



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 02:23 AM EDT

PDB ID : 2GNU
Title : The crystallization of reaction center from Rhodobacter sphaeroides occurs via a new route
Authors : Wadsten, P.; Woehri, A.B.; Snijder, A.; Katona, G.; Gardiner, A.T.; Cogdell, R.J.; Neutze, R.; Engstroem, S.
Deposited on : 2006-04-11
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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

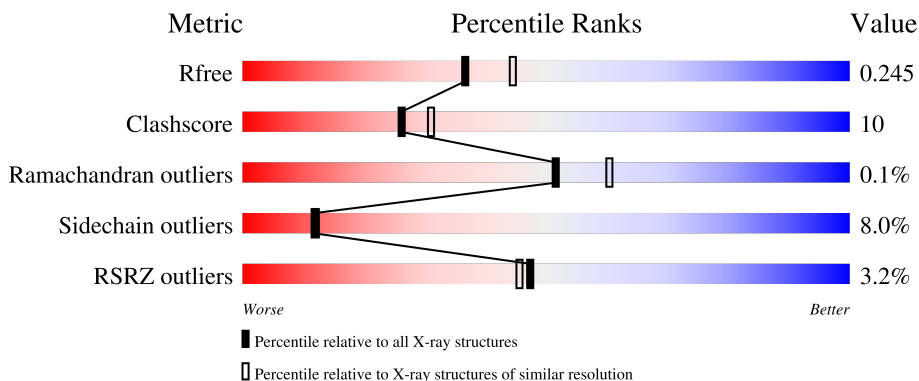
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


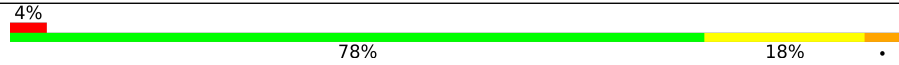
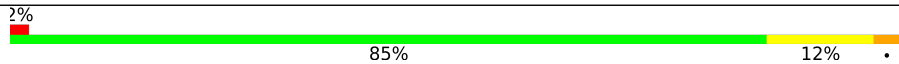
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	235	
2	L	281	
3	M	300	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1282	X	-	-	-
5	BCL	L	1283	X	-	-	-
5	BCL	M	1303	X	-	-	-
9	BPH	M	1284	X	-	-	-
9	BPH	M	1304	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7045 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	235	1787	1143	304	331	9	0	0	0

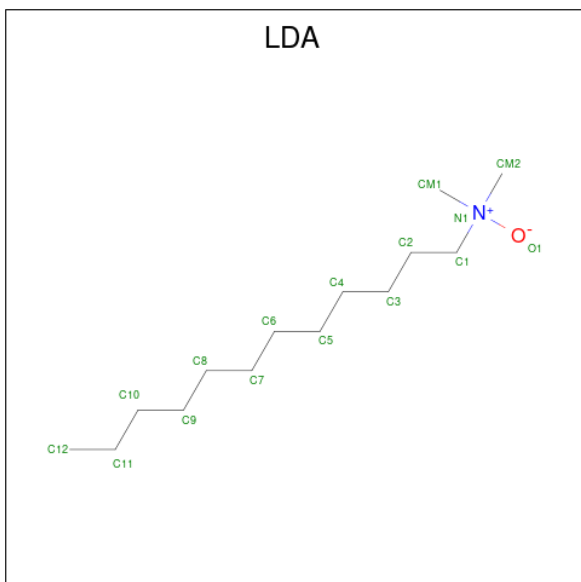
- Molecule 2 is a protein called Reaction center protein L chain.

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

- Molecule 3 is a protein called Reaction center protein M chain.

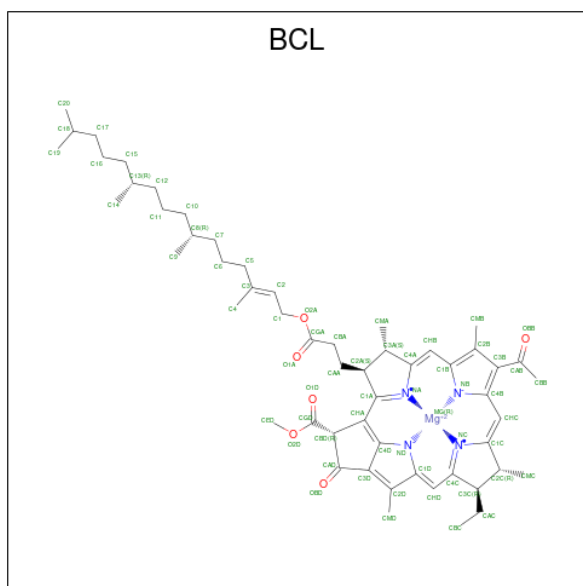
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	300	2400	1602	392	396	10	0	0	0

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



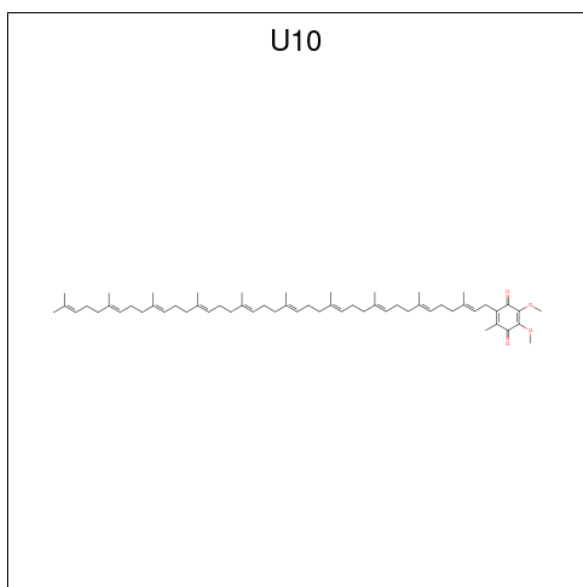
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	14	12	1	1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
5	L	1	66	55	1	4	6	0	0
5	M	1	48	37	1	4	6	0	0
5	M	1	66	55	1	4	6	0	0

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			24	20	4		
6	M	1	Total	C	O	0	0
			45	41	4		

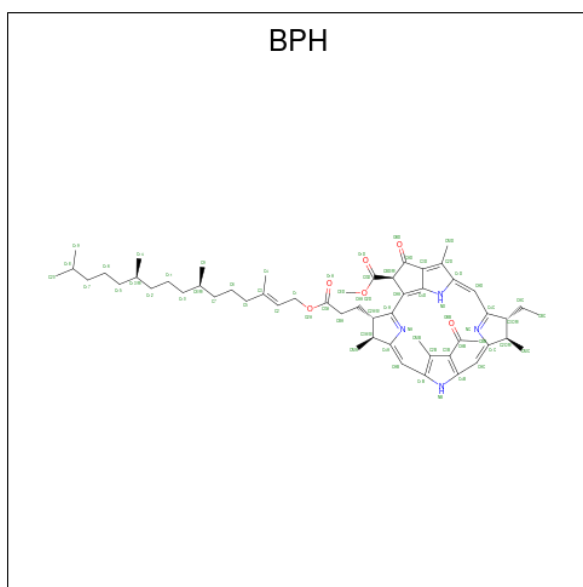
- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

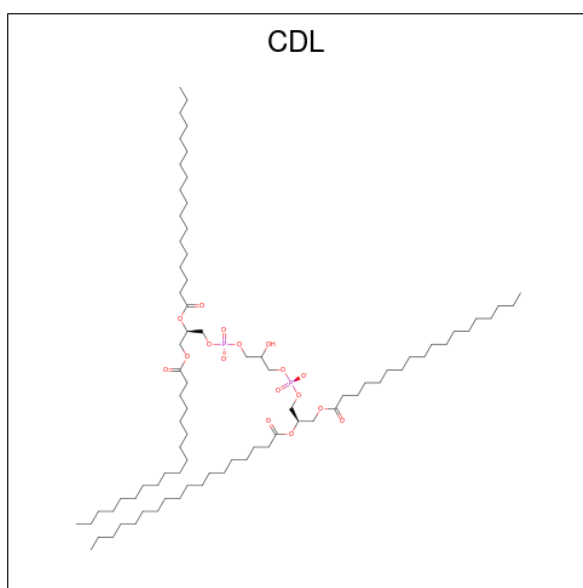
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Cl	0	0
			1	1		

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
10	M	1	10	8	2	0	0

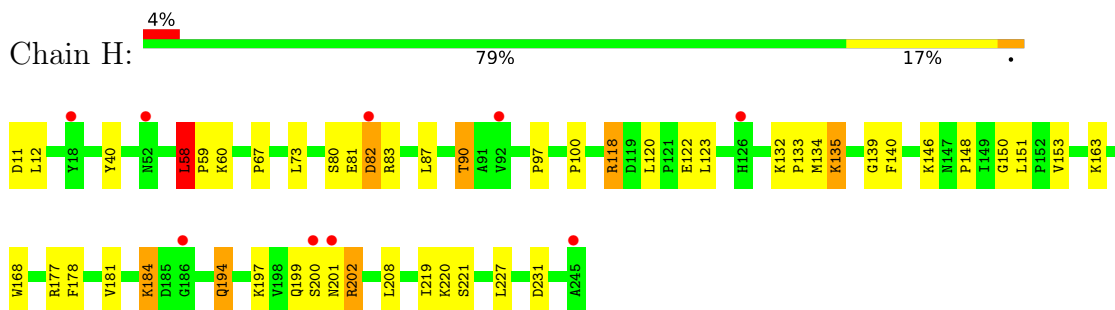
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	64	Total 64	O 64	0	0
11	L	43	Total 43	O 43	0	0
11	M	48	Total 48	O 48	0	0

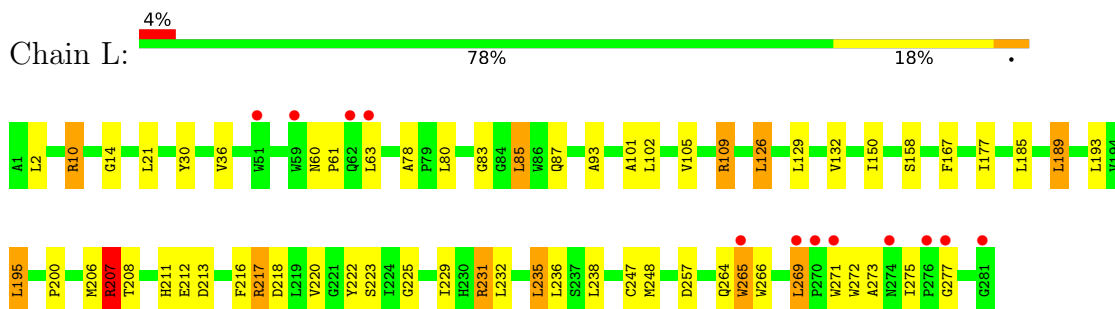
3 Residue-property plots [i](#)

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.

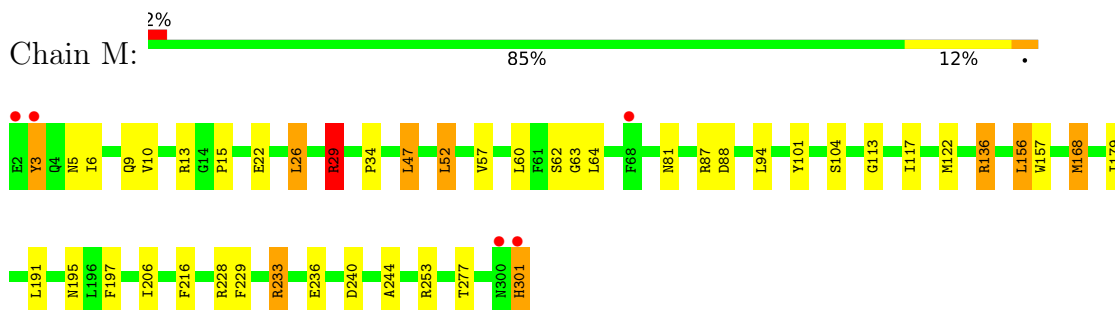
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.42Å 100.42Å 235.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.20 19.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.80-2.20) 99.6 (19.80-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.19Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.246 0.201 , 0.245	Depositor DCC
R_{free} test set	3129 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BCL, CDL, FE2, CL, LDA, U10, BPH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.92	2/1834 (0.1%)	0.89	5/2497 (0.2%)
2	L	0.92	1/2320 (0.0%)	0.98	13/3175 (0.4%)
3	M	0.91	0/2492	0.92	10/3401 (0.3%)
All	All	0.91	3/6646 (0.0%)	0.94	28/9073 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	30	TYR	CD1-CE1	-5.93	1.30	1.39
1	H	132	LYS	CE-NZ	5.41	1.62	1.49
1	H	132	LYS	CD-CE	5.15	1.64	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	207	ARG	NE-CZ-NH2	-14.31	113.14	120.30
3	M	136	ARG	NE-CZ-NH2	-12.97	113.81	120.30
3	M	136	ARG	NE-CZ-NH1	11.77	126.19	120.30
2	L	217	ARG	NE-CZ-NH1	10.68	125.64	120.30
3	M	253	ARG	NE-CZ-NH2	-10.07	115.26	120.30
2	L	207	ARG	NE-CZ-NH1	9.75	125.17	120.30
3	M	233	ARG	NE-CZ-NH1	-9.60	115.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	29	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	L	195	LEU	CB-CG-CD1	7.97	124.56	111.00
3	M	29	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	L	217	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	L	10	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	H	132	LYS	CD-CE-NZ	6.90	127.58	111.70
2	L	10	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	H	58	LEU	CA-CB-CG	6.56	130.38	115.30
3	M	240	ASP	CB-CG-OD1	6.43	124.09	118.30
1	H	118	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	L	235	LEU	CA-CB-CG	6.36	129.92	115.30
2	L	231	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	L	126	LEU	CB-CG-CD1	6.23	121.59	111.00
1	H	118	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	H	83	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	109	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	231	ARG	NE-CZ-NH1	5.59	123.10	120.30
3	M	26	LEU	CA-CB-CG	5.52	127.99	115.30
3	M	233	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	L	217	ARG	CB-CG-CD	5.30	125.39	111.60
3	M	240	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	80	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1787	0	1785	42	0
2	L	2232	0	2187	47	0
3	M	2400	0	2310	43	0
4	H	14	0	24	3	0
5	L	132	0	147	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	114	0	111	13	0
6	L	24	0	25	14	0
6	M	45	0	59	3	0
7	M	1	0	0	0	0
8	M	1	0	0	0	0
9	M	130	0	152	17	0
10	M	10	0	0	0	0
11	H	64	0	0	3	0
11	L	43	0	0	3	0
11	M	48	0	0	1	0
All	All	7045	0	6800	142	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 10.

All (142) 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:L:1306:U10:O3	6:L:1306:U10:H4M3	1.42	1.14
1:H:118:ARG:HD3	1:H:120:LEU:HD12	1.28	1.13
2:L:206:MET:O	11:L:1348:HOH:O	1.69	1.08
6:L:1306:U10:O3	6:L:1306:U10:C4M	2.14	0.95
1:H:90:THR:HB	1:H:97:PRO:O	1.65	0.95
3:M:122:MET:HE3	3:M:157:TRP:HE1	1.32	0.95
3:M:168:MET:HA	3:M:168:MET:CE	2.05	0.86
5:M:1303:BCL:HHC	5:M:1303:BCL:CBB	2.09	0.82
2:L:269:LEU:O	2:L:273:ALA:HB2	1.80	0.80
9:M:1304:BPH:H162	9:M:1304:BPH:H111	1.61	0.80
3:M:168:MET:HA	3:M:168:MET:HE3	1.65	0.77
1:H:118:ARG:CD	1:H:120:LEU:HD12	2.11	0.77
2:L:223:SER:OG	6:L:1306:U10:H4M1	1.85	0.77
3:M:197:PHE:CZ	5:M:1303:BCL:HBB2	2.20	0.76
1:H:194:GLN:CG	3:M:228:ARG:HA	2.16	0.76
5:M:1303:BCL:HHC	5:M:1303:BCL:HBB2	1.68	0.75
1:H:67:PRO:HG3	11:L:1348:HOH:O	1.88	0.74
1:H:81:GLU:HA	11:H:1339:HOH:O	1.87	0.73
1:H:40:TYR:OH	4:H:1310:LDA:CM1	2.36	0.72
1:H:194:GLN:HG3	3:M:228:ARG:HA	1.71	0.72
3:M:197:PHE:HZ	5:M:1303:BCL:HBB2	1.55	0.70
2:L:223:SER:OG	6:L:1306:U10:C4M	2.40	0.70
2:L:275:ILE:HG21	3:M:81:ASN:HD21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:177:ILE:HG12	5:L:1282:BCL:HMB3	1.73	0.69
5:M:1302:BCL:HBB3	5:M:1302:BCL:HMB1	1.74	0.69
1:H:150:GLY:HA2	1:H:163:LYS:HE2	1.75	0.69
2:L:269:LEU:HG	2:L:271:TRP:CZ2	2.27	0.69
3:M:63:GLY:HA3	9:M:1304:BPH:H5C2	1.75	0.69
1:H:40:TYR:OH	4:H:1310:LDA:HM13	1.93	0.68
3:M:122:MET:CE	3:M:157:TRP:HE1	2.06	0.68
3:M:64:LEU:CD2	9:M:1304:BPH:H121	2.24	0.67
2:L:189:LEU:HD13	9:M:1304:BPH:HMD2	1.76	0.67
3:M:64:LEU:HD23	9:M:1304:BPH:H102	1.78	0.66
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.77	0.65
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.12	0.65
1:H:146:LYS:NZ	1:H:200:SER:O	2.29	0.65
9:M:1304:BPH:H162	9:M:1304:BPH:C11	2.26	0.64
3:M:122:MET:HE3	3:M:157:TRP:NE1	2.09	0.63
1:H:184:LYS:HE3	1:H:184:LYS:HA	1.79	0.63
1:H:82:ASP:N	11:H:1339:HOH:O	2.33	0.62
2:L:211:HIS:HE1	3:M:22:GLU:OE1	1.82	0.61
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.82	0.60
1:H:140:PHE:HA	3:M:13:ARG:O	2.01	0.59
1:H:81:GLU:CA	11:H:1339:HOH:O	2.47	0.59
3:M:3:TYR:HD2	3:M:3:TYR:H	1.51	0.58
6:L:1306:U10:H3M2	11:L:1327:HOH:O	2.05	0.57
1:H:197:LYS:HA	3:M:9:GLN:HE22	1.69	0.56
3:M:52:LEU:HD13	3:M:57:VAL:HG23	1.85	0.56
3:M:64:LEU:HD23	9:M:1304:BPH:H121	1.86	0.56
9:M:1304:BPH:HBC2	9:M:1304:BPH:HHD	1.87	0.56
6:L:1306:U10:H4M3	6:L:1306:U10:C3M	2.32	0.56
1:H:184:LYS:HA	1:H:184:LYS:CE	2.36	0.56
2:L:264:GLN:C	2:L:266:TRP:H	2.08	0.56
1:H:11:ASP:HB3	3:M:301:HIS:HD2	1.71	0.55
2:L:277:GLY:O	3:M:87:ARG:NH2	2.39	0.55
5:M:1303:BCL:HHC	5:M:1303:BCL:HBB3	1.87	0.55
1:H:194:GLN:HG3	3:M:228:ARG:CA	2.35	0.54
1:H:40:TYR:OH	4:H:1310:LDA:HM11	2.06	0.54
3:M:168:MET:HA	3:M:168:MET:HE2	1.87	0.54
2:L:217:ARG:HD2	11:M:1318:HOH:O	2.07	0.54
5:M:1302:BCL:OBB	5:M:1302:BCL:HHC	2.08	0.54
1:H:122:GLU:HG3	3:M:236:GLU:HG3	1.90	0.54
1:H:194:GLN:HG2	3:M:228:ARG:HA	1.87	0.53
2:L:101:ALA:O	2:L:105:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:PRO:O	1:H:151:LEU:HB2	2.10	0.52
2:L:14:GLY:O	2:L:109:ARG:HD3	2.08	0.52
2:L:208:THR:H	2:L:211:HIS:CD2	2.27	0.52
3:M:101:TYR:O	3:M:104:SER:HB3	2.10	0.52
1:H:184:LYS:HE3	1:H:184:LYS:CA	2.39	0.52
5:L:1283:BCL:C4A	5:L:1283:BCL:HBA1	2.39	0.51
2:L:264:GLN:C	2:L:266:TRP:N	2.64	0.51
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.93	0.51
2:L:193:LEU:HD21	2:L:212:GLU:HB3	1.93	0.51
2:L:231:ARG:HD3	3:M:5:ASN:O	2.10	0.51
5:L:1282:BCL:H142	5:L:1283:BCL:HMB1	1.93	0.51
5:L:1282:BCL:NC	5:M:1303:BCL:HBB3	2.25	0.51
6:M:1305:U10:H4M2	6:M:1305:U10:O3	2.11	0.51
2:L:213:ASP:OD2	6:L:1306:U10:H4M1	2.11	0.50
2:L:225:GLY:C	6:L:1306:U10:H3M3	2.32	0.50
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.93	0.50
2:L:248:MET:HE2	5:L:1282:BCL:OBD	2.12	0.50
2:L:265:TRP:O	2:L:269:LEU:HD13	2.12	0.50
6:L:1306:U10:H1M1	6:L:1306:U10:C8	2.41	0.50
1:H:201:ASN:OD1	1:H:201:ASN:N	2.44	0.50
2:L:150:ILE:HG23	5:L:1283:BCL:HED1	1.93	0.49
1:H:11:ASP:HB3	3:M:301:HIS:CD2	2.47	0.49
2:L:105:VAL:O	2:L:109:ARG:HG3	2.13	0.49
2:L:208:THR:H	2:L:211:HIS:HD2	1.60	0.49
2:L:269:LEU:O	2:L:273:ALA:CB	2.57	0.49
3:M:87:ARG:HG2	3:M:88:ASP:OD1	2.13	0.48
1:H:194:GLN:HG3	3:M:228:ARG:N	2.28	0.48
2:L:264:GLN:O	2:L:266:TRP:N	2.47	0.48
2:L:80:LEU:HD22	2:L:85:LEU:HD13	1.95	0.47
2:L:222:TYR:HD2	6:L:1306:U10:H13	1.80	0.47
1:H:90:THR:CB	1:H:97:PRO:O	2.52	0.46
2:L:60:ASN:ND2	2:L:63:LEU:HD23	2.30	0.46
1:H:139:GLY:HA3	3:M:15:PRO:HD3	1.96	0.46
2:L:93:ALA:HA	9:M:1284:BPH:H9C2	1.98	0.46
2:L:229:ILE:HD13	6:L:1306:U10:H8	1.97	0.45
9:M:1284:BPH:HBB3	9:M:1284:BPH:CMB	2.46	0.45
3:M:206:ILE:HG12	5:M:1303:BCL:HMB3	1.99	0.45
9:M:1284:BPH:NC	9:M:1284:BPH:ND	2.64	0.45
2:L:61:PRO:O	2:L:150:ILE:HD12	2.17	0.45
2:L:185:LEU:HD13	9:M:1304:BPH:ND	2.31	0.45
1:H:11:ASP:CB	3:M:301:HIS:HD2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:225:GLY:O	6:L:1306:U10:H3M3	2.16	0.45
5:L:1282:BCL:OBB	5:L:1282:BCL:HHC	2.17	0.45
3:M:156:LEU:HD13	5:M:1303:BCL:H43	1.99	0.45
2:L:218:ASP:OD1	3:M:29:ARG:HD2	2.17	0.45
2:L:223:SER:HG	6:L:1306:U10:H4M1	1.81	0.44
2:L:231:ARG:HD2	3:M:6:ILE:O	2.18	0.44
5:L:1283:BCL:HBB3	9:M:1284:BPH:H141	1.98	0.44
1:H:153:VAL:HG21	1:H:181:VAL:HG22	1.99	0.44
2:L:207:ARG:N	2:L:207:ARG:HD2	2.31	0.44
2:L:207:ARG:HD2	2:L:207:ARG:HA	1.86	0.44
9:M:1304:BPH:CHD	9:M:1304:BPH:CBC	2.96	0.44
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.98	0.43
1:H:194:GLN:H	1:H:194:GLN:CD	2.20	0.43
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.00	0.43
2:L:189:LEU:CD1	9:M:1304:BPH:HMD2	2.44	0.43
5:L:1282:BCL:HMB1	5:L:1282:BCL:HBB3	2.00	0.43
2:L:78:ALA:H	2:L:87:GLN:HE22	1.67	0.43
3:M:34:PRO:O	3:M:47:LEU:HB2	2.18	0.43
9:M:1304:BPH:HHD	9:M:1304:BPH:CBC	2.49	0.42
6:M:1305:U10:O3	6:M:1305:U10:C4M	2.68	0.42
1:H:177:ARG:CZ	3:M:233:ARG:HD2	2.49	0.42
5:L:1282:BCL:H193	6:M:1305:U10:H252	2.01	0.42
5:L:1282:BCL:H2C	5:M:1303:BCL:H2C	2.02	0.42
2:L:223:SER:OG	6:L:1306:U10:O4	2.38	0.42
3:M:156:LEU:HD12	3:M:277:THR:HG22	2.02	0.42
1:H:58:LEU:HD22	1:H:59:PRO:HD2	2.02	0.42
5:M:1303:BCL:CBB	5:M:1303:BCL:CHC	2.82	0.42
1:H:219:ILE:HD12	1:H:221:SER:O	2.20	0.41
9:M:1284:BPH:H7C1	9:M:1284:BPH:H112	1.80	0.41
1:H:133:PRO:HB2	1:H:135:LYS:HE3	2.02	0.41
2:L:83:GLY:O	2:L:87:GLN:HG3	2.20	0.41
3:M:179:ILE:HG23	5:M:1302:BCL:HED1	2.02	0.41
5:L:1283:BCL:OBB	5:L:1283:BCL:HHC	2.21	0.40
3:M:113:GLY:O	3:M:117:ILE:HG13	2.20	0.40
2:L:232:LEU:O	2:L:236:LEU:HG	2.21	0.40
1:H:60:LYS:CD	1:H:60:LYS:N	2.85	0.40
1:H:199:GLN:OE1	1:H:202:ARG:HD3	2.20	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	233/235 (99%)	225 (97%)	8 (3%)	0	100	100
2	L	279/281 (99%)	265 (95%)	13 (5%)	1 (0%)	34	37
3	M	298/300 (99%)	288 (97%)	10 (3%)	0	100	100
All	All	810/816 (99%)	778 (96%)	31 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	265	TRP

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	190/190 (100%)	176 (93%)	14 (7%)	13	14
2	L	220/220 (100%)	198 (90%)	22 (10%)	7	7
3	M	236/236 (100%)	220 (93%)	16 (7%)	16	17
All	All	646/646 (100%)	594 (92%)	52 (8%)	12	12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	58	LEU

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Mol	Chain	Res	Type
1	H	73	LEU
1	H	82	ASP
1	H	90	THR
1	H	123	LEU
1	H	134	MET
1	H	135	LYS
1	H	184	LYS
1	H	194	GLN
1	H	202	ARG
1	H	208	LEU
1	H	220	LYS
1	H	231	ASP
2	L	2	LEU
2	L	10	ARG
2	L	21	LEU
2	L	36	VAL
2	L	85	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	132	VAL
2	L	158	SER
2	L	167	PHE
2	L	189	LEU
2	L	195	LEU
2	L	207	ARG
2	L	216	PHE
2	L	220	VAL
2	L	235	LEU
2	L	238	LEU
2	L	247	CYS
2	L	257	ASP
2	L	269	LEU
2	L	272	TRP
3	M	3	TYR
3	M	10	VAL
3	M	26	LEU
3	M	29	ARG
3	M	47	LEU
3	M	52	LEU
3	M	60	LEU
3	M	62	SER

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Mol	Chain	Res	Type
3	M	94	LEU
3	M	136	ARG
3	M	156	LEU
3	M	168	MET
3	M	191	LEU
3	M	195	ASN
3	M	216	PHE
3	M	301	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	194	GLN
2	L	87	GLN
2	L	211	HIS
2	L	258	GLN
3	M	9	GLN
3	M	195	ASN
3	M	301	HIS

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CDL	M	1309	-	8,8,99	1.77	3 (37%)	12,12,111	1.50	3 (25%)
9	BPH	M	1304	-	51,70,70	1.27	5 (9%)	52,101,101	2.05	15 (28%)
6	U10	M	1305	-	45,45,63	2.57	11 (24%)	54,57,79	1.90	16 (29%)
5	BCL	L	1283	2	64,74,74	1.85	12 (18%)	78,115,115	2.17	30 (38%)
5	BCL	M	1302	3	46,56,74	1.86	12 (26%)	56,93,115	2.31	19 (33%)
9	BPH	M	1284	-	51,70,70	1.34	4 (7%)	52,101,101	1.79	18 (34%)
6	U10	L	1306	-	24,24,63	2.55	7 (29%)	29,32,79	2.70	14 (48%)
5	BCL	L	1282	2	64,74,74	1.48	10 (15%)	78,115,115	2.07	22 (28%)
5	BCL	M	1303	3	64,74,74	1.81	9 (14%)	78,115,115	2.18	23 (29%)
4	LDA	H	1310	-	10,13,15	2.11	1 (10%)	12,15,17	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BPH	M	1304	-	1/1/18/22	17/37/105/105	0/5/6/6
6	U10	M	1305	-	-	10/42/66/87	0/1/1/1
5	BCL	L	1283	2	2/2/21/25	10/37/137/137	-
5	BCL	M	1302	3	-	2/16/116/137	-
9	BPH	M	1284	-	1/1/18/22	11/37/105/105	0/5/6/6
6	U10	L	1306	-	-	6/17/41/87	0/1/1/1
5	BCL	L	1282	2	2/2/21/25	15/37/137/137	-
5	BCL	M	1303	3	2/2/21/25	6/37/137/137	-
4	LDA	H	1310	-	-	4/11/11/13	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1305	U10	C28-C29	6.88	1.49	1.33
5	M	1303	BCL	MG-NA	6.86	2.22	2.06
4	H	1310	LDA	O1-N1	-6.54	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1305	U10	C33-C34	6.52	1.48	1.33
5	L	1283	BCL	MG-NC	-6.21	1.91	2.06
6	L	1306	U10	C13-C14	6.17	1.47	1.33
5	M	1303	BCL	MG-ND	-6.01	1.93	2.05
6	M	1305	U10	C18-C19	5.91	1.47	1.33
6	M	1305	U10	C8-C9	5.83	1.47	1.33
6	L	1306	U10	C8-C9	5.69	1.46	1.33
6	L	1306	U10	O4-C4	-5.59	1.23	1.36
6	M	1305	U10	C23-C24	5.55	1.46	1.33
6	M	1305	U10	C13-C14	5.51	1.46	1.33
5	L	1283	BCL	MG-NA	5.35	2.19	2.06
5	M	1302	BCL	O2A-CGA	5.31	1.48	1.33
5	L	1282	BCL	MG-NA	5.10	2.18	2.06
9	M	1304	BPH	O2D-CGD	4.97	1.45	1.33
5	M	1303	BCL	O2D-CGD	4.89	1.45	1.33
9	M	1284	BPH	O2D-CGD	4.87	1.45	1.33
5	M	1302	BCL	O2D-CGD	4.68	1.44	1.33
5	L	1283	BCL	O2A-CGA	4.65	1.46	1.33
5	L	1282	BCL	O2D-CGD	4.62	1.44	1.33
5	L	1282	BCL	C3D-C4D	-4.61	1.33	1.44
5	M	1302	BCL	C3D-C4D	-4.58	1.33	1.44
9	M	1284	BPH	OBD-CAD	4.58	1.28	1.22
6	M	1305	U10	O4-C4	-4.57	1.25	1.36
5	M	1303	BCL	C3D-C4D	-4.26	1.34	1.44
5	L	1283	BCL	OBD-CAD	4.23	1.29	1.22
9	M	1304	BPH	OBD-CAD	4.22	1.28	1.22
5	L	1283	BCL	C3D-C4D	-4.20	1.34	1.44
5	L	1283	BCL	O2D-CGD	4.17	1.43	1.33
6	L	1306	U10	O3-C3	-4.09	1.26	1.36
9	M	1284	BPH	C3A-C2A	-4.05	1.51	1.54
5	M	1303	BCL	O2A-CGA	4.05	1.45	1.33
9	M	1284	BPH	O2A-CGA	3.84	1.44	1.33
6	M	1305	U10	O3-C3	-3.72	1.27	1.36
5	M	1302	BCL	OBD-CAD	3.34	1.28	1.22
5	M	1303	BCL	C4D-ND	-3.31	1.33	1.37
9	M	1304	BPH	O2A-CGA	3.27	1.42	1.33
6	M	1305	U10	C6-C1	3.13	1.40	1.35
6	L	1306	U10	C6-C1	3.11	1.40	1.35
5	L	1282	BCL	O2A-CGA	3.07	1.42	1.33
5	L	1283	BCL	C4B-NB	3.06	1.37	1.35
5	L	1282	BCL	C4D-CHA	3.00	1.49	1.38
5	M	1303	BCL	C1B-NB	2.98	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1283	BCL	C4D-ND	-2.95	1.33	1.37
5	L	1283	BCL	CAA-C2A	2.95	1.59	1.54
5	M	1303	BCL	C4D-CHA	2.91	1.48	1.38
5	L	1283	BCL	C3C-C4C	-2.78	1.48	1.51
5	L	1282	BCL	C3C-C4C	-2.76	1.48	1.51
5	M	1302	BCL	MG-ND	-2.70	2.00	2.05
5	L	1282	BCL	C1B-NB	2.66	1.37	1.35
9	M	1304	BPH	C2C-C3C	-2.66	1.52	1.54
10	M	1309	CDL	PB2-OB5	2.66	1.62	1.54
6	M	1305	U10	C3-C2	-2.51	1.41	1.48
10	M	1309	CDL	PA1-OA3	-2.47	1.45	1.50
9	M	1304	BPH	C3A-C2A	-2.46	1.52	1.54
5	M	1303	BCL	OBD-CAD	2.41	1.26	1.22
5	M	1302	BCL	C1B-NB	2.41	1.37	1.35
5	L	1282	BCL	MG-NC	2.40	2.12	2.06
5	M	1302	BCL	C3C-C4C	-2.36	1.48	1.51
5	M	1302	BCL	C4D-CHA	2.33	1.46	1.38
5	M	1302	BCL	C4D-ND	-2.33	1.34	1.37
5	L	1283	BCL	C2A-C1A	-2.28	1.47	1.52
5	L	1283	BCL	C4D-CHA	2.20	1.46	1.38
6	M	1305	U10	C6-C5	-2.20	1.40	1.46
6	L	1306	U10	O5-C5	2.20	1.28	1.23
10	M	1309	CDL	PA1-OA4	-2.19	1.48	1.54
5	M	1302	BCL	MG-NA	2.17	2.11	2.06
5	L	1282	BCL	C2A-C1A	-2.16	1.47	1.52
5	L	1282	BCL	C4D-ND	-2.14	1.34	1.37
5	M	1302	BCL	MG-NC	2.13	2.11	2.06
6	L	1306	U10	C4-C5	-2.07	1.42	1.48
5	M	1302	BCL	C2A-C1A	-2.03	1.47	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1304	BPH	O2D-CGD-CBD	7.20	120.12	111.00
5	L	1282	BCL	CMB-C2B-C1B	-6.82	117.98	128.46
5	L	1283	BCL	CMB-C2B-C1B	-6.57	118.36	128.46
9	M	1284	BPH	O2D-CGD-CBD	6.53	119.28	111.00
5	M	1302	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
5	L	1282	BCL	CMB-C2B-C3B	6.17	136.23	124.68
5	L	1282	BCL	CAC-C3C-C4C	-6.14	98.97	112.58
5	M	1302	BCL	CMB-C2B-C3B	6.09	136.08	124.68
6	L	1306	U10	C15-C14-C16	6.07	122.92	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	C4A-NA-C1A	5.82	109.32	106.71
5	L	1283	BCL	O2D-CGD-CBD	5.74	121.47	111.27
6	L	1306	U10	C7-C8-C9	-5.63	117.42	126.79
5	L	1283	BCL	CMB-C2B-C3B	5.20	134.41	124.68
9	M	1304	BPH	C4-C3-C5	5.20	124.02	115.27
5	M	1303	BCL	O2D-CGD-O1D	-5.07	113.93	123.84
5	M	1303	BCL	CED-O2D-CGD	5.06	127.38	115.94
5	M	1303	BCL	O2D-CGD-CBD	5.04	120.22	111.27
5	M	1303	BCL	CAC-C3C-C2C	-5.02	101.72	114.26
5	M	1303	BCL	CMB-C2B-C1B	-4.99	120.79	128.46
6	M	1305	U10	C25-C24-C26	4.94	123.57	115.27
6	L	1306	U10	C6-C1-C2	4.90	123.05	119.18
5	M	1302	BCL	C1-O2A-CGA	4.69	130.37	116.73
5	L	1283	BCL	C2C-C3C-C4C	4.66	108.32	101.34
5	L	1283	BCL	CAC-C3C-C2C	-4.48	103.07	114.26
5	M	1303	BCL	CMB-C2B-C3B	4.48	133.05	124.68
5	M	1302	BCL	O2D-CGD-CBD	4.38	119.05	111.27
6	L	1306	U10	C1M-C1-C6	-4.35	117.31	124.40
9	M	1304	BPH	CMA-C3A-C4A	-4.33	104.90	114.38
5	L	1282	BCL	C2D-C1D-ND	-4.28	106.95	110.10
9	M	1304	BPH	CED-O2D-CGD	4.25	125.55	115.94
9	M	1304	BPH	C5-C3-C2	-4.15	112.73	121.12
6	M	1305	U10	C15-C14-C16	4.12	122.20	115.27
5	M	1302	BCL	O2A-CGA-CBA	4.02	124.53	111.91
5	M	1303	BCL	CMC-C2C-C1C	-4.01	101.00	111.77
5	M	1303	BCL	C1C-NC-C4C	3.99	108.50	106.71
6	M	1305	U10	C17-C18-C19	-3.95	118.15	127.66
5	L	1282	BCL	C2A-C3A-C4A	3.82	108.05	101.87
5	M	1303	BCL	CAC-C3C-C4C	-3.73	104.31	112.58
5	L	1283	BCL	CAA-C2A-C3A	-3.72	102.58	112.78
6	L	1306	U10	C10-C9-C11	3.72	121.53	115.27
5	M	1303	BCL	CMC-C2C-C3C	-3.62	99.24	113.83
5	M	1302	BCL	C2D-C1D-ND	-3.60	107.45	110.10
5	M	1302	BCL	C3A-C2A-C1A	3.57	106.68	101.34
5	M	1303	BCL	C2D-C1D-ND	-3.53	107.50	110.10
6	M	1305	U10	C36-C34-C33	3.48	128.16	121.12
5	L	1282	BCL	C1-O2A-CGA	3.43	125.43	116.44
5	L	1283	BCL	C1-O2A-CGA	3.38	125.31	116.44
6	L	1306	U10	O3-C3-C2	3.36	127.93	116.56
5	M	1302	BCL	CAA-C2A-C3A	-3.33	103.66	112.78
5	M	1303	BCL	O2A-CGA-CBA	3.33	122.34	111.91
6	L	1306	U10	C3M-O3-C3	3.31	128.20	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C2C-C3C-C4C	3.30	106.28	101.34
6	M	1305	U10	C35-C34-C33	-3.27	115.30	123.68
5	M	1302	BCL	C4B-C3B-CAB	-3.26	120.83	127.13
5	L	1283	BCL	O2A-CGA-CBA	3.24	122.07	111.91
6	L	1306	U10	C7-C6-C5	3.17	122.29	118.48
5	M	1302	BCL	CMA-C3A-C2A	-3.16	101.09	113.83
5	L	1283	BCL	CMC-C2C-C3C	-3.16	101.10	113.83
5	L	1283	BCL	CAA-CBA-CGA	3.14	122.43	113.25
5	L	1283	BCL	C2D-C1D-ND	-3.12	107.80	110.10
5	L	1282	BCL	CMA-C3A-C4A	-3.11	103.41	111.77
5	L	1282	BCL	CMA-C3A-C2A	-3.09	101.38	113.83
5	M	1302	BCL	O2A-C1-C2	3.08	119.75	108.42
5	L	1282	BCL	CAC-C3C-C2C	-3.07	106.59	114.26
6	L	1306	U10	O3-C3-C4	-3.06	112.09	123.64
9	M	1284	BPH	C1-O2A-CGA	3.04	124.42	116.44
9	M	1284	BPH	O2D-CGD-O1D	-3.03	117.91	123.84
6	M	1305	U10	C4M-O4-C4	3.00	127.09	116.47
5	M	1303	BCL	C3C-C2C-C1C	2.98	106.69	101.87
6	M	1305	U10	C37-C36-C34	2.98	119.49	114.62
5	L	1282	BCL	C4B-C3B-CAB	-2.97	121.39	127.13
5	L	1283	BCL	CMA-C3A-C2A	-2.97	101.85	113.83
9	M	1304	BPH	CAC-C3C-C4C	2.96	120.36	113.73
9	M	1304	BPH	C1-O2A-CGA	2.90	124.06	116.44
9	M	1304	BPH	CMB-C2B-C3B	2.90	130.10	124.68
5	M	1303	BCL	C2A-C3A-C4A	2.88	106.53	101.87
6	L	1306	U10	O4-C4-C3	-2.88	112.77	123.64
9	M	1304	BPH	O1D-CGD-CBD	-2.84	120.00	124.74
5	L	1283	BCL	C1C-NC-C4C	2.83	107.98	106.71
5	M	1303	BCL	CHA-C1A-NA	-2.80	119.98	126.40
5	L	1282	BCL	O2A-CGA-CBA	2.79	120.67	111.91
5	L	1283	BCL	C4-C3-C5	2.77	119.93	115.27
5	M	1302	BCL	O1D-CGD-CBD	-2.77	118.82	124.48
5	L	1283	BCL	O2A-CGA-O1A	-2.73	116.69	123.59
5	L	1282	BCL	CHA-C1A-NA	-2.73	120.14	126.40
6	M	1305	U10	C3M-O3-C3	2.73	126.13	116.47
5	L	1283	BCL	CHD-C1D-ND	-2.72	121.95	124.45
9	M	1284	BPH	CAA-C2A-C3A	-2.72	105.33	112.78
6	M	1305	U10	C16-C14-C13	-2.70	115.64	121.12
5	M	1302	BCL	C3C-C2C-C1C	2.67	106.17	101.87
5	L	1282	BCL	C4-C3-C5	2.66	119.75	115.27
5	M	1302	BCL	C2A-C1A-CHA	2.66	128.51	123.86
5	M	1302	BCL	CBB-CAB-C3B	-2.66	112.45	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1283	BCL	CAC-C3C-C4C	-2.65	106.69	112.58
5	M	1303	BCL	C2A-C1A-CHA	2.65	128.50	123.86
5	L	1283	BCL	C3D-C4D-ND	2.65	114.52	110.24
9	M	1304	BPH	O2A-CGA-O1A	-2.65	116.91	123.59
10	M	1309	CDL	OB5-PB2-OB2	-2.62	99.56	107.97
5	L	1283	BCL	O1D-CGD-CBD	-2.61	119.15	124.48
5	L	1282	BCL	CHA-C4D-ND	2.61	137.95	132.50
6	L	1306	U10	C12-C13-C14	-2.58	121.46	127.66
5	L	1283	BCL	C1D-ND-C4D	-2.56	104.52	106.33
5	L	1282	BCL	O2D-CGD-CBD	2.55	115.79	111.27
6	L	1306	U10	C15-C14-C13	-2.54	117.15	123.68
9	M	1284	BPH	CED-O2D-CGD	2.53	121.66	115.94
5	L	1282	BCL	C1C-NC-C4C	2.53	107.84	106.71
9	M	1304	BPH	OBD-CAD-CBD	-2.50	122.16	125.82
9	M	1284	BPH	C6-C7-C8	-2.49	107.87	115.92
9	M	1304	BPH	C4B-NB-C1B	-2.49	101.99	107.09
5	M	1303	BCL	C2C-C3C-C4C	2.48	105.06	101.34
6	M	1305	U10	C30-C29-C31	2.48	119.44	115.27
9	M	1284	BPH	O2A-CGA-CBA	2.46	119.62	111.91
9	M	1284	BPH	CMA-C3A-C4A	-2.46	108.99	114.38
6	M	1305	U10	C1M-C1-C6	-2.45	120.40	124.40
5	L	1282	BCL	C4A-NA-C1A	2.43	107.80	106.71
5	L	1283	BCL	C4B-C3B-CAB	-2.43	122.44	127.13
6	M	1305	U10	C27-C28-C29	-2.42	121.82	127.66
5	M	1303	BCL	CGD-CBD-CAD	-2.42	102.91	110.73
9	M	1284	BPH	C4C-C3C-C2C	-2.34	100.62	102.84
5	L	1282	BCL	O2A-CGA-O1A	-2.32	117.73	123.59
10	M	1309	CDL	OA5-PA1-OA3	-2.32	102.41	110.89
6	M	1305	U10	C32-C33-C34	-2.31	122.10	127.66
9	M	1284	BPH	CMB-C2B-C3B	2.30	128.98	124.68
5	L	1283	BCL	O2D-CGD-O1D	-2.30	119.35	123.84
5	M	1302	BCL	O2A-CGA-O1A	-2.29	117.81	123.59
9	M	1284	BPH	C4-C3-C5	2.29	119.12	115.27
5	L	1283	BCL	C16-C17-C18	-2.29	105.19	115.98
5	L	1283	BCL	CHD-C4C-NC	2.28	127.60	125.08
9	M	1304	BPH	C4A-C3A-C2A	-2.26	100.69	102.84
5	M	1302	BCL	OBB-CAB-C3B	2.26	124.01	119.99
5	L	1283	BCL	CHD-C1D-C2D	2.26	130.22	125.48
10	M	1309	CDL	OA4-PA1-OA2	2.25	115.20	107.97
5	L	1283	BCL	C5-C3-C2	-2.25	116.56	121.12
5	M	1303	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
6	L	1306	U10	C8-C7-C6	2.22	118.04	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1284	BPH	C1C-C2C-C3C	-2.22	100.73	102.84
5	L	1283	BCL	C1B-CHB-C4A	-2.21	125.73	130.12
5	L	1282	BCL	C14-C13-C12	2.20	119.27	111.29
9	M	1284	BPH	CBA-CAA-C2A	-2.19	107.41	113.81
5	M	1303	BCL	O2A-CGA-O1A	-2.16	118.14	123.59
9	M	1304	BPH	C3D-CAD-CBD	2.16	110.44	107.61
6	M	1305	U10	C7-C8-C9	-2.15	123.21	126.79
9	M	1284	BPH	C4B-NB-C1B	-2.15	102.69	107.09
5	L	1283	BCL	C2A-C3A-C4A	2.14	105.33	101.87
5	L	1282	BCL	C16-C15-C13	2.13	122.79	115.92
5	L	1283	BCL	C3A-C2A-C1A	2.12	104.51	101.34
9	M	1284	BPH	O2A-CGA-O1A	-2.12	118.25	123.59
6	M	1305	U10	C26-C24-C23	-2.11	116.84	121.12
5	M	1303	BCL	CHC-C1C-NC	2.10	127.42	124.51
5	L	1283	BCL	CAA-C2A-C1A	-2.10	105.09	111.97
6	L	1306	U10	O4-C4-C5	2.10	123.66	116.56
5	L	1282	BCL	C11-C12-C13	2.09	122.69	115.92
9	M	1284	BPH	C4A-C3A-C2A	-2.09	100.85	102.84
5	M	1303	BCL	C7-C6-C5	-2.07	107.75	113.36
5	M	1302	BCL	CHA-C1A-NA	-2.06	121.68	126.40
9	M	1284	BPH	C5-C3-C2	-2.05	116.98	121.12
9	M	1284	BPH	OBD-CAD-CBD	-2.04	122.83	125.82
9	M	1304	BPH	O2D-CGD-O1D	-2.03	119.88	123.84
6	M	1305	U10	C22-C23-C24	-2.02	122.81	127.66
5	M	1302	BCL	C3D-C4D-ND	2.00	113.48	110.24

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1283	BCL	C8
5	L	1283	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13
9	M	1284	BPH	C8
9	M	1304	BPH	C8

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1310	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
4	H	1310	LDA	C2-C1-N1-CM2
5	L	1282	BCL	C14-C13-C15-C16
5	M	1303	BCL	C6-C7-C8-C10
6	L	1306	U10	C7-C8-C9-C10
6	L	1306	U10	C7-C8-C9-C11
6	L	1306	U10	C12-C13-C14-C15
6	L	1306	U10	C12-C13-C14-C16
6	M	1305	U10	C32-C33-C34-C35
6	M	1305	U10	C32-C33-C34-C36
6	M	1305	U10	C34-C36-C37-C38
9	M	1304	BPH	C4C-C3C-CAC-CBC
9	M	1304	BPH	C2-C3-C5-C6
9	M	1304	BPH	C4-C3-C5-C6
9	M	1304	BPH	C3-C5-C6-C7
9	M	1284	BPH	C3-C5-C6-C7
5	L	1283	BCL	CBD-CGD-O2D-CED
6	M	1305	U10	C29-C31-C32-C33
5	L	1282	BCL	C11-C12-C13-C14
5	L	1283	BCL	C6-C7-C8-C9
9	M	1304	BPH	C13-C15-C16-C17
9	M	1304	BPH	C15-C16-C17-C18
9	M	1284	BPH	C8-C10-C11-C12
5	L	1282	BCL	C11-C10-C8-C7
9	M	1284	BPH	C11-C10-C8-C7
9	M	1304	BPH	C8-C10-C11-C12
5	L	1282	BCL	C15-C16-C17-C18
9	M	1284	BPH	C5-C6-C7-C8
5	L	1283	BCL	C16-C17-C18-C20
5	M	1303	BCL	C6-C7-C8-C9
5	M	1303	BCL	C14-C13-C15-C16
9	M	1284	BPH	C11-C12-C13-C14
4	H	1310	LDA	C6-C7-C8-C9
6	M	1305	U10	C35-C34-C36-C37
6	M	1305	U10	C33-C34-C36-C37
5	L	1282	BCL	C5-C6-C7-C8
9	M	1284	BPH	C2-C3-C5-C6
9	M	1284	BPH	C11-C12-C13-C15
9	M	1304	BPH	C6-C7-C8-C10
5	L	1283	BCL	C16-C17-C18-C19
5	L	1282	BCL	C10-C11-C12-C13
9	M	1304	BPH	C6-C7-C8-C9
9	M	1304	BPH	C2C-C3C-CAC-CBC

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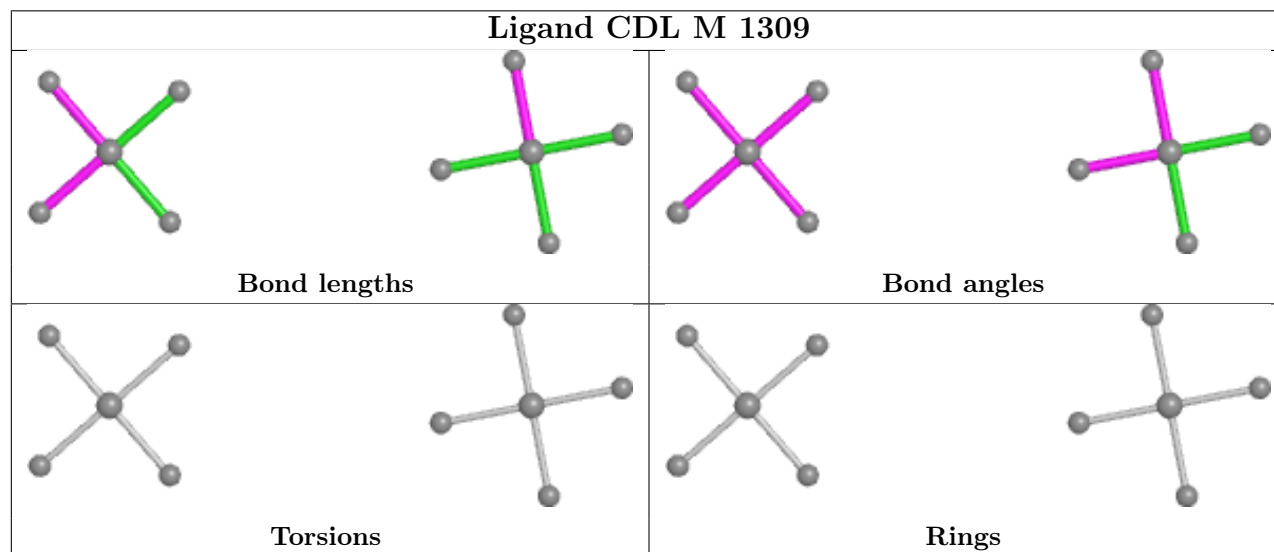
Mol	Chain	Res	Type	Atoms
5	L	1282	BCL	C13-C15-C16-C17
5	L	1283	BCL	C3-C5-C6-C7
9	M	1284	BPH	C4-C3-C5-C6
5	L	1283	BCL	O1D-CGD-O2D-CED
9	M	1284	BPH	C11-C10-C8-C9
5	M	1303	BCL	C12-C13-C15-C16
5	L	1282	BCL	CAD-CBD-CGD-O2D
9	M	1284	BPH	CAD-CBD-CGD-O2D
9	M	1304	BPH	CAD-CBD-CGD-O2D
5	L	1282	BCL	C11-C10-C8-C9
5	L	1282	BCL	C2A-CAA-CBA-CGA
5	L	1283	BCL	C2-C1-O2A-CGA
4	H	1310	LDA	C2-C1-N1-O1
5	L	1282	BCL	C8-C10-C11-C12
9	M	1304	BPH	C5-C6-C7-C8
9	M	1304	BPH	C12-C13-C15-C16
5	L	1283	BCL	C5-C6-C7-C8
6	M	1305	U10	C14-C16-C17-C18
5	L	1283	BCL	C13-C15-C16-C17
5	L	1282	BCL	C6-C7-C8-C9
9	M	1284	BPH	O2A-C1-C2-C3
9	M	1304	BPH	O2A-C1-C2-C3
6	M	1305	U10	C30-C29-C31-C32
5	L	1282	BCL	C11-C12-C13-C15
6	M	1305	U10	C5-C4-O4-C4M
6	L	1306	U10	C15-C14-C16-C17
5	L	1282	BCL	C16-C17-C18-C20
6	L	1306	U10	C5-C4-O4-C4M
9	M	1304	BPH	C11-C10-C8-C9
5	M	1302	BCL	CAD-CBD-CGD-O2D
5	L	1282	BCL	C2-C1-O2A-CGA
5	M	1302	BCL	C2-C1-O2A-CGA
9	M	1304	BPH	O1D-CGD-O2D-CED
5	L	1283	BCL	CHA-CBD-CGD-O2D
5	M	1303	BCL	CAA-CBA-CGA-O2A
9	M	1304	BPH	C2-C1-O2A-CGA
5	M	1303	BCL	CAD-CBD-CGD-O1D
6	M	1305	U10	C28-C29-C31-C32

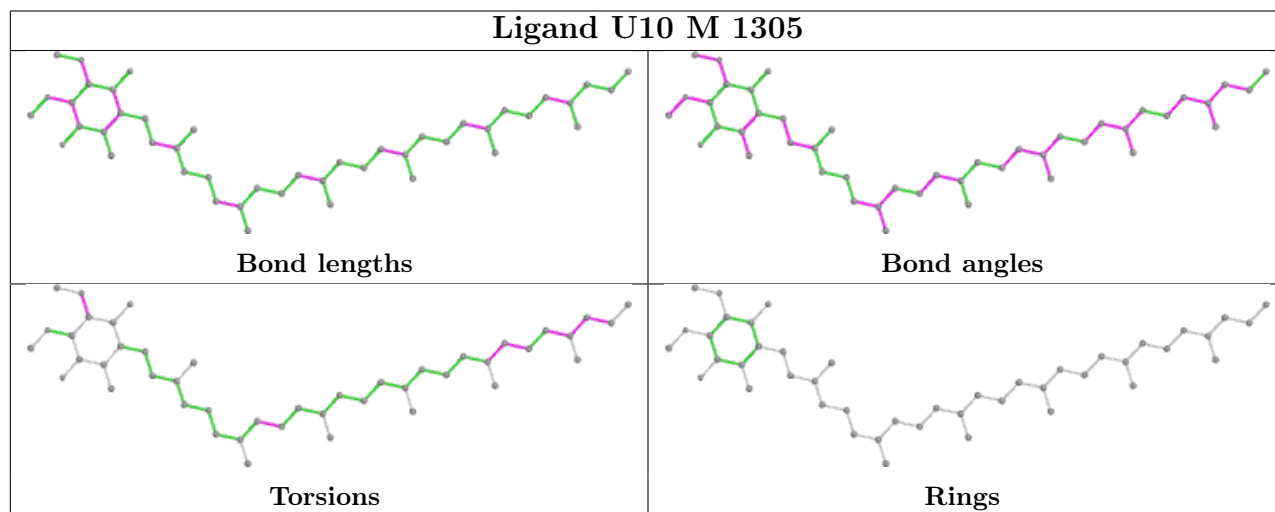
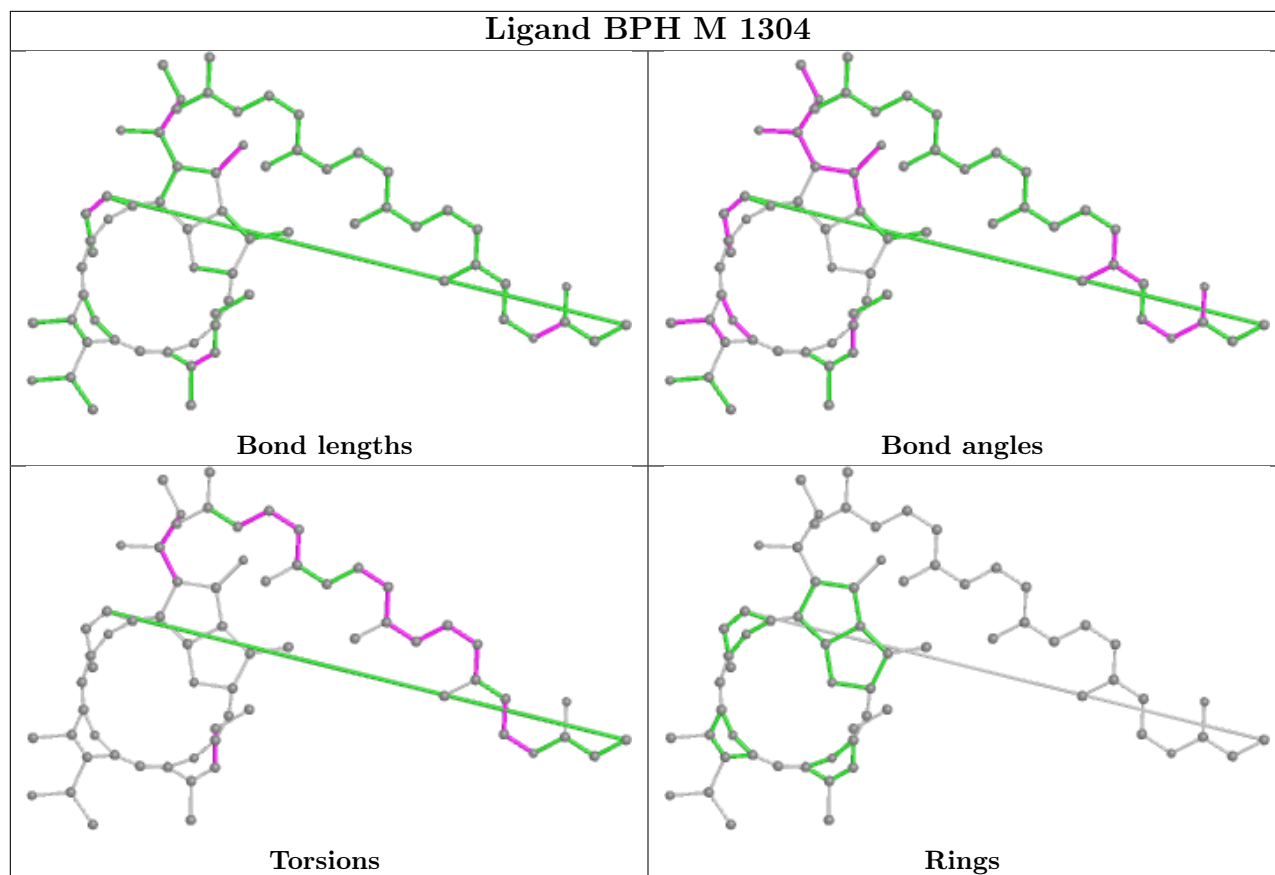
There are no ring outliers.

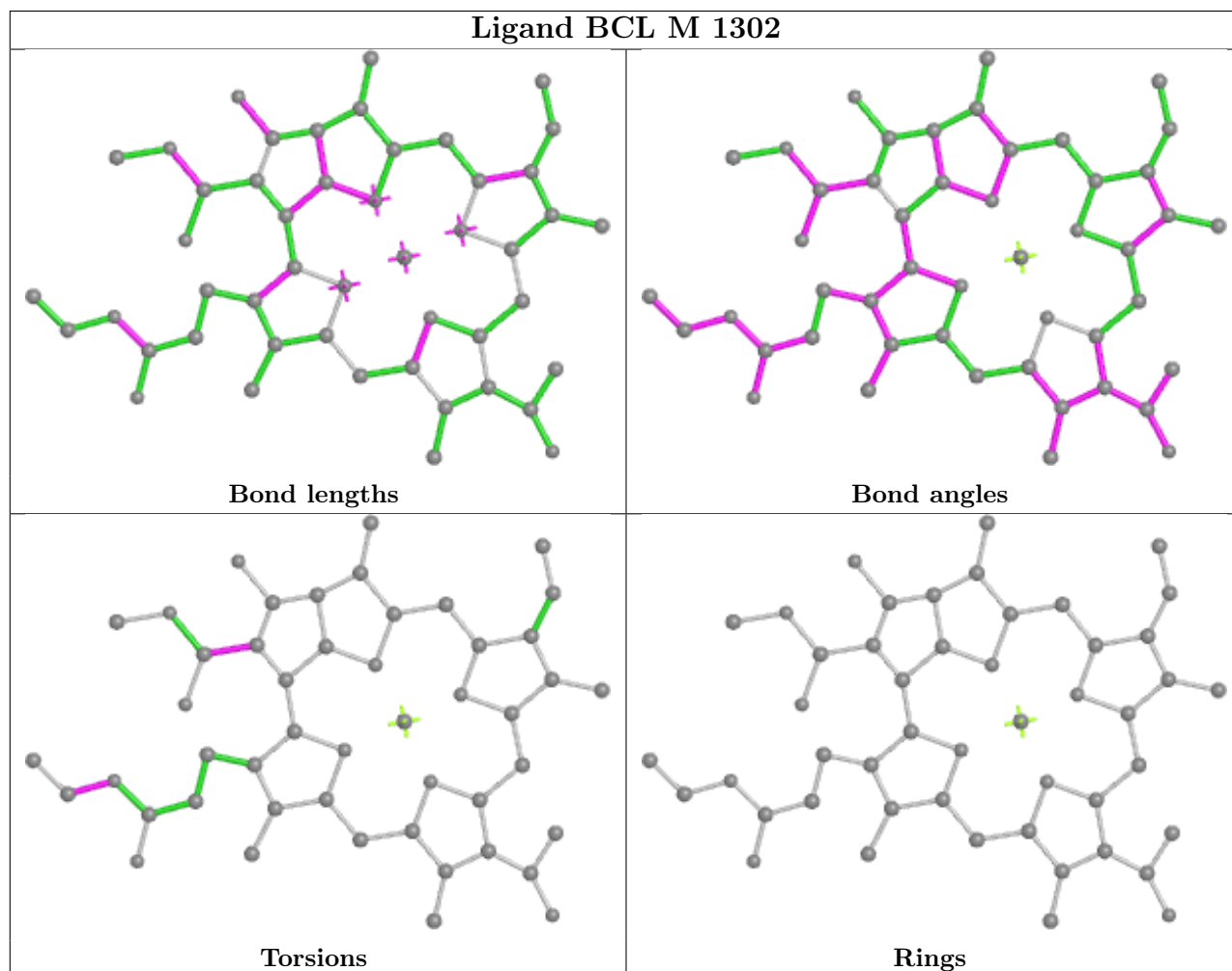
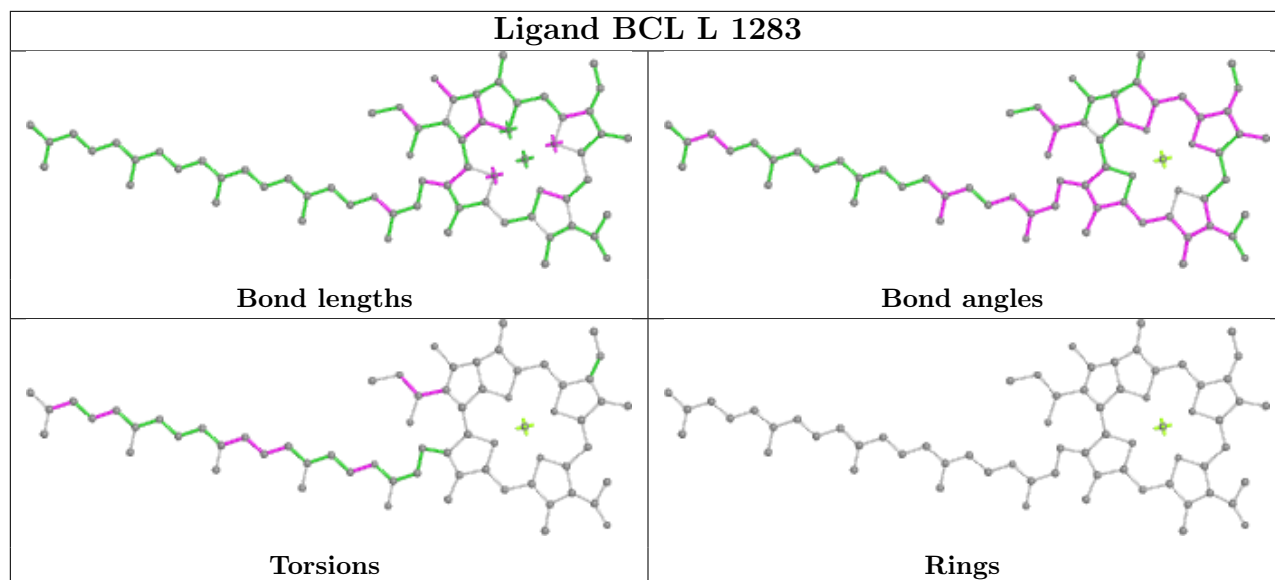
9 monomers are involved in 58 short contacts:

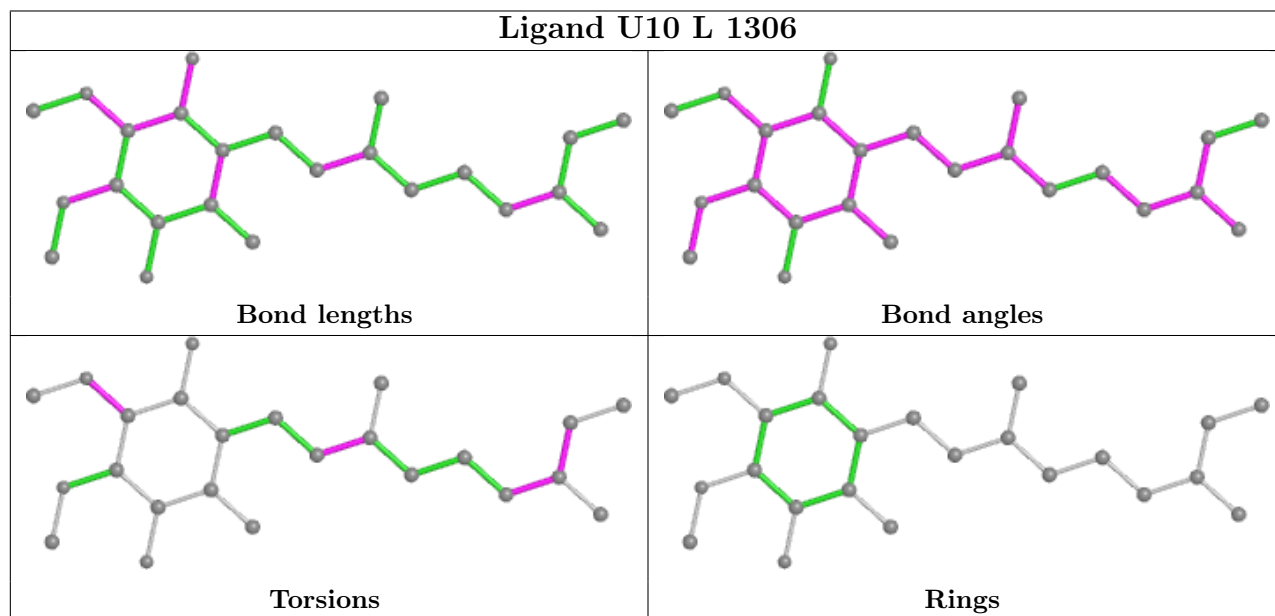
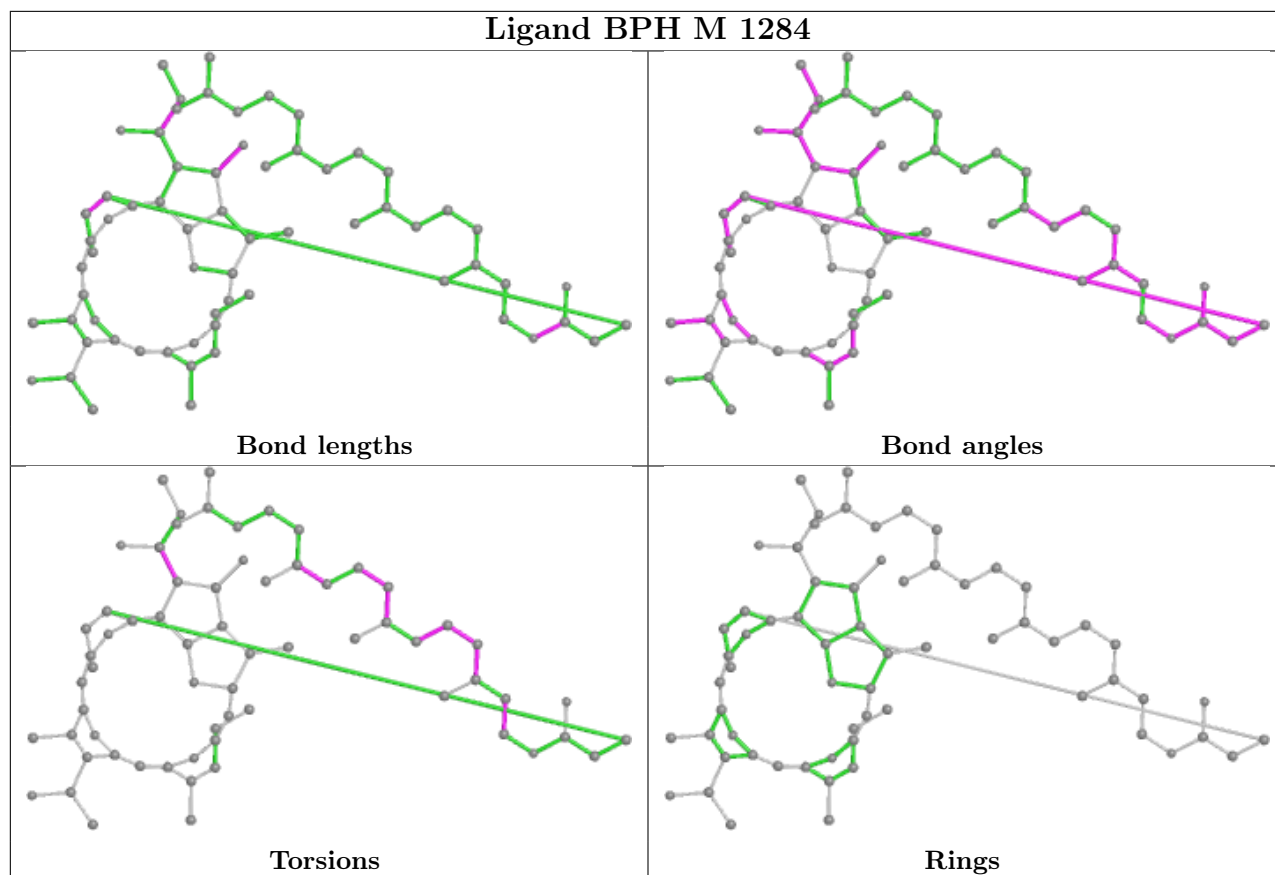
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1304	BPH	12	0
6	M	1305	U10	3	0
5	L	1283	BCL	5	0
5	M	1302	BCL	3	0
9	M	1284	BPH	5	0
6	L	1306	U10	14	0
5	L	1282	BCL	8	0
5	M	1303	BCL	10	0
4	H	1310	LDA	3	0

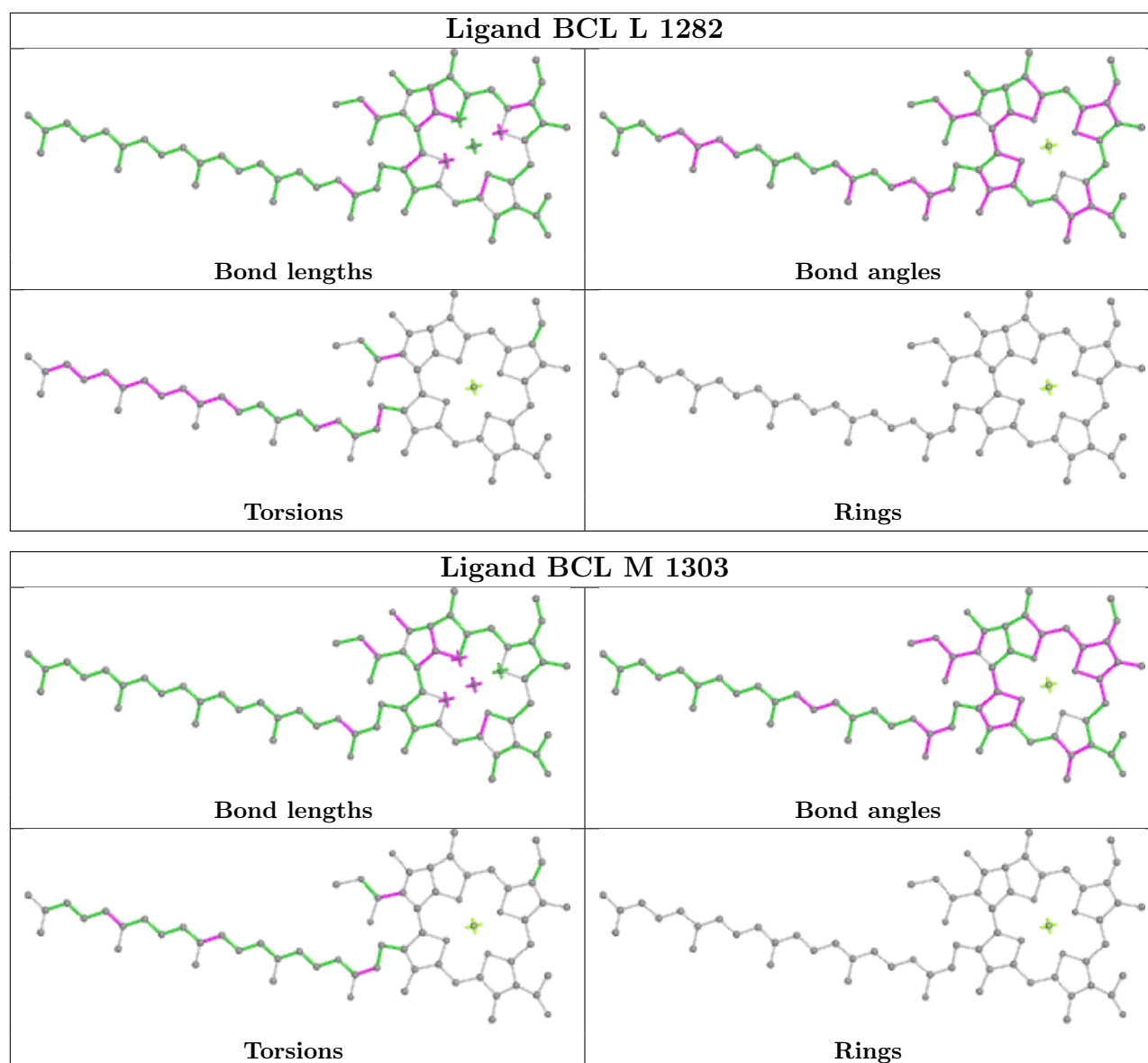
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.











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

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, 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	235/235 (100%)	-0.20	9 (3%) 40 38	13, 28, 45, 50	0
2	L	281/281 (100%)	-0.30	12 (4%) 35 33	9, 24, 59, 65	0
3	M	300/300 (100%)	-0.51	5 (1%) 70 68	9, 23, 46, 68	0
All	All	816/816 (100%)	-0.35	26 (3%) 47 45	9, 25, 47, 68	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	281	GLY	6.6
2	L	59	TRP	5.9
3	M	301	HIS	5.6
2	L	276	PRO	5.0
3	M	300	ASN	4.4
1	H	245	ALA	4.3
2	L	265	TRP	4.2
2	L	270	PRO	3.8
2	L	277	GLY	3.8
1	H	92	VAL	3.7
2	L	274	ASN	3.4
2	L	51	TRP	3.1
2	L	62	GLN	2.8
1	H	186	GLY	2.8
3	M	2	GLU	2.7
1	H	52	ASN	2.6
3	M	68	PHE	2.6
1	H	126	HIS	2.5
1	H	82	ASP	2.5
3	M	3	TYR	2.5
2	L	63	LEU	2.5
1	H	201	ASN	2.4
1	H	200	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	269	LEU	2.2
1	H	18	TYR	2.2
2	L	271	TRP	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](#)

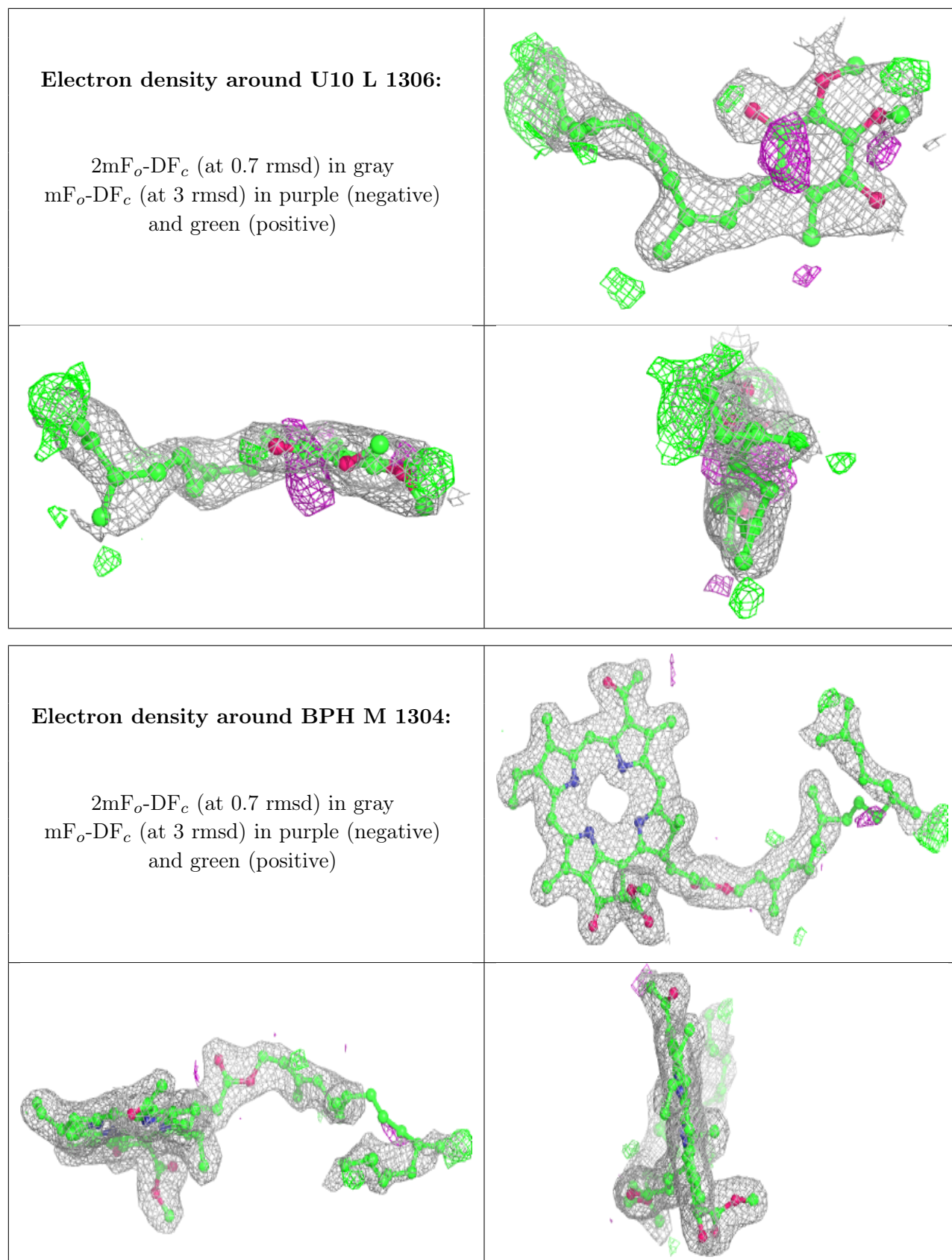
There are no monosaccharides in this entry.

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.

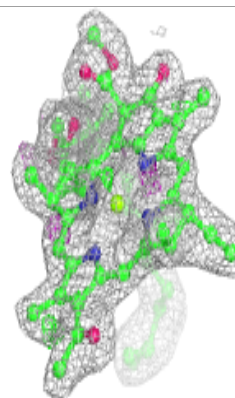
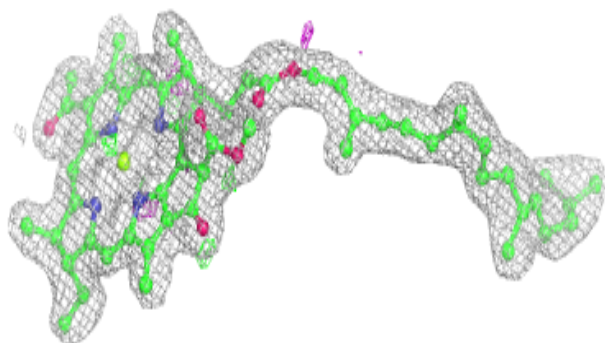
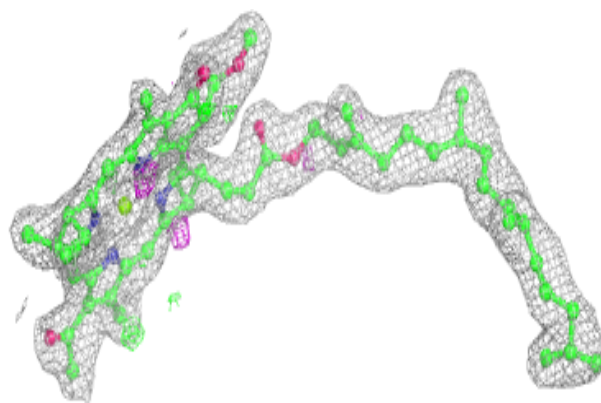
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	U10	L	1306	24/63	0.75	0.21	46,49,55,56	0
4	LDA	H	1310	14/16	0.89	0.12	30,38,42,45	0
9	BPH	M	1304	65/65	0.91	0.14	11,19,73,74	0
5	BCL	L	1282	66/66	0.92	0.14	15,22,28,37	0
6	U10	M	1305	45/63	0.93	0.11	14,25,46,48	0
5	BCL	M	1303	66/66	0.93	0.13	11,19,38,43	0
5	BCL	M	1302	48/66	0.94	0.09	14,19,27,29	0
5	BCL	L	1283	66/66	0.95	0.09	17,19,32,41	0
9	BPH	M	1284	65/65	0.96	0.10	9,15,31,33	0
8	CL	M	1308	1/1	0.98	0.05	38,38,38,38	0
10	CDL	M	1309	10/100	0.98	0.12	15,27,34,36	0
7	FE2	M	1307	1/1	1.00	0.05	14,14,14,14	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.

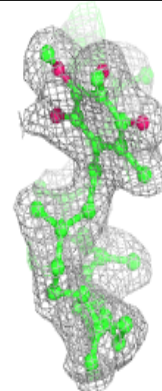
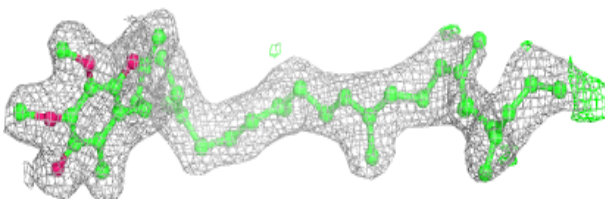
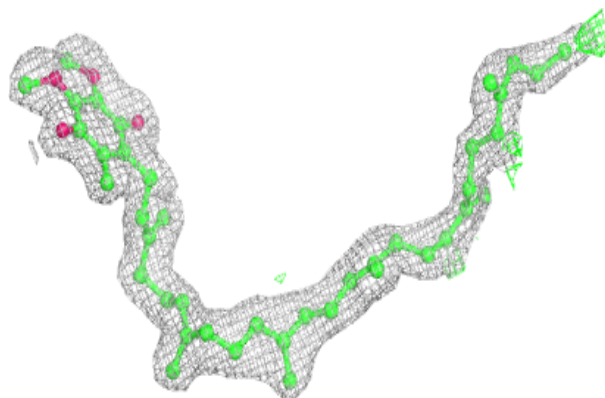


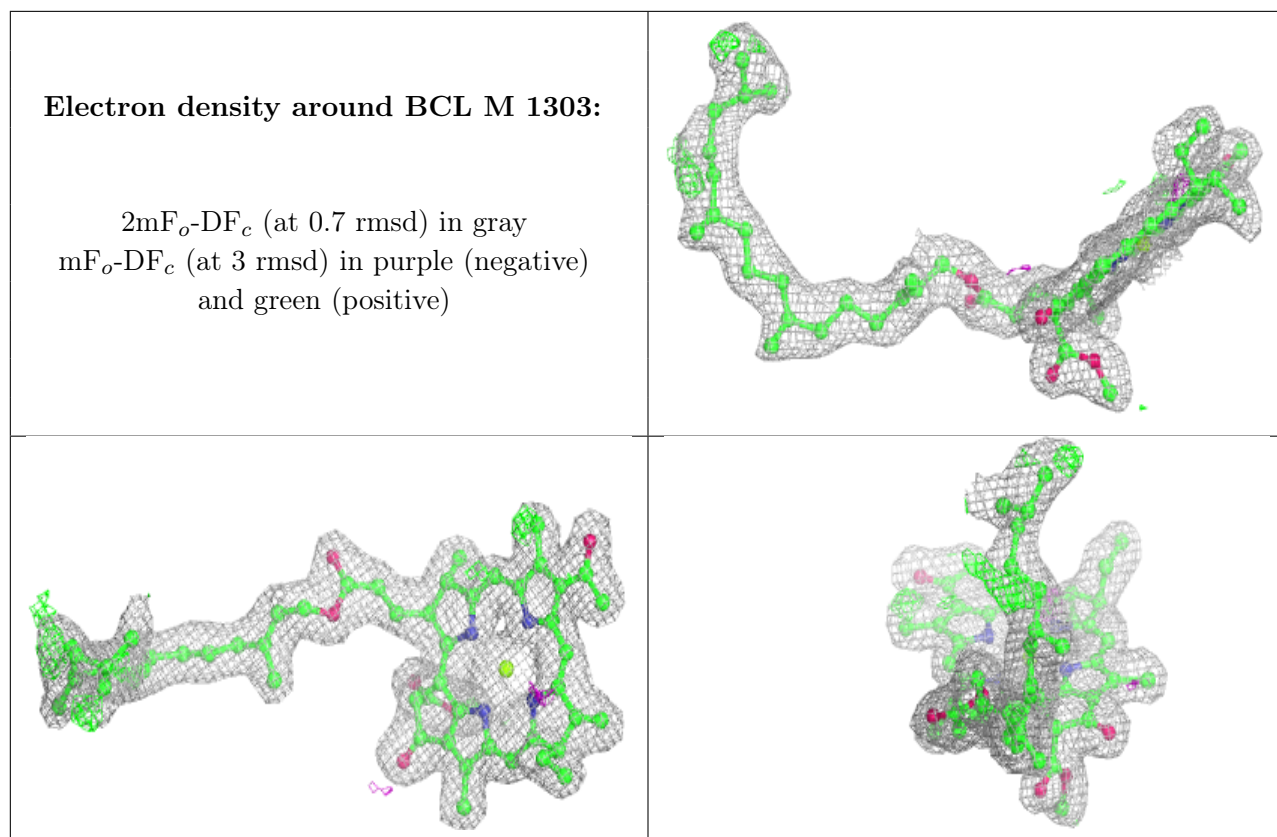
Electron density around BCL L 1282:

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

**Electron density around U10 M 1305:**

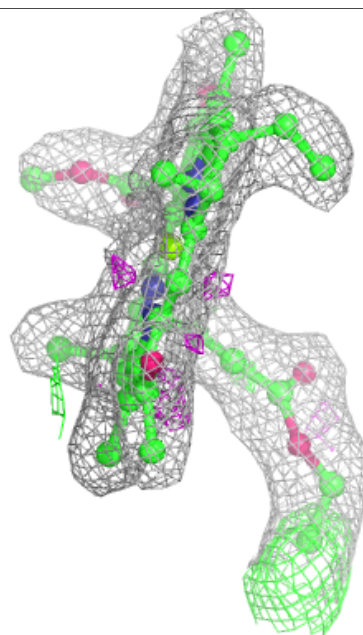
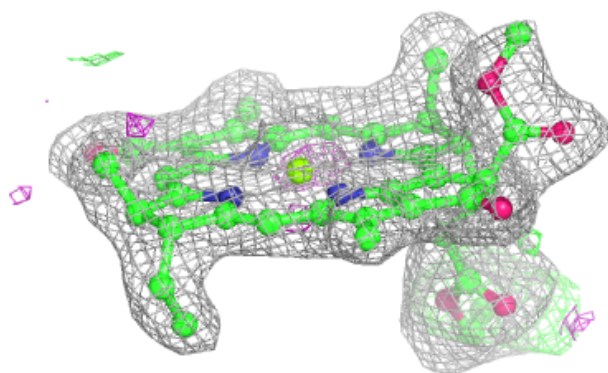
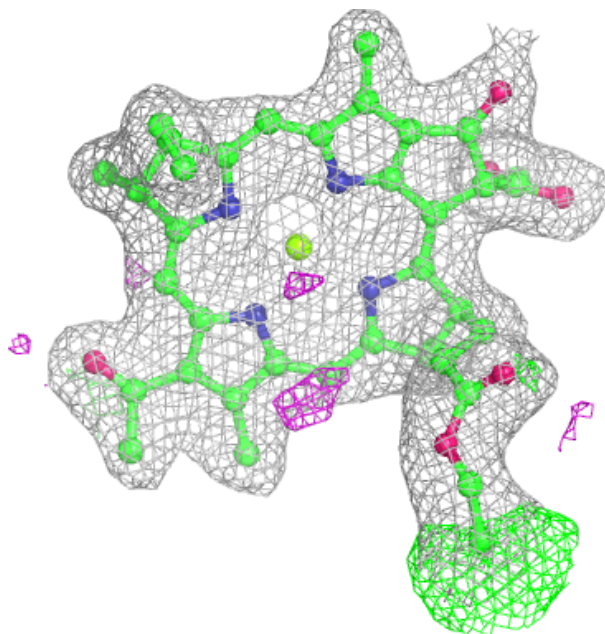
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

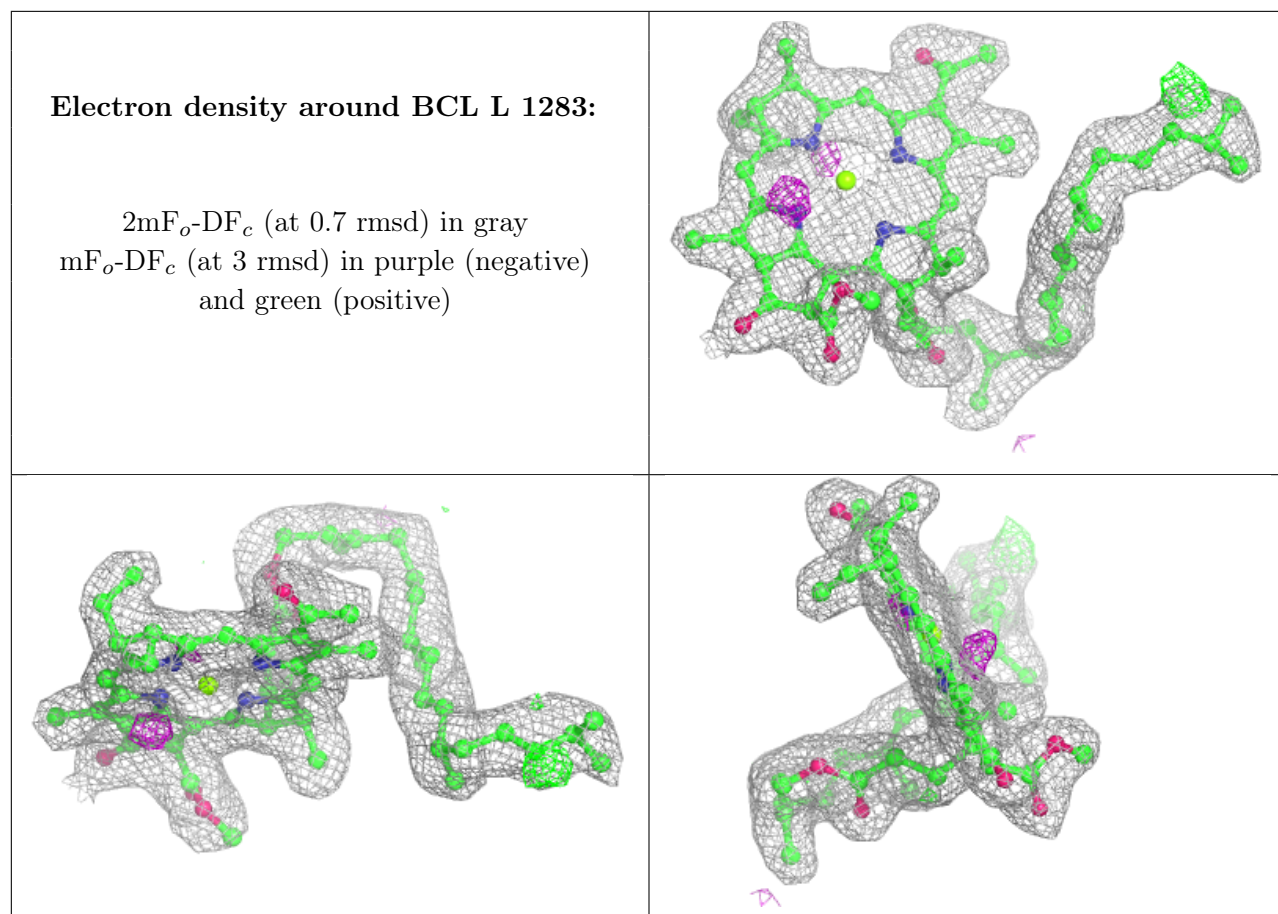




Electron density around BCL M 1302:

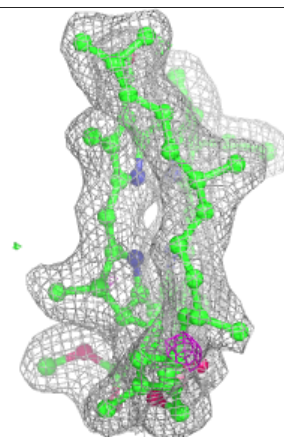
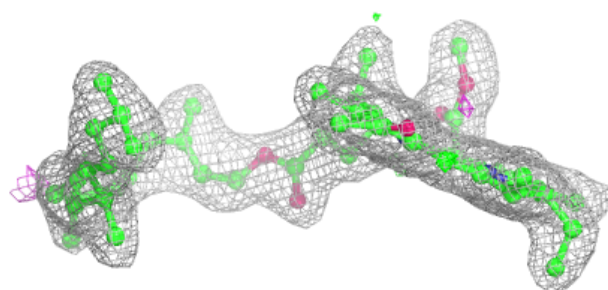
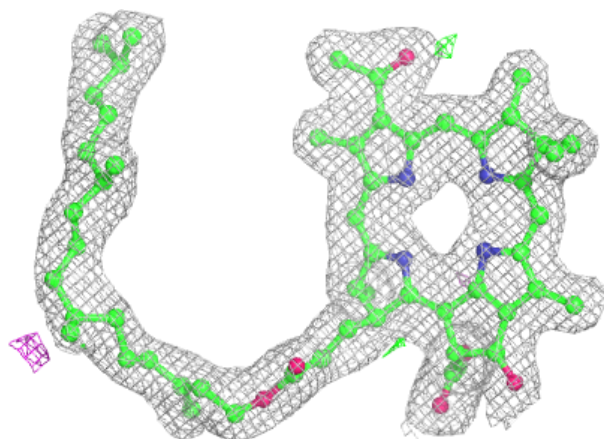
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



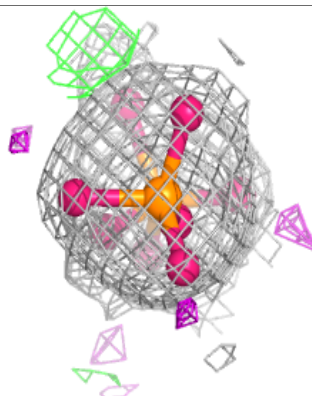
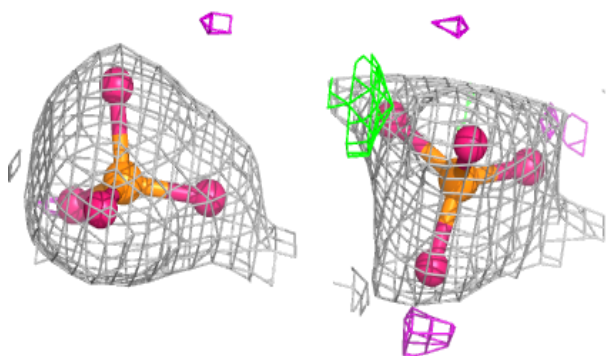
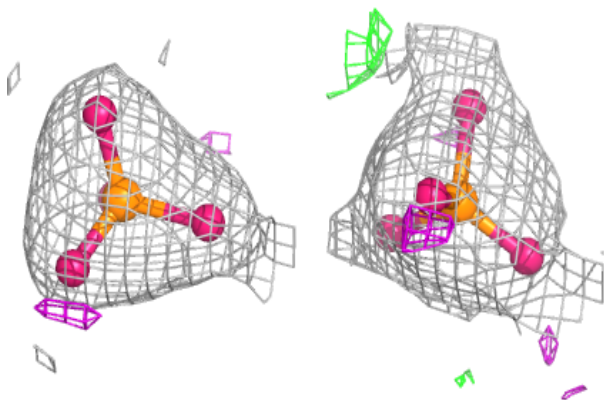


Electron density around BPH M 1284:

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

**Electron density around CDL M 1309:**

$2mF_o-DF_c$ (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.