Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:39 pm BST

PDB ID	:	3ZUM
Title	:	Photosynthetic Reaction Centre Mutant with Phe L146 replaced with Ala
Authors	:	Gibasiewicz, K.; Pajzderska, M.; Potter, J.A.; Fyfe, P.K.; Dobek, A.; Brettel, K.; Jones, M.R.
Deposited on	:	2011-07-19
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

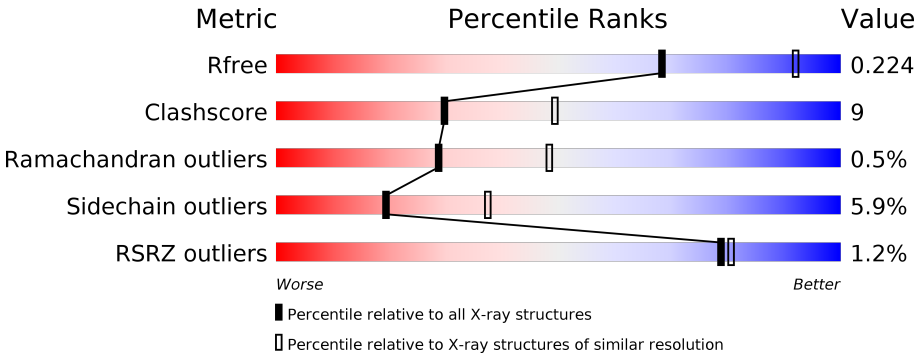
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	% 76% 12% • 10%
2	L	281	2% 86% 12% •
3	M	307	% 84% 12% • •

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
7	BPH	L	1284	X	-	-	-
7	BPH	M	1305	X	-	-	-
8	U10	L	1285	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7265 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	235	Total	C	N	O	S	0	0	0
			1787	1143	304	331	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2226	1501	355	362	8			

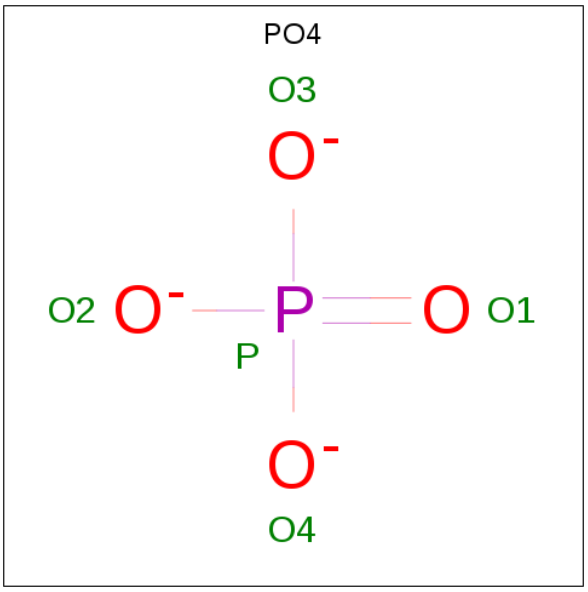
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	146	ALA	PHE	engineered mutation	UNP P0C0Y8

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

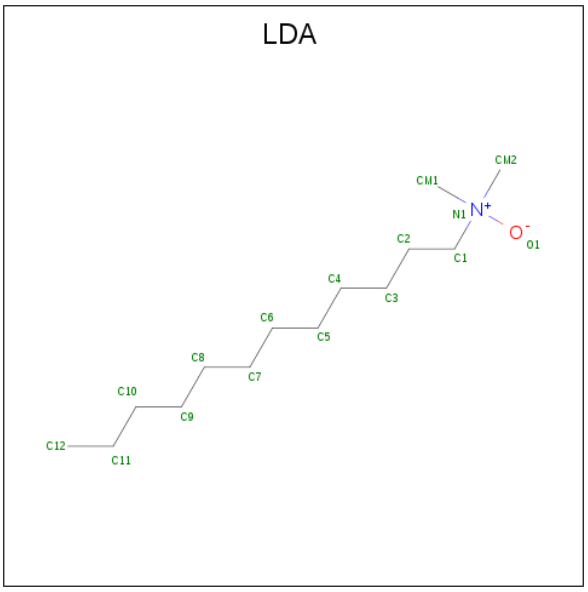
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2404	1605	393	396	10			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0

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



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

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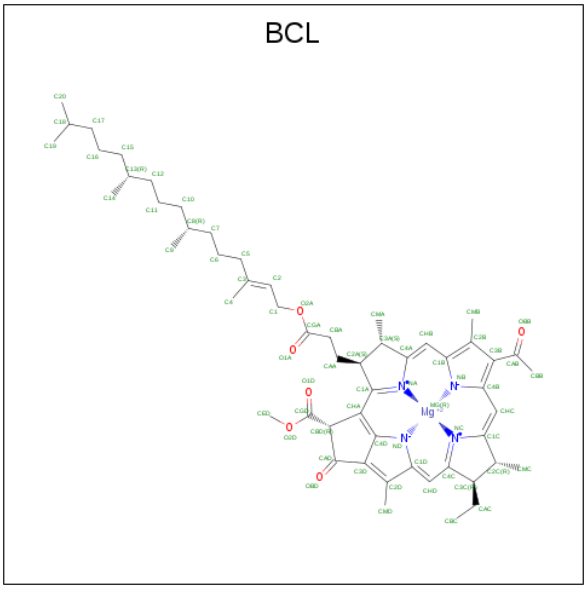
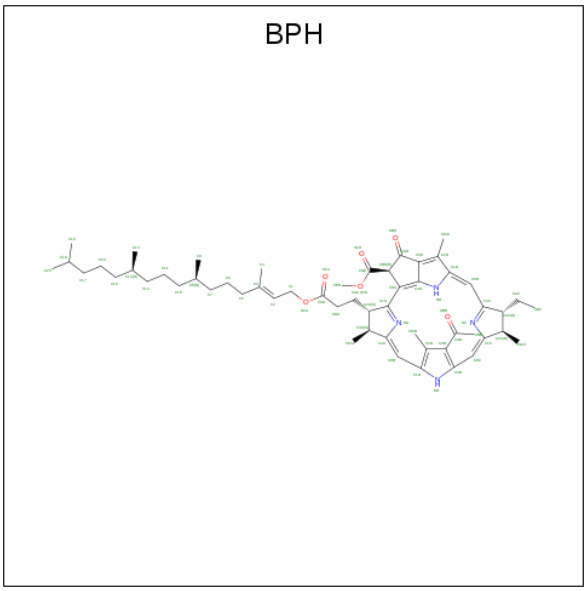
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C N O 16 14 1 1	0	0
5	L	1	Total C N O 16 14 1 1	0	0
5	L	1	Total C N O 16 14 1 1	0	0
5	L	1	Total C N O 16 14 1 1	0	0
5	L	1	Total C 11 11	0	0
5	L	1	Total C 7 7	0	0

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



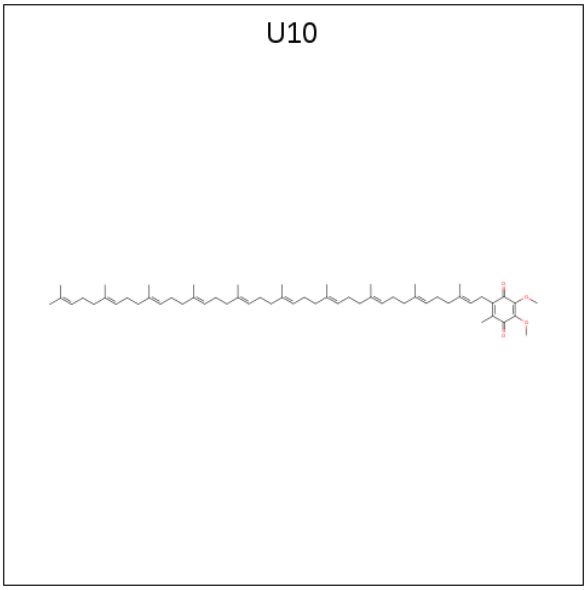
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



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

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

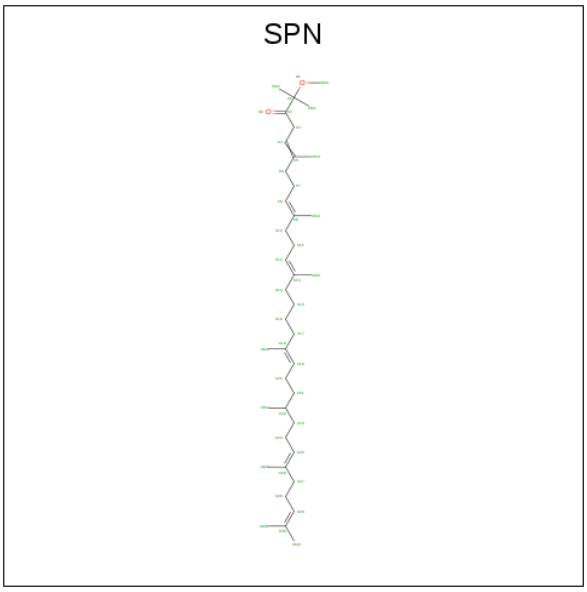


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			48	44	4		
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 11 is water.

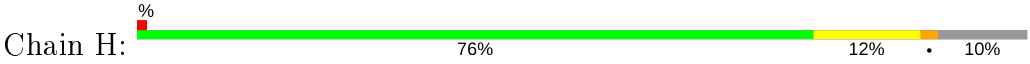
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	109	Total O 109 109	0	0
11	L	49	Total O 49 49	0	0
11	M	48	Total O 48 48	0	0

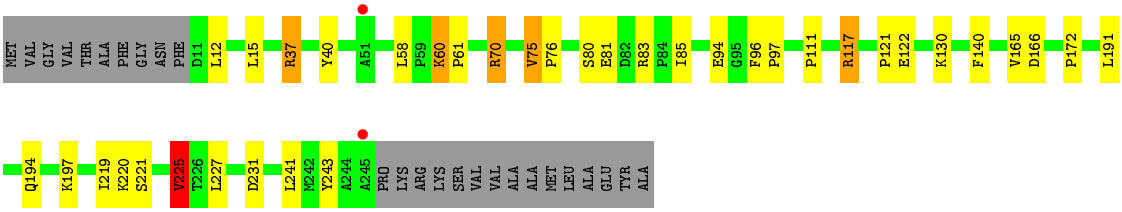
3 Residue-property plots (i)

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

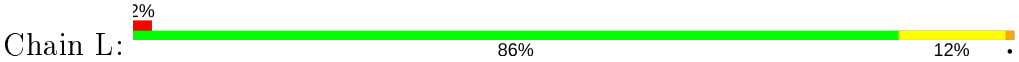
Chain H:

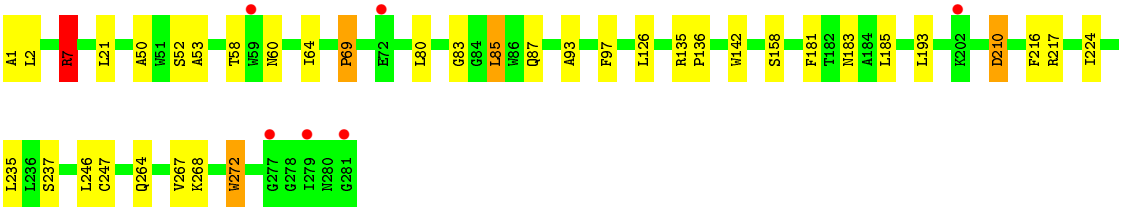




- Molecule 2: REACTION CENTER PROTEIN L CHAIN

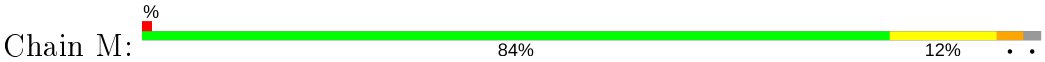
Chain L:

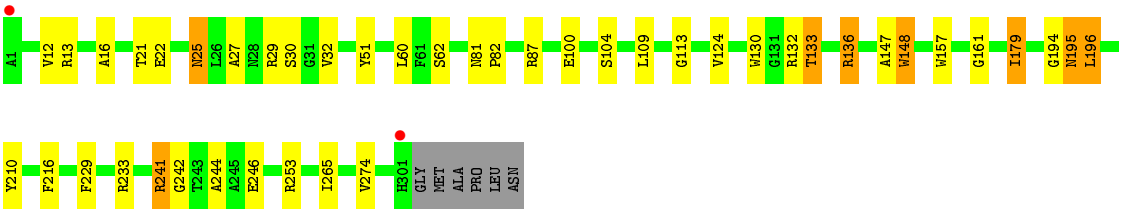




- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.46Å 139.46Å 185.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (119.52-2.50) 99.4 (15.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.228 0.192 , 0.224	Depositor DCC
R_{free} test set	3528 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7265	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, LDA, BPH, PO4, FE, SPN, 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	0.86	1/1834 (0.1%)	0.86	5/2497 (0.2%)
2	L	0.83	0/2313	0.79	4/3166 (0.1%)
3	M	0.80	0/2496	0.80	6/3408 (0.2%)
All	All	0.83	1/6643 (0.0%)	0.81	15/9071 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	94	GLU	CG-CD	5.37	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	241	ARG	NE-CZ-NH2	-9.62	115.49	120.30
3	M	241	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	L	7	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	H	37	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	L	7	ARG	NE-CZ-NH1	7.56	124.08	120.30
3	M	253	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	L	217	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	L	210	ASP	CB-CG-OD1	6.80	124.42	118.30
3	M	29	ARG	NE-CZ-NH2	-6.78	116.91	120.30
3	M	136	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	H	117	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	H	225	VAL	CB-CA-C	-5.74	100.49	111.40
3	M	233	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	H	117	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	H	37	ARG	CG-CD-NE	-5.33	100.61	111.80

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	1787	0	1785	23	0
2	L	2226	0	2183	27	0
3	M	2404	0	2318	41	0
4	H	5	0	0	1	0
4	M	5	0	0	0	0
5	L	98	0	183	7	0
6	L	132	0	148	7	0
6	M	132	0	148	14	0
7	L	65	0	76	8	0
7	M	65	0	76	5	0
8	L	48	0	63	17	0
8	M	48	0	63	2	0
9	M	1	0	0	0	0
10	M	43	0	70	7	0
11	H	109	0	0	3	0
11	L	49	0	0	2	0
11	M	48	0	0	0	0
All	All	7265	0	7113	133	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 9.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1285:U10:H303	8:L:1285:U10:C40	1.66	1.24
5:L:702:LDA:HM21	11:L:2048:HOH:O	1.38	1.21
5:L:701:LDA:H91	5:L:702:LDA:H121	1.22	1.16
8:L:1285:U10:H303	8:L:1285:U10:H402	1.25	1.15
8:L:1285:U10:C40	8:L:1285:U10:C30	2.27	1.10
8:L:1285:U10:H301	8:L:1285:U10:H372	1.32	1.10
8:L:1285:U10:C30	8:L:1285:U10:H402	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ILE:H	8:L:1285:U10:H103	1.19	1.02
8:L:1285:U10:H1M1	8:L:1285:U10:H8	1.46	0.97
7:L:1284:BPH:HBB3	7:L:1284:BPH:HHC	1.46	0.94
8:L:1285:U10:H403	8:L:1285:U10:C30	1.97	0.93
8:L:1285:U10:H1M1	8:L:1285:U10:C8	1.98	0.92
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.52	0.92
6:L:1283:BCL:HMB1	6:L:1283:BCL:HBB2	1.51	0.90
7:M:1305:BPH:HBB3	7:M:1305:BPH:HHC	1.52	0.89
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.56	0.87
6:M:1302:BCL:HMB1	6:M:1302:BCL:CBB	2.05	0.86
6:L:1283:BCL:HMB1	6:L:1283:BCL:CBB	2.12	0.80
8:L:1285:U10:C40	8:L:1285:U10:H301	2.13	0.78
1:H:70:ARG:NH2	1:H:121:PRO:O	2.17	0.78
3:M:133:THR:HG22	3:M:147:ALA:HB2	1.64	0.78
2:L:224:ILE:N	8:L:1285:U10:H103	1.98	0.77
6:M:1302:BCL:HMB1	6:M:1302:BCL:HBB2	1.65	0.76
7:L:1284:BPH:HHC	7:L:1284:BPH:CBB	2.17	0.74
3:M:133:THR:HG21	3:M:147:ALA:HA	1.69	0.74
3:M:25:ASN:ND2	3:M:27:ALA:H	1.87	0.71
2:L:181:PHE:HB3	7:M:1305:BPH:HBB2	1.72	0.71
1:H:117:ARG:HD3	3:M:242:GLY:HA2	1.73	0.70
2:L:69:PRO:HG2	2:L:142:TRP:CB	2.21	0.70
1:H:37:ARG:NH2	1:H:60:LYS:O	2.24	0.69
6:M:1303:BCL:CBB	6:M:1303:BCL:HMB1	2.22	0.69
3:M:25:ASN:HD22	3:M:25:ASN:C	1.95	0.68
1:H:40:TYR:OH	5:L:702:LDA:HM23	1.95	0.67
2:L:69:PRO:HD3	2:L:83:GLY:O	1.95	0.67
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.77	0.66
3:M:133:THR:CG2	3:M:147:ALA:HB2	2.24	0.66
3:M:161:GLY:HA3	10:M:1307:SPN:H201	1.75	0.66
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.27	0.65
6:M:1303:BCL:HAA2	6:M:1303:BCL:HBD	1.78	0.65
6:M:1303:BCL:HBB3	6:M:1303:BCL:HMB1	1.77	0.64
1:H:194:GLN:NE2	4:H:1246:PO4:O1	2.28	0.64
6:L:1282:BCL:HMB1	6:L:1282:BCL:CBB	2.28	0.63
8:L:1285:U10:H303	8:L:1285:U10:H403	1.57	0.63
7:M:1305:BPH:HHC	7:M:1305:BPH:CBB	2.29	0.62
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.82	0.62
3:M:133:THR:HG22	3:M:147:ALA:CB	2.29	0.62
2:L:87:GLN:NE2	2:L:142:TRP:CD1	2.68	0.62
3:M:133:THR:CG2	3:M:147:ALA:HA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:51:TYR:O	3:M:132:ARG:NH2	2.33	0.60
6:M:1302:BCL:H72	6:M:1302:BCL:C4	2.32	0.59
3:M:157:TRP:CE2	10:M:1307:SPN:HM73	2.37	0.59
6:M:1302:BCL:CAB	10:M:1307:SPN:H162	2.32	0.59
8:L:1285:U10:C37	8:L:1285:U10:H301	2.20	0.59
3:M:25:ASN:HD21	3:M:27:ALA:HB3	1.67	0.59
1:H:40:TYR:OH	5:L:702:LDA:CM2	2.51	0.59
3:M:25:ASN:HD22	3:M:27:ALA:H	1.51	0.59
3:M:25:ASN:ND2	3:M:25:ASN:C	2.57	0.58
6:M:1302:BCL:HMB1	6:M:1302:BCL:HBB3	1.85	0.57
2:L:181:PHE:CD2	7:M:1305:BPH:HBB1	2.39	0.56
2:L:52:SER:HB2	2:L:85:LEU:HD23	1.87	0.56
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.41	0.56
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.41	0.56
3:M:133:THR:CG2	3:M:147:ALA:CB	2.83	0.56
3:M:194:GLY:O	3:M:195:ASN:HB3	2.07	0.55
3:M:16:ALA:CB	3:M:32:VAL:HG21	2.37	0.55
2:L:7:ARG:O	2:L:7:ARG:HG3	2.07	0.54
2:L:1:ALA:O	2:L:2:LEU:HD23	2.08	0.53
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.23	0.53
1:H:40:TYR:HB3	1:H:58:LEU:HD21	1.92	0.52
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.73	0.52
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.92	0.52
1:H:140:PHE:HA	3:M:13:ARG:O	2.11	0.51
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.51
2:L:50:ALA:O	2:L:53:ALA:HB3	2.11	0.51
3:M:133:THR:CG2	3:M:147:ALA:CA	2.89	0.50
2:L:60:ASN:O	2:L:64:ILE:HG13	2.11	0.50
1:H:220:LYS:HG2	11:H:2067:HOH:O	2.11	0.50
6:M:1303:BCL:HAA2	6:M:1303:BCL:CBD	2.42	0.49
5:L:701:LDA:H91	5:L:702:LDA:C12	2.16	0.49
3:M:21:THR:O	3:M:22:GLU:C	2.49	0.48
7:L:1284:BPH:CBB	3:M:210:TYR:HB3	2.35	0.48
2:L:93:ALA:HA	7:L:1284:BPH:C9	2.44	0.48
2:L:97:PHE:CE1	6:L:1282:BCL:H121	2.49	0.48
3:M:25:ASN:HD21	3:M:27:ALA:CB	2.27	0.48
8:M:1308:U10:H4M2	8:M:1308:U10:H3M3	1.95	0.48
2:L:181:PHE:HB3	7:M:1305:BPH:CBB	2.41	0.47
1:H:121:PRO:HB3	1:H:225:VAL:O	2.14	0.47
2:L:135:ARG:HB3	2:L:136:PRO:CD	2.44	0.47
3:M:157:TRP:CZ2	10:M:1307:SPN:HM73	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:GLN:NE2	2:L:142:TRP:NE1	2.62	0.47
5:L:701:LDA:C9	5:L:702:LDA:H121	2.16	0.45
1:H:130:LYS:NZ	1:H:172:PRO:HG2	2.31	0.45
6:L:1282:BCL:HMB1	6:L:1282:BCL:HBB3	1.99	0.45
3:M:136:ARG:NE	3:M:136:ARG:HA	2.31	0.45
7:L:1284:BPH:H112	7:L:1284:BPH:H7C2	1.60	0.45
2:L:52:SER:CB	2:L:85:LEU:HD23	2.46	0.45
8:L:1285:U10:H403	8:L:1285:U10:H301	1.81	0.44
1:H:60:LYS:HA	1:H:61:PRO:HD3	1.84	0.44
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.32	0.44
3:M:196:LEU:HD12	3:M:196:LEU:HA	1.61	0.44
3:M:241:ARG:HD2	3:M:246:GLU:OE2	2.17	0.44
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.98	0.44
6:M:1303:BCL:HHC	6:M:1303:BCL:OBB	2.17	0.44
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.52	0.44
3:M:109:LEU:HA	3:M:113:GLY:HA3	2.00	0.43
1:H:165:VAL:O	1:H:166:ASP:HB2	2.19	0.43
1:H:220:LYS:NZ	11:H:2066:HOH:O	2.48	0.43
1:H:241:LEU:HB2	11:H:2108:HOH:O	2.17	0.43
2:L:83:GLY:HA2	11:L:2011:HOH:O	2.17	0.43
1:H:111:PRO:HD2	1:H:243:TYR:CE2	2.54	0.43
2:L:264:GLN:O	2:L:268:LYS:HB2	2.18	0.43
3:M:130:TRP:O	3:M:133:THR:HB	2.18	0.43
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.43
6:M:1302:BCL:H171	10:M:1307:SPN:H72	1.99	0.43
8:L:1285:U10:H8	8:L:1285:U10:C1M	2.33	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.43
1:H:81:GLU:HG3	1:H:85:ILE:HD11	2.01	0.43
1:H:81:GLU:O	1:H:83:ARG:HG2	2.19	0.42
7:L:1284:BPH:CHC	7:L:1284:BPH:CBB	2.88	0.42
8:M:1308:U10:H8	8:M:1308:U10:H1M1	2.01	0.42
3:M:241:ARG:HD3	3:M:246:GLU:HG2	2.00	0.42
6:L:1282:BCL:HMB1	6:L:1282:BCL:HBB2	1.99	0.42
6:M:1302:BCL:H72	6:M:1302:BCL:H41	2.02	0.42
6:M:1302:BCL:OBB	10:M:1307:SPN:H162	2.19	0.42
8:L:1285:U10:C33	8:L:1285:U10:H301	2.46	0.42
6:L:1283:BCL:H193	6:L:1283:BCL:H161	1.77	0.41
3:M:179:ILE:HG23	6:M:1302:BCL:HED1	2.03	0.41
2:L:246:LEU:HA	2:L:246:LEU:HD12	1.91	0.41
5:L:704:LDA:H21	5:L:704:LDA:HM22	1.80	0.41
3:M:194:GLY:O	3:M:195:ASN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:LEU:HD23	8:L:1285:U10:C2	2.51	0.40
10:M:1307:SPN:H111	10:M:1307:SPN:HM41	1.90	0.40
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.90	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	233/260 (90%)	224 (96%)	9 (4%)	0	100	100
2	L	279/281 (99%)	258 (92%)	19 (7%)	2 (1%)	22	39
3	M	299/307 (97%)	281 (94%)	16 (5%)	2 (1%)	22	39
All	All	811/848 (96%)	763 (94%)	44 (5%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	80	LEU
3	M	30	SER
3	M	195	ASN
2	L	69	PRO

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	190/208 (91%)	179 (94%)	11 (6%)	20	38
2	L	219/219 (100%)	206 (94%)	13 (6%)	19	37
3	M	236/240 (98%)	222 (94%)	14 (6%)	19	37
All	All	645/667 (97%)	607 (94%)	38 (6%)	19	37

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	15	LEU
1	H	60	LYS
1	H	70	ARG
1	H	75	VAL
1	H	80	SER
1	H	191	LEU
1	H	197	LYS
1	H	221	SER
1	H	225	VAL
1	H	231	ASP
2	L	7	ARG
2	L	21	LEU
2	L	58	THR
2	L	85	LEU
2	L	126	LEU
2	L	158	SER
2	L	185	LEU
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	267	VAL
2	L	272	TRP
3	M	12	VAL
3	M	25	ASN
3	M	60	LEU
3	M	62	SER
3	M	100	GLU
3	M	104	SER
3	M	124	VAL
3	M	133	THR
3	M	148	TRP
3	M	179	ILE

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Mol	Chain	Res	Type
3	M	196	LEU
3	M	216	PHE
3	M	265	ILE
3	M	274	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
3	M	25	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

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LDA	L	701	-	12,15,15	2.24	1 (8%)	14,17,17	1.02	1 (7%)
4	PO4	H	1246	-	4,4,4	0.94	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	SPN	M	1307	-	40,42,42	0.64	0	50,52,52	1.63	10 (20%)
5	LDA	L	705	-	12,15,15	2.05	1 (8%)	14,17,17	0.62	0
6	BCL	M	1302	3	58,74,74	1.49	4 (6%)	69,115,115	1.62	12 (17%)
7	BPH	L	1284	-	64,70,70	1.41	7 (10%)	76,101,101	1.37	10 (13%)
4	PO4	M	1306	-	4,4,4	0.78	0	6,6,6	0.59	0
5	LDA	L	702	-	12,15,15	1.95	1 (8%)	14,17,17	0.70	0
7	BPH	M	1305	-	64,70,70	1.36	7 (10%)	76,101,101	1.79	16 (21%)
5	LDA	L	703	-	12,15,15	2.00	1 (8%)	14,17,17	0.48	0
5	LDA	L	706	-	10,10,15	0.47	0	9,9,17	0.38	0
6	BCL	L	1283	2	58,74,74	1.75	6 (10%)	69,115,115	1.97	19 (27%)
5	LDA	L	707	-	6,6,15	0.44	0	5,5,17	0.18	0
8	U10	M	1308	-	48,48,63	2.76	13 (27%)	58,61,79	1.89	13 (22%)
6	BCL	L	1282	2	58,74,74	1.46	2 (3%)	69,115,115	1.43	9 (13%)
5	LDA	L	704	-	12,15,15	2.01	1 (8%)	14,17,17	0.47	0
6	BCL	M	1303	3	58,74,74	1.34	2 (3%)	69,115,115	1.63	14 (20%)
8	U10	L	1285	-	48,48,63	2.67	12 (25%)	58,61,79	2.24	19 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	L	701	-	-	3/13/13/13	-
10	SPN	M	1307	-	-	15/50/51/51	-
5	LDA	L	705	-	-	4/13/13/13	-
6	BCL	M	1302	3	-	10/37/137/137	-
7	BPH	L	1284	-	2/2/18/22	14/54/105/105	0/5/6/6
5	LDA	L	702	-	-	8/13/13/13	-
7	BPH	M	1305	-	2/2/18/22	17/54/105/105	0/5/6/6
5	LDA	L	703	-	-	6/13/13/13	-
5	LDA	L	706	-	-	2/8/8/13	-
6	BCL	L	1283	2	-	5/37/137/137	-
5	LDA	L	707	-	-	2/4/4/13	-
8	U10	M	1308	-	-	12/45/69/87	0/1/1/1
6	BCL	L	1282	2	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	L	704	-	-	5/13/13/13	-
6	BCL	M	1303	3	-	2/37/137/137	-
8	U10	L	1285	-	-	19/45/69/87	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BCL	C4B-NB	8.77	1.43	1.35
6	M	1302	BCL	C1B-NB	7.90	1.42	1.35
6	L	1282	BCL	C4B-NB	7.40	1.41	1.35
5	L	701	LDA	O1-N1	-7.37	1.24	1.42
6	L	1283	BCL	C1B-NB	7.09	1.41	1.35
6	M	1303	BCL	C4B-NB	7.07	1.41	1.35
5	L	705	LDA	O1-N1	-6.98	1.25	1.42
5	L	704	LDA	O1-N1	-6.81	1.26	1.42
5	L	703	LDA	O1-N1	-6.77	1.26	1.42
5	L	702	LDA	O1-N1	-6.72	1.26	1.42
8	M	1308	U10	C13-C14	6.68	1.49	1.33
8	L	1285	U10	C28-C29	6.62	1.48	1.33
8	M	1308	U10	C18-C19	6.54	1.48	1.33
6	L	1282	BCL	C1B-NB	6.45	1.41	1.35
8	M	1308	U10	C33-C34	6.42	1.48	1.33
8	L	1285	U10	C18-C19	6.39	1.48	1.33
8	L	1285	U10	C23-C24	6.39	1.48	1.33
8	L	1285	U10	C33-C34	6.16	1.47	1.33
8	L	1285	U10	C13-C14	6.15	1.47	1.33
8	M	1308	U10	C28-C29	6.11	1.47	1.33
8	M	1308	U10	C8-C9	6.02	1.47	1.33
8	M	1308	U10	C23-C24	5.89	1.47	1.33
8	M	1308	U10	C38-C39	5.80	1.49	1.32
8	L	1285	U10	C8-C9	5.58	1.46	1.33
8	L	1285	U10	C38-C39	5.52	1.48	1.32
6	M	1303	BCL	C1B-NB	5.40	1.40	1.35
6	M	1302	BCL	C4B-NB	5.22	1.39	1.35
7	L	1284	BPH	CHA-C1A	5.16	1.49	1.38
7	M	1305	BPH	CHA-C1A	4.84	1.48	1.38
8	L	1285	U10	O4-C4	-4.80	1.25	1.36
8	M	1308	U10	O3-C3	-4.72	1.25	1.36
7	L	1284	BPH	CHD-C4C	4.42	1.49	1.38
7	M	1305	BPH	CHD-C4C	4.38	1.49	1.38
8	M	1308	U10	O4-C4	-4.31	1.26	1.36
8	L	1285	U10	O3-C3	-3.71	1.27	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1305	BPH	C1A-NA	-3.59	1.30	1.37
7	L	1284	BPH	CHB-C1B	3.42	1.45	1.38
7	L	1284	BPH	C1A-NA	-3.29	1.31	1.37
7	M	1305	BPH	C4C-NC	-3.22	1.30	1.37
6	L	1283	BCL	MG-NA	-3.18	1.98	2.06
7	L	1284	BPH	C1B-C2B	-3.12	1.39	1.45
8	L	1285	U10	C6-C5	-3.12	1.37	1.46
8	M	1308	U10	C4-C5	-3.01	1.40	1.48
7	M	1305	BPH	C1B-C2B	-3.01	1.39	1.45
7	L	1284	BPH	C4C-NC	-2.99	1.31	1.37
8	L	1285	U10	C4-C5	-2.92	1.40	1.48
8	M	1308	U10	C6-C1	2.81	1.40	1.35
8	M	1308	U10	C3-C2	-2.81	1.40	1.48
8	L	1285	U10	C3-C2	-2.81	1.40	1.48
6	L	1283	BCL	MG-NC	-2.50	2.00	2.06
6	M	1302	BCL	MG-NC	-2.38	2.00	2.06
7	M	1305	BPH	C3C-C4C	2.35	1.54	1.50
6	M	1302	BCL	C4B-CHC	-2.29	1.34	1.41
6	L	1283	BCL	CHD-C4C	-2.22	1.34	1.41
7	M	1305	BPH	CHB-C1B	2.15	1.42	1.38
6	L	1283	BCL	O2D-CGD	2.12	1.38	1.33
8	M	1308	U10	O2-C2	2.04	1.27	1.23
7	L	1284	BPH	C3D-C2D	-2.03	1.35	1.39

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1285	U10	C7-C8-C9	-7.15	114.90	126.79
8	L	1285	U10	C1M-C1-C6	-6.99	113.00	124.40
6	L	1283	BCL	O2D-CGD-CBD	5.31	120.71	111.27
7	M	1305	BPH	C4D-C3D-CAD	-5.29	104.52	107.87
6	L	1283	BCL	C1C-NC-C4C	5.24	109.06	106.71
7	M	1305	BPH	CAC-C3C-C4C	5.10	125.76	112.67
8	M	1308	U10	C17-C18-C19	-5.02	115.58	127.66
7	M	1305	BPH	C4-C3-C5	-5.02	106.83	115.27
6	L	1283	BCL	C1D-CHD-C4C	-4.93	118.61	125.88
6	M	1302	BCL	C1C-NC-C4C	4.84	108.88	106.71
8	M	1308	U10	C30-C29-C31	4.63	123.07	115.27
7	M	1305	BPH	C5-C3-C2	4.61	130.44	121.12
6	L	1283	BCL	CHD-C4C-NC	4.57	130.15	125.08
10	M	1307	SPN	CM5-C13-C14	4.56	122.94	115.27
8	L	1285	U10	C35-C34-C36	4.53	122.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1308	U10	C35-C34-C36	4.48	122.80	115.27
8	L	1285	U10	O5-C5-C6	-4.46	113.72	121.55
7	L	1284	BPH	C4D-CHA-C1A	-4.43	119.59	130.51
6	M	1302	BCL	CHD-C4C-NC	4.39	129.95	125.08
6	M	1303	BCL	CHD-C4C-NC	4.30	129.86	125.08
6	M	1302	BCL	C1-O2A-CGA	4.21	127.49	116.44
7	M	1305	BPH	C4D-CHA-C1A	-3.96	120.74	130.51
6	L	1283	BCL	CHB-C4A-NA	3.90	129.91	124.51
8	L	1285	U10	C30-C29-C31	3.89	121.82	115.27
10	M	1307	SPN	CM3-C5-C6	3.88	121.80	115.27
6	M	1303	BCL	O2D-CGD-CBD	3.88	118.16	111.27
6	L	1282	BCL	C1-O2A-CGA	3.70	126.16	116.44
6	L	1283	BCL	OBD-CAD-C3D	-3.68	121.86	127.98
6	M	1303	BCL	O2D-CGD-O1D	-3.53	116.94	123.84
6	L	1283	BCL	O1D-CGD-CBD	-3.51	117.30	124.48
6	L	1282	BCL	C11-C12-C13	-3.49	104.64	115.92
6	L	1282	BCL	CED-O2D-CGD	3.49	123.83	115.94
8	M	1308	U10	C10-C9-C11	3.47	121.10	115.27
8	L	1285	U10	C15-C14-C16	3.43	121.04	115.27
6	L	1283	BCL	OBD-CAD-CBD	3.34	130.66	125.89
6	M	1302	BCL	CHB-C4A-NA	3.33	129.11	124.51
7	L	1284	BPH	C4D-C3D-CAD	-3.33	105.76	107.87
8	L	1285	U10	C3M-O3-C3	3.28	128.10	116.47
6	M	1302	BCL	C1B-CHB-C4A	-3.28	123.63	130.12
6	L	1282	BCL	C1D-CHD-C4C	-3.25	121.08	125.88
8	M	1308	U10	C32-C33-C34	-3.25	119.83	127.66
7	M	1305	BPH	CMD-C2D-C3D	3.25	130.76	124.68
8	M	1308	U10	C27-C28-C29	-3.23	119.89	127.66
6	L	1283	BCL	C5-C3-C2	-3.21	114.61	121.12
10	M	1307	SPN	CM4-C9-C10	3.13	120.53	115.27
6	L	1283	BCL	CED-O2D-CGD	3.12	123.00	115.94
6	M	1303	BCL	O2A-CGA-CBA	3.09	121.61	111.91
6	M	1303	BCL	CHB-C4A-NA	3.09	128.79	124.51
6	M	1303	BCL	C11-C10-C8	-3.07	105.99	115.92
7	M	1305	BPH	CAC-C3C-C2C	-3.07	106.59	114.26
6	L	1283	BCL	C1B-CHB-C4A	-3.04	124.10	130.12
6	M	1303	BCL	C4D-C3D-CAD	-3.01	106.79	108.47
6	M	1302	BCL	C4-C3-C2	-2.99	116.00	123.68
6	M	1303	BCL	C1C-NC-C4C	2.91	108.01	106.71
8	M	1308	U10	C12-C13-C14	-2.90	120.67	127.66
7	M	1305	BPH	OBB-CAB-C3B	2.89	125.76	120.41
6	M	1303	BCL	C1D-CHD-C4C	-2.87	121.65	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1305	BPH	CHD-C4C-NC	-2.87	121.79	125.20
7	L	1284	BPH	OBB-CAB-C3B	2.86	125.70	120.41
8	L	1285	U10	C22-C23-C24	-2.86	120.78	127.66
6	L	1282	BCL	O2D-CGD-CBD	2.84	116.32	111.27
6	M	1302	BCL	C1D-CHD-C4C	-2.84	121.69	125.88
7	M	1305	BPH	C1-O2A-CGA	2.83	123.88	116.44
6	L	1282	BCL	CHD-C4C-NC	2.82	128.21	125.08
7	L	1284	BPH	C2B-C1B-NB	-2.81	105.55	109.79
6	L	1282	BCL	O2A-CGA-CBA	2.79	120.67	111.91
7	L	1284	BPH	C1C-NC-C4C	-2.78	108.09	110.54
6	L	1283	BCL	O2A-CGA-CBA	2.76	120.57	111.91
10	M	1307	SPN	CM6-C18-C17	2.69	119.80	115.27
8	M	1308	U10	C22-C23-C24	-2.69	121.19	127.66
6	M	1302	BCL	C3C-C4C-CHD	-2.68	117.67	123.39
6	M	1302	BCL	CBC-CAC-C3C	-2.67	107.52	113.47
5	L	701	LDA	CM1-N1-C1	2.66	115.82	110.23
6	L	1283	BCL	C3C-C4C-CHD	-2.63	117.76	123.39
8	M	1308	U10	C31-C29-C28	-2.62	115.82	121.12
8	L	1285	U10	C20-C19-C21	2.60	119.64	115.27
10	M	1307	SPN	C24-C25-C26	-2.60	121.40	127.66
7	L	1284	BPH	CMD-C2D-C3D	2.59	129.53	124.68
8	M	1308	U10	C15-C14-C16	2.56	119.58	115.27
8	M	1308	U10	C41-C39-C40	2.55	120.24	114.60
8	L	1285	U10	C1M-C1-C2	2.55	126.20	116.99
6	L	1282	BCL	C4-C3-C5	2.54	119.55	115.27
8	L	1285	U10	C10-C9-C11	2.53	119.53	115.27
6	M	1302	BCL	O2D-CGD-CBD	2.52	115.75	111.27
7	L	1284	BPH	OBB-CAB-CBB	-2.52	114.15	119.73
8	L	1285	U10	C27-C28-C29	-2.52	121.60	127.66
10	M	1307	SPN	C21-C20-C19	-2.51	105.61	112.23
7	M	1305	BPH	C1B-NB-C4B	2.50	111.22	106.51
8	M	1308	U10	C26-C27-C28	-2.50	103.67	111.88
7	M	1305	BPH	C2B-C1B-NB	-2.49	106.04	109.79
6	M	1303	BCL	C16-C15-C13	-2.47	107.93	115.92
7	L	1284	BPH	C1B-NB-C4B	2.40	111.03	106.51
6	M	1303	BCL	C4A-NA-C1A	2.36	107.77	106.71
8	L	1285	U10	C32-C33-C34	-2.31	122.11	127.66
6	L	1283	BCL	C2A-C1A-CHA	-2.29	119.86	123.86
6	M	1302	BCL	O2A-CGA-CBA	2.28	119.07	111.91
6	L	1283	BCL	C1-O2A-CGA	2.27	122.41	116.44
6	L	1283	BCL	CAC-C3C-C2C	-2.27	108.58	114.26
7	L	1284	BPH	CHC-C1C-NC	2.24	127.86	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1303	BCL	C2A-C1A-CHA	-2.23	119.96	123.86
7	L	1284	BPH	C7-C6-C5	-2.23	107.31	113.36
8	L	1285	U10	C36-C34-C33	-2.22	116.62	121.12
10	M	1307	SPN	CM8-C26-C27	2.20	118.98	115.27
10	M	1307	SPN	C28-C29-C30	-2.19	120.25	127.75
10	M	1307	SPN	C6-C5-C4	-2.18	116.70	121.12
7	M	1305	BPH	OBB-CAB-CBB	-2.16	114.95	119.73
6	L	1283	BCL	C4B-CHC-C1C	-2.16	125.85	130.12
10	M	1307	SPN	C7-C8-C9	-2.16	122.47	127.66
7	M	1305	BPH	CBA-CAA-C2A	-2.15	107.51	113.86
6	M	1303	BCL	C11-C12-C13	-2.14	109.01	115.92
7	M	1305	BPH	CMA-C3A-C4A	-2.13	106.02	112.36
8	L	1285	U10	C10-C9-C8	-2.13	118.23	123.68
8	L	1285	U10	C12-C13-C14	-2.11	122.59	127.66
6	L	1283	BCL	CMB-C2B-C1B	-2.09	125.25	128.46
6	M	1302	BCL	C5-C3-C2	2.09	125.34	121.12
8	L	1285	U10	C15-C14-C13	-2.08	118.34	123.68
8	L	1285	U10	C20-C19-C18	-2.08	118.34	123.68
6	L	1283	BCL	CHC-C1C-NC	2.05	127.35	124.51
8	M	1308	U10	C7-C8-C9	-2.05	123.39	126.79
8	L	1285	U10	C17-C18-C19	-2.04	122.75	127.66
7	M	1305	BPH	CHB-C1B-C2B	2.03	130.85	125.73
6	M	1303	BCL	C3C-C4C-CHD	-2.03	119.05	123.39
6	L	1282	BCL	C1B-CHB-C4A	-2.00	126.15	130.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	1284	BPH	C8
7	L	1284	BPH	C13
7	M	1305	BPH	C8
7	M	1305	BPH	C13

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	M	1307	SPN	O1-C1-C2-O2
10	M	1307	SPN	C4-C5-C6-C7
10	M	1307	SPN	CM3-C5-C6-C7
10	M	1307	SPN	C12-C13-C14-C15
10	M	1307	SPN	CM5-C13-C14-C15
6	M	1302	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
7	L	1284	BPH	C4C-C3C-CAC-CBC
7	L	1284	BPH	C11-C12-C13-C15
5	L	702	LDA	N1-C1-C2-C3
7	M	1305	BPH	C4C-C3C-CAC-CBC
7	M	1305	BPH	C4B-C3B-CAB-OBB
7	M	1305	BPH	C11-C12-C13-C15
5	L	703	LDA	C2-C1-N1-CM1
8	M	1308	U10	C27-C28-C29-C30
8	M	1308	U10	C27-C28-C29-C31
8	M	1308	U10	C32-C33-C34-C35
8	M	1308	U10	C32-C33-C34-C36
8	M	1308	U10	C37-C38-C39-C41
5	L	704	LDA	C2-C1-N1-CM2
8	L	1285	U10	C32-C33-C34-C35
8	L	1285	U10	C32-C33-C34-C36
7	M	1305	BPH	C3-C5-C6-C7
8	L	1285	U10	C17-C18-C19-C20
8	M	1308	U10	C37-C38-C39-C40
10	M	1307	SPN	C14-C15-C16-C17
10	M	1307	SPN	C11-C10-C9-CM4
10	M	1307	SPN	C16-C17-C18-CM6
7	M	1305	BPH	C4-C3-C5-C6
8	L	1285	U10	C30-C29-C31-C32
10	M	1307	SPN	C11-C10-C9-C8
10	M	1307	SPN	C16-C17-C18-C19
7	M	1305	BPH	C2-C3-C5-C6
8	L	1285	U10	C28-C29-C31-C32
8	M	1308	U10	C24-C26-C27-C28
8	L	1285	U10	C34-C36-C37-C38
6	M	1302	BCL	C13-C15-C16-C17
7	M	1305	BPH	C8-C10-C11-C12
6	M	1302	BCL	C8-C10-C11-C12
6	M	1302	BCL	C6-C7-C8-C10
6	L	1283	BCL	C15-C16-C17-C18
5	L	702	LDA	C11-C10-C9-C8
6	L	1282	BCL	C16-C17-C18-C20
5	L	702	LDA	C2-C3-C4-C5
5	L	705	LDA	C4-C5-C6-C7
7	M	1305	BPH	C16-C17-C18-C19
7	L	1284	BPH	C11-C12-C13-C14
5	L	701	LDA	C3-C4-C5-C6
7	M	1305	BPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	L	1284	BPH	O2A-C1-C2-C3
8	L	1285	U10	C18-C19-C21-C22
5	L	701	LDA	C11-C10-C9-C8
8	L	1285	U10	C17-C18-C19-C21
8	L	1285	U10	C20-C19-C21-C22
7	M	1305	BPH	C12-C13-C15-C16
6	L	1282	BCL	C16-C17-C18-C19
5	L	701	LDA	C1-C2-C3-C4
5	L	704	LDA	C1-C2-C3-C4
6	L	1283	BCL	C16-C17-C18-C20
5	L	702	LDA	C1-C2-C3-C4
7	M	1305	BPH	C14-C13-C15-C16
8	L	1285	U10	C37-C38-C39-C41
5	L	705	LDA	C5-C6-C7-C8
6	L	1283	BCL	C13-C15-C16-C17
7	M	1305	BPH	C16-C17-C18-C20
7	M	1305	BPH	C2C-C3C-CAC-CBC
5	L	702	LDA	C6-C7-C8-C9
5	L	702	LDA	C5-C6-C7-C8
8	L	1285	U10	C5-C6-C7-C8
5	L	707	LDA	C2-C3-C4-C5
7	L	1284	BPH	C11-C10-C8-C7
6	M	1302	BCL	C6-C7-C8-C9
7	M	1305	BPH	C11-C12-C13-C14
5	L	704	LDA	N1-C1-C2-C3
7	L	1284	BPH	C8-C10-C11-C12
5	L	706	LDA	C2-C3-C4-C5
6	L	1283	BCL	C16-C17-C18-C19
7	L	1284	BPH	C2-C3-C5-C6
8	M	1308	U10	C23-C24-C26-C27
5	L	703	LDA	C6-C7-C8-C9
5	L	704	LDA	C3-C4-C5-C6
6	M	1302	BCL	C16-C17-C18-C20
8	L	1285	U10	C25-C24-C26-C27
5	L	705	LDA	C2-C3-C4-C5
5	L	703	LDA	C11-C10-C9-C8
7	L	1284	BPH	C4-C3-C5-C6
8	M	1308	U10	C25-C24-C26-C27
10	M	1307	SPN	C21-C22-C23-C24
6	L	1282	BCL	C11-C12-C13-C15
7	M	1305	BPH	C4B-C3B-CAB-CBB
7	L	1284	BPH	CAD-CBD-CGD-O2D

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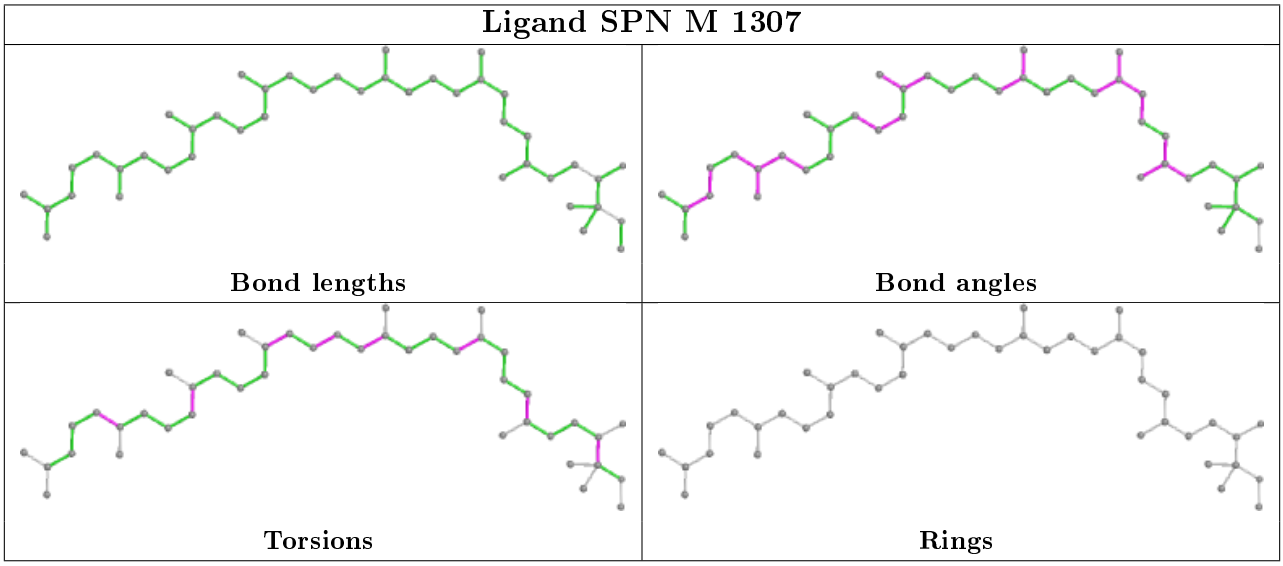
Mol	Chain	Res	Type	Atoms
7	M	1305	BPH	CAD-CBD-CGD-O2D
6	L	1282	BCL	CAD-CBD-CGD-O2D
8	L	1285	U10	C15-C14-C16-C17
8	L	1285	U10	C5-C4-O4-C4M
6	L	1282	BCL	C15-C16-C17-C18
5	L	703	LDA	C2-C1-N1-CM2
8	L	1285	U10	C13-C14-C16-C17
8	L	1285	U10	C37-C38-C39-C40
6	M	1302	BCL	C5-C6-C7-C8
7	L	1284	BPH	C6-C7-C8-C9
8	L	1285	U10	C19-C21-C22-C23
8	L	1285	U10	C23-C24-C26-C27
6	M	1302	BCL	C16-C17-C18-C19
5	L	704	LDA	C5-C6-C7-C8
10	M	1307	SPN	CM7-C22-C23-C24
6	L	1282	BCL	C11-C12-C13-C14
7	M	1305	BPH	C13-C15-C16-C17
5	L	705	LDA	C1-C2-C3-C4
6	M	1302	BCL	C15-C16-C17-C18
10	M	1307	SPN	CM1-C1-C2-C3
8	M	1308	U10	C5-C4-O4-C4M
6	M	1303	BCL	CAA-CBA-CGA-O2A
5	L	707	LDA	C3-C4-C5-C6
5	L	703	LDA	C2-C3-C4-C5
8	M	1308	U10	C3-C4-O4-C4M
5	L	702	LDA	C3-C4-C5-C6
5	L	706	LDA	C6-C7-C8-C9
7	L	1284	BPH	C5-C6-C7-C8
10	M	1307	SPN	CM8-C26-C27-C28
8	M	1308	U10	C14-C16-C17-C18
10	M	1307	SPN	C25-C26-C27-C28
7	L	1284	BPH	C11-C10-C8-C9
5	L	703	LDA	C5-C6-C7-C8
6	M	1302	BCL	CAD-CBD-CGD-O2D
6	L	1283	BCL	CAD-CBD-CGD-O2D
6	M	1303	BCL	CAD-CBD-CGD-O2D
5	L	702	LDA	C9-C10-C11-C12
7	L	1284	BPH	C16-C17-C18-C20
7	L	1284	BPH	C14-C13-C15-C16
8	L	1285	U10	C16-C17-C18-C19

There are no ring outliers.

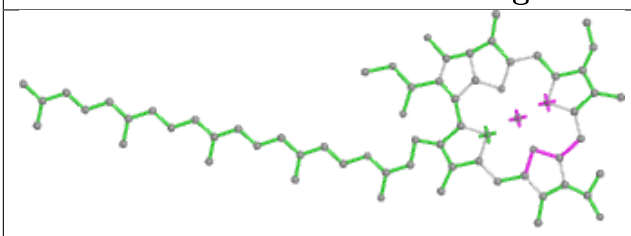
13 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	701	LDA	3	0
4	H	1246	PO4	1	0
10	M	1307	SPN	7	0
6	M	1302	BCL	9	0
7	L	1284	BPH	8	0
5	L	702	LDA	6	0
7	M	1305	BPH	5	0
6	L	1283	BCL	3	0
8	M	1308	U10	2	0
6	L	1282	BCL	4	0
5	L	704	LDA	1	0
6	M	1303	BCL	5	0
8	L	1285	U10	17	0

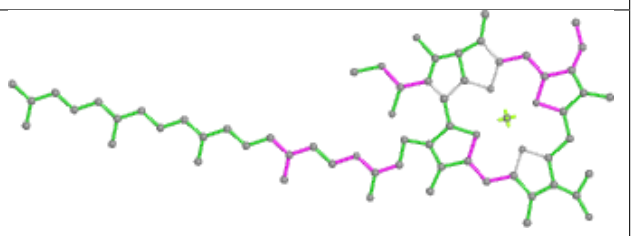
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



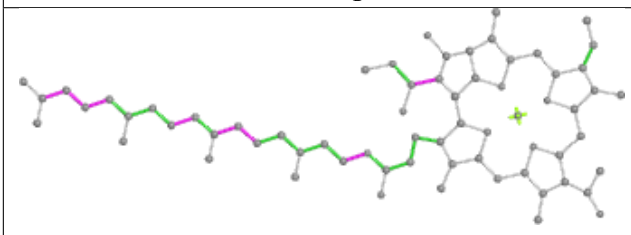
Ligand BCL M 1302



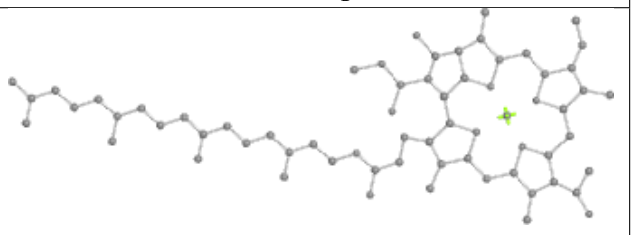
Bond lengths



Bond angles

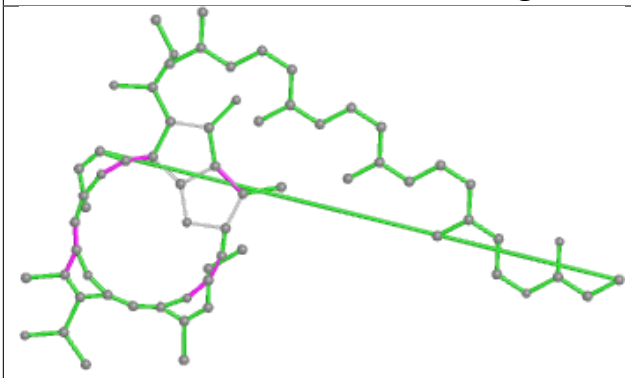


Torsions

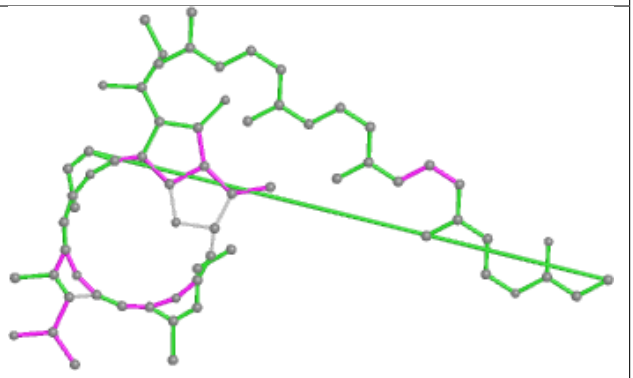


Rings

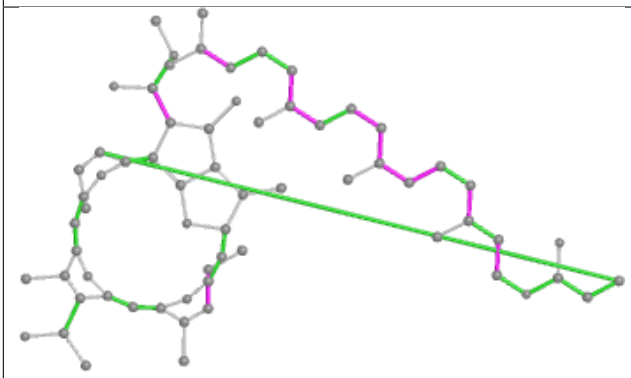
Ligand BPH L 1284



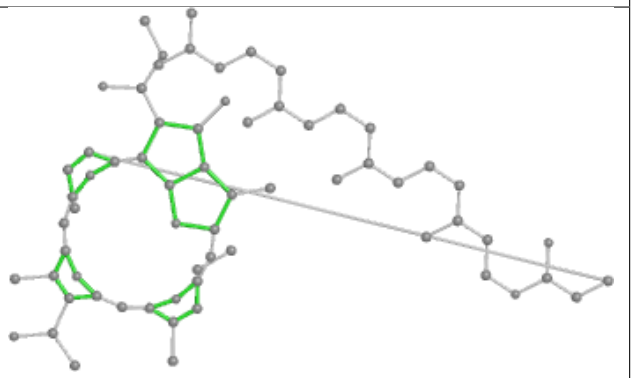
Bond lengths



Bond angles

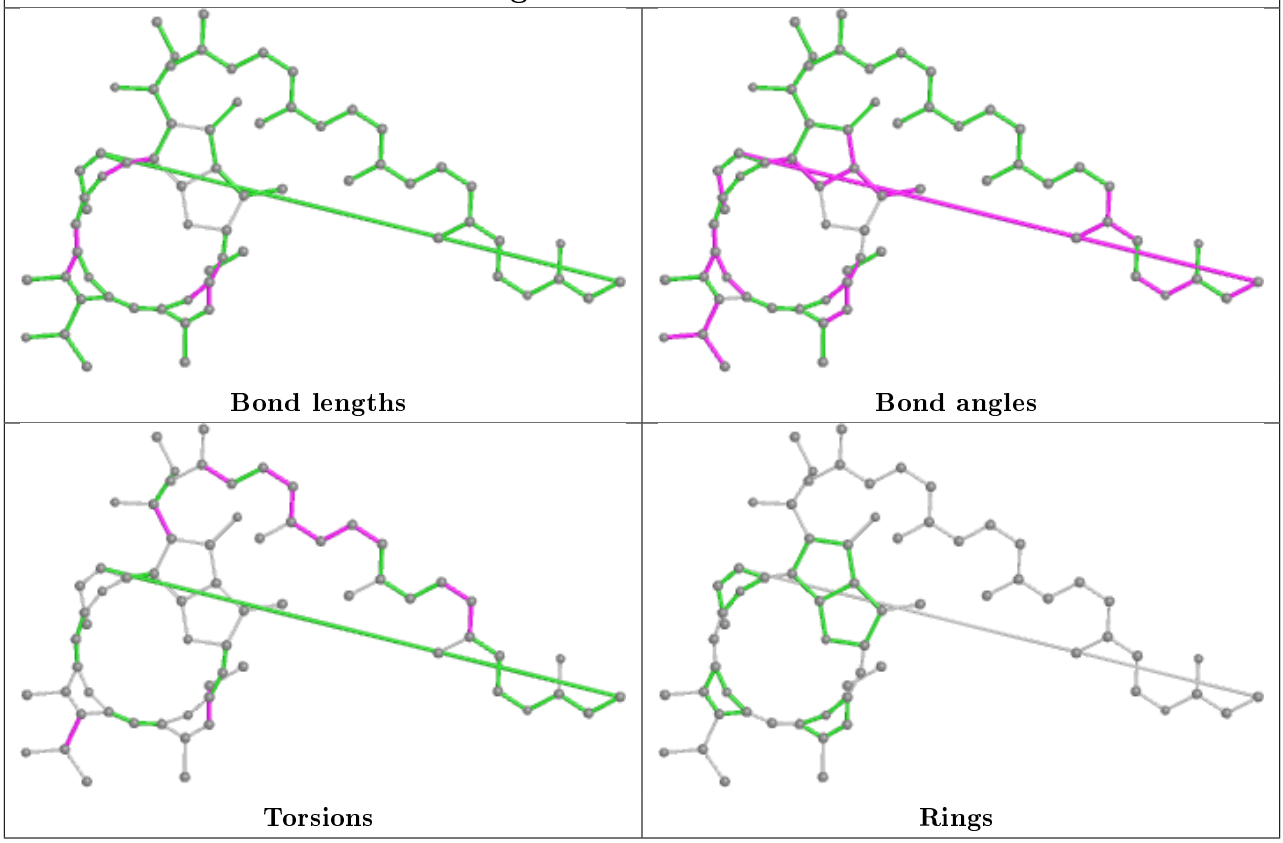


Torsions

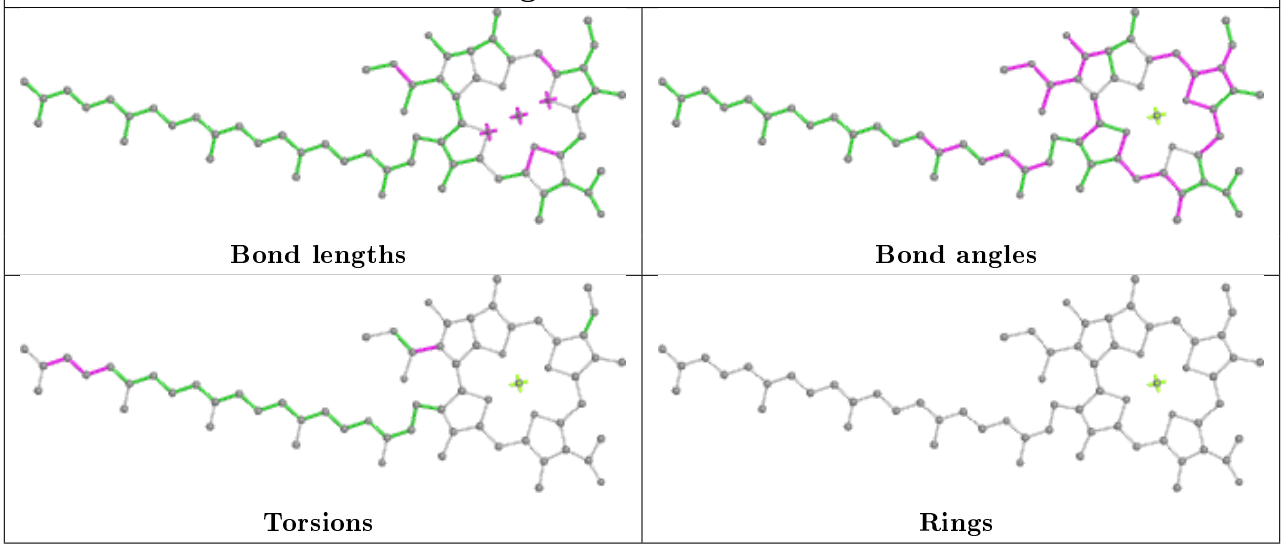


Rings

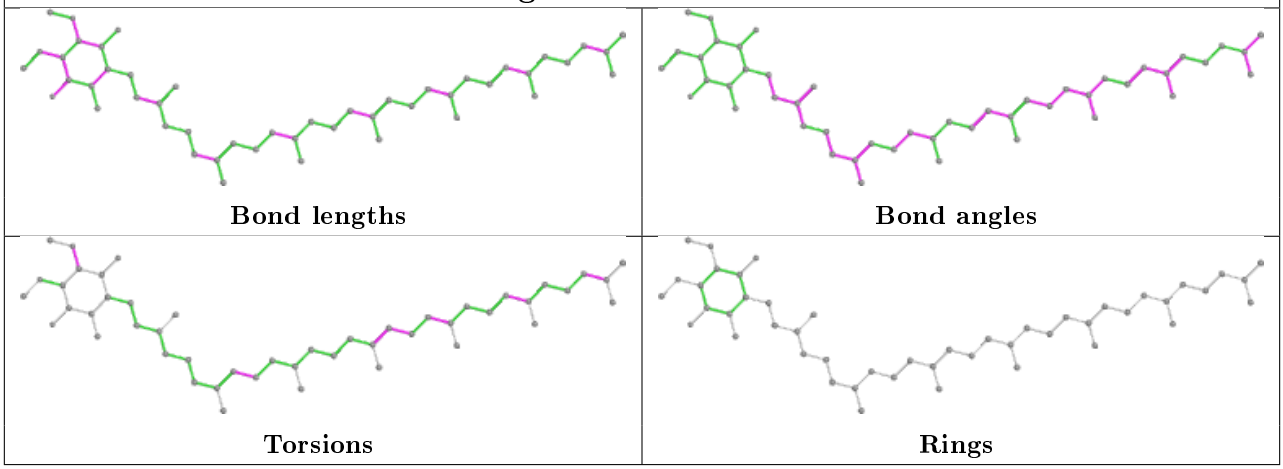
Ligand BPH M 1305



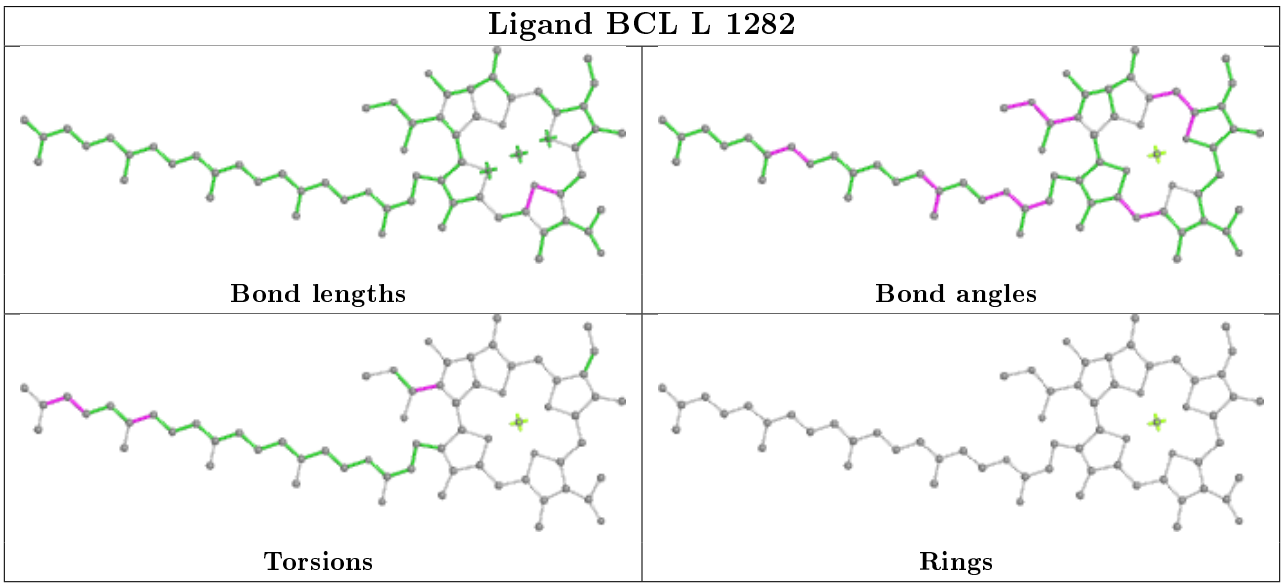
Ligand BCL L 1283



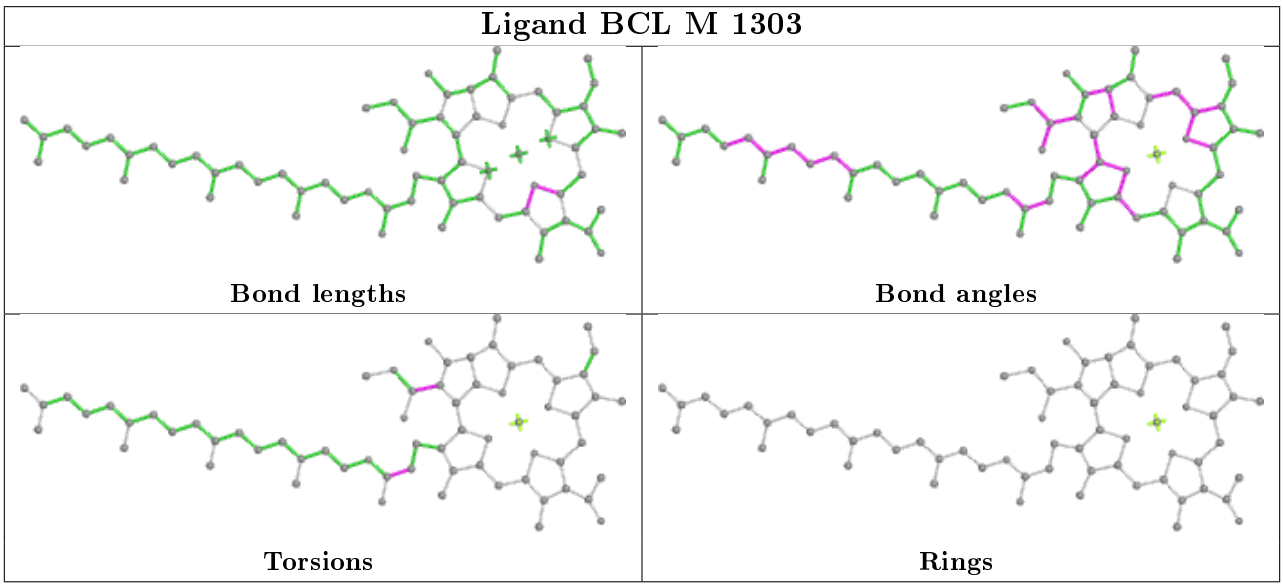
Ligand U10 M 1308

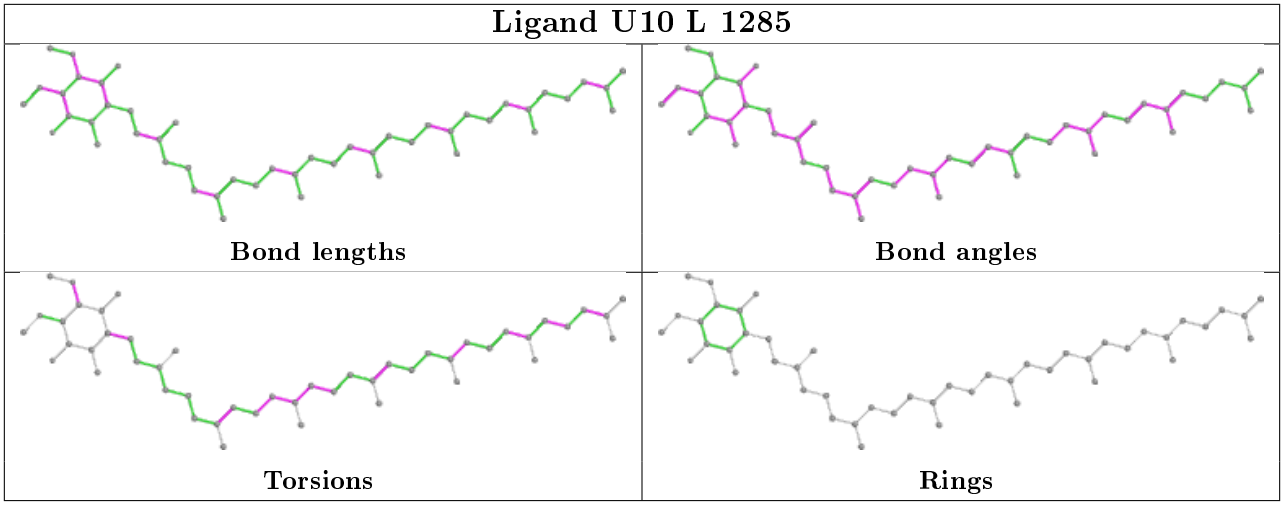


Ligand BCL L 1282



Ligand BCL M 1303





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, 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	235/260 (90%)	-0.56	2 (0%)	84	86	34, 44, 60, 69	0
2	L	281/281 (100%)	-0.52	6 (2%)	63	66	32, 45, 82, 101	0
3	M	301/307 (98%)	-0.60	2 (0%)	87	89	29, 46, 76, 83	0
All	All	817/848 (96%)	-0.56	10 (1%)	79	80	29, 45, 76, 101	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.6
2	L	281	GLY	5.5
2	L	59	TRP	5.0
1	H	245	ALA	4.3
2	L	202	LYS	2.8
2	L	277	GLY	2.6
2	L	72	GLU	2.3
3	M	301	HIS	2.2
1	H	51	ALA	2.2
2	L	279	ILE	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands (i)

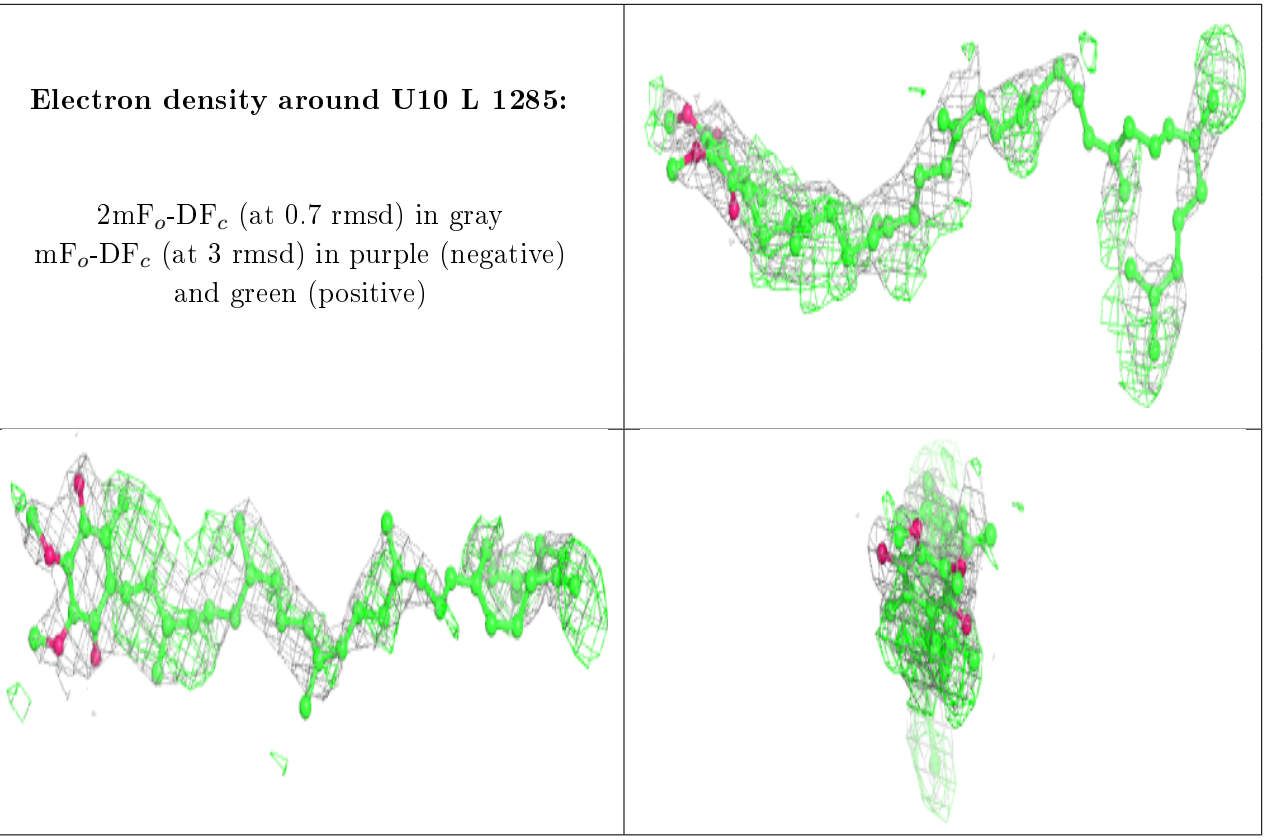
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	LDA	L	703	16/16	0.36	0.30	87,89,122,123	0
8	U10	L	1285	48/63	0.60	0.41	17,49,60,62	48
5	LDA	L	704	16/16	0.65	0.29	94,97,116,117	0
5	LDA	L	707	7/16	0.67	0.23	75,81,81,82	0
5	LDA	L	705	16/16	0.68	0.31	100,104,109,110	0
5	LDA	L	706	11/16	0.75	0.30	73,77,83,83	0
5	LDA	L	701	16/16	0.87	0.19	41,63,74,77	0
5	LDA	L	702	16/16	0.93	0.12	71,73,88,89	0
10	SPN	M	1307	43/43	0.93	0.14	33,53,79,83	0
8	U10	M	1308	48/63	0.94	0.12	26,43,74,77	0
7	BPH	M	1305	65/65	0.94	0.12	34,47,121,123	0
4	PO4	H	1246	5/5	0.94	0.22	92,96,101,102	0
4	PO4	M	1306	5/5	0.97	0.25	73,78,80,81	0
6	BCL	L	1283	66/66	0.97	0.08	14,30,66,73	0
6	BCL	M	1302	66/66	0.97	0.10	28,38,81,82	0
7	BPH	L	1284	65/65	0.98	0.10	16,34,54,60	0
6	BCL	M	1303	66/66	0.98	0.08	30,40,59,70	0
6	BCL	L	1282	66/66	0.98	0.08	29,40,48,50	0
9	FE	M	1304	1/1	1.00	0.04	33,33,33,33	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.

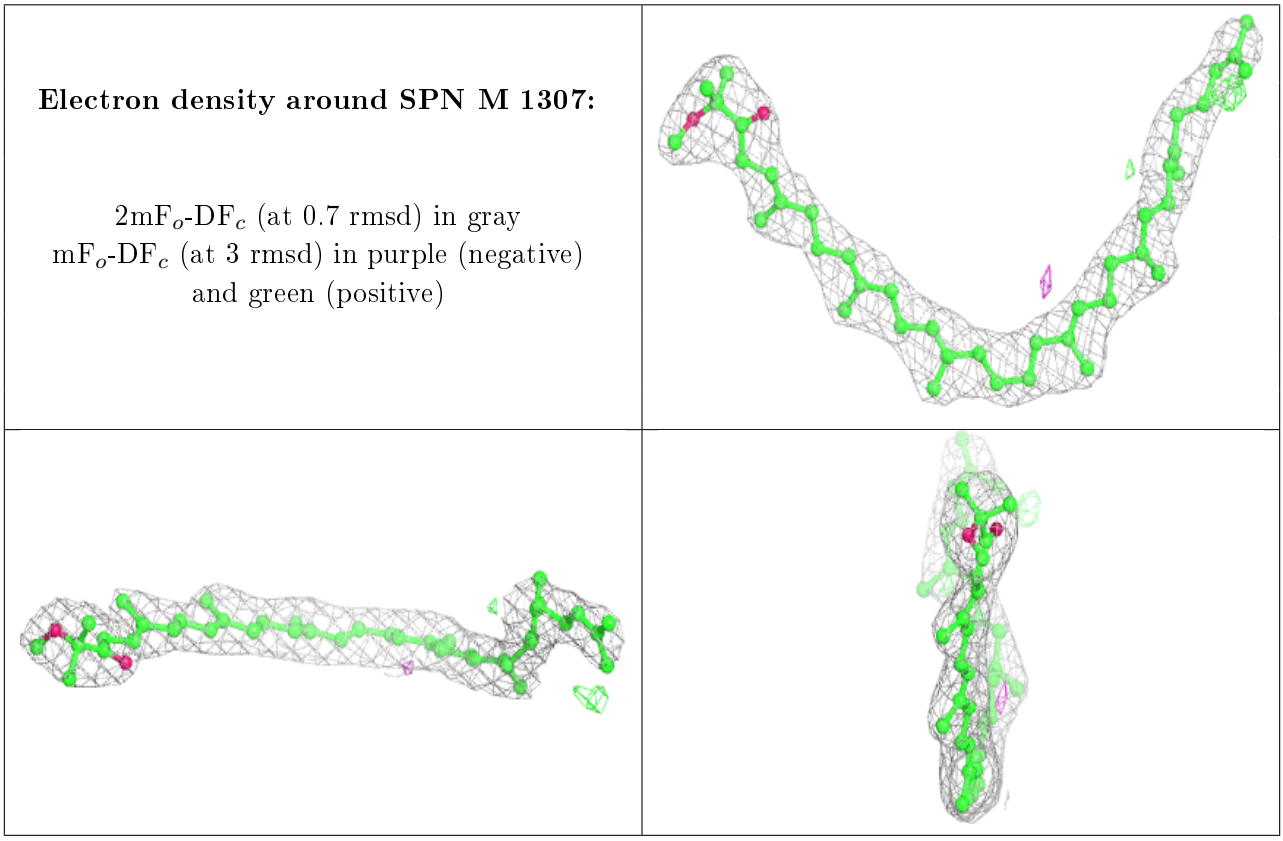
Electron density around U10 L 1285:

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



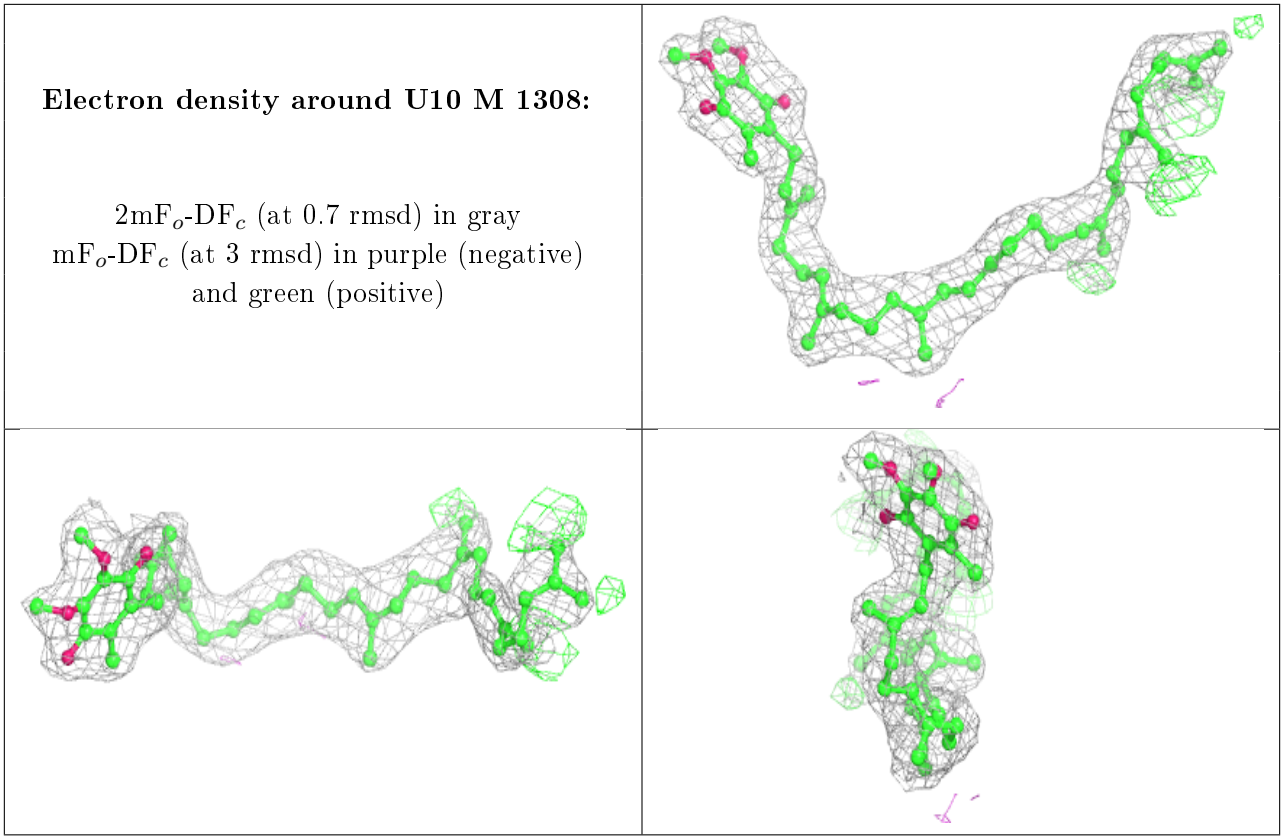
Electron density around SPN M 1307:

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



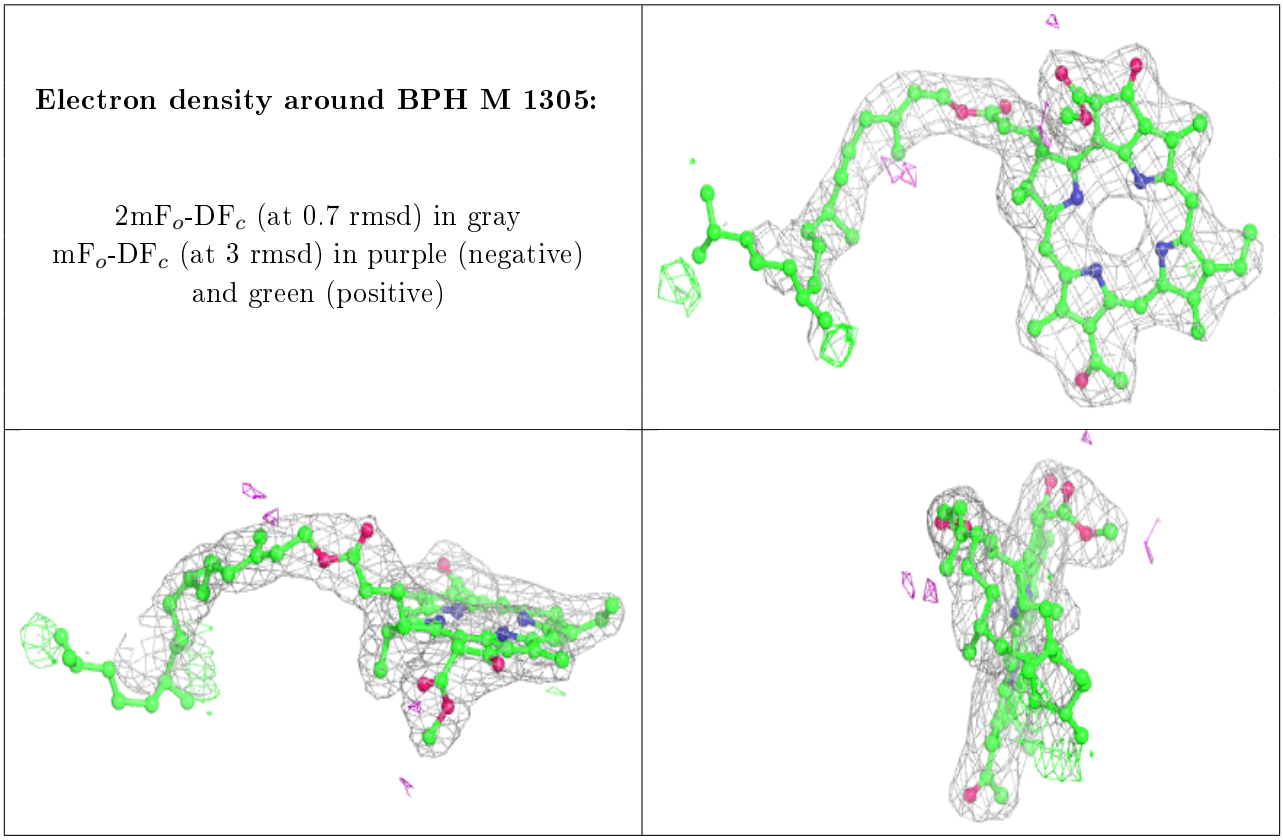
Electron density around U10 M 1308:

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



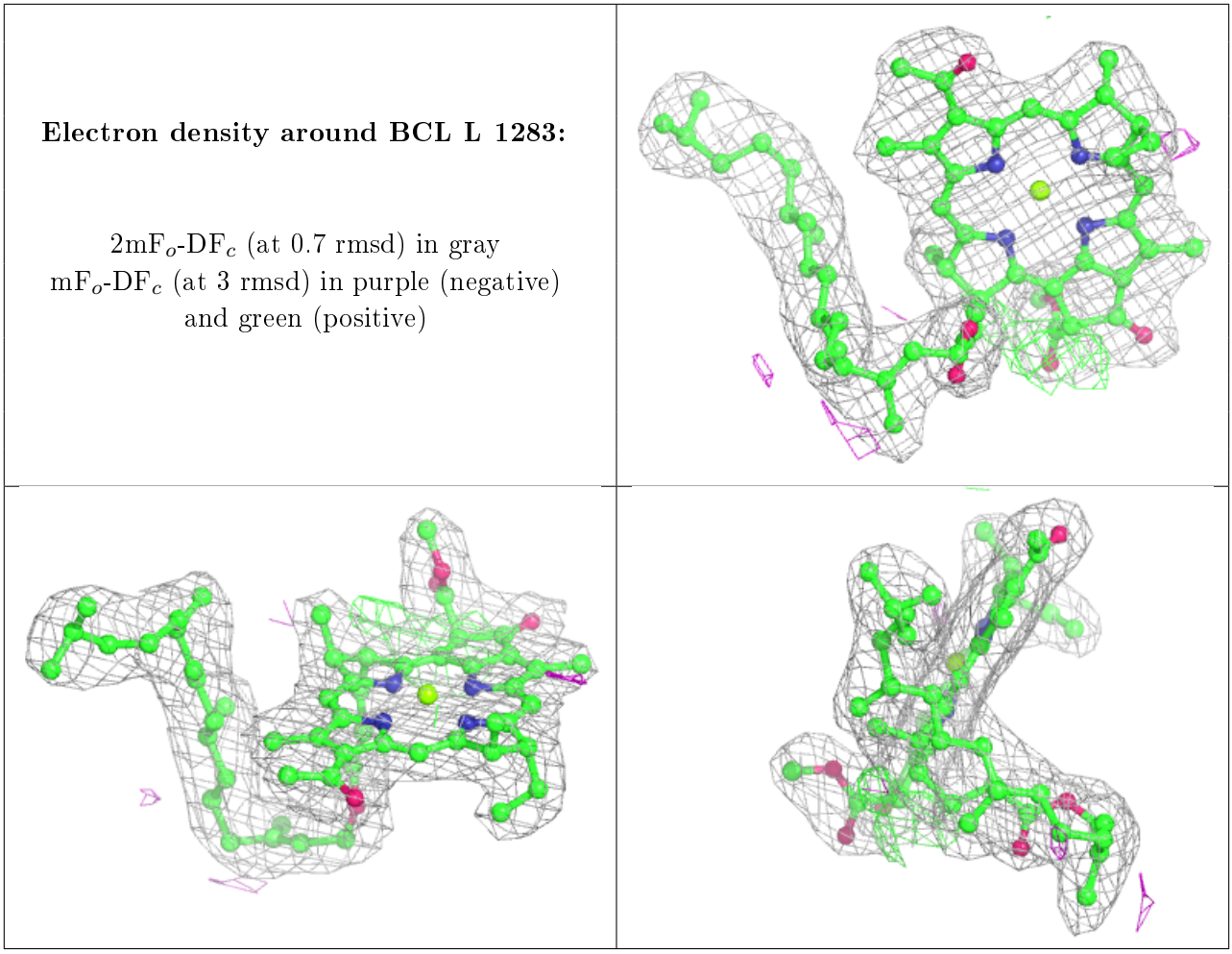
Electron density around BPH M 1305:

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



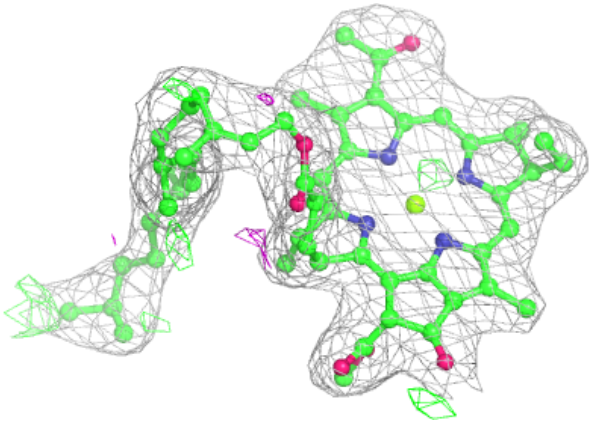
Electron density around BCL L 1283:

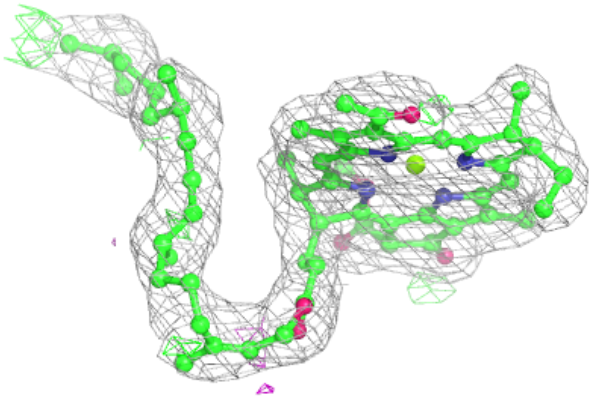
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

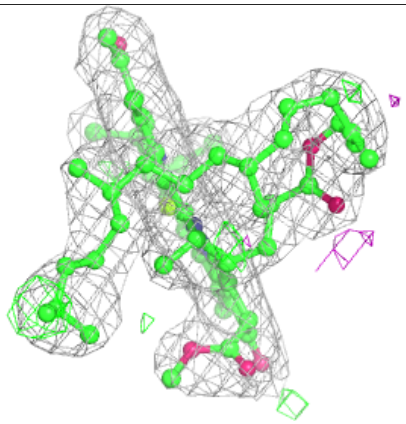


Electron density around BCL M 1302:

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

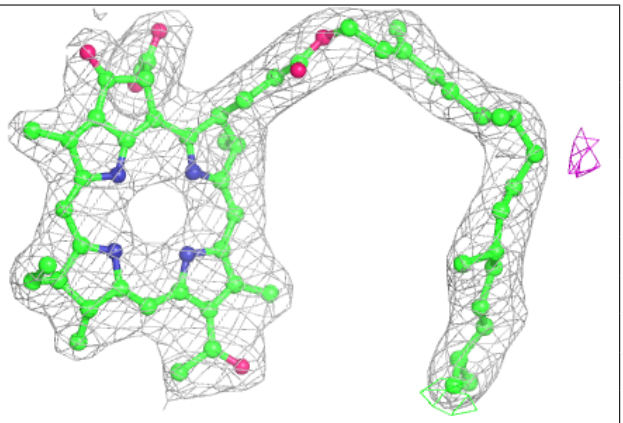


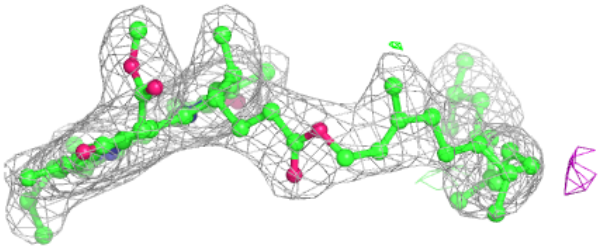


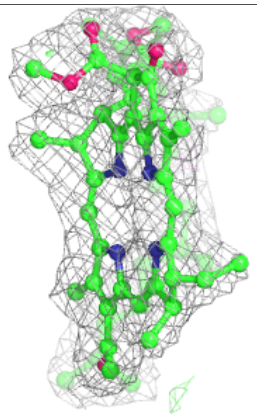


Electron density around BPH L 1284:

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

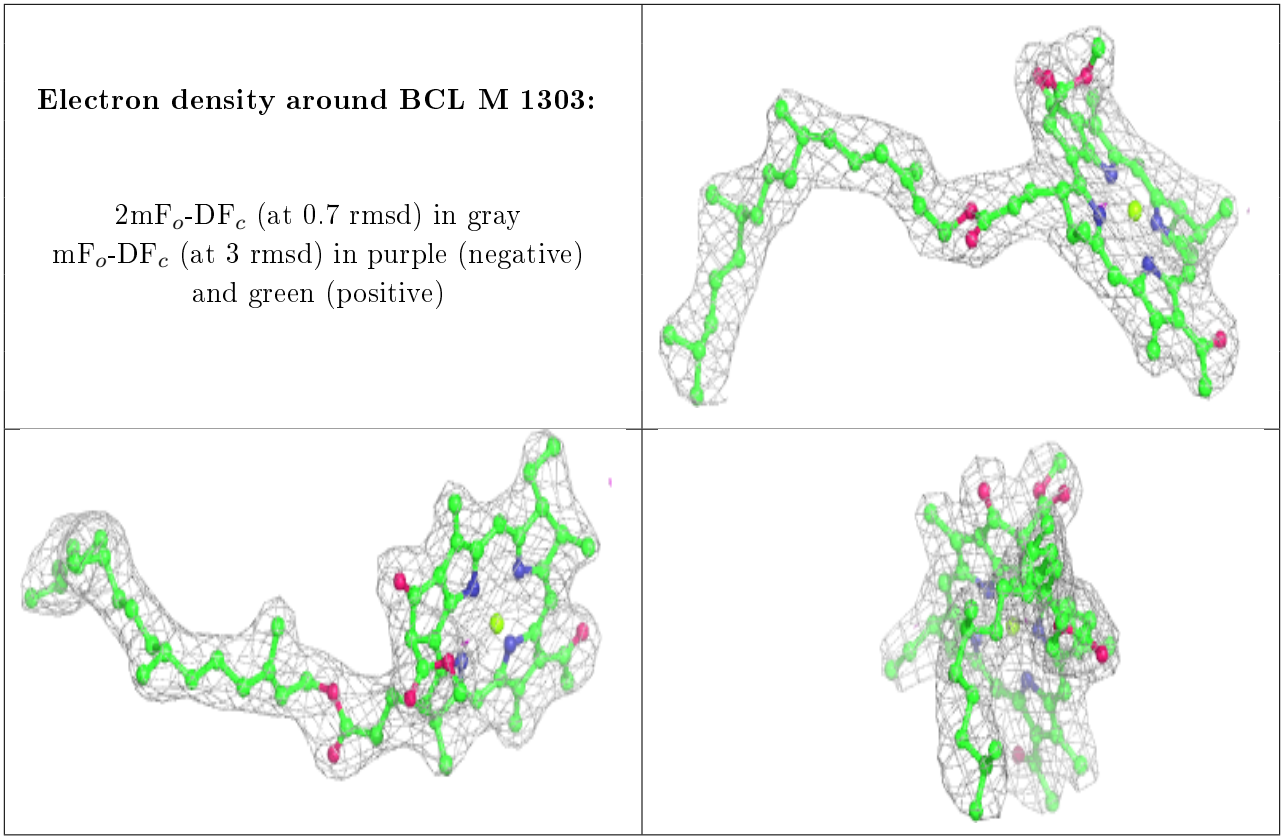






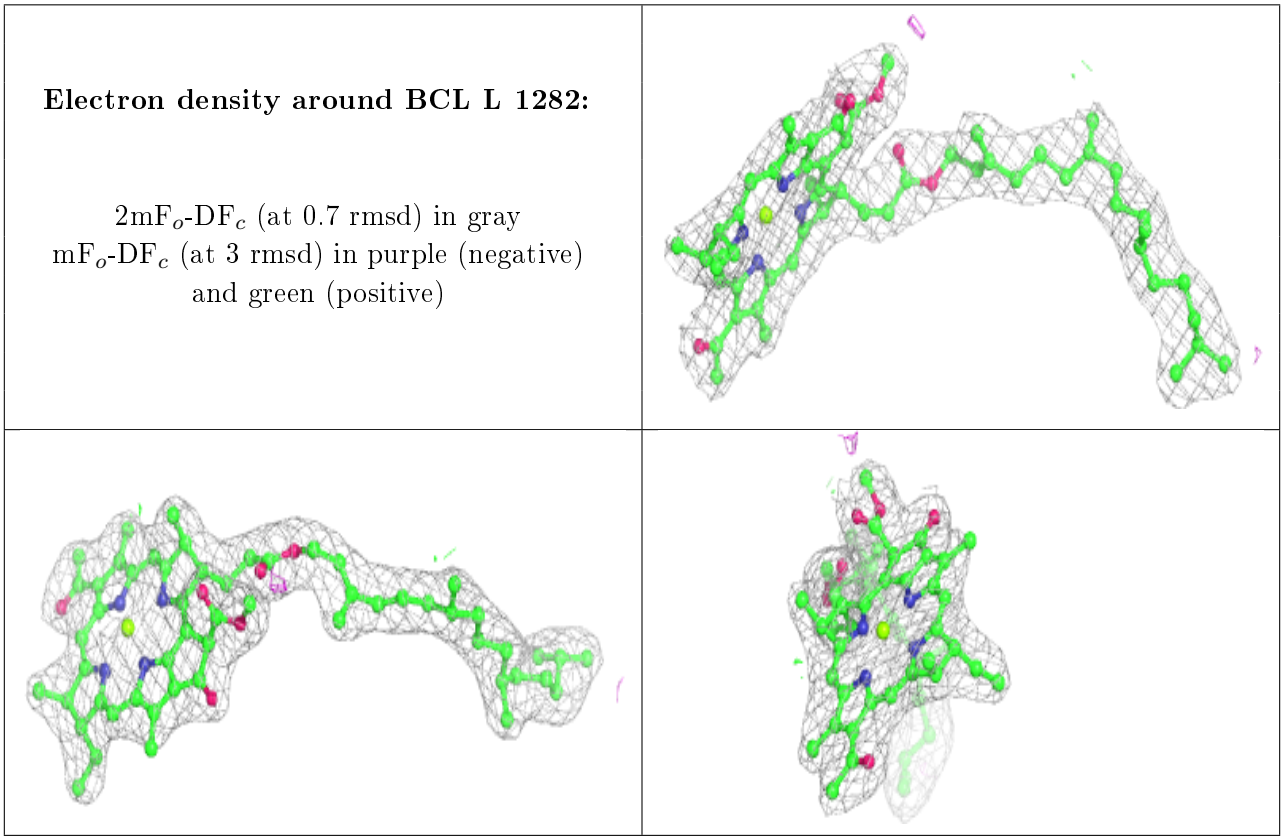
Electron density around BCL M 1303:

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



Electron density around BCL L 1282:

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



6.5 Other polymers (i)

There are no such residues in this entry.