Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 05:39 PM EDT

PDB ID	:	5V33
Title	:	R. sphaeroides photosythetic reaction center mutant - Residue L223, Ser to Trp - Room Temperature Structure Solved on X-ray Transparent Microfluidic Chip
Authors	:	Schieferstein, J.M.; Pawate, A.S.; Sun, C.; Wan, F.; Broecker, J.; Ernst, O.P.; Gennis, R.B.; Kenis, P.J.A.
Deposited on	:	2017-03-06
Resolution	:	3.49 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

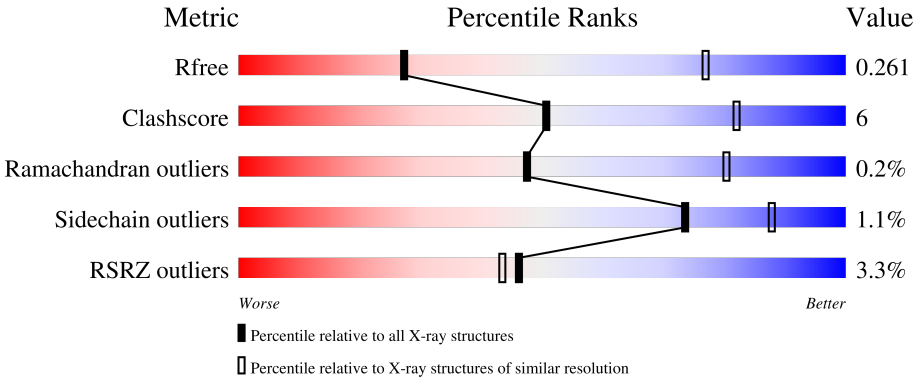
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.49 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	240	4% 85% 15%
2	L	281	5% 89% 11%
3	M	302	% 85% 15%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6919 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2239	1515	356	360	8			

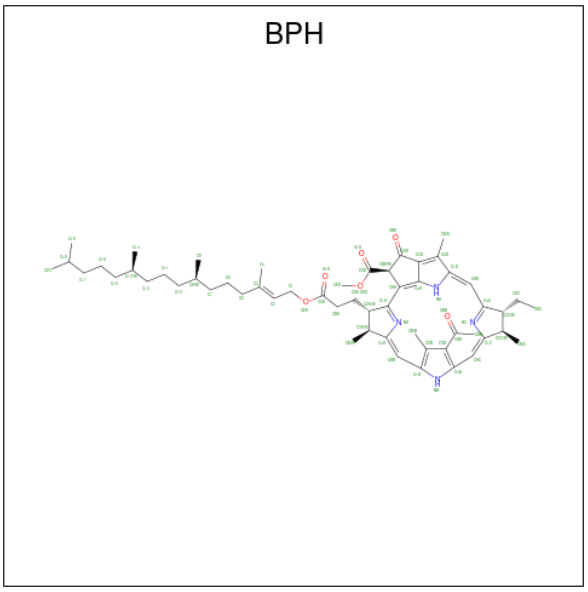
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	223	TRP	SER	engineered mutation	UNP P0C0Y8

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

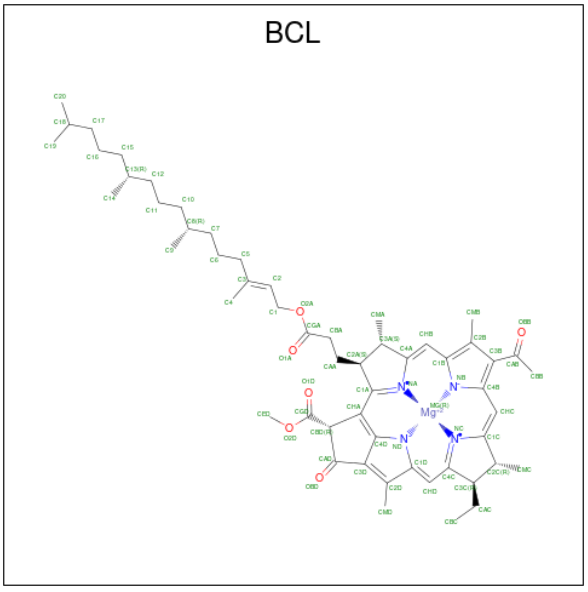
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

- Molecule 4 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

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



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

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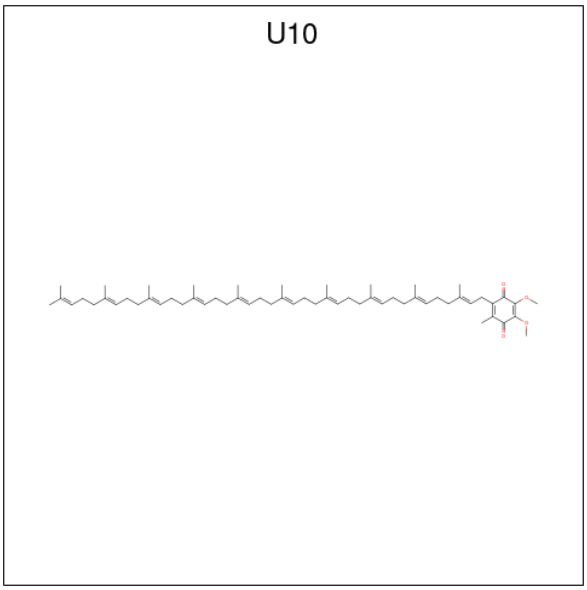
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Fe	0	0
			1	1		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

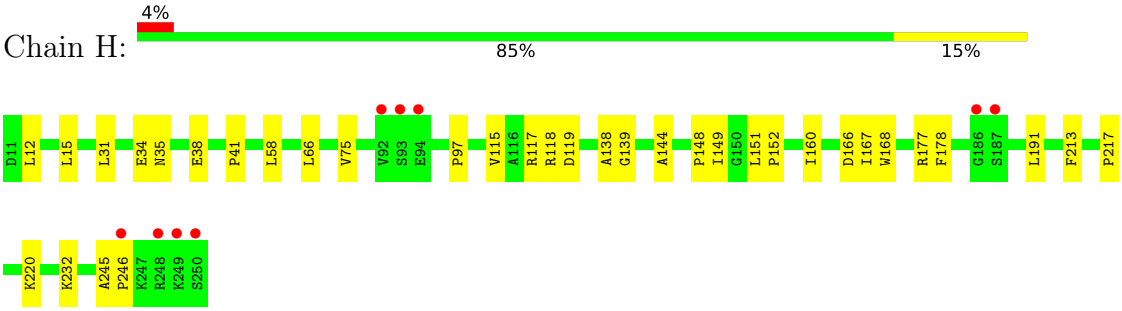


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			63	59	4		

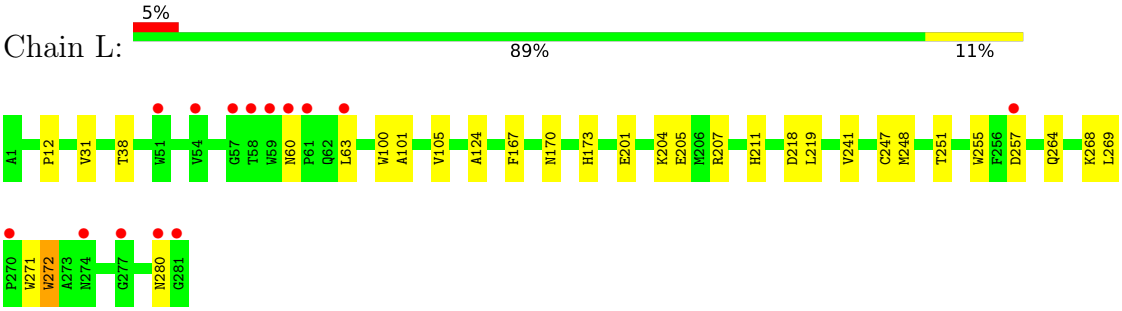
3 Residue-property plots (i)

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.

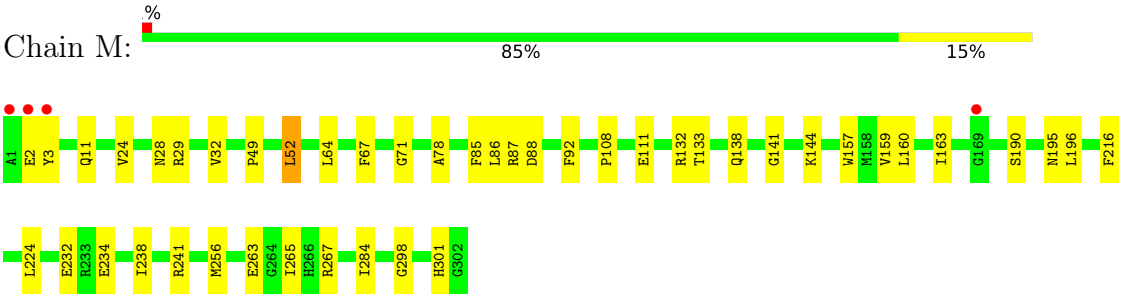
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.33Å 102.33Å 240.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.08 – 3.49 47.08 – 3.49	Depositor EDS
% Data completeness (in resolution range)	83.7 (47.08-3.49) 82.1 (47.08-3.49)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.262 0.226 , 0.261	Depositor DCC
R_{free} test set	1506 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, U10, FE, BPH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	H	0.22	0/1877	0.39	0/2553
2	L	0.23	0/2329	0.36	0/3190
3	M	0.23	0/2500	0.37	0/3413
All	All	0.23	0/6706	0.37	0/9156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	21	0
2	L	2239	0	2192	21	0
3	M	2408	0	2321	31	0
4	L	65	0	76	5	0
4	M	65	0	76	4	0
5	L	183	0	189	12	0
5	M	66	0	74	7	0
6	L	1	0	0	0	0
7	M	63	0	90	4	0
All	All	6919	0	6854	78	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 6.

All (78) 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)
3:M:67:PHE:HZ	4:M:403:BPH:H7C2	1.42	0.82
2:L:241:VAL:HG21	4:L:301:BPH:HAC2	1.63	0.79
3:M:3:TYR:OH	3:M:224:LEU:O	2.09	0.69
2:L:170:ASN:HB3	2:L:173:HIS:HB2	1.75	0.68
1:H:119:ASP:OD2	1:H:220:LYS:NZ	2.25	0.67
3:M:265:ILE:HD13	7:M:401:U10:H8	1.79	0.64
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.80	0.64
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.81	0.62
1:H:149:ILE:HD11	1:H:167:ILE:HG13	1.81	0.61
3:M:67:PHE:CZ	4:M:403:BPH:H7C2	2.32	0.60
2:L:204:LYS:HD2	2:L:207:ARG:HH22	1.67	0.59
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.32	0.58
1:H:41:PRO:HG3	1:H:58:LEU:HD11	1.85	0.58
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.88	0.56
7:M:401:U10:H103	7:M:401:U10:H1M1	1.86	0.56
2:L:207:ARG:HH21	3:M:141:GLY:HA3	1.72	0.55
2:L:218:ASP:O	3:M:132:ARG:NH1	2.39	0.55
1:H:31:LEU:O	1:H:35:ASN:ND2	2.26	0.55
4:L:301:BPH:HHC	4:L:301:BPH:HBB3	1.88	0.54
2:L:269:LEU:HB3	2:L:271:TRP:HE3	1.72	0.54
3:M:85:PHE:HD2	3:M:86:LEU:HD12	1.73	0.53
3:M:159:VAL:HA	3:M:163:ILE:HB	1.90	0.52
5:L:304:BCL:HBB2	5:M:402:BCL:H62	1.90	0.52
1:H:12:LEU:HA	1:H:15:LEU:HD12	1.91	0.52
1:H:152:PRO:HB2	1:H:160:ILE:HD12	1.91	0.52
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.93	0.51
1:H:245:ALA:N	1:H:246:PRO:HD2	2.26	0.51
2:L:255:TRP:NE1	2:L:257:ASP:O	2.44	0.51
3:M:238:ILE:HD12	3:M:263:GLU:HB2	1.92	0.51
5:M:402:BCL:H202	4:M:403:BPH:H111	1.93	0.50
5:M:402:BCL:H2	4:M:403:BPH:HHC	1.92	0.50
3:M:234:GLU:O	3:M:238:ILE:HG12	2.11	0.49
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.78	0.49
7:M:401:U10:H272	7:M:401:U10:H251	1.47	0.48
4:L:301:BPH:H3A	5:L:303:BCL:H122	1.96	0.48
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.77	0.48
2:L:205:GLU:O	2:L:207:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:280:ASN:ND2	3:M:88:ASP:OD1	2.48	0.47
4:L:301:BPH:HMB3	5:L:302:BCL:HMB2	1.95	0.47
5:L:304:BCL:HBB1	3:M:157:TRP:CD1	2.50	0.46
5:M:402:BCL:OBB	5:M:402:BCL:HHC	2.16	0.46
5:L:303:BCL:HBC2	5:M:402:BCL:HBC2	1.97	0.46
3:M:298:GLY:O	3:M:301:HIS:ND1	2.49	0.46
3:M:67:PHE:O	3:M:71:GLY:N	2.33	0.45
5:L:302:BCL:HBC1	5:L:303:BCL:CGA	2.47	0.45
5:L:302:BCL:HMD2	5:M:402:BCL:HBB3	1.98	0.44
1:H:66:LEU:HD13	1:H:118:ARG:HH12	1.83	0.44
2:L:201:GLU:OE2	3:M:144:LYS:NZ	2.51	0.44
2:L:60:ASN:OD1	2:L:63:LEU:HB2	2.19	0.43
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.50	0.43
3:M:32:VAL:HG12	3:M:49:PRO:HG3	1.99	0.43
2:L:248:MET:HA	2:L:251:THR:HG22	2.00	0.43
2:L:264:GLN:HB3	2:L:268:LYS:HE2	2.01	0.42
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.54	0.42
2:L:124:ALA:HB2	4:L:301:BPH:HAC1	2.00	0.42
3:M:28:ASN:HB3	3:M:52:LEU:HG	2.01	0.42
3:M:64:LEU:HA	3:M:67:PHE:HD2	1.84	0.42
1:H:97:PRO:HB2	2:L:12:PRO:HG3	2.02	0.42
3:M:265:ILE:CD1	7:M:401:U10:H8	2.49	0.42
2:L:272:TRP:O	3:M:87:ARG:NH1	2.47	0.42
1:H:217:PRO:HG2	1:H:232:LYS:HB3	2.02	0.42
3:M:190:SER:HA	3:M:196:LEU:HG	2.00	0.42
1:H:115:VAL:HG23	1:H:117:ARG:HG3	2.01	0.42
1:H:166:ASP:OD1	1:H:167:ILE:N	2.51	0.41
2:L:167:PHE:HB3	5:L:303:BCL:HMC3	2.02	0.41
1:H:220:LYS:HE2	1:H:220:LYS:HB3	1.91	0.41
3:M:138:GLN:HA	3:M:144:LYS:HZ2	1.84	0.41
2:L:207:ARG:HD2	2:L:211:HIS:CD2	2.55	0.41
5:L:303:BCL:H61	5:L:303:BCL:H41	1.92	0.41
1:H:177:ARG:NH1	3:M:232:GLU:OE2	2.52	0.41
3:M:24:VAL:HG21	3:M:29:ARG:NH1	2.36	0.41
3:M:160:LEU:HD21	3:M:284:ILE:HD13	2.03	0.40
5:L:302:BCL:HMB1	5:L:302:BCL:HBB2	2.02	0.40
2:L:101:ALA:O	2:L:105:VAL:HG23	2.22	0.40
5:L:303:BCL:HBB3	5:L:303:BCL:HMB1	2.02	0.40
1:H:144:ALA:HB3	3:M:11:GLN:HB2	2.02	0.40
1:H:34:GLU:HG2	3:M:267:ARG:HD2	2.04	0.40
5:L:304:BCL:HAC1	5:M:402:BCL:CAD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	238/240 (99%)	236 (99%)	2 (1%)	0	100 100
2	L	279/281 (99%)	268 (96%)	10 (4%)	1 (0%)	34 70
3	M	300/302 (99%)	289 (96%)	10 (3%)	1 (0%)	41 75
All	All	817/823 (99%)	793 (97%)	22 (3%)	2 (0%)	47 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN
2	L	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	195/195 (100%)	194 (100%)	1 (0%)	88 95
2	L	220/220 (100%)	218 (99%)	2 (1%)	78 91
3	M	236/236 (100%)	232 (98%)	4 (2%)	60 82
All	All	651/651 (100%)	644 (99%)	7 (1%)	73 88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	75	VAL
2	L	247	CYS
2	L	272	TRP
3	M	2	GLU
3	M	52	LEU
3	M	216	PHE
3	M	256	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	56	GLN

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	BCL	L	302	-	64,74,74	1.25	5 (7%)	78,115,115	1.46	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BPH	M	403	-	51,70,70	0.85	2 (3%)	52,101,101	1.24	6 (11%)
5	BCL	L	303	-	64,74,74	1.25	5 (7%)	78,115,115	1.48	9 (11%)
7	U10	M	401	-	63,63,63	2.68	17 (26%)	76,79,79	1.81	20 (26%)
4	BPH	L	301	-	51,70,70	0.94	2 (3%)	52,101,101	1.06	4 (7%)
5	BCL	M	402	-	64,74,74	1.28	6 (9%)	78,115,115	1.56	11 (14%)
5	BCL	L	304	-	49,59,74	1.42	4 (8%)	60,97,115	1.62	9 (15%)

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	BCL	L	302	-	-	2/37/137/137	-
4	BPH	M	403	-	-	5/37/105/105	0/5/6/6
5	BCL	L	303	-	-	3/37/137/137	-
7	U10	M	401	-	-	26/63/87/87	0/1/1/1
4	BPH	L	301	-	-	6/37/105/105	0/5/6/6
5	BCL	M	402	-	-	0/37/137/137	-
5	BCL	L	304	-	-	0/19/119/137	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	U10	C8-C9	6.11	1.47	1.33
7	M	401	U10	C13-C14	6.01	1.47	1.33
7	M	401	U10	C48-C49	6.00	1.47	1.33
7	M	401	U10	C33-C34	6.00	1.47	1.33
7	M	401	U10	C38-C39	5.98	1.47	1.33
7	M	401	U10	C18-C19	5.96	1.47	1.33
7	M	401	U10	C43-C44	5.95	1.47	1.33
7	M	401	U10	C28-C29	5.94	1.47	1.33
7	M	401	U10	C23-C24	5.93	1.47	1.33
7	M	401	U10	O4-C4	-5.35	1.23	1.36
7	M	401	U10	O3-C3	-5.28	1.24	1.36
7	M	401	U10	C53-C54	5.26	1.47	1.32
5	L	303	BCL	C1B-NB	5.01	1.39	1.35
5	L	304	BCL	C1B-NB	4.97	1.39	1.35
5	L	302	BCL	C1B-NB	4.88	1.39	1.35
5	M	402	BCL	C1B-NB	4.87	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	402	BCL	MG-NA	4.85	2.17	2.06
5	L	304	BCL	MG-NA	4.71	2.17	2.06
4	L	301	BPH	CBD-CGD	-4.64	1.46	1.52
5	L	302	BCL	MG-NA	4.61	2.17	2.06
5	L	303	BCL	MG-NA	4.45	2.16	2.06
4	M	403	BPH	CBD-CGD	-3.65	1.47	1.52
5	L	304	BCL	MG-NC	3.29	2.14	2.06
5	M	402	BCL	MG-NC	3.20	2.13	2.06
5	L	303	BCL	MG-NC	3.15	2.13	2.06
5	L	302	BCL	MG-NC	3.14	2.13	2.06
7	M	401	U10	C4-C5	-3.10	1.39	1.48
7	M	401	U10	C3-C2	-3.09	1.40	1.48
7	M	401	U10	C6-C5	-2.56	1.39	1.46
5	L	304	BCL	CHD-C1D	2.50	1.43	1.38
5	L	302	BCL	CHD-C1D	2.48	1.43	1.38
5	L	303	BCL	CHD-C1D	2.47	1.43	1.38
5	M	402	BCL	CHD-C1D	2.40	1.43	1.38
5	M	402	BCL	C1D-ND	2.37	1.40	1.37
5	M	402	BCL	C4B-NB	2.28	1.37	1.35
4	L	301	BPH	OBD-CAD	2.28	1.25	1.22
7	M	401	U10	C6-C1	2.27	1.39	1.35
7	M	401	U10	C1-C2	-2.25	1.39	1.47
4	M	403	BPH	OBD-CAD	2.20	1.25	1.22
5	L	302	BCL	C1D-ND	2.19	1.40	1.37
5	L	303	BCL	C4B-NB	2.04	1.37	1.35

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	304	BCL	CHD-C1D-ND	-5.45	119.44	124.45
5	L	302	BCL	CHD-C1D-ND	-5.31	119.57	124.45
5	M	402	BCL	CHD-C1D-ND	-5.29	119.59	124.45
5	M	402	BCL	C4D-CHA-C1A	5.23	127.61	121.25
5	L	303	BCL	CHD-C1D-ND	-5.13	119.74	124.45
5	L	302	BCL	C4D-CHA-C1A	5.03	127.37	121.25
5	L	304	BCL	C4D-CHA-C1A	4.97	127.30	121.25
5	L	303	BCL	C4D-CHA-C1A	4.83	127.13	121.25
5	M	402	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
4	M	403	BPH	C11-C10-C8	4.12	129.23	115.92
7	M	401	U10	C7-C8-C9	-4.09	119.98	126.79
5	M	402	BCL	C1D-ND-C4D	-3.93	103.54	106.33
5	L	303	BCL	CMB-C2B-C1B	-3.86	122.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	302	BCL	C1D-ND-C4D	-3.83	103.61	106.33
5	M	402	BCL	C4A-NA-C1A	3.67	108.35	106.71
5	L	304	BCL	C1D-ND-C4D	-3.61	103.77	106.33
5	L	304	BCL	C4A-NA-C1A	3.59	108.32	106.71
5	L	302	BCL	CMB-C2B-C1B	-3.57	122.98	128.46
7	M	401	U10	C40-C39-C41	3.55	121.25	115.27
5	L	303	BCL	C1D-ND-C4D	-3.55	103.81	106.33
7	M	401	U10	C47-C48-C49	-3.40	119.47	127.66
7	M	401	U10	C37-C38-C39	-3.35	119.59	127.66
7	M	401	U10	C22-C23-C24	-3.30	119.70	127.66
5	L	302	BCL	C4A-NA-C1A	3.26	108.17	106.71
4	M	403	BPH	O2A-C1-C2	-3.26	100.07	108.64
4	M	403	BPH	OBD-CAD-CBD	-3.24	121.07	125.82
7	M	401	U10	C42-C43-C44	-3.20	119.95	127.66
5	L	304	BCL	CMB-C2B-C1B	-3.20	123.55	128.46
7	M	401	U10	C10-C9-C11	3.18	120.62	115.27
7	M	401	U10	C12-C13-C14	-3.15	120.07	127.66
7	M	401	U10	C30-C29-C31	3.11	120.51	115.27
5	M	402	BCL	CHA-C1A-NA	-3.09	119.33	126.40
5	M	402	BCL	CMB-C2B-C3B	3.08	130.44	124.68
7	M	401	U10	C20-C19-C21	3.07	120.44	115.27
4	L	301	BPH	CED-O2D-CGD	3.06	122.86	115.94
4	L	301	BPH	OBD-CAD-CBD	-3.06	121.34	125.82
7	M	401	U10	C35-C34-C36	3.04	120.39	115.27
5	L	303	BCL	CHA-C1A-NA	-3.00	119.52	126.40
7	M	401	U10	C27-C28-C29	-2.99	120.46	127.66
5	L	303	BCL	C2A-C1A-CHA	2.98	129.06	123.86
5	L	302	BCL	CHA-C1A-NA	-2.92	119.72	126.40
7	M	401	U10	C25-C24-C26	2.91	120.17	115.27
7	M	401	U10	C45-C44-C46	2.87	120.11	115.27
5	L	303	BCL	CMB-C2B-C3B	2.83	129.96	124.68
5	L	304	BCL	CHA-C1A-NA	-2.78	120.03	126.40
7	M	401	U10	C32-C33-C34	-2.78	120.97	127.66
7	M	401	U10	C50-C49-C51	2.68	119.78	115.27
7	M	401	U10	C15-C14-C16	2.66	119.75	115.27
5	L	304	BCL	C2A-C1A-CHA	2.65	128.50	123.86
5	L	302	BCL	CMB-C2B-C3B	2.60	129.55	124.68
5	M	402	BCL	C4B-C3B-CAB	-2.58	122.14	127.13
5	M	402	BCL	C2A-C1A-CHA	2.56	128.34	123.86
4	L	301	BPH	CMD-C2D-C3D	2.50	129.36	124.68
5	L	302	BCL	C2A-C1A-CHA	2.49	128.21	123.86
5	M	402	BCL	OBB-CAB-CBB	-2.47	114.61	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	301	BPH	CMB-C2B-C3B	2.40	129.16	124.68
7	M	401	U10	C17-C18-C19	-2.37	121.96	127.66
4	M	403	BPH	CMD-C2D-C3D	2.36	129.09	124.68
4	M	403	BPH	CMB-C2B-C3B	2.35	129.08	124.68
7	M	401	U10	C56-C54-C55	2.33	119.76	114.60
5	L	304	BCL	CMB-C2B-C3B	2.31	129.00	124.68
5	L	303	BCL	C4B-C3B-CAB	-2.23	122.83	127.13
5	L	304	BCL	C1C-NC-C4C	2.16	107.67	106.71
5	L	303	BCL	OBB-CAB-CBB	-2.14	115.36	120.17
5	L	302	BCL	C4B-C3B-CAB	-2.12	123.03	127.13
5	M	402	BCL	C4D-C3D-CAD	-2.09	105.63	108.10
4	M	403	BPH	O2D-CGD-CBD	2.09	113.64	111.00
7	M	401	U10	C1M-C1-C6	-2.06	121.03	124.40

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	BPH	C4C-C3C-CAC-CBC
4	L	301	BPH	C2C-C3C-CAC-CBC
5	L	303	BCL	C2-C3-C5-C6
5	L	303	BCL	C4-C3-C5-C6
7	M	401	U10	C12-C13-C14-C15
7	M	401	U10	C12-C13-C14-C16
7	M	401	U10	C23-C24-C26-C27
7	M	401	U10	C25-C24-C26-C27
7	M	401	U10	C29-C31-C32-C33
7	M	401	U10	C34-C36-C37-C38
7	M	401	U10	C38-C39-C41-C42
7	M	401	U10	C40-C39-C41-C42
7	M	401	U10	C39-C41-C42-C43
7	M	401	U10	C14-C16-C17-C18
7	M	401	U10	C19-C21-C22-C23
7	M	401	U10	C49-C51-C52-C53
7	M	401	U10	C37-C38-C39-C40
7	M	401	U10	C42-C43-C44-C45
7	M	401	U10	C37-C38-C39-C41
7	M	401	U10	C24-C26-C27-C28
4	L	301	BPH	C4-C3-C5-C6
7	M	401	U10	C42-C43-C44-C46
4	L	301	BPH	C2-C3-C5-C6
4	M	403	BPH	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	M	401	U10	C35-C34-C36-C37
7	M	401	U10	C33-C34-C36-C37
5	L	302	BCL	C12-C13-C15-C16
4	L	301	BPH	CAD-CBD-CGD-O2D
4	M	403	BPH	CAD-CBD-CGD-O2D
7	M	401	U10	C30-C29-C31-C32
4	M	403	BPH	C4C-C3C-CAC-CBC
5	L	302	BCL	C14-C13-C15-C16
7	M	401	U10	C28-C29-C31-C32
7	M	401	U10	C5-C4-O4-C4M
4	M	403	BPH	C14-C13-C15-C16
4	M	403	BPH	C2A-CAA-CBA-CGA
5	L	303	BCL	C10-C11-C12-C13
7	M	401	U10	C45-C44-C46-C47
7	M	401	U10	C44-C46-C47-C48
7	M	401	U10	C43-C44-C46-C47
4	L	301	BPH	O2A-C1-C2-C3
7	M	401	U10	C3-C4-O4-C4M

There are no ring outliers.

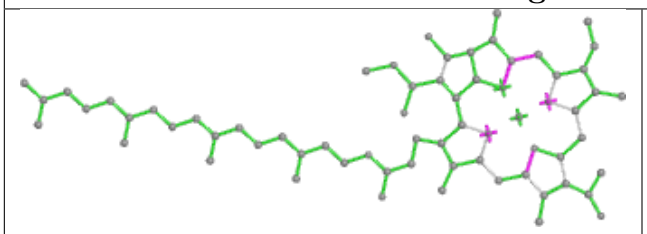
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	BCL	4	0
4	M	403	BPH	4	0
5	L	303	BCL	6	0
7	M	401	U10	4	0
4	L	301	BPH	5	0
5	M	402	BCL	7	0
5	L	304	BCL	3	0

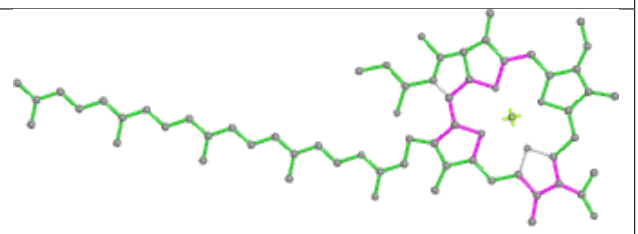
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

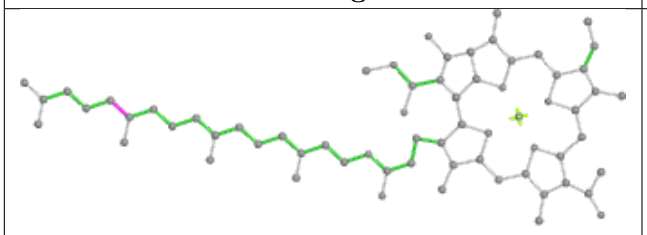
Ligand BCL L 302



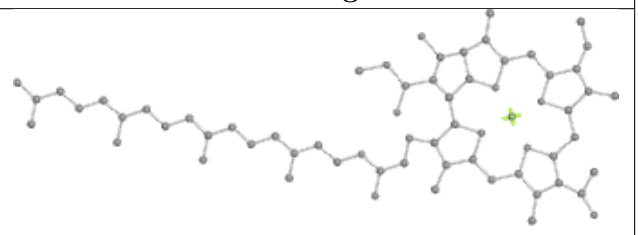
Bond lengths



Bond angles

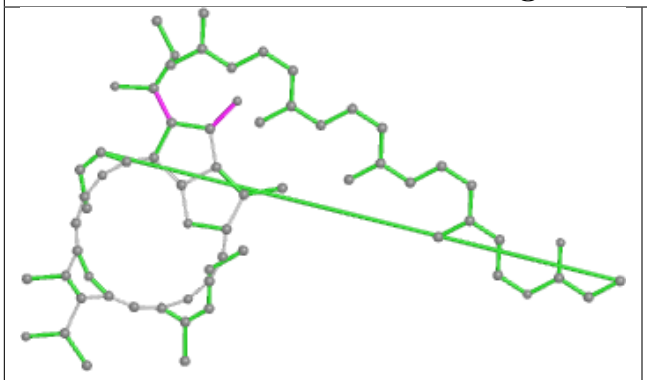


Torsions

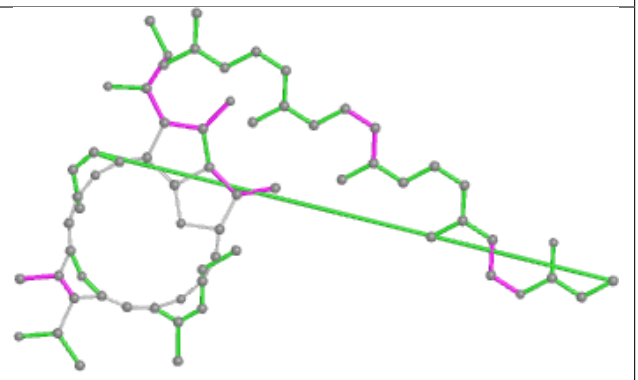


Rings

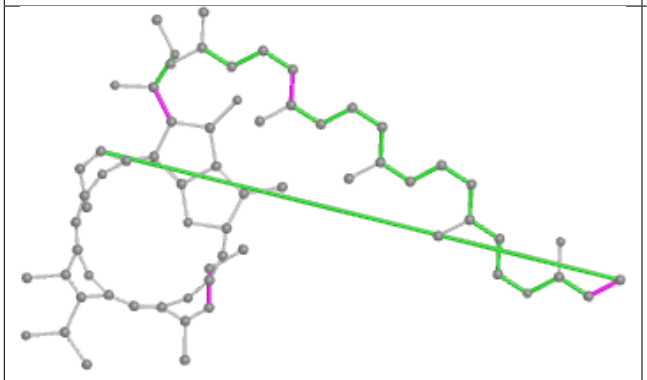
Ligand BPH M 403



Bond lengths



Bond angles



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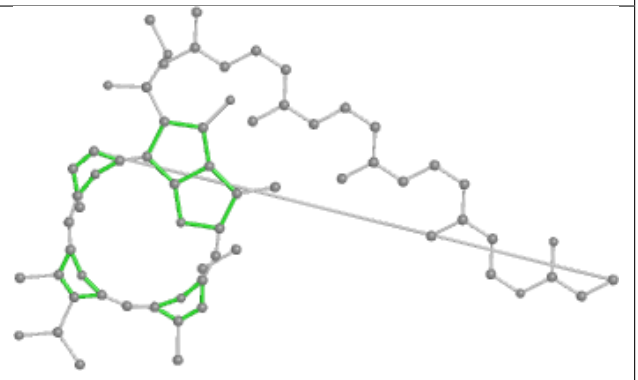
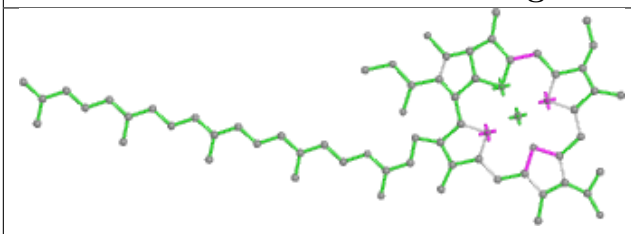
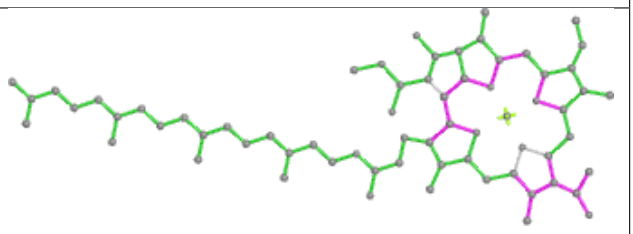


Rings

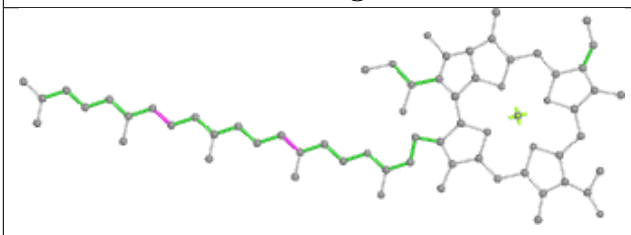
Ligand BCL L 303



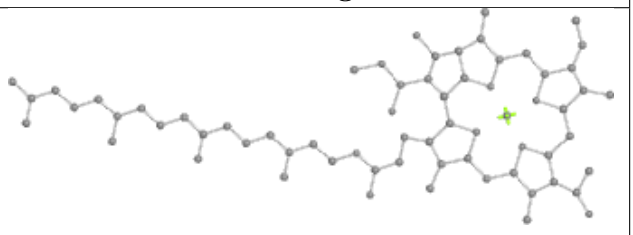
Bond lengths



Bond angles

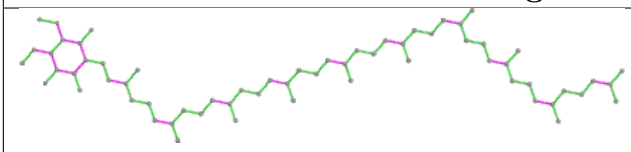


Torsions

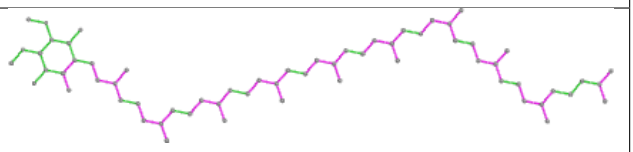


Rings

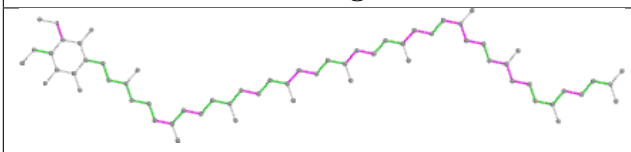
Ligand U10 M 401



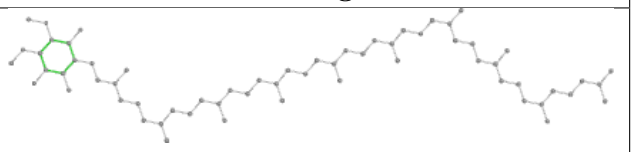
Bond lengths



Bond angles

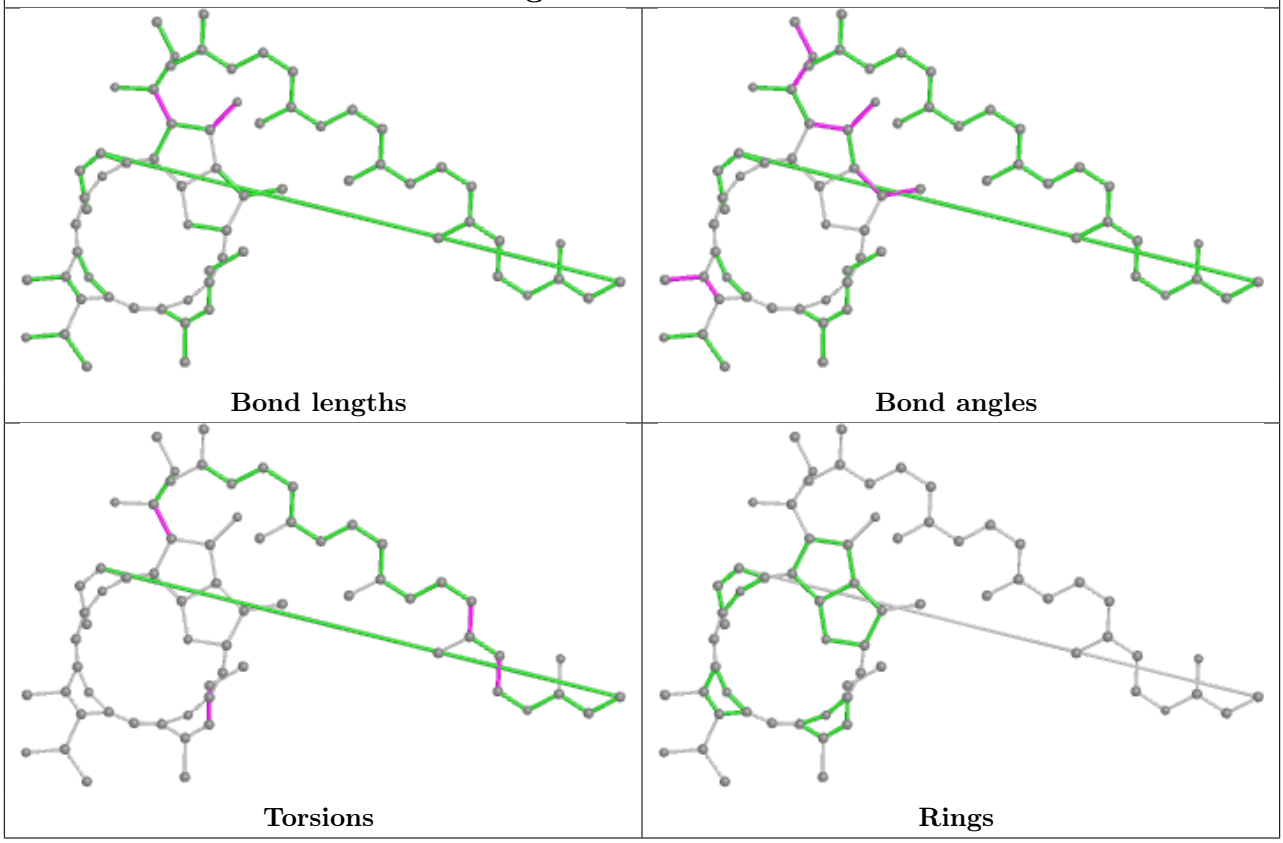


Torsions

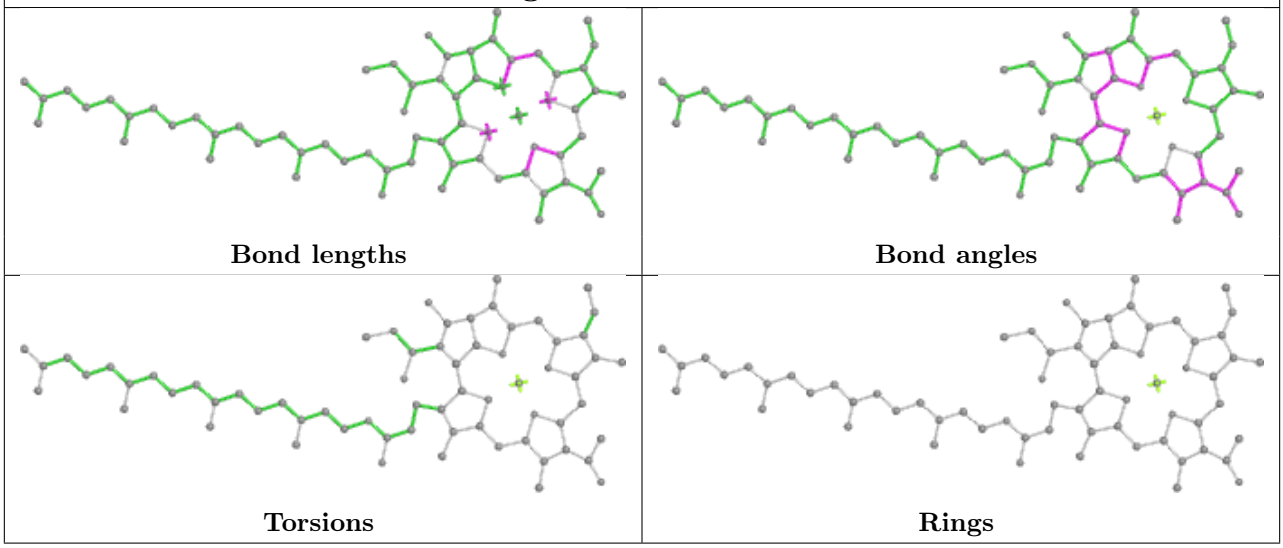


Rings

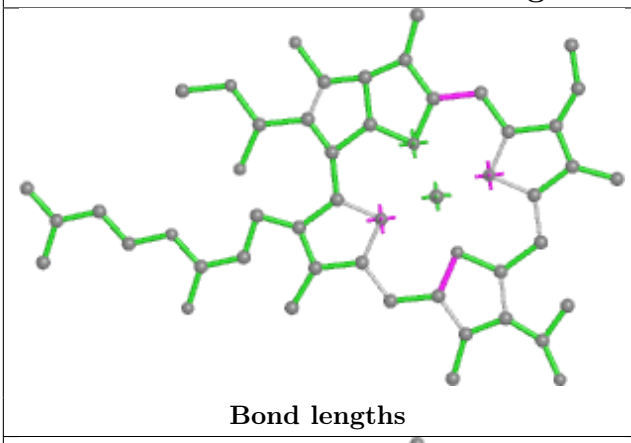
Ligand BPH L 301



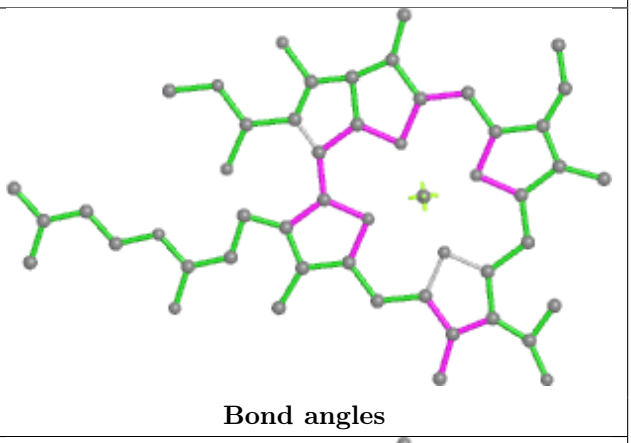
Ligand BCL M 402



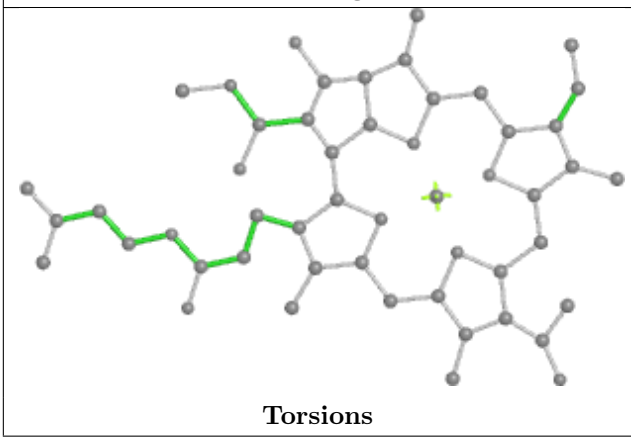
Ligand BCL L 304



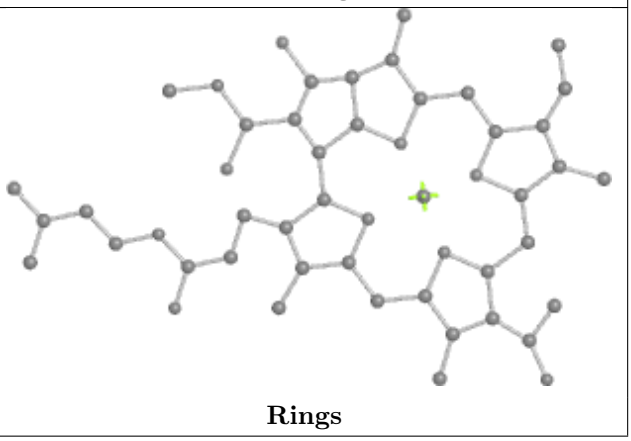
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	H	240/240 (100%)	0.17	9 (3%) 40 37	27, 45, 76, 115	0
2	L	281/281 (100%)	-0.22	14 (4%) 28 27	25, 40, 82, 95	0
3	M	302/302 (100%)	-0.18	4 (1%) 77 73	24, 43, 73, 112	0
All	All	823/823 (100%)	-0.09	27 (3%) 46 43	24, 42, 78, 115	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	6.9
1	H	249	LYS	4.8
1	H	246	PRO	4.7
1	H	187	SER	4.1
1	H	93	SER	3.7
2	L	270	PRO	3.5
2	L	281	GLY	3.4
3	M	1	ALA	3.2
2	L	59	TRP	3.1
1	H	94	GLU	3.1
2	L	51	TRP	3.0
1	H	248	ARG	3.0
3	M	3	TYR	3.0
3	M	2	GLU	2.9
2	L	257	ASP	2.7
1	H	92	VAL	2.5
2	L	61	PRO	2.3
2	L	57	GLY	2.3
1	H	186	GLY	2.2
2	L	58	THR	2.2
2	L	54	VAL	2.2
2	L	280	ASN	2.1
3	M	169	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	277	GLY	2.1
2	L	60	ASN	2.0
2	L	274	ASN	2.0
2	L	63	LEU	2.0

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)

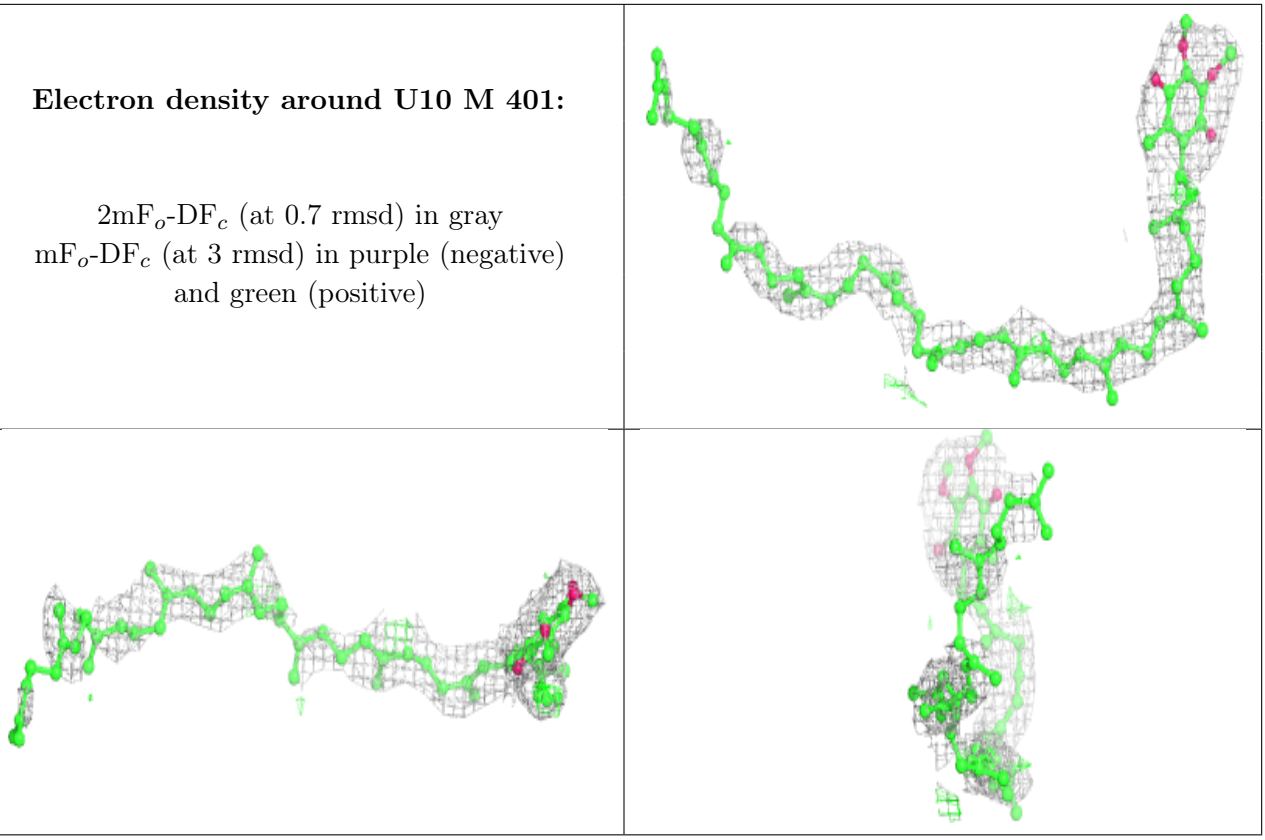
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	U10	M	401	63/63	0.83	0.33	51,61,82,84	0
4	BPH	M	403	65/65	0.89	0.28	36,40,95,103	0
5	BCL	M	402	66/66	0.93	0.21	31,35,43,66	0
5	BCL	L	303	66/66	0.95	0.19	37,44,51,52	0
5	BCL	L	304	51/66	0.95	0.18	31,36,38,40	0
4	BPH	L	301	65/65	0.95	0.18	25,28,35,40	0
5	BCL	L	302	66/66	0.95	0.18	26,31,34,38	0
6	FE	L	305	1/1	0.98	0.12	24,24,24,24	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.

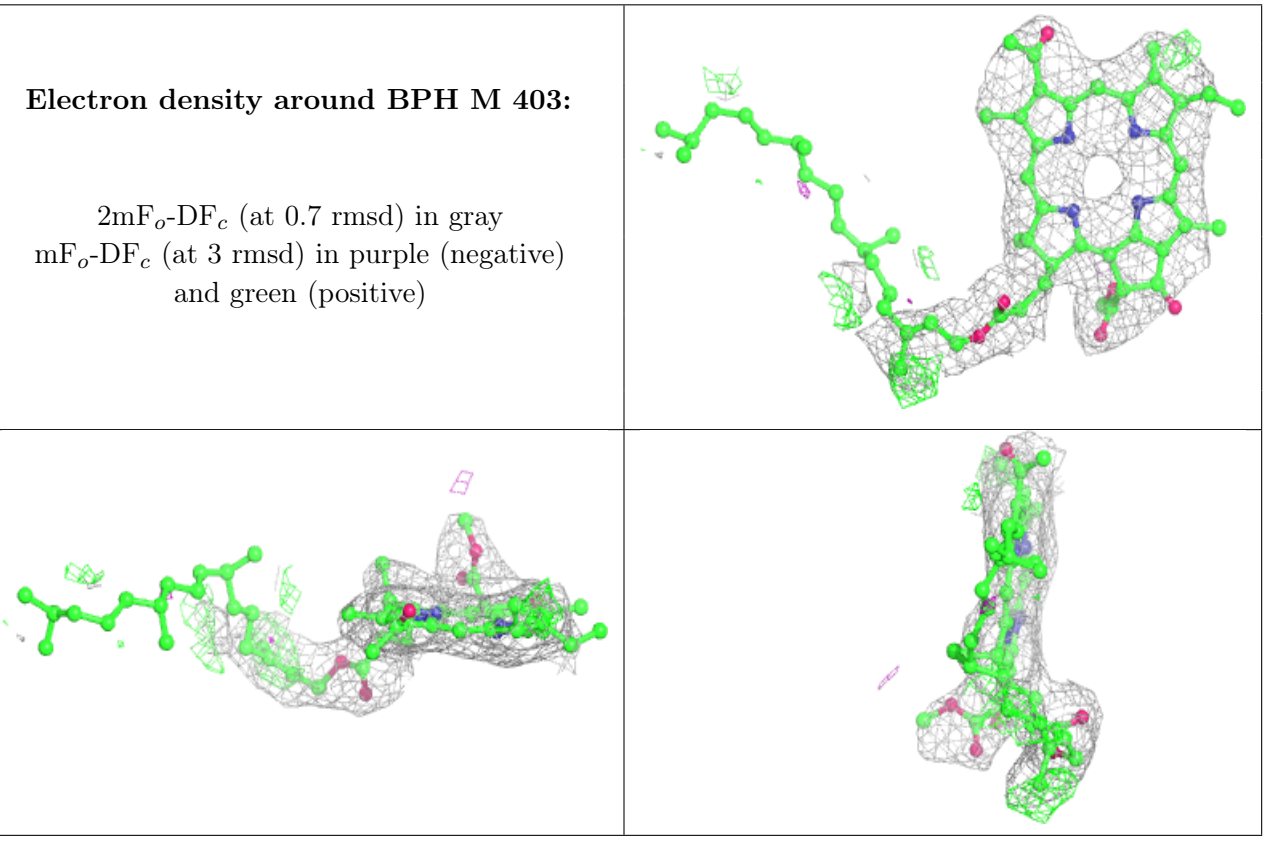
Electron density around U10 M 401:

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



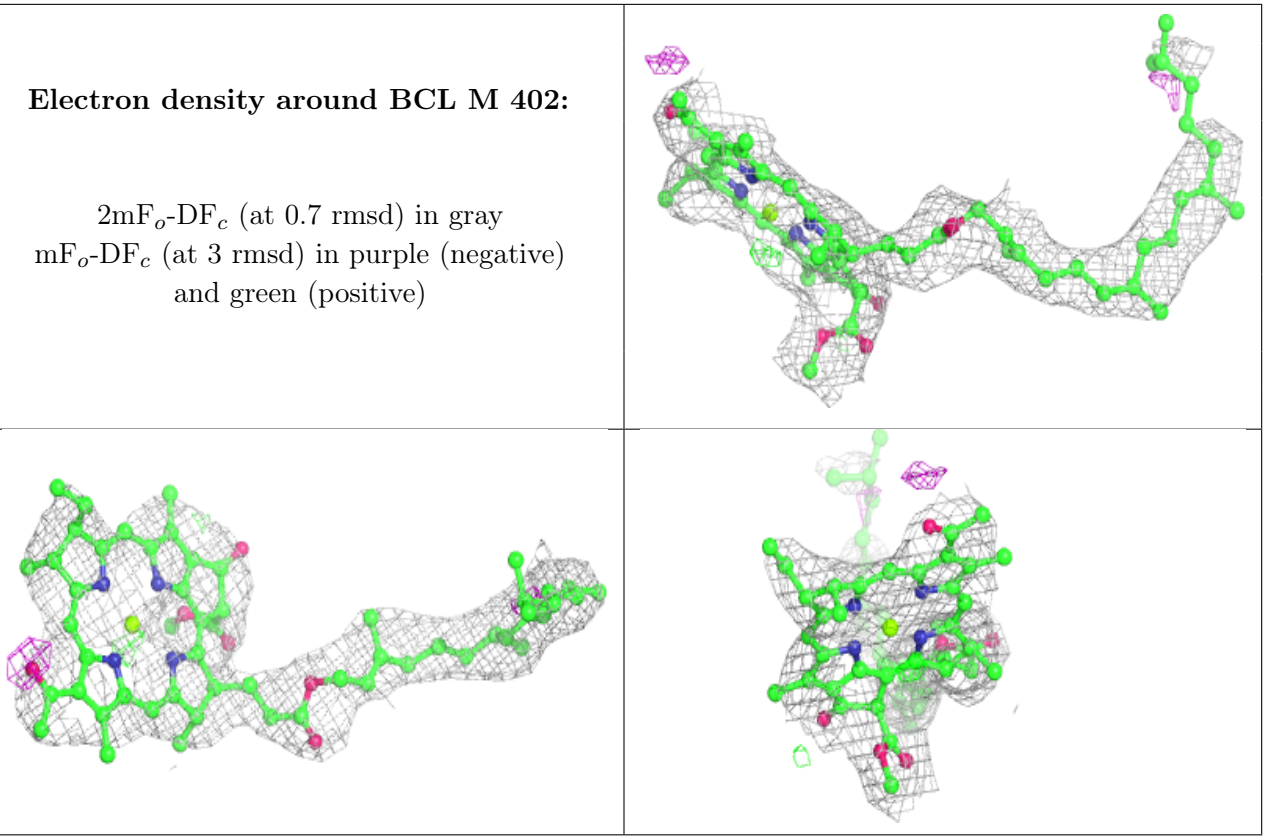
Electron density around BPH M 403:

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



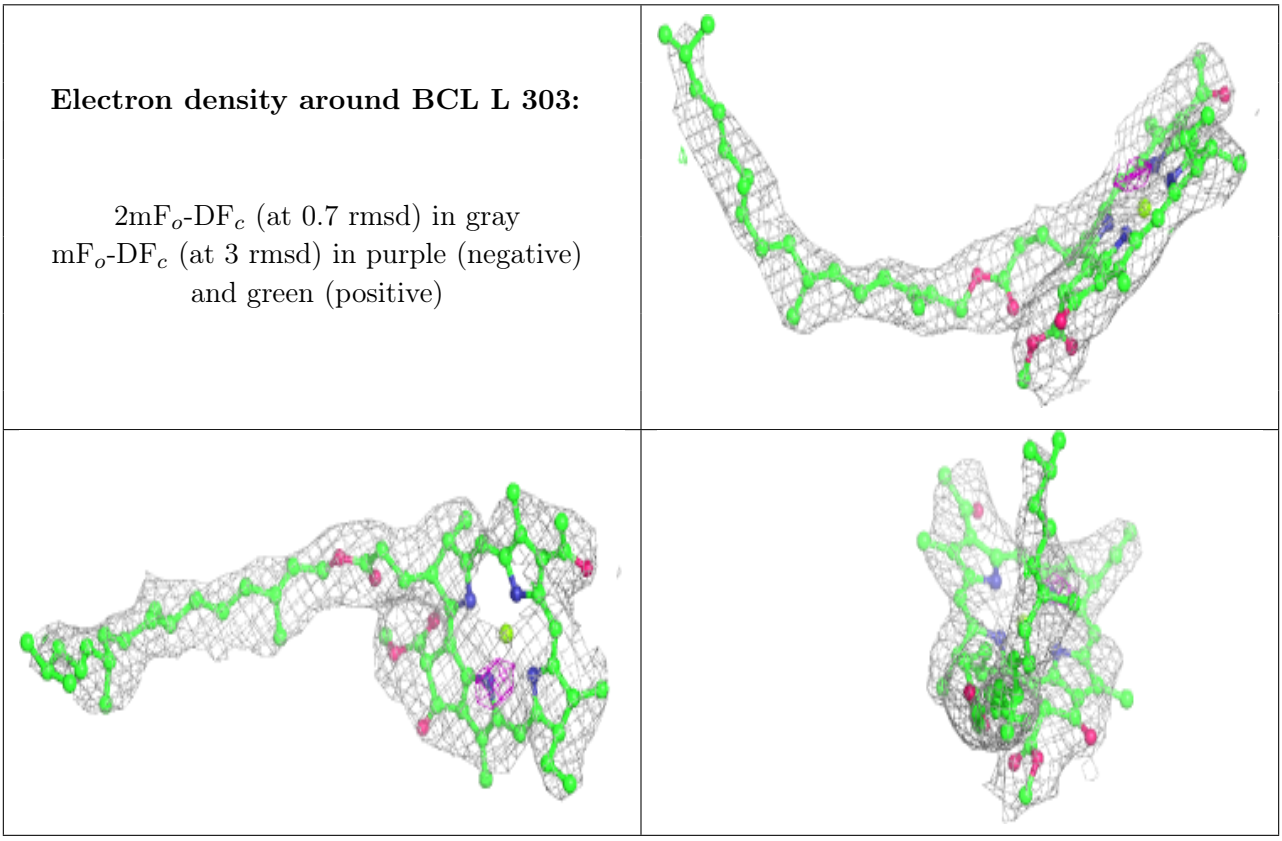
Electron density around BCL M 402:

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



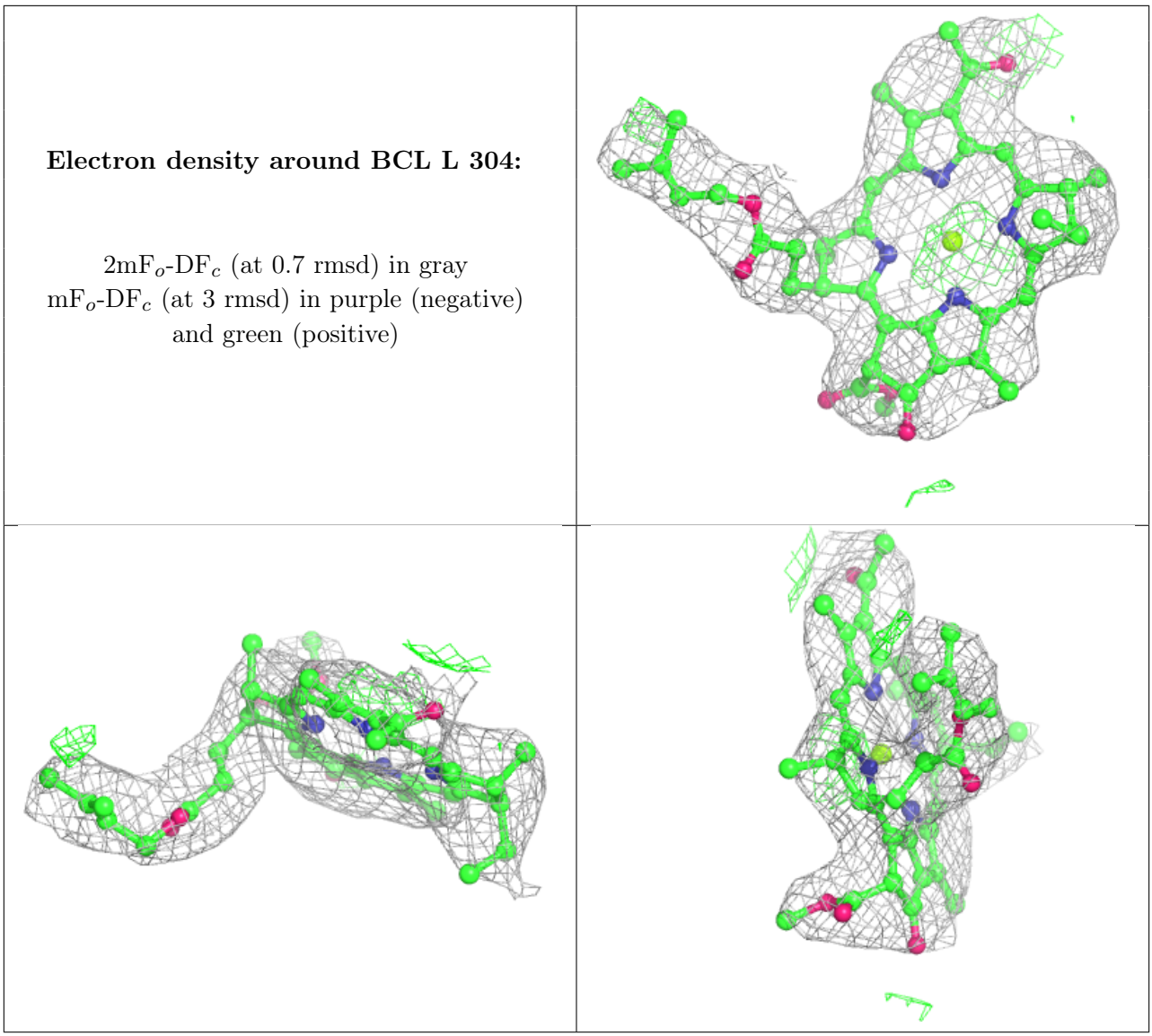
Electron density around BCL L 303:

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



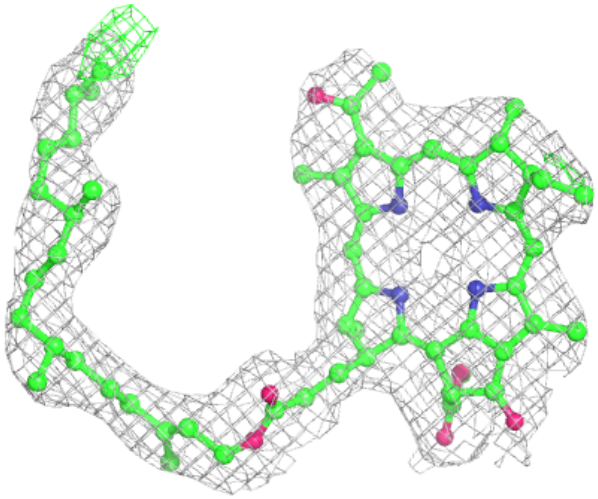
Electron density around BCL L 304:

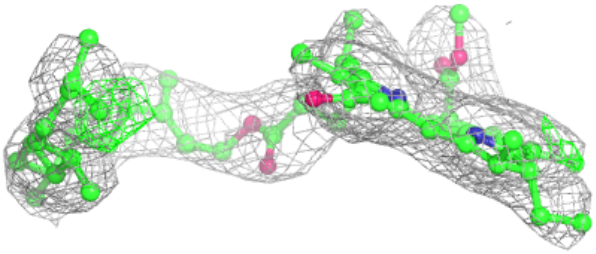
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

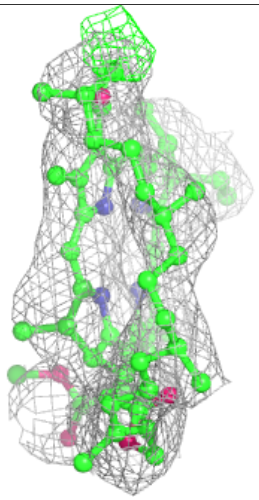


Electron density around BPH L 301:

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

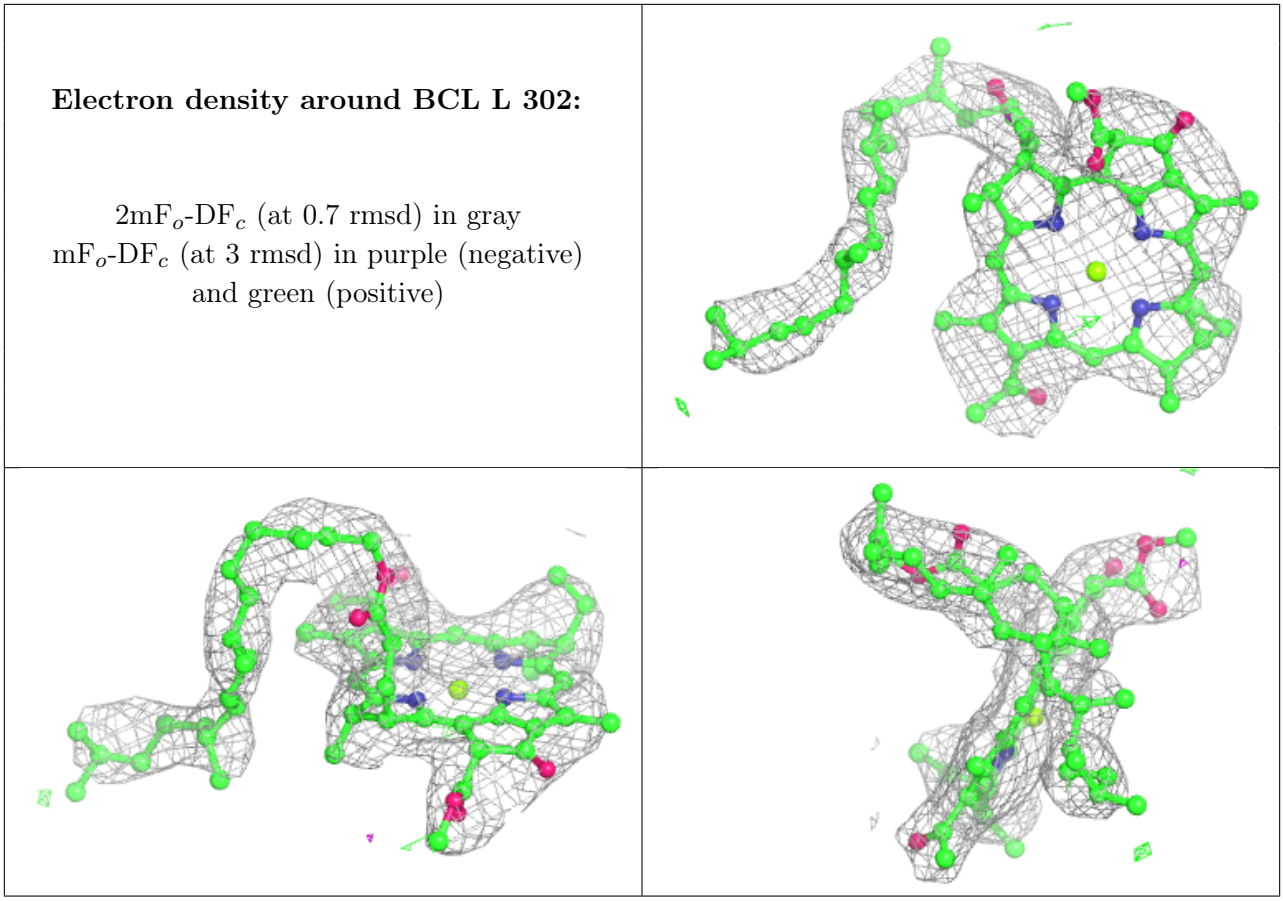






Electron density around BCL L 302:

$2mF_o$-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

There are no such residues in this entry.