Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 04:57 AM EDT

PDB ID	:	8VTK / pdb_00008vtk
Title	:	Crystal structure of R.sphaeroides Photosynthetic Reaction Center variant Y (M210)2-chlorophenylalanine
Authors	:	Tran, K.; Mathews, I.; Boxer, S.G.
Deposited on	:	2024-01-26
Resolution	:	3.07 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:

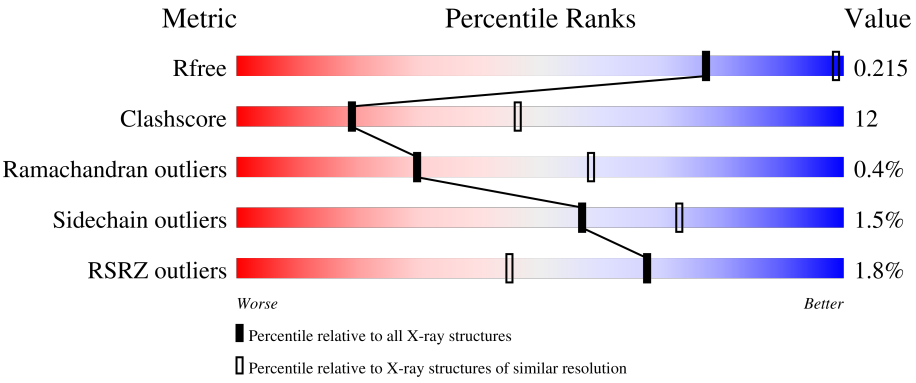
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.07 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	2% 80% 18%
2	L	281	2% 78% 21%
3	M	301	2% 76% 22%

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
11	CDL	M	405	X	-	-	-
8	CL	L	307	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7024 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	2	0
			2248	1517	357	366	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	301	Total	C	Cl	N	O	S	0	0	0
			2396	1598	1	392	395	10			

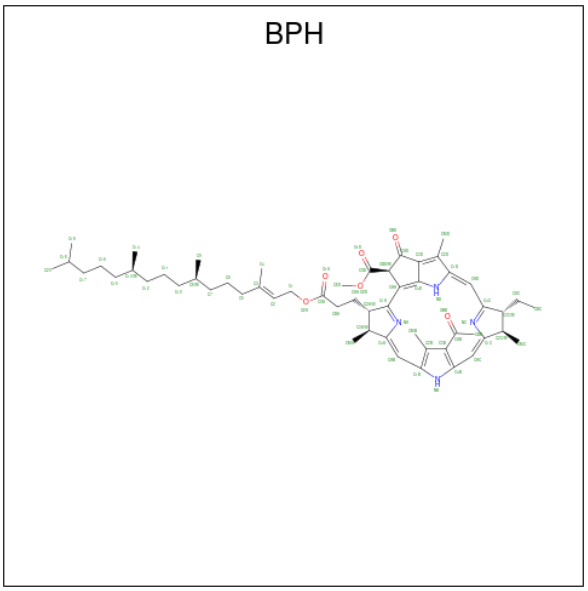
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	210	2L5	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

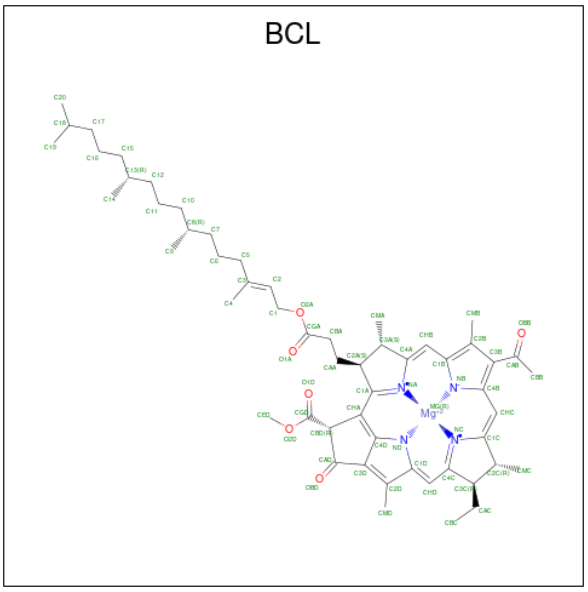
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			55	45	4	6		
5	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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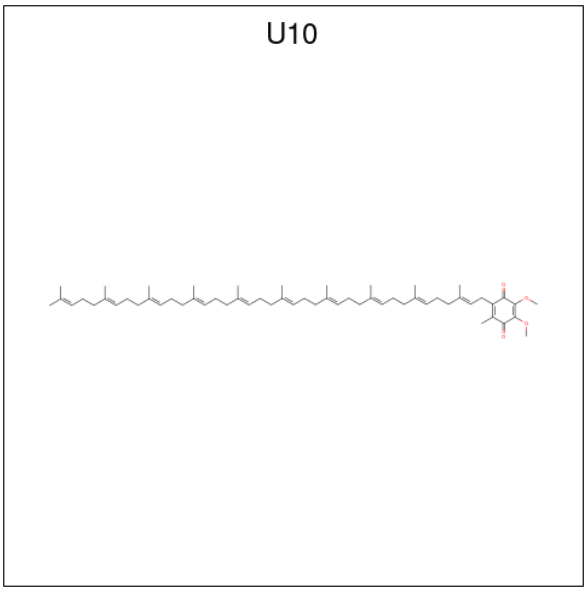
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

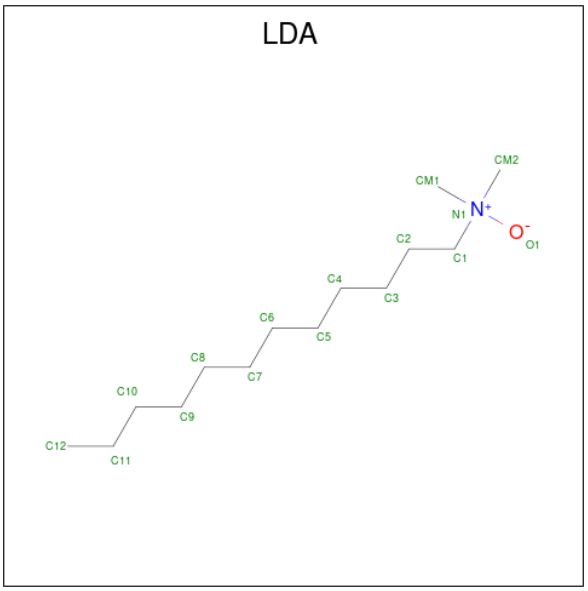


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

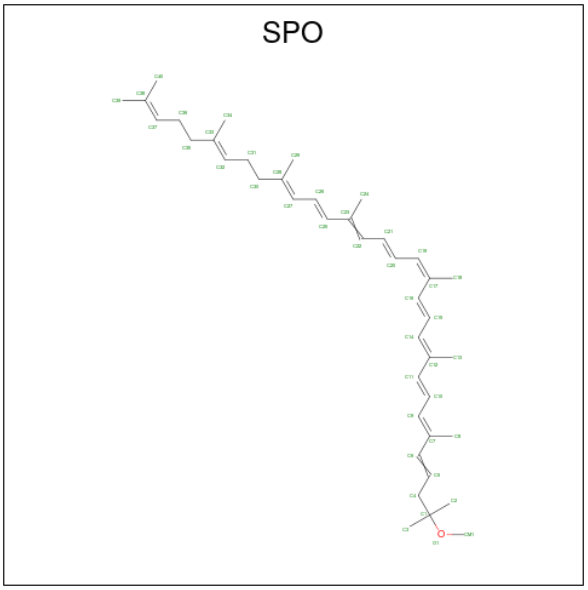
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Cl	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



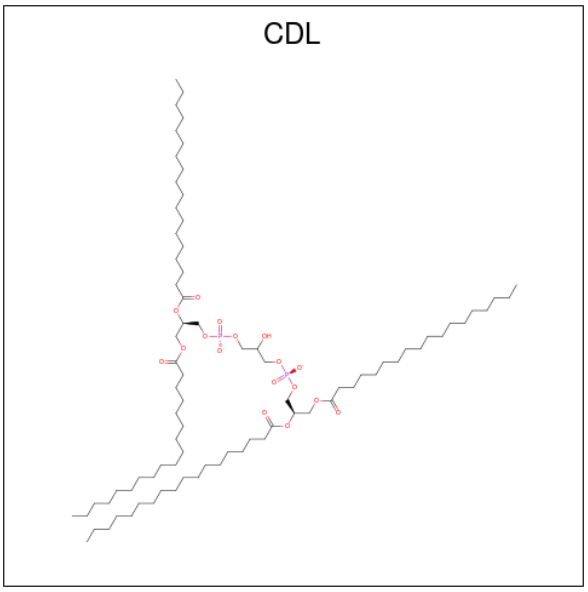
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			69	50	17	2		

- Molecule 12 is water.

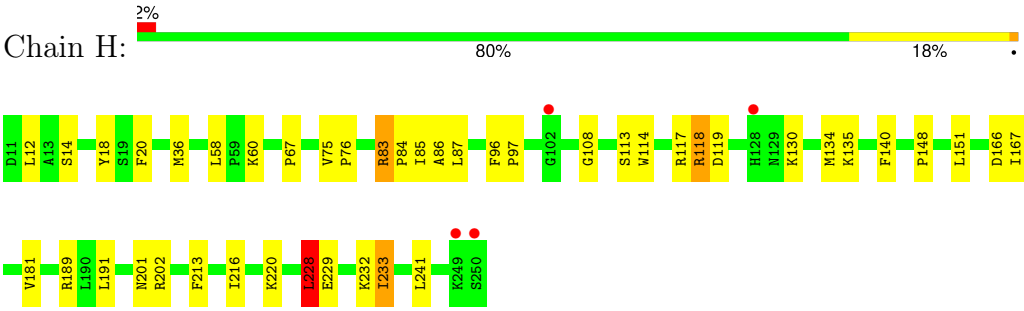
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	5	Total	O	0	0
			5	5		
12	L	4	Total	O	0	0
			4	4		
12	M	10	Total	O	0	0
			10	10		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

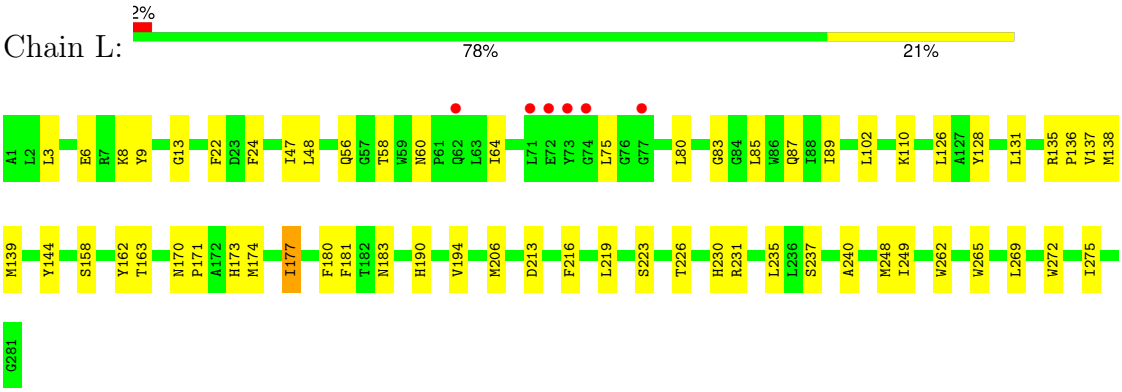
• Molecule 1: Reaction center protein H chain

Chain H:



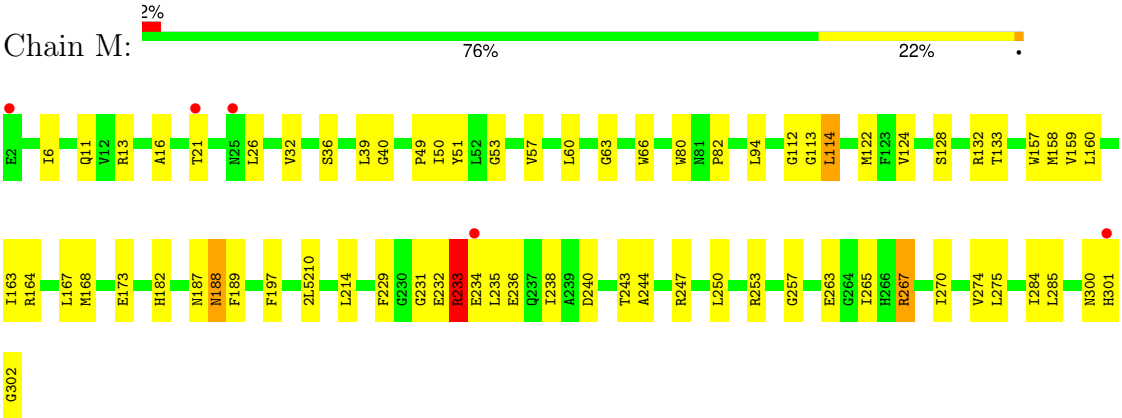
• Molecule 2: Reaction center protein L chain

Chain L:



• Molecule 3: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.95Å 140.95Å 186.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.76 – 3.07 39.76 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.76-3.07) 91.1 (39.76-3.07)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.177 , 0.213 0.182 , 0.215	Depositor DCC
R_{free} test set	2036 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: SPO, CL, U10, BPH, BCL, FE, LDA, CDL, 2L5

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	0.65	0/1877	0.75	1/2553 (0.0%)
2	L	0.54	1/2336 (0.0%)	0.65	0/3197
3	M	0.62	1/2472 (0.0%)	0.75	4/3372 (0.1%)
All	All	0.60	2/6685 (0.0%)	0.72	5/9122 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	177	ILE	CG1-CD1	-5.39	1.30	1.51
3	M	233	ARG	CA-C	-5.13	1.47	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	235	LEU	N-CA-C	9.19	122.99	111.69
1	H	228	LEU	N-CA-C	-6.17	104.19	111.03
3	M	267	ARG	N-CA-C	-6.01	104.65	112.23
3	M	257	GLY	CA-C-N	-5.72	111.99	123.09
3	M	257	GLY	C-N-CA	-5.72	111.99	123.09

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	51	0
2	L	2248	0	2200	46	0
3	M	2396	0	2307	58	0
4	L	1	0	0	0	0
5	L	120	0	129	12	0
6	L	132	0	148	9	0
6	M	117	0	115	11	0
7	L	18	0	15	3	0
8	L	1	0	0	2	0
9	M	32	0	62	3	0
10	M	42	0	60	1	0
11	M	69	0	82	3	0
12	H	5	0	0	0	0
12	L	4	0	0	1	0
12	M	10	0	0	1	0
All	All	7024	0	6954	164	0

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

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:ASP:OD2	1:H:220:LYS:NZ	1.68	1.26
2:L:230:HIS:NE2	3:M:234:GLU:OE2	1.72	1.22
1:H:83:ARG:NH2	1:H:108:GLY:O	1.75	1.19
1:H:229:GLU:O	1:H:233:ILE:HD12	1.59	1.02
1:H:117:ARG:O	1:H:228:LEU:HD12	1.62	0.99
1:H:118:ARG:HG3	1:H:118:ARG:HH11	1.24	0.99
1:H:118:ARG:HH12	3:M:240:ASP:HB2	1.35	0.88
3:M:112:GLY:O	3:M:114:LEU:N	2.07	0.87
11:M:405:CDL:HB4	11:M:405:CDL:HA61	1.55	0.86
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.57	0.85
1:H:119:ASP:CG	1:H:220:LYS:NZ	2.35	0.83
1:H:117:ARG:O	1:H:228:LEU:CD1	2.26	0.83
1:H:119:ASP:CG	1:H:220:LYS:HZ2	1.86	0.83
3:M:238:ILE:HD13	3:M:263:GLU:HB2	1.61	0.82
1:H:118:ARG:HG3	1:H:118:ARG:NH1	1.94	0.81
2:L:162:TYR:OH	3:M:187:ASN:OD1	2.00	0.79
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.63	0.79
6:L:303:BCL:HBB3	6:L:306:BCL:H52	1.63	0.78
2:L:56:GLN:HG2	2:L:58:THR:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:405:CDL:H312	11:M:405:CDL:H511	1.66	0.76
1:H:118:ARG:NH1	3:M:240:ASP:HB2	2.03	0.74
3:M:265:ILE:O	3:M:265:ILE:HG13	1.87	0.74
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.70	0.74
2:L:219:LEU:O	3:M:132:ARG:NH2	2.21	0.74
1:H:83:ARG:NH1	1:H:114:TRP:O	2.20	0.73
5:L:304:BPH:HHC	5:L:304:BPH:HBB3	1.70	0.72
1:H:189:ARG:HD2	1:H:216:ILE:HB	1.72	0.71
3:M:197:PHE:HZ	6:M:401:BCL:HBB2	1.54	0.71
1:H:60:LYS:H	1:H:60:LYS:HD2	1.56	0.69
3:M:300:ASN:C	3:M:302:GLY:H	2.02	0.68
2:L:230:HIS:CE1	3:M:234:GLU:OE2	2.46	0.67
1:H:229:GLU:O	1:H:233:ILE:CD1	2.40	0.67
3:M:231:GLY:C	3:M:233:ARG:H	2.02	0.65
2:L:138:MET:HE3	2:L:249:ILE:HD11	1.79	0.65
6:L:303:BCL:HHC	6:L:303:BCL:HBB2	1.80	0.64
1:H:14:SER:O	1:H:18:TYR:HD1	1.81	0.63
1:H:118:ARG:HH12	3:M:240:ASP:CB	2.12	0.62
5:L:302:BPH:H6C1	6:M:401:BCL:H192	1.81	0.61
1:H:220:LYS:HE3	1:H:229:GLU:OE2	2.01	0.61
5:L:302:BPH:H5C1	3:M:63:GLY:HA3	1.84	0.59
1:H:83:ARG:HH12	1:H:114:TRP:H	1.50	0.59
2:L:85:LEU:O	2:L:89:ILE:HG13	2.02	0.58
5:L:302:BPH:H4C1	3:M:60:LEU:HD12	1.85	0.58
5:L:302:BPH:HBC3	5:L:302:BPH:HHD	1.86	0.57
3:M:197:PHE:CZ	6:M:401:BCL:HBB2	2.39	0.56
3:M:231:GLY:C	3:M:233:ARG:N	2.61	0.56
6:M:406:BCL:HBB2	6:M:406:BCL:HHC	1.88	0.55
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.89	0.55
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.89	0.54
1:H:220:LYS:CE	1:H:229:GLU:OE2	2.56	0.54
2:L:171:PRO:HA	2:L:174:MET:HG3	1.89	0.53
8:L:307:CL:CL	12:L:404:HOH:O	2.56	0.53
1:H:140:PHE:HA	3:M:13:ARG:O	2.09	0.53
3:M:36:SER:HB3	3:M:39:LEU:HB2	1.90	0.52
7:L:305:U10:H4M3	9:M:403:LDA:H122	1.91	0.52
6:M:401:BCL:HBB2	6:M:401:BCL:HHC	1.92	0.51
3:M:300:ASN:C	3:M:302:GLY:N	2.68	0.51
3:M:160:LEU:HD23	3:M:284:ILE:HG21	1.93	0.51
3:M:53:GLY:O	3:M:57:VAL:HG23	2.11	0.51
1:H:117:ARG:O	1:H:118:ARG:C	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:177:ILE:HD11	6:L:306:BCL:C1B	2.41	0.51
2:L:190:HIS:NE2	3:M:234:GLU:OE2	2.42	0.51
2:L:272:TRP:HA	2:L:275:ILE:HG13	1.93	0.51
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.46	0.51
3:M:188:ASN:O	3:M:189:PHE:C	2.53	0.51
1:H:113:SER:HB3	2:L:8:LYS:HD2	1.92	0.51
2:L:262:TRP:O	2:L:265:TRP:HD1	1.94	0.51
7:L:305:U10:H71	9:M:402:LDA:H121	1.93	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.93	0.50
2:L:181:PHE:HB3	5:L:302:BPH:HBB2	1.93	0.50
2:L:75:LEU:HD21	2:L:137:VAL:HA	1.92	0.50
3:M:267:ARG:NH1	12:M:501:HOH:O	2.44	0.50
7:L:305:U10:C11	8:L:307:CL:CL	2.97	0.50
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.49
2:L:8:LYS:HE2	2:L:9:TYR:CE2	2.48	0.49
3:M:94:LEU:HD11	3:M:114:LEU:HB3	1.95	0.49
2:L:83:GLY:O	2:L:87:GLN:HG3	2.13	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
3:M:231:GLY:O	3:M:233:ARG:N	2.46	0.48
3:M:300:ASN:O	3:M:302:GLY:N	2.46	0.48
2:L:60:ASN:O	2:L:64:ILE:HG13	2.13	0.48
1:H:20:PHE:HD2	11:M:405:CDL:H401	1.78	0.48
2:L:163:THR:O	2:L:163:THR:HG22	2.12	0.48
5:L:302:BPH:HBB3	5:L:302:BPH:HHC	1.95	0.48
1:H:134:MET:CE	1:H:167:ILE:HB	2.44	0.48
2:L:170:ASN:HB3	2:L:173:HIS:HB2	1.95	0.47
1:H:118:ARG:NH1	3:M:240:ASP:CB	2.76	0.47
2:L:13:GLY:O	2:L:110:LYS:NZ	2.29	0.47
6:M:406:BCL:HHC	6:M:406:BCL:CBB	2.44	0.47
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.47
1:H:118:ARG:NH1	1:H:118:ARG:CG	2.72	0.47
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.15	0.47
2:L:47:ILE:HG22	2:L:48:LEU:HD23	1.97	0.47
1:H:228:LEU:HD23	1:H:232:LYS:HE3	1.95	0.47
2:L:216:PHE:HB2	2:L:223:SER:HB2	1.97	0.47
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.30	0.47
1:H:36:MET:HE2	1:H:58:LEU:HD23	1.97	0.46
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.50	0.46
6:L:306:BCL:C1C	6:M:401:BCL:HBB3	2.46	0.46
2:L:213:ASP:OD1	2:L:223:SER:OG	2.32	0.46
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:PHE:O	1:H:216:ILE:HG13	2.15	0.46
6:L:306:BCL:OBB	6:L:306:BCL:HHC	2.16	0.46
3:M:236:GLU:O	3:M:236:GLU:HG3	2.16	0.45
6:M:401:BCL:HAA2	6:M:401:BCL:HBD	1.99	0.45
3:M:50:ILE:HG12	3:M:51:TYR:N	2.32	0.45
2:L:226:THR:O	2:L:230:HIS:ND1	2.50	0.45
3:M:243:THR:O	3:M:247:ARG:HG3	2.17	0.45
1:H:67:PRO:HG3	2:L:206:MET:O	2.17	0.44
9:M:402:LDA:HM13	9:M:402:LDA:H21	1.79	0.44
5:L:304:BPH:HHC	5:L:304:BPH:CBB	2.44	0.44
3:M:124:VAL:O	3:M:128:SER:OG	2.29	0.44
3:M:275:LEU:HD23	3:M:275:LEU:HA	1.87	0.44
1:H:135:LYS:HB3	1:H:135:LYS:HE2	1.76	0.44
2:L:181:PHE:HB3	5:L:302:BPH:CBB	2.48	0.43
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.00	0.43
10:M:404:SPO:H243	6:M:406:BCL:CBB	2.48	0.43
2:L:190:HIS:O	2:L:194:VAL:HG23	2.19	0.43
1:H:12:LEU:HD23	1:H:12:LEU:O	2.18	0.43
5:L:304:BPH:ND	3:M:214:LEU:HD13	2.33	0.43
1:H:134:MET:HE3	1:H:167:ILE:HB	2.00	0.43
1:H:135:LYS:HE2	1:H:166:ASP:OD2	2.17	0.43
2:L:158:SER:HA	6:L:306:BCL:HBC1	2.01	0.43
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.53	0.43
2:L:102:LEU:HD23	2:L:102:LEU:HA	1.71	0.43
2:L:190:HIS:HE2	3:M:234:GLU:CD	2.26	0.42
3:M:80:TRP:O	3:M:82:PRO:HD3	2.19	0.42
3:M:159:VAL:HA	3:M:163:ILE:HB	2.01	0.42
3:M:164:ARG:NH1	3:M:173:GLU:OE1	2.49	0.42
3:M:167:LEU:CD1	3:M:285:LEU:HD11	2.49	0.42
2:L:131:LEU:HD21	2:L:248:MET:HG2	2.00	0.42
3:M:32:VAL:HG12	3:M:49:PRO:HD3	2.01	0.42
1:H:75:VAL:HA	1:H:76:PRO:C	2.45	0.42
1:H:118:ARG:HG3	3:M:240:ASP:OD2	2.19	0.42
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.89	0.42
1:H:86:ALA:O	1:H:87:LEU:HD23	2.20	0.42
2:L:131:LEU:HD23	2:L:131:LEU:HA	1.85	0.42
1:H:201:ASN:OD1	1:H:201:ASN:N	2.53	0.41
3:M:253:ARG:HH11	3:M:253:ARG:HG3	1.85	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.20	0.41
2:L:3:LEU:HB2	2:L:6:GLU:HB2	2.02	0.41
3:M:32:VAL:H	3:M:32:VAL:HG22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:51:TYR:O	3:M:132:ARG:NH1	2.38	0.41
2:L:128:TYR:HD1	6:L:303:BCL:HBB1	1.84	0.41
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.51	0.41
2:L:181:PHE:CD2	5:L:302:BPH:HBB1	2.55	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.01	0.41
2:L:183:ASN:OD1	2:L:237:SER:HB3	2.20	0.41
2:L:139:MET:HB3	2:L:144:TYR:CD2	2.56	0.41
2:L:231:ARG:HD3	3:M:6:ILE:O	2.20	0.41
1:H:241:LEU:HD23	1:H:241:LEU:HA	1.95	0.41
2:L:80:LEU:HD22	2:L:85:LEU:HD23	2.03	0.41
3:M:164:ARG:NH2	3:M:168:MET:HE2	2.36	0.41
6:M:401:BCL:HHC	6:M:401:BCL:CBB	2.51	0.41
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.70	0.41
1:H:201:ASN:HD21	1:H:202:ARG:NH2	2.19	0.40
6:L:306:BCL:NC	6:M:401:BCL:HBB3	2.36	0.40
1:H:83:ARG:HA	1:H:84:PRO:HD3	1.90	0.40
5:L:302:BPH:H3A	5:L:302:BPH:HBA2	1.79	0.40
3:M:112:GLY:C	3:M:114:LEU:N	2.76	0.40
1:H:84:PRO:C	1:H:85:ILE:HD13	2.46	0.40
1:H:119:ASP:OD1	1:H:220:LYS:NZ	2.45	0.40
6:L:303:BCL:HHC	6:L:303:BCL:CBB	2.49	0.40
3:M:11:GLN:NE2	3:M:40:GLY:C	2.80	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%)	228 (96%)	10 (4%)	0	100	100
2	L	281/281 (100%)	271 (96%)	10 (4%)	0	100	100
3	M	298/301 (99%)	280 (94%)	15 (5%)	3 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	817/822 (99%)	779 (95%)	35 (4%)	3 (0%)	30 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	113	GLY
3	M	301	HIS
3	M	232	GLU

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%)	191 (98%)	4 (2%)	47 68
2	L	222/220 (101%)	219 (99%)	3 (1%)	59 73
3	M	235/235 (100%)	231 (98%)	4 (2%)	53 71
All	All	652/650 (100%)	641 (98%)	11 (2%)	57 71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	83	ARG
1	H	118	ARG
1	H	228	LEU
1	H	233	ILE
2	L	126[A]	LEU
2	L	126[B]	LEU
2	L	235	LEU
3	M	114	LEU
3	M	182	HIS
3	M	188	ASN
3	M	233	ARG

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

Mol	Chain	Res	Type
1	H	32	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
3	2L5	M	210	3	11,12,13	0.96	1 (9%)	9,15,17	0.17	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
3	2L5	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	2L5	O-C	3.12	1.31	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	2L5	CA-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	M	210	2L5	CA-C13-C14-C16

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
6	BCL	M	406	3	54,59,74	1.60	11 (20%)	61,97,115	1.67	10 (16%)
6	BCL	L	306	2	69,74,74	1.26	6 (8%)	79,115,115	1.46	10 (12%)
11	CDL	M	405	-	68,68,99	1.27	10 (14%)	74,80,111	1.03	6 (8%)
6	BCL	M	401	3	69,74,74	1.17	6 (8%)	79,115,115	1.39	7 (8%)
9	LDA	M	402	-	13,15,15	2.32	2 (15%)	14,17,17	0.53	0
10	SPO	M	404	-	41,41,41	0.34	0	47,50,50	0.58	0
9	LDA	M	403	-	13,15,15	2.04	2 (15%)	14,17,17	0.71	0
6	BCL	L	303	2	69,74,74	1.46	11 (15%)	79,115,115	1.47	12 (15%)
5	BPH	L	302	-	49,60,70	1.23	6 (12%)	47,89,101	2.27	10 (21%)
7	U10	L	305	-	18,18,63	2.45	8 (44%)	24,25,79	1.67	5 (20%)
5	BPH	L	304	-	59,70,70	1.28	3 (5%)	59,101,101	2.29	15 (25%)

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
6	BCL	M	406	3	-	0/23/119/137	-
6	BCL	L	306	2	-	4/41/137/137	-
11	CDL	M	405	-	1/1/9/9	32/79/79/110	-
6	BCL	M	401	3	-	1/41/137/137	-
9	LDA	M	402	-	-	6/13/13/13	-
10	SPO	M	404	-	-	6/47/47/47	-
9	LDA	M	403	-	-	6/13/13/13	-
6	BCL	L	303	2	-	8/41/137/137	-
5	BPH	L	302	-	-	4/25/93/105	0/5/6/6
7	U10	L	305	-	-	2/9/33/87	0/1/1/1
5	BPH	L	304	-	-	3/37/105/105	0/5/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	402	LDA	O1-N1	-6.65	1.25	1.42
9	M	403	LDA	O1-N1	-6.27	1.26	1.42
5	L	304	BPH	CBD-CGD	-5.11	1.46	1.52
6	M	406	BCL	MG-NA	5.10	2.18	2.06
6	L	306	BCL	MG-NA	5.07	2.18	2.06
7	L	305	U10	O3-C3	-4.95	1.24	1.36
9	M	402	LDA	C1-N1	-4.92	1.46	1.51
6	L	303	BCL	MG-NA	4.76	2.17	2.06
7	L	305	U10	O4-C4	-4.74	1.25	1.36
6	M	401	BCL	MG-NA	4.73	2.17	2.06
7	L	305	U10	C8-C9	4.72	1.46	1.32
5	L	304	BPH	C3D-CAD	-4.53	1.39	1.47
6	L	303	BCL	MG-NC	4.16	2.16	2.06
6	M	406	BCL	C1-C2	3.91	1.60	1.49
9	M	403	LDA	C1-N1	-3.75	1.47	1.51
6	M	401	BCL	MG-NC	3.63	2.14	2.06
6	L	303	BCL	O1A-CGA	-3.53	1.12	1.22
11	M	405	CDL	PA1-OA5	3.52	1.73	1.59
6	M	406	BCL	MG-NC	3.43	2.14	2.06
6	M	406	BCL	O2A-CGA	3.36	1.43	1.33
6	L	306	BCL	C3B-C4B	3.31	1.47	1.41
6	M	406	BCL	OBD-CAD	3.24	1.28	1.22
11	M	405	CDL	PB2-OB5	3.15	1.71	1.59
11	M	405	CDL	PA1-OA4	-3.13	1.40	1.55
6	L	306	BCL	MG-NC	3.07	2.13	2.06
7	L	305	U10	C6-C1	2.97	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	405	CDL	PA1-OA3	-2.95	1.40	1.50
6	M	406	BCL	C3B-C4B	2.85	1.46	1.41
5	L	304	BPH	C3B-C4B	2.85	1.46	1.41
5	L	302	BPH	C1D-C2D	2.84	1.42	1.39
11	M	405	CDL	PB2-OB4	-2.80	1.42	1.55
5	L	302	BPH	CBD-CGD	-2.77	1.49	1.52
6	L	303	BCL	CHD-C1D	2.74	1.43	1.38
5	L	302	BPH	C3D-CAD	-2.70	1.42	1.47
6	L	306	BCL	CMB-C2B	2.67	1.56	1.50
11	M	405	CDL	PB2-OB3	-2.67	1.41	1.50
6	L	303	BCL	C3B-C4B	2.66	1.46	1.41
5	L	302	BPH	CHA-CBD	2.62	1.54	1.51
6	M	406	BCL	CHD-C1D	2.61	1.43	1.38
7	L	305	U10	C4-C5	-2.59	1.41	1.48
11	M	405	CDL	CA3-CA4	2.54	1.58	1.50
6	M	406	BCL	C1B-NB	2.48	1.41	1.37
11	M	405	CDL	OB8-CB7	2.41	1.40	1.33
6	M	401	BCL	C3B-C4B	2.38	1.45	1.41
6	M	401	BCL	C3D-C4D	-2.37	1.38	1.44
7	L	305	U10	C3-C2	-2.32	1.42	1.48
6	L	303	BCL	C1D-C2D	-2.26	1.40	1.45
11	M	405	CDL	OB6-CB5	2.23	1.40	1.34
6	L	303	BCL	OBD-CAD	2.22	1.26	1.22
7	L	305	U10	C6-C5	-2.22	1.40	1.46
6	M	401	BCL	OBD-CAD	2.21	1.26	1.22
5	L	302	BPH	C4D-CHA	2.19	1.42	1.39
6	M	406	BCL	C1D-ND	2.19	1.40	1.37
6	L	303	BCL	CAC-C3C	2.18	1.58	1.54
6	M	401	BCL	C1D-C2D	-2.18	1.41	1.45
11	M	405	CDL	OA6-CA5	2.16	1.40	1.34
6	M	406	BCL	CAA-CBA	2.14	1.59	1.52
6	L	306	BCL	C3D-C4D	-2.12	1.39	1.44
6	L	306	BCL	C5-C3	2.12	1.55	1.51
6	L	303	BCL	C5-C3	2.12	1.55	1.51
5	L	302	BPH	C1D-ND	2.11	1.42	1.38
6	L	303	BCL	C1D-ND	2.09	1.40	1.37
6	L	303	BCL	C4-C3	2.09	1.55	1.50
7	L	305	U10	C1-C2	-2.05	1.40	1.47
6	M	406	BCL	O2A-C1	2.00	1.51	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	304	BPH	C4D-CHA-CBD	-12.62	102.40	108.45
5	L	302	BPH	C4D-CHA-CBD	-9.39	103.95	108.45
5	L	302	BPH	C1-C2-C3	-6.13	116.15	126.20
6	M	406	BCL	C1-O2A-CGA	5.08	128.94	116.65
6	M	406	BCL	C4D-CHA-C1A	5.00	127.20	121.24
6	M	401	BCL	C4D-CHA-C1A	4.82	127.00	121.24
6	L	303	BCL	C1D-ND-C4D	-4.62	103.07	106.31
6	L	306	BCL	C4D-CHA-C1A	4.48	126.59	121.24
5	L	304	BPH	C4D-ND-C1D	-4.45	103.54	108.87
6	M	406	BCL	C1D-ND-C4D	-4.20	103.36	106.31
6	L	306	BCL	C15-C13-C12	-4.05	91.55	112.07
6	L	303	BCL	C4D-CHA-C1A	4.02	126.04	121.24
6	M	406	BCL	CHD-C1D-ND	-3.94	119.26	124.80
6	L	303	BCL	O2D-CGD-CBD	3.94	118.11	111.23
6	L	306	BCL	C1D-ND-C4D	-3.93	103.55	106.31
6	L	306	BCL	C16-C15-C13	-3.90	102.99	115.97
5	L	302	BPH	C4D-ND-C1D	-3.90	104.20	108.87
7	L	305	U10	C7-C8-C9	-3.80	116.50	127.25
6	M	401	BCL	C1D-ND-C4D	-3.74	103.69	106.31
6	M	401	BCL	CHD-C1D-ND	-3.64	119.68	124.80
5	L	304	BPH	C11-C10-C8	-3.57	104.11	115.97
5	L	302	BPH	OBD-CAD-CBD	-3.56	120.60	125.82
6	L	303	BCL	CHD-C1D-ND	-3.54	119.82	124.80
6	L	303	BCL	C16-C17-C18	-3.53	100.18	115.94
6	L	306	BCL	CHD-C1D-ND	-3.49	119.89	124.80
5	L	302	BPH	C3D-C4D-ND	3.49	112.18	107.71
7	L	305	U10	C11-C9-C10	3.46	122.56	114.59
6	L	303	BCL	CED-O2D-CGD	3.22	123.23	115.92
5	L	302	BPH	CBA-CAA-C2A	-3.21	104.33	113.78
6	M	401	BCL	CHA-C1A-NA	-3.15	119.25	126.39
6	L	306	BCL	CHA-C1A-NA	-3.09	119.40	126.39
5	L	304	BPH	OBB-CAB-C3B	3.07	125.11	119.99
5	L	304	BPH	C3D-C4D-ND	3.06	111.63	107.71
5	L	302	BPH	O2D-CGD-CBD	3.04	114.29	110.95
5	L	304	BPH	C2D-C1D-ND	3.04	111.63	109.43
5	L	304	BPH	C1-C2-C3	-3.02	121.25	126.20
6	M	406	BCL	CHA-C1A-NA	-2.97	119.66	126.39
5	L	304	BPH	OBD-CAD-CBD	-2.97	121.46	125.82
6	M	401	BCL	C11-C10-C8	-2.96	106.11	115.97
5	L	304	BPH	OBB-CAB-CBB	-2.95	113.91	120.19
6	L	303	BCL	CHA-C1A-NA	-2.88	119.86	126.39
11	M	405	CDL	OA4-PA1-OA3	2.88	125.83	112.44
6	L	303	BCL	C2A-C1A-CHA	2.87	128.86	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	305	U10	O5-C5-C6	-2.85	116.27	121.79
6	L	306	BCL	C2A-C1A-CHA	2.79	128.70	123.87
7	L	305	U10	C1M-C1-C6	-2.75	119.93	124.45
11	M	405	CDL	CB4-OB6-CB5	2.70	124.27	117.80
6	M	406	BCL	O2D-CGD-CBD	2.65	115.87	111.23
6	L	306	BCL	C11-C10-C8	-2.63	107.24	115.97
11	M	405	CDL	OB4-PB2-OB3	2.60	124.52	112.44
6	L	306	BCL	CED-O2D-CGD	2.58	121.77	115.92
11	M	405	CDL	OA6-CA5-OA7	-2.53	117.80	123.70
11	M	405	CDL	OA6-CA5-C11	2.50	116.90	111.48
6	M	406	BCL	O2D-CGD-O1D	-2.50	118.97	123.85
6	M	406	BCL	C2A-C1A-CHA	2.50	128.20	123.87
6	L	303	BCL	C4A-NA-C1A	2.50	107.82	106.68
5	L	304	BPH	C4C-C3C-C2C	-2.41	100.54	102.84
11	M	405	CDL	OB8-CB6-CB4	2.40	115.32	108.40
5	L	302	BPH	C2D-C1D-ND	2.39	111.16	109.43
5	L	304	BPH	C16-C15-C13	-2.37	108.08	115.97
5	L	302	BPH	CMD-C2D-C3D	2.36	129.41	124.68
5	L	304	BPH	CMD-C2D-C3D	2.35	129.38	124.68
6	M	401	BCL	C2A-C1A-CHA	2.34	127.92	123.87
6	L	303	BCL	O2D-CGD-O1D	-2.30	119.38	123.85
7	L	305	U10	C7-C6-C1	-2.28	120.99	124.89
6	L	306	BCL	C17-C16-C15	2.26	123.40	113.28
6	M	406	BCL	C4-C3-C2	2.25	129.39	122.66
6	M	401	BCL	CHC-C1C-NC	-2.24	121.17	124.40
6	M	406	BCL	C5-C3-C4	-2.20	109.53	114.59
5	L	302	BPH	CMA-C3A-C4A	-2.18	109.91	114.61
5	L	304	BPH	CMA-C3A-C4A	-2.13	110.02	114.61
6	L	303	BCL	OBB-CAB-CBB	-2.09	115.09	119.77
6	L	303	BCL	C2D-C1D-ND	2.06	112.16	110.13
5	L	304	BPH	O2D-CGD-CBD	2.03	113.17	110.95
5	L	304	BPH	CMB-C2B-C3B	2.01	128.71	124.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	405	CDL	CA4

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	403	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
9	M	403	LDA	C2-C1-N1-CM1
11	M	405	CDL	CA3-OA5-PA1-OA4
11	M	405	CDL	CB2-OB2-PB2-OB4
11	M	405	CDL	CB2-OB2-PB2-OB5
11	M	405	CDL	CB3-OB5-PB2-OB2
11	M	405	CDL	CB3-OB5-PB2-OB3
11	M	405	CDL	OB5-CB3-CB4-OB6
7	L	305	U10	C7-C8-C9-C11
7	L	305	U10	C7-C8-C9-C10
11	M	405	CDL	C51-CB5-OB6-CB4
11	M	405	CDL	C71-CB7-OB8-CB6
11	M	405	CDL	O1-C1-CA2-OA2
5	L	302	BPH	C5-C6-C7-C8
11	M	405	CDL	OB7-CB5-OB6-CB4
6	L	303	BCL	C15-C16-C17-C18
11	M	405	CDL	OB9-CB7-OB8-CB6
5	L	304	BPH	C15-C16-C17-C18
11	M	405	CDL	C31-CA7-OA8-CA6
10	M	404	SPO	C5-C6-C7-C8
11	M	405	CDL	C11-CA5-OA6-CA4
11	M	405	CDL	O1-C1-CB2-OB2
9	M	403	LDA	C6-C7-C8-C9
11	M	405	CDL	OA9-CA7-OA8-CA6
9	M	403	LDA	C5-C6-C7-C8
11	M	405	CDL	C51-C52-C53-C54
11	M	405	CDL	OA7-CA5-OA6-CA4
9	M	402	LDA	C1-C2-C3-C4
5	L	304	BPH	C4-C3-C5-C6
6	L	306	BCL	C13-C15-C16-C17
9	M	403	LDA	C2-C3-C4-C5
11	M	405	CDL	OA6-CA4-CA6-OA8
11	M	405	CDL	C39-C40-C41-C42
5	L	304	BPH	C2-C3-C5-C6
10	M	404	SPO	C2-C1-C4-C5
11	M	405	CDL	C76-C77-C78-C79
9	M	403	LDA	C1-C2-C3-C4
9	M	402	LDA	C4-C5-C6-C7
5	L	302	BPH	C2-C3-C5-C6
5	L	302	BPH	C4-C3-C5-C6
11	M	405	CDL	C14-C15-C16-C17
11	M	405	CDL	OB5-CB3-CB4-CB6
10	M	404	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
6	L	306	BCL	C15-C16-C17-C18
11	M	405	CDL	C34-C35-C36-C37
6	L	303	BCL	CHA-CBD-CGD-O1D
6	L	303	BCL	CHA-CBD-CGD-O2D
11	M	405	CDL	CA3-OA5-PA1-OA2
11	M	405	CDL	CB2-OB2-PB2-OB3
11	M	405	CDL	CB3-OB5-PB2-OB4
10	M	404	SPO	C29-C28-C30-C31
9	M	402	LDA	C9-C10-C11-C12
9	M	402	LDA	N1-C1-C2-C3
11	M	405	CDL	C12-C13-C14-C15
11	M	405	CDL	C72-C73-C74-C75
10	M	404	SPO	C27-C28-C30-C31
6	L	303	BCL	C16-C17-C18-C19
11	M	405	CDL	CA3-CA4-CA6-OA8
11	M	405	CDL	CB3-CB4-CB6-OB8
6	L	303	BCL	C2B-C3B-CAB-OBB
6	L	303	BCL	C2B-C3B-CAB-CBB
10	M	404	SPO	C34-C33-C35-C36
6	L	303	BCL	C4B-C3B-CAB-OBB
6	L	306	BCL	C2A-CAA-CBA-CGA
9	M	402	LDA	C7-C8-C9-C10
9	M	402	LDA	C5-C6-C7-C8
5	L	302	BPH	C2-C1-O2A-CGA
11	M	405	CDL	CB2-C1-CA2-OA2
6	L	303	BCL	C4B-C3B-CAB-CBB
6	M	401	BCL	CAA-CBA-CGA-O2A
6	L	306	BCL	CAD-CBD-CGD-O2D
11	M	405	CDL	CB7-C71-C72-C73

There are no ring outliers.

11 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	406	BCL	3	0
6	L	306	BCL	6	0
11	M	405	CDL	3	0
6	M	401	BCL	8	0
9	M	402	LDA	2	0
10	M	404	SPO	1	0
9	M	403	LDA	1	0
6	L	303	BCL	4	0

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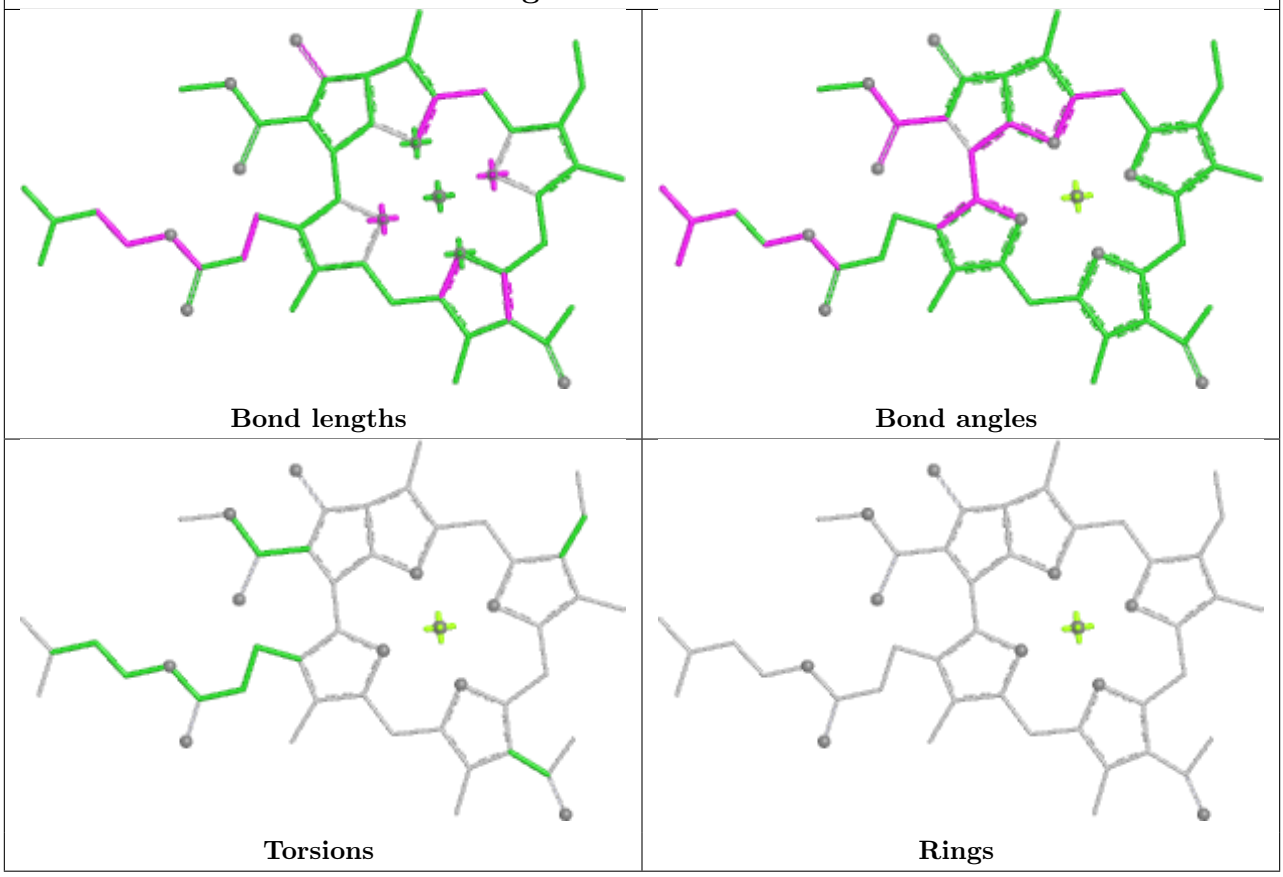
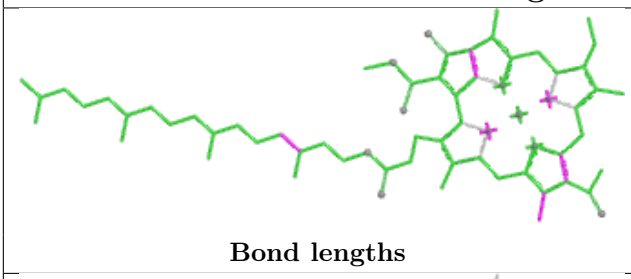
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	BPH	9	0
7	L	305	U10	3	0
5	L	304	BPH	3	0

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.

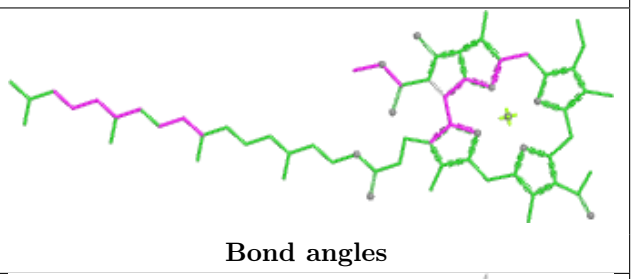
Ligand BCL M 406



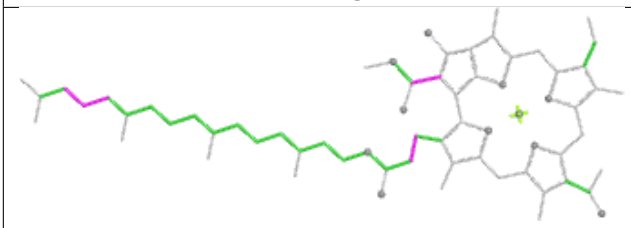
Ligand BCL L 306



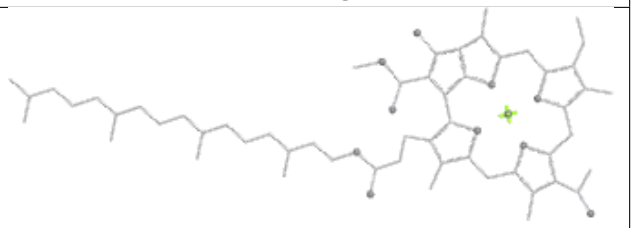
Bond lengths



Bond angles

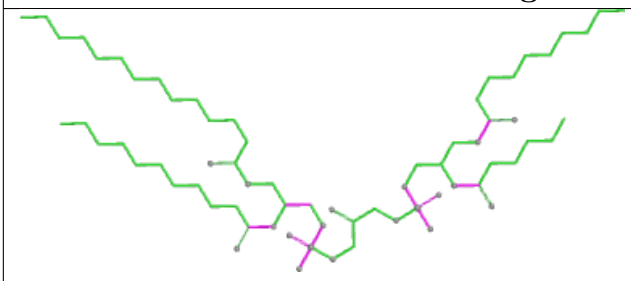


Torsions

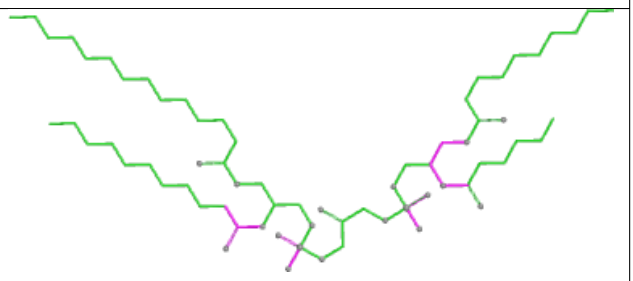


Rings

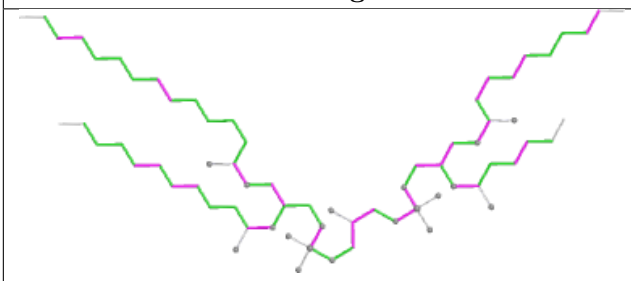
Ligand CDL M 405



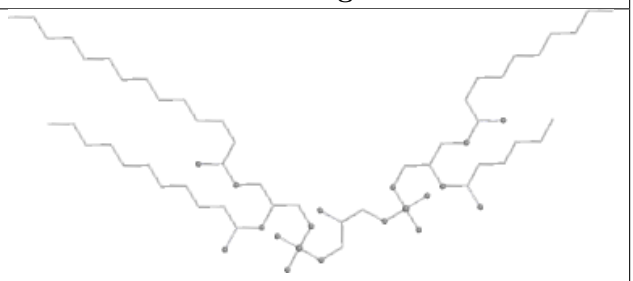
Bond lengths



Bond angles

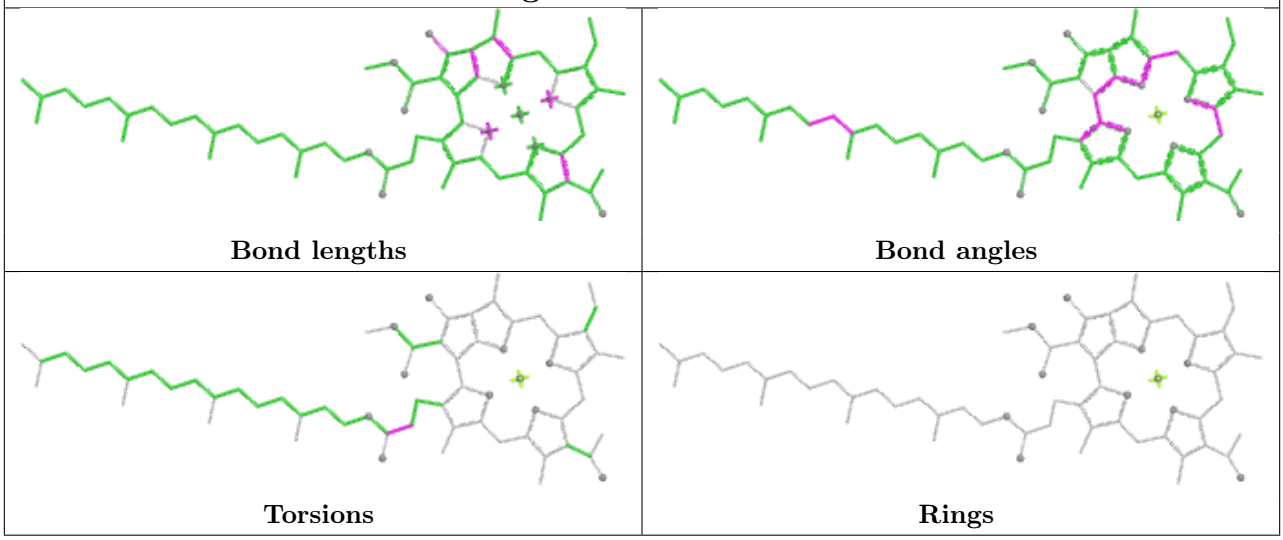


Torsions

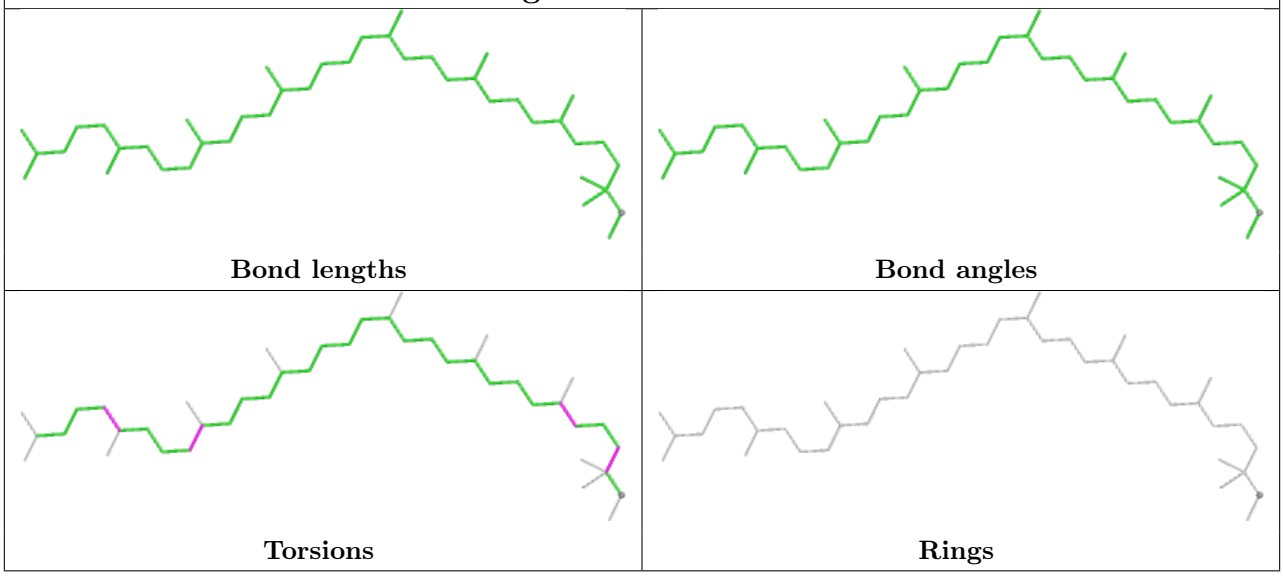


Rings

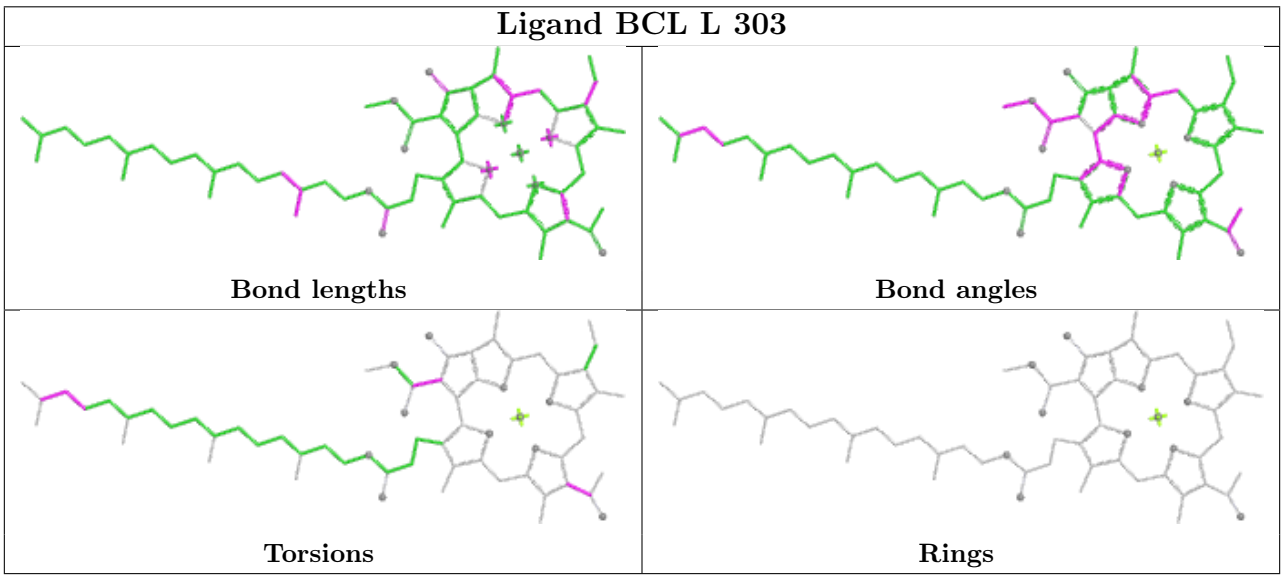
Ligand BCL M 401



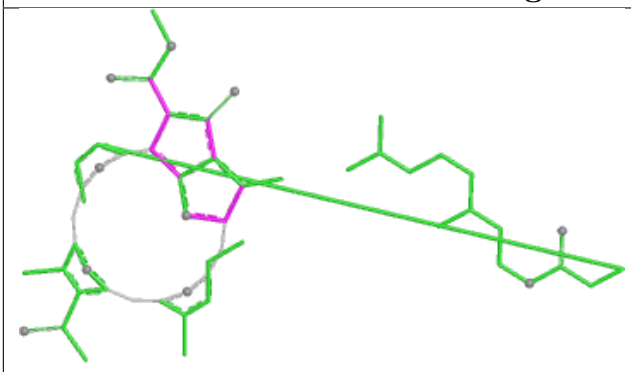
Ligand SPO M 404



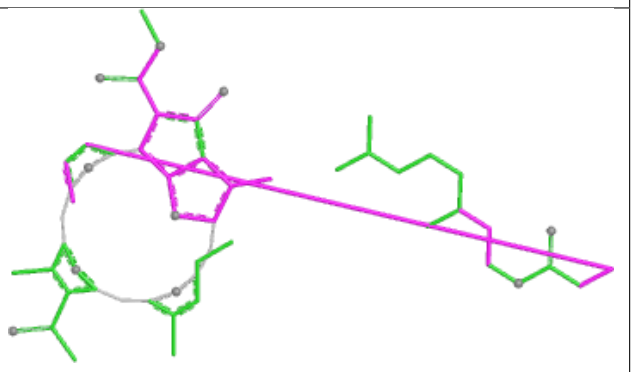
Ligand BCL L 303



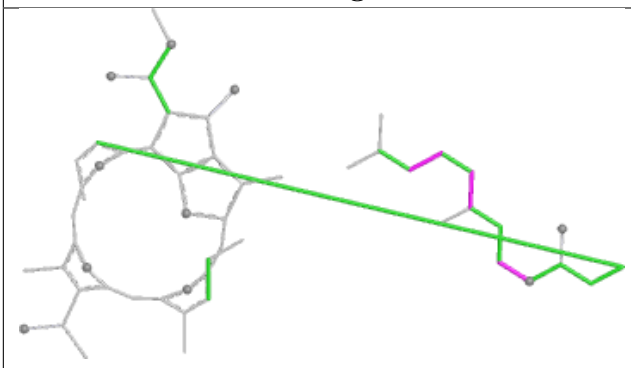
Ligand BPH L 302



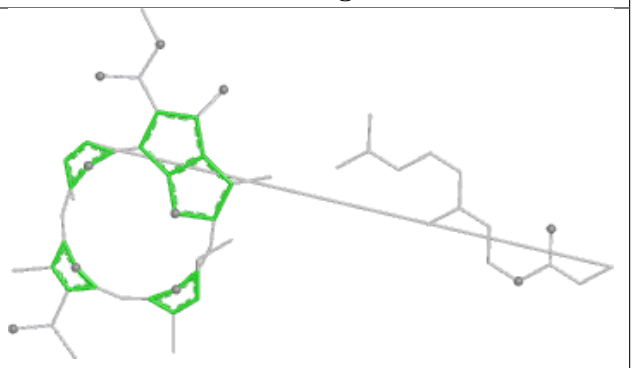
Bond lengths



Bond angles

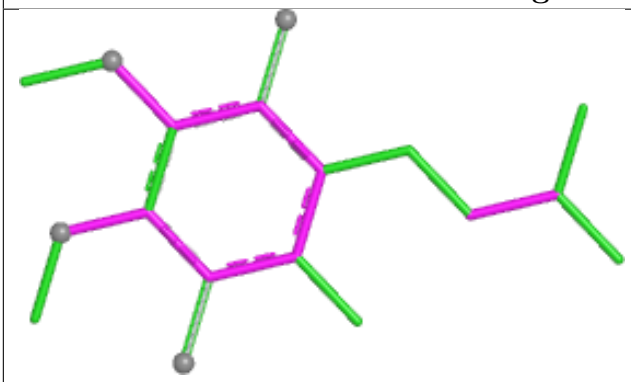


Torsions

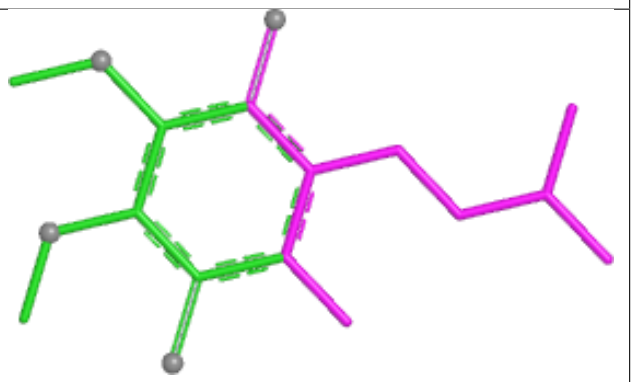


Rings

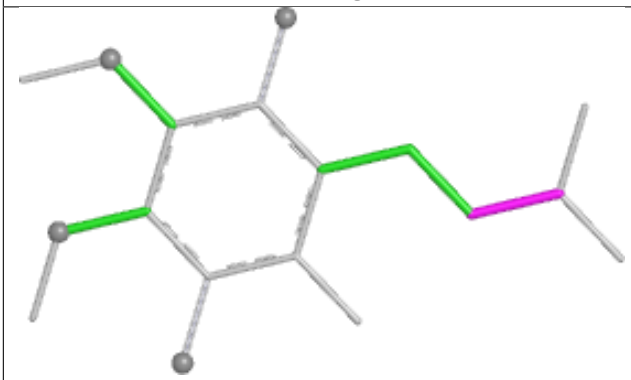
Ligand U10 L 305



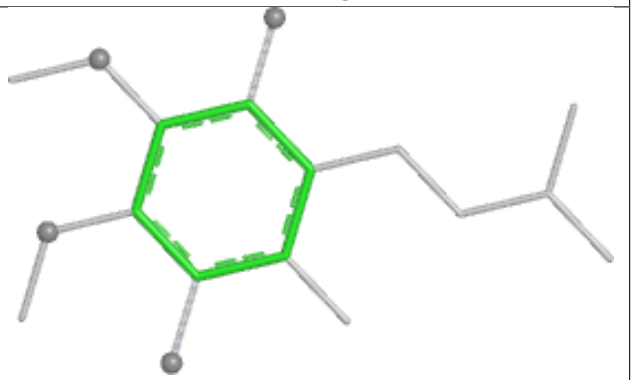
Bond lengths



Bond angles

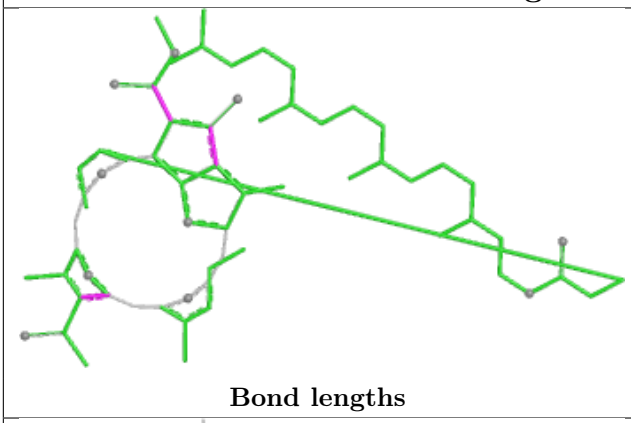


Torsions

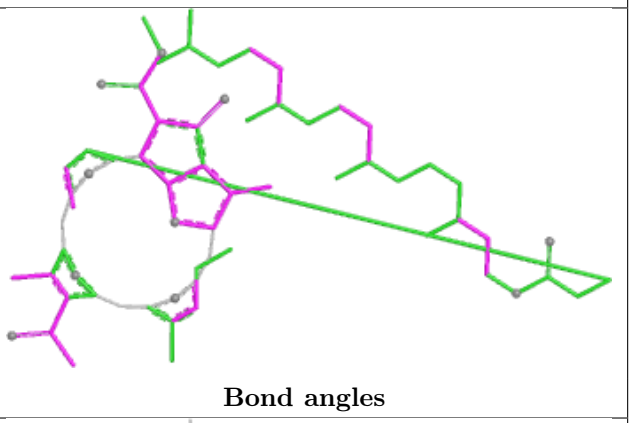


Rings

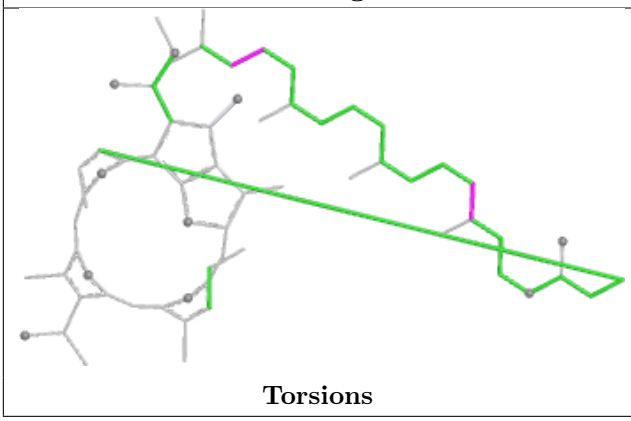
Ligand BPH L 304



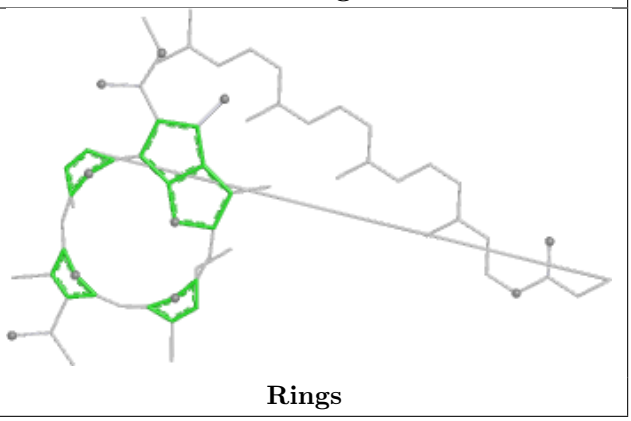
Bond lengths



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%)	-0.32	4 (1%)	69	46	50, 62, 89, 132	0
2	L	281/281 (100%)	-0.26	6 (2%)	63	41	31, 57, 93, 117	2 (0%)
3	M	300/301 (99%)	-0.30	5 (1%)	69	46	43, 62, 91, 120	0
All	All	821/822 (99%)	-0.29	15 (1%)	67	45	31, 60, 91, 132	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	7.8
2	L	73	TYR	4.9
3	M	301	HIS	3.6
2	L	62	GLN	3.5
2	L	74	GLY	3.5
2	L	77	GLY	3.1
3	M	25	ASN	3.0
1	H	250	SER	2.8
3	M	2	GLU	2.6
2	L	71	LEU	2.5
1	H	102	GLY	2.4
3	M	21	THR	2.3
1	H	249	LYS	2.2
1	H	128	HIS	2.1
3	M	234	GLU	2.0

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

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
3	2L5	M	210	12/13	0.97	0.10	44,49,52,53	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

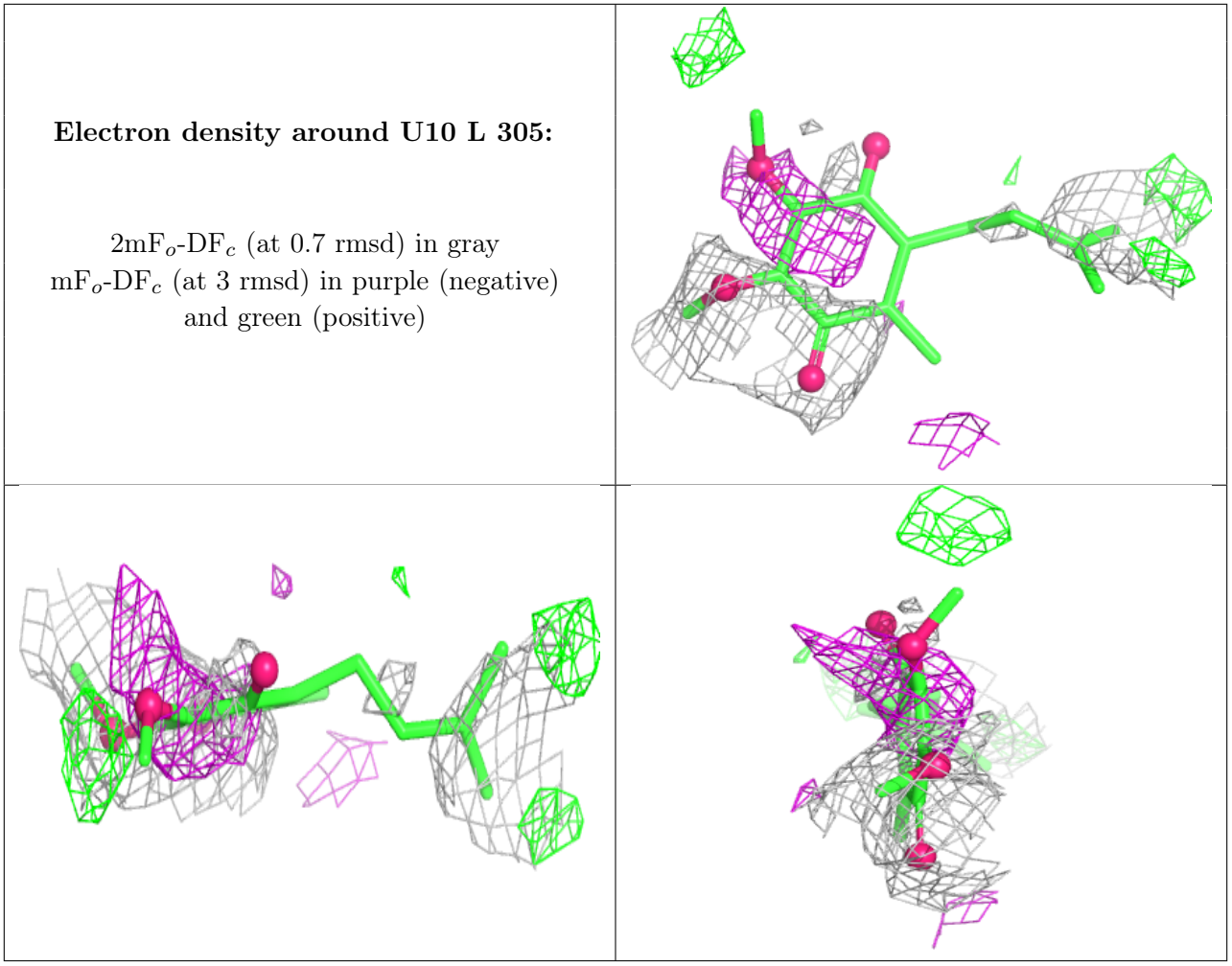
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	L	305	18/63	0.80	0.32	117,136,151,152	0
8	CL	L	307	1/1	0.84	0.20	109,109,109,109	0
11	CDL	M	405	69/100	0.85	0.19	64,93,116,123	0
9	LDA	M	402	16/16	0.86	0.24	82,86,103,105	0
9	LDA	M	403	16/16	0.88	0.20	66,86,111,111	0
10	SPO	M	404	42/42	0.93	0.17	49,66,82,92	0
4	FE	L	301	1/1	0.95	0.22	130,130,130,130	0
5	BPH	L	304	65/65	0.95	0.11	36,50,59,64	0
5	BPH	L	302	55/65	0.96	0.10	36,54,71,85	0
6	BCL	M	406	51/66	0.96	0.09	41,50,66,71	0
6	BCL	M	401	66/66	0.97	0.09	36,49,66,83	0
6	BCL	L	303	66/66	0.97	0.08	42,49,66,68	0
6	BCL	L	306	66/66	0.98	0.07	42,50,59,66	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.

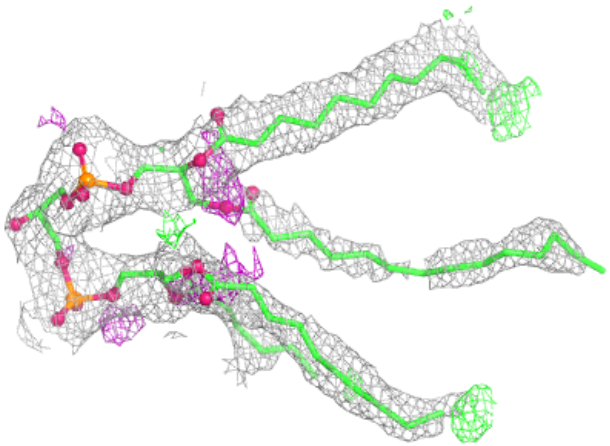
Electron density around U10 L 305:

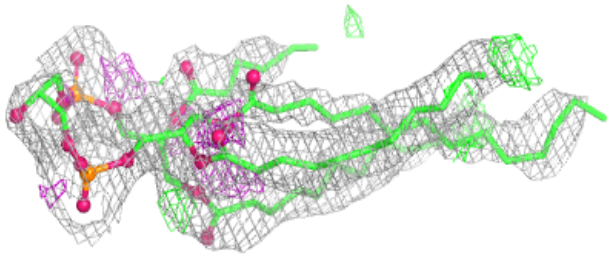
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CDL M 405:

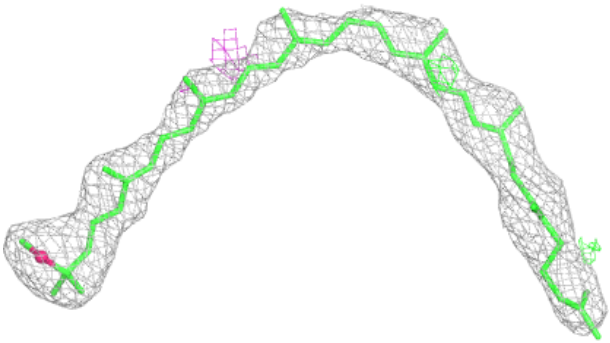
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

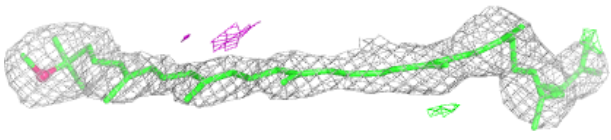


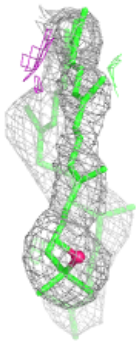


Electron density around SPO M 404:

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

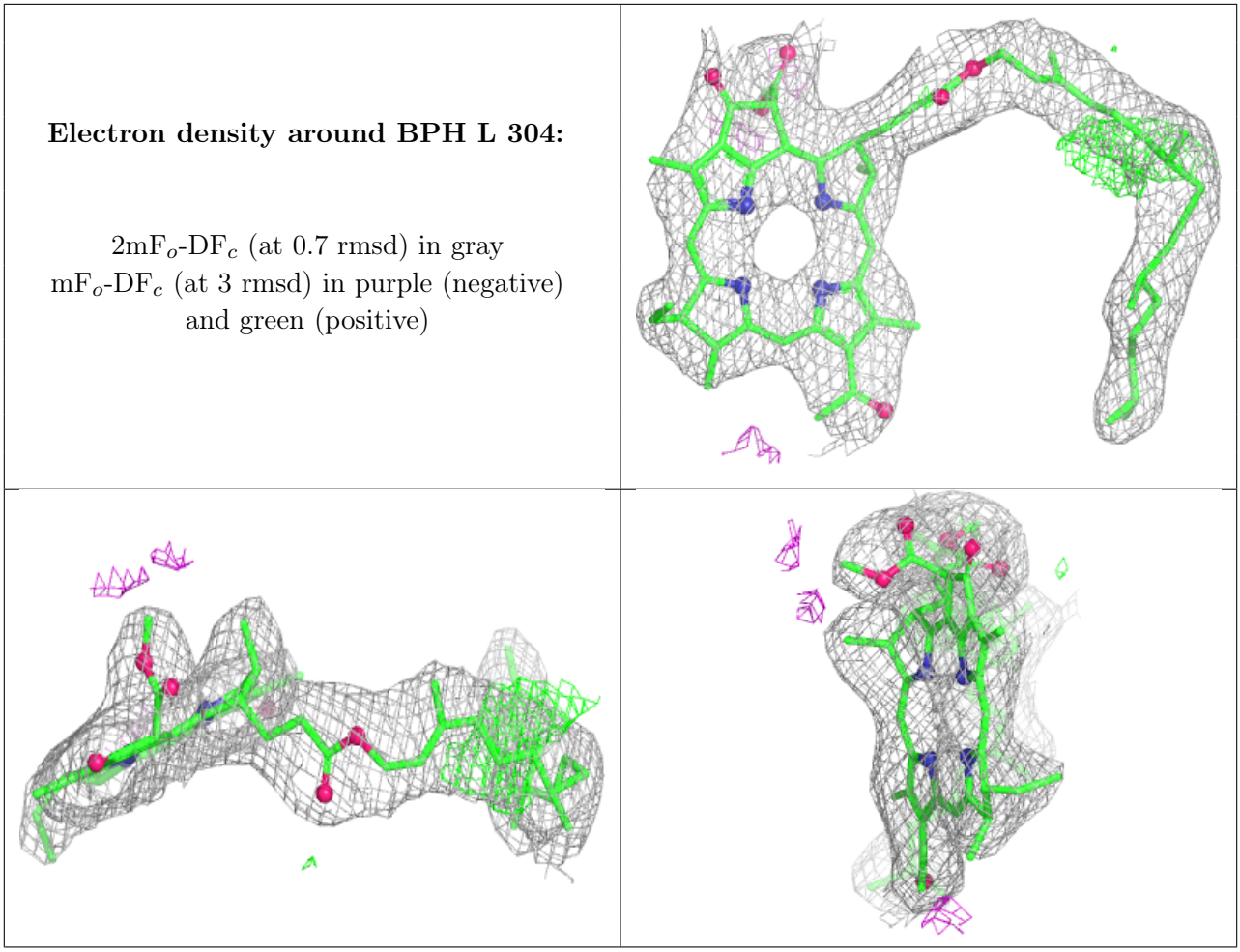






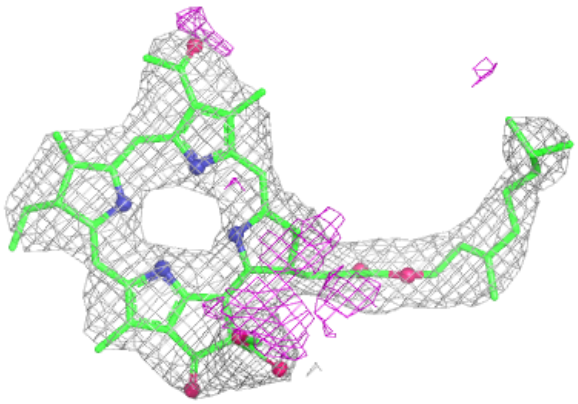
Electron density around BPH L 304:

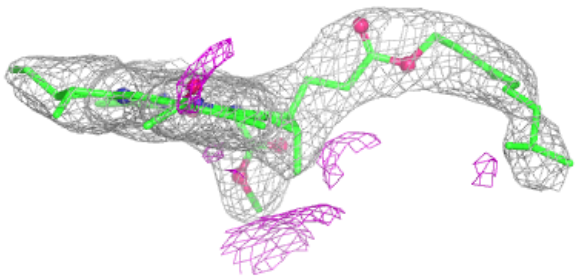
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

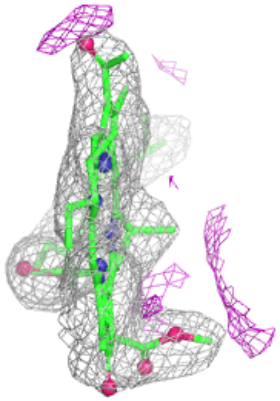


Electron density around BPH L 302:

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

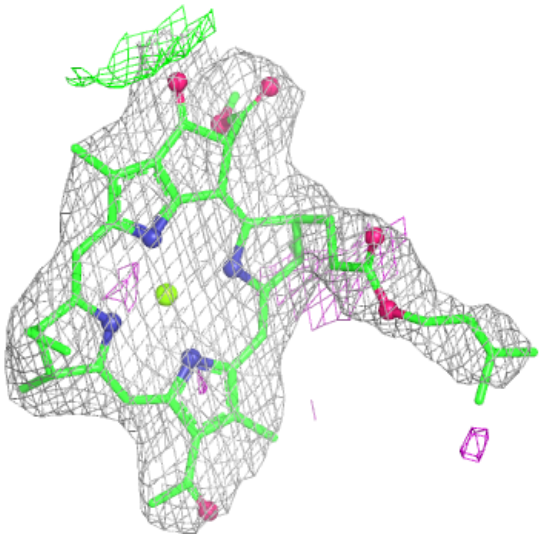


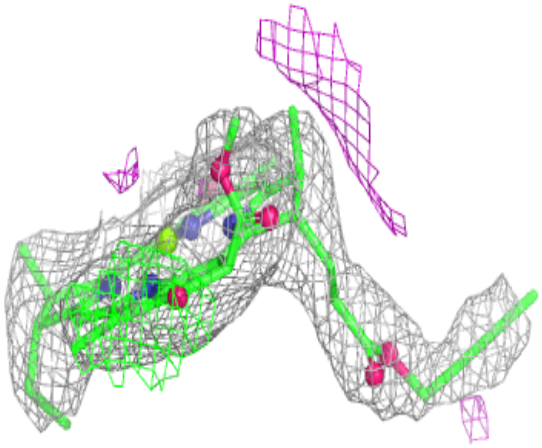


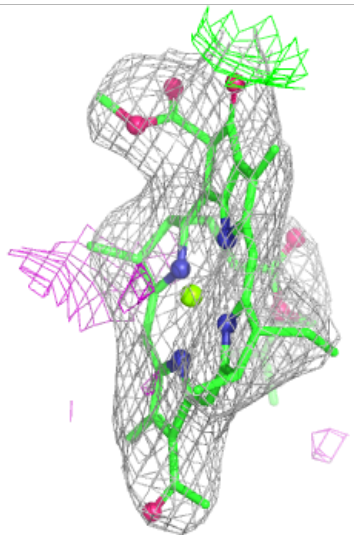


Electron density around BCL M 406:

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

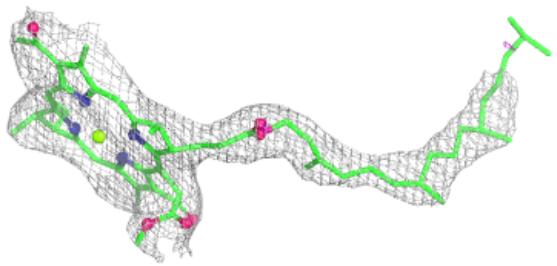


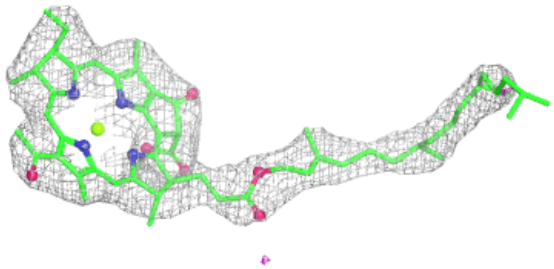


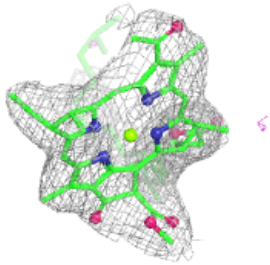


Electron density around BCL M 401:

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

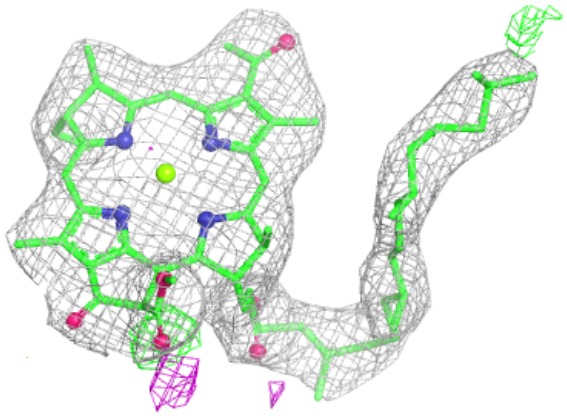


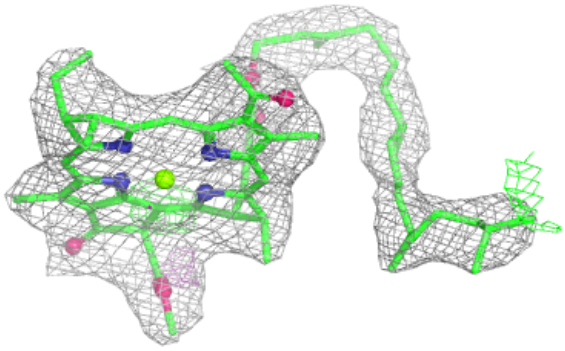


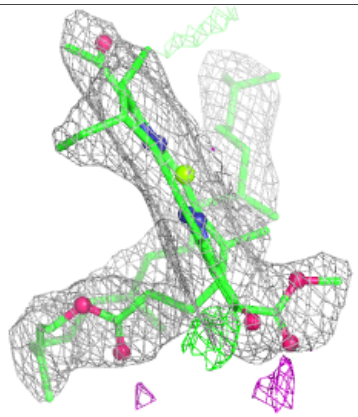


Electron density around BCL L 303:

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

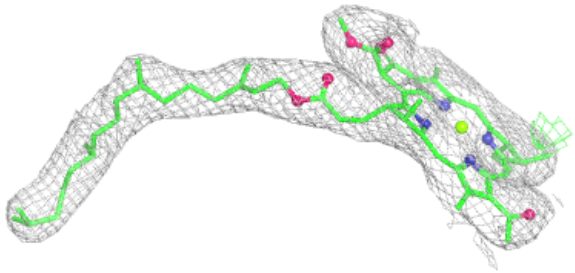


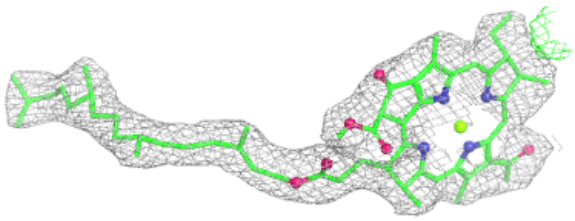


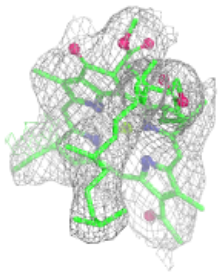


Electron density around BCL L 306:

$2mF_o$-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.