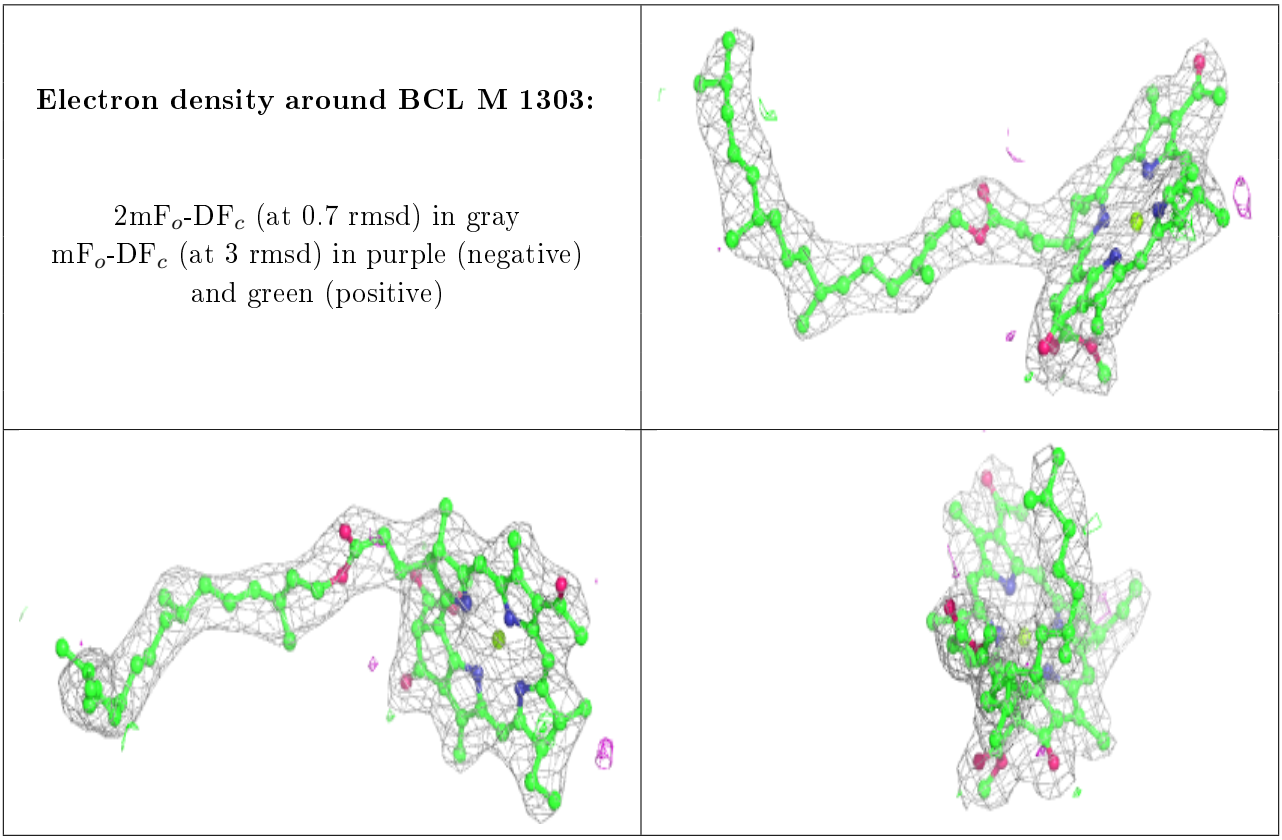
Electron density around BPH L 1288:

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



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.