



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:50 pm BST

PDB ID : 3V3Y
Title : Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.
Deposited on : 2011-12-14
Resolution : 2.80 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

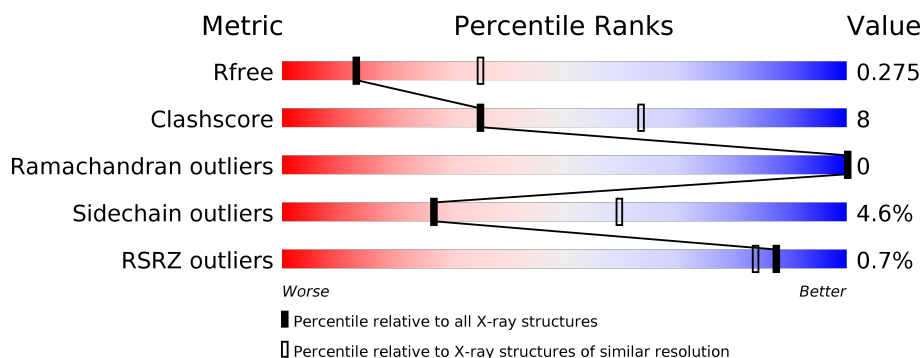
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	241	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> </div>
2	L	281	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
3	M	302	<div> <div></div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>

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
6	BPH	L	402	X	-	-	-
6	BPH	M	401	X	-	-	-
7	U10	L	502	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7270 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	241	Total	C	N	O	S	0	0	0
			1840	1178	315	338	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
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

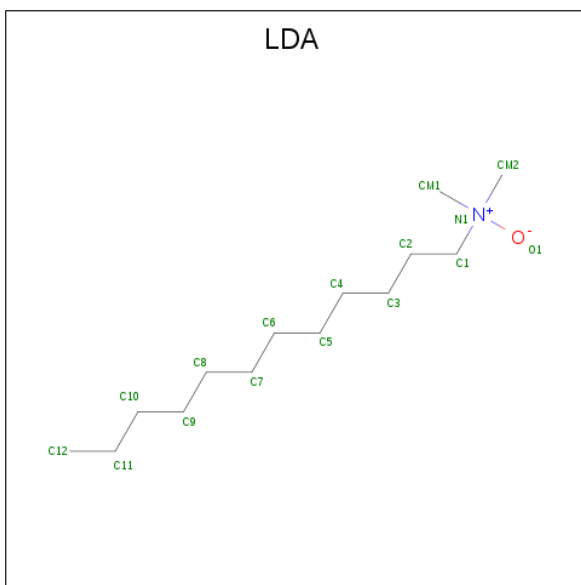
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

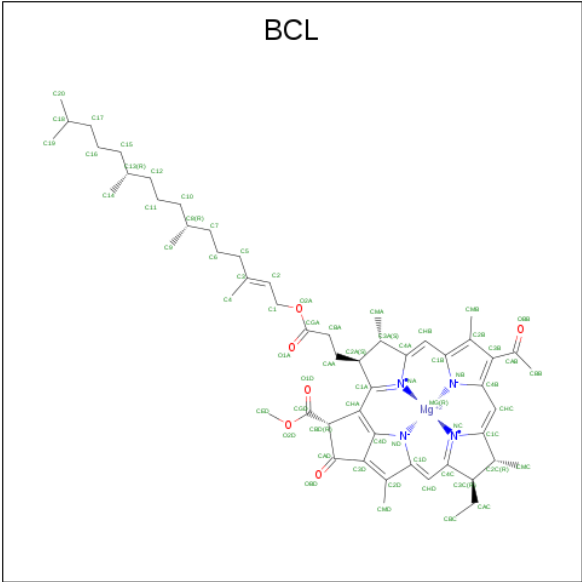
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



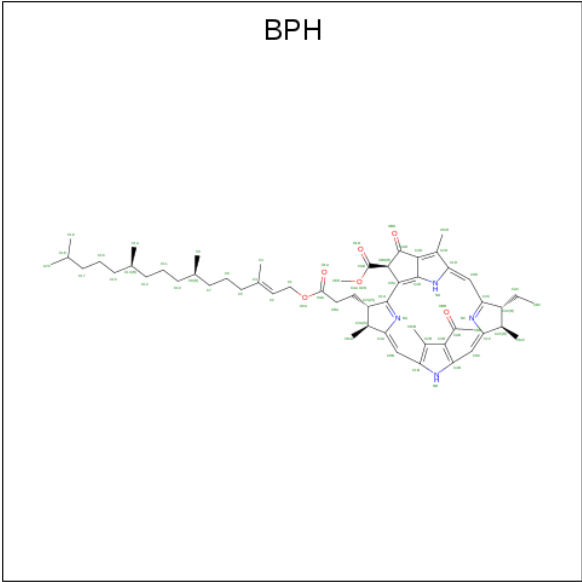
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

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



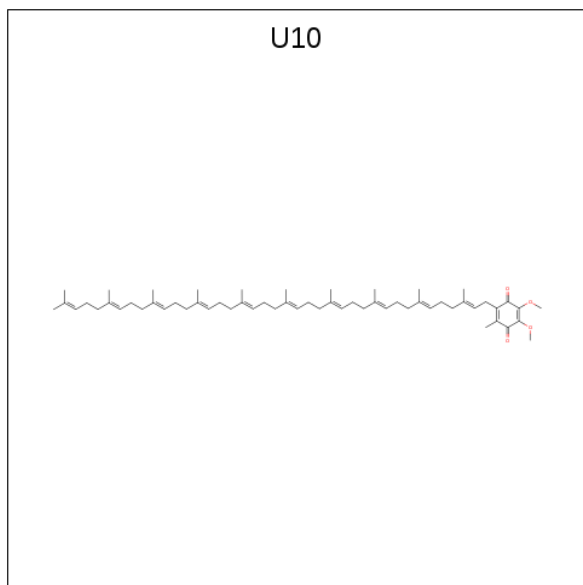
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



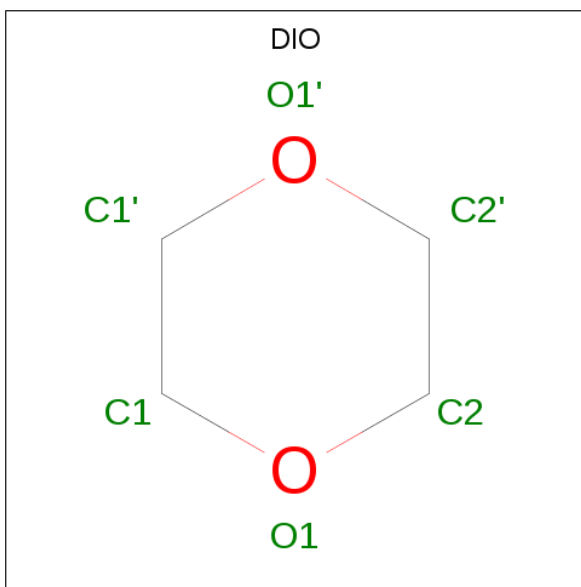
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 8 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).

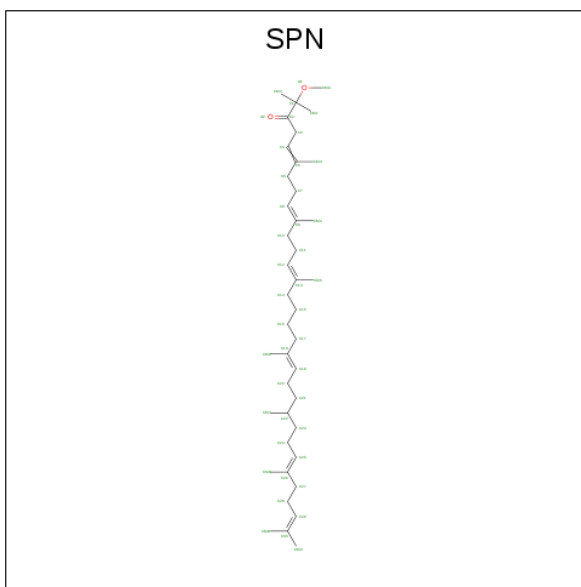


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			6	4	2		
8	L	1	Total	C	O	0	0
			6	4	2		
8	M	1	Total	C	O	0	0
			6	4	2		

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

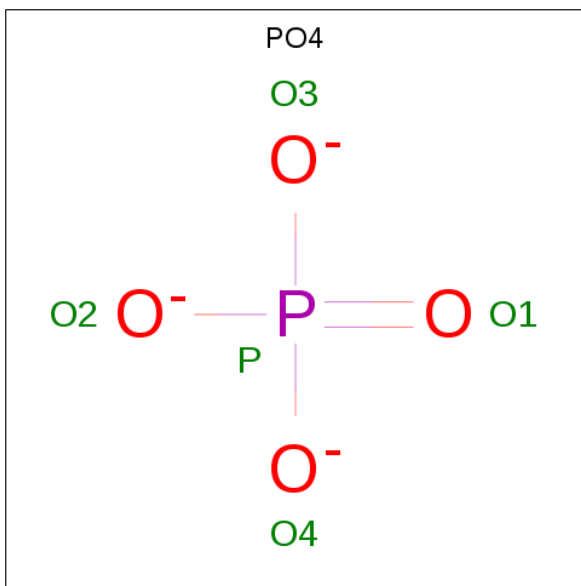
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

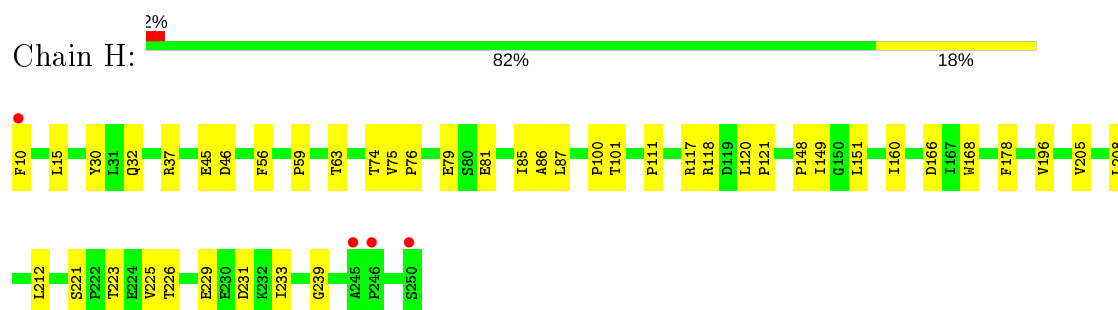
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	40	Total	O	0	0
			40	40		
13	L	21	Total	O	0	0
			21	21		
13	M	31	Total	O	0	0
			31	31		

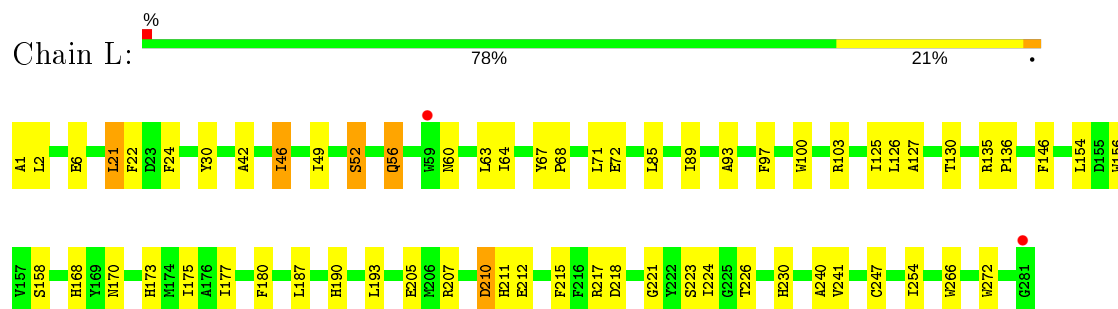
3 Residue-property plots [i](#)

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.

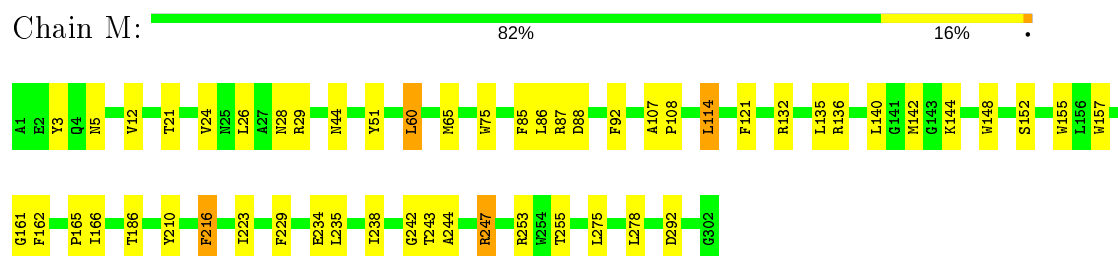
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.75Å 139.75Å 185.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.80 26.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.94-2.80) 99.2 (26.60-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.244 , 0.284 0.239 , 0.275	Depositor DCC
R_{free} test set	2645 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, DIO, CL, 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	0.48	0/1889	0.67	0/2569
2	L	0.47	0/2321	0.61	0/3177
3	M	0.48	0/2501	0.60	0/3415
All	All	0.48	0/6711	0.62	0/9161

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 [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	1840	0	1845	24	0
2	L	2233	0	2189	40	0
3	M	2409	0	2323	40	0
4	H	48	0	93	5	0
4	M	80	0	155	3	0
5	L	66	0	74	4	0
5	M	198	0	222	13	0
6	L	65	0	76	6	0
6	M	65	0	76	5	0
7	L	48	0	63	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	48	0	63	1	0
8	L	12	0	16	2	0
8	M	6	0	8	0	0
9	M	1	0	0	0	0
10	M	43	0	70	6	0
11	M	15	0	0	0	0
12	M	1	0	0	0	0
13	H	40	0	0	0	0
13	L	21	0	0	0	0
13	M	31	0	0	1	0
All	All	7270	0	7273	119	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 8.

All (119) 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)
5:M:303:BCL:H62	5:M:304:BCL:H202	1.62	0.82
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.66	0.78
1:H:63:THR:HG1	1:H:74:THR:HG1	1.33	0.77
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.72	0.72
2:L:30:TYR:O	2:L:103:ARG:NH2	2.26	0.69
6:L:402:BPH:HH C	6:L:402:BPH:HBB3	1.76	0.68
6:L:402:BPH:HBB2	3:M:210:TYR:HB3	1.78	0.65
2:L:190:HIS:HD1	7:L:502:U10:H4M1	1.61	0.65
4:H:702:LDA:HM22	3:M:253:ARG:HH22	1.62	0.64
1:H:111:PRO:O	3:M:247:ARG:NH2	2.31	0.64
3:M:234:GLU:O	3:M:238:ILE:HG13	1.99	0.63
1:H:30:TYR:CZ	4:H:704:LDA:H12	2.34	0.62
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.82	0.61
3:M:136:ARG:NH2	13:M:336:HOH:O	2.33	0.61
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.83	0.60
5:M:304:BCL:H192	6:M:401:BPH:H7C2	1.84	0.60
2:L:71:LEU:H	2:L:71:LEU:HD12	1.69	0.58
1:H:120:LEU:N	1:H:226:THR:HB	2.19	0.57
3:M:161:GLY:HA3	10:M:600:SPN:H201	1.86	0.57
2:L:266:TRP:CG	8:L:900:DIO:H21	2.42	0.55
1:H:120:LEU:H	1:H:226:THR:HB	1.72	0.55
2:L:60:ASN:O	2:L:64:ILE:HG13	2.07	0.55
5:L:302:BCL:HBB2	5:M:304:BCL:NA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:401:BPH:HHC	6:M:401:BPH:HBB3	1.88	0.55
5:L:302:BCL:NA	5:M:304:BCL:HBB2	2.23	0.53
3:M:157:TRP:CD1	10:M:600:SPN:H202	2.43	0.53
2:L:97:PHE:HB3	2:L:125:ILE:HG12	1.90	0.53
6:L:402:BPH:HHC	6:L:402:BPH:CBB	2.39	0.53
3:M:243:THR:O	3:M:247:ARG:HG2	2.09	0.53
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.91	0.52
2:L:210:ASP:OD1	2:L:210:ASP:N	2.43	0.52
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.92	0.52
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.93	0.51
2:L:266:TRP:CD2	8:L:900:DIO:H21	2.47	0.50
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.47	0.49
5:M:305:BCL:HMB1	5:M:305:BCL:HBB2	1.95	0.48
2:L:127:ALA:O	2:L:130:THR:HB	2.12	0.48
7:L:502:U10:H122	7:L:502:U10:H101	1.52	0.48
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.49	0.48
5:M:303:BCL:H111	5:M:303:BCL:H142	1.69	0.48
1:H:149:ILE:HD13	1:H:166:ASP:HA	1.95	0.48
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.49	0.48
2:L:193:LEU:HG	2:L:212:GLU:HG2	1.96	0.48
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.95	0.47
1:H:86:ALA:HB1	1:H:101:THR:OG1	2.13	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.97	0.47
2:L:224:ILE:HG22	7:L:502:U10:C2	2.44	0.47
5:M:303:BCL:C4B	10:M:600:SPN:H152	2.45	0.47
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.96	0.47
1:H:37:ARG:HB3	1:H:75:VAL:HB	1.97	0.46
2:L:175:ILE:HG12	7:L:502:U10:H261	1.97	0.46
2:L:103:ARG:NH1	3:M:255:THR:O	2.42	0.46
5:M:303:BCL:CAB	10:M:600:SPN:H162	2.46	0.46
4:M:703:LDA:H11	4:M:703:LDA:H41	1.60	0.46
2:L:170:ASN:O	2:L:173:HIS:HB3	2.15	0.46
2:L:1:ALA:C	2:L:2:LEU:HD23	2.37	0.45
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.98	0.45
5:M:303:BCL:H2	6:M:401:BPH:CMB	2.46	0.45
3:M:60:LEU:HA	6:M:401:BPH:H4C2	1.98	0.45
3:M:85:PHE:HD2	3:M:86:LEU:HD12	1.81	0.45
1:H:121:PRO:HB3	1:H:225:VAL:O	2.17	0.45
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.52	0.44
5:L:302:BCL:CGA	5:M:305:BCL:HBC1	2.48	0.44
1:H:81:GLU:HG3	1:H:85:ILE:CD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:107:ALA:HA	3:M:108:PRO:HD3	1.86	0.44
3:M:75:TRP:HE1	10:M:600:SPN:HMA2	1.82	0.44
2:L:205:GLU:O	2:L:207:ARG:NH1	2.51	0.43
2:L:215:PHE:HB2	3:M:142:MET:HE1	2.00	0.43
2:L:217:ARG:O	2:L:221:GLY:HA2	2.18	0.43
3:M:114:LEU:HD13	3:M:114:LEU:HA	1.80	0.43
3:M:162:PHE:O	3:M:166:ILE:HG12	2.18	0.43
2:L:223:SER:O	3:M:44:ASN:ND2	2.48	0.43
3:M:223:ILE:HD13	3:M:223:ILE:HA	1.87	0.43
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.53	0.43
7:L:502:U10:H72	7:L:502:U10:H1M1	1.81	0.43
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.54	0.43
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.75	0.43
1:H:59:PRO:HG2	1:H:76:PRO:HD3	2.00	0.43
4:H:704:LDA:HM11	4:H:704:LDA:H22	1.79	0.43
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.19	0.43
2:L:93:ALA:HB2	6:L:402:BPH:H122	2.01	0.43
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.53	0.43
5:M:304:BCL:HHC	5:M:304:BCL:OBB	2.19	0.43
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.54	0.42
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.55	0.42
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.01	0.42
1:H:229:GLU:O	1:H:233:ILE:HG13	2.20	0.42
1:H:118:ARG:HD3	1:H:120:LEU:HD12	2.02	0.42
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.55	0.42
2:L:42:ALA:O	2:L:46:ILE:HB	2.19	0.42
5:M:303:BCL:HHC	5:M:303:BCL:OBB	2.19	0.42
4:M:705:LDA:HM13	4:M:705:LDA:H21	1.73	0.42
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.87	0.42
2:L:100:TRP:CH2	7:M:501:U10:H261	2.54	0.42
3:M:135:LEU:HD23	3:M:135:LEU:HA	1.92	0.42
2:L:52:SER:O	2:L:56:GLN:HB2	2.20	0.42
5:M:303:BCL:H102	5:M:303:BCL:H61	1.93	0.41
3:M:24:VAL:HG11	3:M:29:ARG:NH1	2.36	0.41
3:M:157:TRP:CE2	10:M:600:SPN:HM73	2.55	0.41
4:H:702:LDA:H121	4:M:701:LDA:H91	2.02	0.41
2:L:67:TYR:HA	2:L:68:PRO:HD3	1.93	0.41
6:M:401:BPH:HBA2	6:M:401:BPH:H3A	1.82	0.41
3:M:140:LEU:HA	3:M:140:LEU:HD23	1.95	0.41
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.56	0.41
1:H:208:LEU:HA	1:H:208:LEU:HD23	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:702:LDA:HM22	3:M:253:ARG:NH2	2.31	0.41
2:L:2:LEU:HB3	2:L:6:GLU:HB3	2.02	0.41
5:L:302:BCL:HBB3	5:L:302:BCL:HMB1	2.03	0.41
3:M:152:SER:O	3:M:155:TRP:HB3	2.21	0.41
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.57	0.40
2:L:168:HIS:HE1	3:M:186:THR:HB	1.87	0.40
2:L:173:HIS:O	2:L:177:ILE:HG13	2.21	0.40
3:M:162:PHE:C	3:M:165:PRO:HD2	2.42	0.40
3:M:88:ASP:HB2	3:M:92:PHE:CZ	2.56	0.40
2:L:21:LEU:HA	2:L:21:LEU:HD13	1.86	0.40
2:L:241:VAL:HG21	6:L:402:BPH:H2C	2.04	0.40
6:L:402:BPH:H112	6:L:402:BPH:H7C2	1.65	0.40
3:M:132:ARG:O	3:M:136:ARG:HG2	2.20	0.40
1:H:160:ILE:HD13	1:H:160:ILE:HA	1.88	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	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/302 (99%)	282 (94%)	18 (6%)	0	100	100
All	All	818/824 (99%)	785 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	196/196 (100%)	188 (96%)	8 (4%)	30	64
2	L	220/220 (100%)	206 (94%)	14 (6%)	17	45
3	M	236/236 (100%)	228 (97%)	8 (3%)	37	71
All	All	652/652 (100%)	622 (95%)	30 (5%)	27	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	10	PHE
1	H	15	LEU
1	H	45	GLU
1	H	46	ASP
1	H	79	GLU
1	H	221	SER
1	H	223	THR
1	H	231	ASP
2	L	21	LEU
2	L	46	ILE
2	L	52	SER
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	85	LEU
2	L	126	LEU
2	L	154	LEU
2	L	158	SER
2	L	210	ASP
2	L	226	THR
2	L	247	CYS
2	L	254	ILE
3	M	12	VAL
3	M	60	LEU
3	M	114	LEU
3	M	144	LYS

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Mol	Chain	Res	Type
3	M	148	TRP
3	M	216	PHE
3	M	247	ARG
3	M	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	M	305	-	58,74,74	1.37	5 (8%)	69,115,115	2.02	18 (26%)
4	LDA	H	702	-	12,15,15	1.97	1 (8%)	14,17,17	0.58	0
8	DIO	L	900	-	6,6,6	0.80	0	6,6,6	0.82	0
4	LDA	M	701	-	12,15,15	2.03	1 (8%)	14,17,17	0.43	0
11	PO4	M	800	-	4,4,4	1.12	0	6,6,6	0.52	0
4	LDA	H	704	-	12,15,15	1.96	1 (8%)	14,17,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	M	707	-	12,15,15	1.97	1 (8%)	14,17,17	0.44	0
7	U10	L	502	-	48,48,63	2.77	13 (27%)	58,61,79	1.66	19 (32%)
4	LDA	M	705	-	12,15,15	2.03	1 (8%)	14,17,17	0.48	0
4	LDA	H	709	-	12,15,15	1.98	1 (8%)	14,17,17	0.61	0
6	BPH	M	401	-	64,70,70	1.44	7 (10%)	76,101,101	1.29	10 (13%)
10	SPN	M	600	-	40,42,42	1.22	6 (15%)	50,52,52	1.69	12 (24%)
11	PO4	M	803	-	4,4,4	0.77	0	6,6,6	0.57	0
5	BCL	L	302	-	58,74,74	1.40	3 (5%)	69,115,115	1.72	19 (27%)
4	LDA	M	708	-	12,15,15	2.06	1 (8%)	14,17,17	0.50	0
7	U10	M	501	-	48,48,63	2.67	14 (29%)	58,61,79	1.66	14 (24%)
8	DIO	L	901	-	6,6,6	0.75	0	6,6,6	0.99	0
11	PO4	M	801	-	4,4,4	0.53	0	6,6,6	0.78	0
5	BCL	M	304	-	58,74,74	1.39	4 (6%)	69,115,115	1.85	19 (27%)
5	BCL	M	303	-	58,74,74	1.45	5 (8%)	69,115,115	1.90	24 (34%)
6	BPH	L	402	-	64,70,70	1.34	7 (10%)	76,101,101	1.50	14 (18%)
8	DIO	M	902	-	6,6,6	0.74	0	6,6,6	0.94	0
4	LDA	M	703	-	12,15,15	1.95	1 (8%)	14,17,17	0.47	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
7	U10	M	501	-	-	15/45/69/87	0/1/1/1
5	BCL	M	305	-	-	3/37/137/137	-
8	DIO	L	900	-	-	-	0/1/1/1
8	DIO	L	901	-	-	-	0/1/1/1
10	SPN	M	600	-	-	18/50/51/51	-
5	BCL	M	304	-	-	3/37/137/137	-
4	LDA	H	702	-	-	7/13/13/13	-
7	U10	L	502	-	-	21/45/69/87	0/1/1/1
4	LDA	M	707	-	-	8/13/13/13	-
4	LDA	H	704	-	-	5/13/13/13	-
4	LDA	M	705	-	-	4/13/13/13	-
4	LDA	M	701	-	-	8/13/13/13	-
4	LDA	M	703	-	-	10/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BPH	L	402	-	2/2/18/22	13/54/105/105	0/5/6/6
5	BCL	M	303	-	-	8/37/137/137	-
8	DIO	M	902	-	-	-	0/1/1/1
4	LDA	H	709	-	-	8/13/13/13	-
5	BCL	L	302	-	-	10/37/137/137	-
6	BPH	M	401	-	2/2/18/22	14/54/105/105	0/5/6/6
4	LDA	M	708	-	-	4/13/13/13	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	708	LDA	O1-N1	-7.02	1.25	1.42
4	M	705	LDA	O1-N1	-6.96	1.25	1.42
4	M	701	LDA	O1-N1	-6.87	1.26	1.42
5	M	305	BCL	C4B-NB	6.87	1.41	1.35
7	L	502	U10	C13-C14	6.85	1.49	1.33
5	L	302	BCL	C4B-NB	6.83	1.41	1.35
7	L	502	U10	C8-C9	6.76	1.49	1.33
4	H	709	LDA	O1-N1	-6.75	1.26	1.42
4	H	702	LDA	O1-N1	-6.73	1.26	1.42
4	M	707	LDA	O1-N1	-6.72	1.26	1.42
5	M	303	BCL	C1B-NB	6.70	1.41	1.35
4	H	704	LDA	O1-N1	-6.69	1.26	1.42
7	M	501	U10	C13-C14	6.69	1.49	1.33
4	M	703	LDA	O1-N1	-6.61	1.26	1.42
5	M	304	BCL	C4B-NB	6.49	1.41	1.35
7	L	502	U10	C18-C19	6.43	1.48	1.33
7	M	501	U10	C33-C34	6.41	1.48	1.33
7	L	502	U10	C28-C29	6.39	1.48	1.33
7	L	502	U10	C23-C24	6.30	1.48	1.33
7	L	502	U10	C33-C34	6.28	1.48	1.33
5	M	303	BCL	C4B-NB	6.28	1.40	1.35
5	M	304	BCL	C1B-NB	6.27	1.40	1.35
7	M	501	U10	C18-C19	6.20	1.47	1.33
5	L	302	BCL	C1B-NB	5.88	1.40	1.35
7	M	501	U10	C8-C9	5.87	1.47	1.33
7	M	501	U10	C28-C29	5.85	1.47	1.33
7	L	502	U10	C38-C39	5.56	1.48	1.32
7	M	501	U10	C23-C24	5.53	1.46	1.33
7	M	501	U10	C38-C39	5.51	1.48	1.32
5	M	305	BCL	C1B-NB	5.37	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	501	U10	O3-C3	-4.98	1.24	1.36
7	L	502	U10	O3-C3	-4.80	1.25	1.36
6	M	401	BPH	CHA-C1A	4.75	1.48	1.38
7	M	501	U10	O4-C4	-4.50	1.25	1.36
6	L	402	BPH	CHD-C4C	4.36	1.49	1.38
6	L	402	BPH	CHA-C1A	4.26	1.47	1.38
6	M	401	BPH	C4C-NC	-4.24	1.28	1.37
6	M	401	BPH	CHD-C4C	4.20	1.48	1.38
7	L	502	U10	O4-C4	-4.17	1.26	1.36
6	M	401	BPH	C1B-C2B	-3.77	1.37	1.45
6	M	401	BPH	C1A-NA	-3.77	1.30	1.37
6	L	402	BPH	C1A-NA	-3.56	1.30	1.37
6	L	402	BPH	C4C-NC	-3.22	1.30	1.37
10	M	600	SPN	C1-C2	-3.20	1.50	1.53
6	L	402	BPH	C1B-C2B	-3.10	1.39	1.45
10	M	600	SPN	C25-C26	2.98	1.40	1.33
7	L	502	U10	C3-C2	-2.83	1.40	1.48
10	M	600	SPN	C8-C9	2.77	1.39	1.33
7	M	501	U10	C4-C5	-2.76	1.40	1.48
7	M	501	U10	C3-C2	-2.67	1.41	1.48
7	L	502	U10	C6-C1	2.63	1.40	1.35
10	M	600	SPN	C19-C18	2.62	1.39	1.33
7	L	502	U10	C4-C5	-2.61	1.41	1.48
5	M	305	BCL	MG-NA	-2.61	2.00	2.06
6	L	402	BPH	CHB-C1B	2.57	1.43	1.38
5	M	303	BCL	MG-NA	-2.49	2.00	2.06
6	L	402	BPH	C3D-C2D	-2.46	1.35	1.39
7	M	501	U10	C1-C2	-2.42	1.38	1.47
6	M	401	BPH	CHB-C4A	-2.41	1.34	1.40
7	M	501	U10	C6-C5	-2.38	1.40	1.46
7	M	501	U10	C6-C1	2.37	1.39	1.35
5	L	302	BCL	CHD-C4C	-2.32	1.34	1.41
5	M	305	BCL	CHD-C4C	-2.27	1.34	1.41
10	M	600	SPN	C12-C13	2.19	1.38	1.33
6	M	401	BPH	C3D-C2D	-2.17	1.35	1.39
5	M	304	BCL	CHD-C4C	-2.13	1.35	1.41
5	M	303	BCL	MG-NC	-2.09	2.01	2.06
5	M	305	BCL	C4B-CHC	-2.08	1.35	1.41
5	M	303	BCL	CHD-C4C	-2.07	1.35	1.41
7	L	502	U10	C1-C2	-2.06	1.39	1.47
5	M	304	BCL	C4B-CHC	-2.05	1.35	1.41
10	M	600	SPN	C4-C5	2.01	1.37	1.33

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	305	BCL	O2D-CGD-CBD	7.55	124.68	111.27
10	M	600	SPN	C3-C4-C5	-5.28	118.00	126.79
5	M	303	BCL	C1C-NC-C4C	5.19	109.04	106.71
5	M	304	BCL	O2D-CGD-CBD	5.02	120.18	111.27
5	M	305	BCL	CHD-C4C-NC	4.93	130.55	125.08
6	L	402	BPH	C1C-NC-C4C	-4.88	106.25	110.54
5	M	305	BCL	C1C-NC-C4C	4.72	108.83	106.71
5	M	305	BCL	C4A-NA-C1A	4.53	108.74	106.71
6	L	402	BPH	C4D-CHA-C1A	-4.44	119.57	130.51
5	M	304	BCL	CHD-C4C-NC	4.20	129.74	125.08
5	M	303	BCL	CHD-C4C-NC	4.09	129.62	125.08
7	M	501	U10	C32-C33-C34	-4.07	117.86	127.66
6	M	401	BPH	C4D-C3D-CAD	-4.00	105.34	107.87
5	L	302	BCL	C1C-NC-C4C	3.97	108.49	106.71
5	L	302	BCL	CMB-C2B-C1B	-3.96	122.38	128.46
5	M	303	BCL	C4-C3-C5	3.94	121.90	115.27
5	M	304	BCL	C1C-NC-C4C	3.93	108.47	106.71
5	L	302	BCL	CHD-C4C-NC	3.83	129.33	125.08
7	M	501	U10	C22-C23-C24	-3.81	118.48	127.66
5	M	303	BCL	O2D-CGD-CBD	3.81	118.03	111.27
6	M	401	BPH	C4D-CHA-C1A	-3.75	121.26	130.51
5	M	305	BCL	O2D-CGD-O1D	-3.71	116.58	123.84
7	L	502	U10	O5-C5-C4	-3.69	113.10	120.93
5	M	303	BCL	C3A-C2A-C1A	-3.65	95.87	101.34
5	M	304	BCL	CMB-C2B-C1B	-3.64	122.87	128.46
7	M	501	U10	C30-C29-C31	3.57	121.27	115.27
7	M	501	U10	C35-C34-C36	3.53	121.21	115.27
5	M	303	BCL	CMB-C2B-C1B	-3.53	123.05	128.46
5	M	304	BCL	CHB-C4A-NA	3.47	129.31	124.51
5	M	303	BCL	C1D-CHD-C4C	-3.37	120.91	125.88
5	M	303	BCL	C1B-CHB-C4A	-3.37	123.44	130.12
5	M	304	BCL	O2D-CGD-O1D	-3.31	117.37	123.84
7	L	502	U10	C7-C6-C5	3.30	122.45	118.48
5	L	302	BCL	CED-O2D-CGD	3.28	123.36	115.94
10	M	600	SPN	CM3-C5-C6	3.23	120.70	115.27
5	L	302	BCL	C4-C3-C5	3.22	120.69	115.27
10	M	600	SPN	C7-C8-C9	-3.21	119.94	127.66
6	M	401	BPH	C6-C5-C3	3.21	121.86	113.45
6	M	401	BPH	CMD-C2D-C3D	3.13	130.54	124.68
6	L	402	BPH	OBB-CAB-C3B	3.12	126.18	120.41
5	M	305	BCL	O2A-CGA-CBA	3.09	121.61	111.91
7	M	501	U10	C25-C24-C26	3.08	120.45	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	402	BPH	C3A-C2A-C1A	-3.08	97.97	101.64
5	M	303	BCL	O1D-CGD-CBD	-3.05	118.24	124.48
7	M	501	U10	C17-C18-C19	-3.04	120.34	127.66
5	M	305	BCL	CMB-C2B-C1B	-3.02	123.82	128.46
5	M	304	BCL	C1-C2-C3	-3.01	120.84	126.04
5	M	305	BCL	C1D-CHD-C4C	-3.01	121.44	125.88
5	M	304	BCL	CMB-C2B-C3B	2.99	130.27	124.68
6	M	401	BPH	CHD-C4C-NC	-2.96	121.69	125.20
5	M	305	BCL	CHB-C4A-NA	2.93	128.56	124.51
5	M	303	BCL	CHB-C4A-NA	2.92	128.55	124.51
10	M	600	SPN	C24-C25-C26	-2.89	120.70	127.66
7	L	502	U10	C22-C23-C24	-2.86	120.77	127.66
5	M	304	BCL	C1D-CHD-C4C	-2.84	121.70	125.88
5	M	304	BCL	C4D-C3D-CAD	-2.83	106.89	108.47
5	M	305	BCL	O1D-CGD-CBD	-2.82	118.72	124.48
5	M	304	BCL	C4A-NA-C1A	2.80	107.97	106.71
7	M	501	U10	C12-C13-C14	-2.79	120.93	127.66
5	M	304	BCL	CAA-C2A-C3A	-2.78	105.15	112.78
10	M	600	SPN	CM6-C18-C17	2.77	119.93	115.27
5	L	302	BCL	O2D-CGD-CBD	2.73	116.11	111.27
7	L	502	U10	C17-C18-C19	-2.72	121.10	127.66
7	L	502	U10	C32-C33-C34	-2.72	121.11	127.66
6	L	402	BPH	C4D-C3D-CAD	-2.71	106.15	107.87
5	M	305	BCL	C3C-C4C-CHD	-2.70	117.62	123.39
5	M	304	BCL	O2A-CGA-CBA	2.69	120.36	111.91
6	L	402	BPH	C6-C5-C3	2.69	120.52	113.45
5	M	304	BCL	CAC-C3C-C2C	-2.69	107.54	114.26
5	L	302	BCL	C1D-CHD-C4C	-2.67	121.94	125.88
5	L	302	BCL	O2A-CGA-CBA	2.67	120.28	111.91
5	M	304	BCL	CGD-CBD-CAD	-2.66	102.11	110.73
10	M	600	SPN	C20-C19-C18	-2.66	121.25	127.66
7	L	502	U10	C20-C19-C21	2.65	119.73	115.27
6	M	401	BPH	OBb-CAB-C3B	2.64	125.29	120.41
5	L	302	BCL	CMB-C2B-C3B	2.64	129.61	124.68
5	M	305	BCL	C11-C12-C13	-2.63	107.42	115.92
5	M	304	BCL	C4-C3-C5	2.61	119.66	115.27
5	M	303	BCL	C6-C5-C3	-2.60	106.62	113.45
7	M	501	U10	C15-C14-C16	2.55	119.55	115.27
6	L	402	BPH	OBb-CAB-CBB	-2.55	114.09	119.73
7	L	502	U10	C35-C34-C36	2.54	119.54	115.27
6	L	402	BPH	C2B-C1B-NB	-2.52	106.00	109.79
7	L	502	U10	C25-C24-C26	2.51	119.49	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	BCL	O2A-CGA-CBA	2.50	119.76	111.91
5	L	302	BCL	C7-C6-C5	-2.49	106.58	113.36
5	L	302	BCL	C1-C2-C3	-2.47	121.78	126.04
6	L	402	BPH	CMD-C2D-C3D	2.45	129.27	124.68
7	L	502	U10	C4M-O4-C4	2.45	125.16	116.47
5	L	302	BCL	OBB-CAB-CBB	-2.44	114.67	120.17
6	L	402	BPH	CHC-C1C-NC	2.43	128.09	125.20
7	L	502	U10	C30-C29-C31	2.43	119.35	115.27
7	L	502	U10	C27-C28-C29	-2.42	121.82	127.66
5	M	303	BCL	OBB-CAB-CBB	-2.42	114.73	120.17
7	L	502	U10	C1M-C1-C6	-2.41	120.47	124.40
7	L	502	U10	O5-C5-C6	-2.41	117.33	121.55
6	L	402	BPH	C1B-NB-C4B	2.40	111.02	106.51
7	L	502	U10	C3M-O3-C3	2.39	124.94	116.47
6	M	401	BPH	CAC-C3C-C4C	2.38	118.78	112.67
7	M	501	U10	C27-C28-C29	-2.37	121.95	127.66
5	L	302	BCL	C1B-CHB-C4A	-2.37	125.42	130.12
5	M	303	BCL	C3C-C4C-CHD	-2.36	118.34	123.39
5	M	305	BCL	C4-C3-C5	2.36	119.24	115.27
5	M	305	BCL	O2A-CGA-O1A	-2.35	117.65	123.59
10	M	600	SPN	C7-C6-C5	2.35	120.71	112.98
5	M	305	BCL	OBD-CAD-CBD	2.35	129.25	125.89
7	M	501	U10	C4M-O4-C4	2.35	124.79	116.47
5	L	302	BCL	C11-C10-C8	-2.34	108.35	115.92
10	M	600	SPN	C11-C12-C13	-2.34	122.03	127.66
5	M	305	BCL	C16-C15-C13	-2.31	108.46	115.92
5	M	303	BCL	CBC-CAC-C3C	-2.29	108.36	113.47
5	L	302	BCL	C11-C12-C13	-2.28	108.55	115.92
7	L	502	U10	O2-C2-C3	-2.27	116.12	120.93
7	M	501	U10	C22-C21-C19	-2.26	105.53	112.98
5	M	305	BCL	C6-C5-C3	-2.26	107.53	113.45
5	M	303	BCL	CMB-C2B-C3B	2.26	128.91	124.68
6	L	402	BPH	C3B-C2B-C1B	2.26	109.16	105.87
6	L	402	BPH	C4-C3-C5	-2.25	111.48	115.27
6	M	401	BPH	OBB-CAB-CBB	-2.24	114.77	119.73
5	M	304	BCL	CBC-CAC-C3C	-2.22	108.52	113.47
6	L	402	BPH	C1-O2A-CGA	-2.21	110.65	116.44
7	L	502	U10	C41-C39-C40	2.21	119.48	114.60
10	M	600	SPN	CM5-C13-C14	2.20	118.97	115.27
5	M	303	BCL	C1-C2-C3	-2.19	122.25	126.04
7	M	501	U10	C25-C24-C23	-2.19	118.07	123.68
5	M	303	BCL	O2A-CGA-O1A	-2.19	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	BCL	CAC-C3C-C2C	-2.19	108.80	114.26
5	L	302	BCL	CHB-C4A-NA	2.18	127.52	124.51
5	M	303	BCL	C11-C12-C13	-2.17	108.92	115.92
5	L	302	BCL	C3C-C4C-CHD	-2.16	118.78	123.39
5	M	303	BCL	O2A-C1-C2	-2.14	103.01	108.64
5	M	304	BCL	C11-C10-C8	-2.14	109.00	115.92
5	M	305	BCL	CMB-C2B-C3B	2.14	128.68	124.68
5	M	303	BCL	C3D-CAD-CBD	-2.13	104.81	107.61
10	M	600	SPN	C28-C29-C30	-2.11	120.53	127.75
7	M	501	U10	C41-C39-C40	2.11	119.27	114.60
5	L	302	BCL	C1-O2A-CGA	2.11	121.98	116.44
5	M	303	BCL	C5-C3-C2	-2.11	116.86	121.12
7	M	501	U10	C10-C9-C11	2.10	118.81	115.27
5	M	304	BCL	OBB-CAB-CBB	-2.10	115.45	120.17
7	L	502	U10	C7-C8-C9	-2.10	123.30	126.79
10	M	600	SPN	O1-C1-C2	-2.07	104.54	108.78
5	L	302	BCL	O2A-CGA-O1A	-2.06	118.39	123.59
7	L	502	U10	C37-C38-C39	-2.04	120.76	127.75
6	M	401	BPH	C1B-NB-C4B	2.02	110.32	106.51
6	M	401	BPH	C1C-NC-C4C	-2.02	108.76	110.54
10	M	600	SPN	C6-C5-C4	-2.02	117.04	121.12
5	M	303	BCL	CMA-C3A-C4A	-2.01	106.36	111.77
7	L	502	U10	C8-C7-C6	2.01	117.45	112.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	401	BPH	C8
6	M	401	BPH	C13
6	L	402	BPH	C8
6	L	402	BPH	C13

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	702	LDA	C2-C1-N1-O1
4	H	702	LDA	C2-C1-N1-CM1
4	H	702	LDA	C2-C1-N1-CM2
4	M	701	LDA	C2-C1-N1-O1
4	M	701	LDA	C2-C1-N1-CM1
4	M	701	LDA	C2-C1-N1-CM2
4	M	707	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
4	M	707	LDA	C2-C1-N1-CM1
4	M	707	LDA	C2-C1-N1-CM2
7	L	502	U10	C7-C8-C9-C10
7	L	502	U10	C7-C8-C9-C11
7	L	502	U10	C32-C33-C34-C35
7	L	502	U10	C32-C33-C34-C36
7	L	502	U10	C34-C36-C37-C38
4	H	709	LDA	C2-C1-N1-O1
4	H	709	LDA	C2-C1-N1-CM1
4	H	709	LDA	C2-C1-N1-CM2
6	M	401	BPH	C4B-C3B-CAB-CBB
6	M	401	BPH	C4B-C3B-CAB-OB
6	M	401	BPH	C4-C3-C5-C6
10	M	600	SPN	CM1-C1-C2-C3
10	M	600	SPN	C4-C5-C6-C7
10	M	600	SPN	C11-C10-C9-C8
10	M	600	SPN	C12-C13-C14-C15
10	M	600	SPN	CM5-C13-C14-C15
10	M	600	SPN	C28-C29-C30-CMB
4	M	708	LDA	C2-C1-N1-CM1
7	M	501	U10	C27-C28-C29-C30
7	M	501	U10	C32-C33-C34-C35
7	M	501	U10	C32-C33-C34-C36
6	L	402	BPH	C14-C13-C15-C16
4	M	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
4	M	703	LDA	C1-C2-C3-C4
10	M	600	SPN	C11-C10-C9-CM4
6	M	401	BPH	C2-C3-C5-C6
7	M	501	U10	C37-C38-C39-C40
7	M	501	U10	C27-C28-C29-C31
7	M	501	U10	C37-C38-C39-C41
7	L	502	U10	C12-C11-C9-C10
10	M	600	SPN	CM3-C5-C6-C7
10	M	600	SPN	C16-C17-C18-CM6
7	L	502	U10	C12-C11-C9-C8
10	M	600	SPN	C16-C17-C18-C19
7	L	502	U10	C9-C11-C12-C13
7	L	502	U10	C24-C26-C27-C28
7	M	501	U10	C29-C31-C32-C33
10	M	600	SPN	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
10	M	600	SPN	CM6-C18-C19-C20
6	L	402	BPH	C10-C11-C12-C13
7	L	502	U10	C37-C38-C39-C40
5	M	305	BCL	C15-C16-C17-C18
4	M	701	LDA	C3-C4-C5-C6
4	M	705	LDA	C5-C6-C7-C8
4	H	704	LDA	C4-C5-C6-C7
4	M	705	LDA	C3-C4-C5-C6
4	M	707	LDA	C7-C8-C9-C10
4	H	709	LDA	C4-C5-C6-C7
4	H	704	LDA	C2-C3-C4-C5
5	L	302	BCL	C15-C16-C17-C18
4	M	707	LDA	C4-C5-C6-C7
4	M	703	LDA	C11-C10-C9-C8
4	M	703	LDA	C7-C8-C9-C10
4	H	704	LDA	C5-C6-C7-C8
4	M	708	LDA	C5-C6-C7-C8
6	L	402	BPH	C4-C3-C5-C6
7	L	502	U10	C37-C38-C39-C41
4	H	702	LDA	C7-C8-C9-C10
6	M	401	BPH	C3-C5-C6-C7
4	M	701	LDA	C1-C2-C3-C4
4	M	707	LDA	C1-C2-C3-C4
4	H	704	LDA	C7-C8-C9-C10
6	L	402	BPH	C2-C3-C5-C6
6	L	402	BPH	C11-C10-C8-C7
6	L	402	BPH	C11-C12-C13-C15
6	M	401	BPH	CBA-CGA-O2A-C1
6	M	401	BPH	CBD-CGD-O2D-CED
4	M	708	LDA	C1-C2-C3-C4
5	M	304	BCL	C2C-C3C-CAC-CBC
6	M	401	BPH	O1A-CGA-O2A-C1
4	M	707	LDA	C5-C6-C7-C8
7	L	502	U10	C35-C34-C36-C37
7	L	502	U10	C33-C34-C36-C37
5	M	303	BCL	C11-C10-C8-C9
4	M	703	LDA	C4-C5-C6-C7
4	M	708	LDA	N1-C1-C2-C3
4	M	703	LDA	C6-C7-C8-C9
10	M	600	SPN	C19-C20-C21-C22
10	M	600	SPN	C28-C29-C30-CM9
4	M	705	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	H	709	LDA	C3-C4-C5-C6
4	H	702	LDA	C9-C10-C11-C12
4	M	707	LDA	C9-C10-C11-C12
5	M	305	BCL	C16-C17-C18-C19
7	M	501	U10	C24-C26-C27-C28
5	L	302	BCL	C13-C15-C16-C17
4	M	703	LDA	C3-C4-C5-C6
6	M	401	BPH	C4C-C3C-CAC-CBC
5	M	305	BCL	C16-C17-C18-C20
4	H	709	LDA	C9-C10-C11-C12
5	M	303	BCL	C11-C10-C8-C7
5	L	302	BCL	CBD-CGD-O2D-CED
6	L	402	BPH	CAD-CBD-CGD-O2D
6	M	401	BPH	C15-C16-C17-C18
7	L	502	U10	C5-C4-O4-C4M
6	M	401	BPH	O1D-CGD-O2D-CED
5	M	303	BCL	C1A-C2A-CAA-CBA
4	M	701	LDA	C9-C10-C11-C12
6	L	402	BPH	C12-C13-C15-C16
6	L	402	BPH	C8-C10-C11-C12
5	L	302	BCL	C16-C17-C18-C20
5	L	302	BCL	C16-C17-C18-C19
7	L	502	U10	C14-C16-C17-C18
4	H	702	LDA	C2-C3-C4-C5
6	M	401	BPH	C2B-C3B-CAB-OB
4	M	701	LDA	C6-C7-C8-C9
4	H	709	LDA	C1-C2-C3-C4
5	M	303	BCL	C2-C1-O2A-CGA
5	L	302	BCL	C11-C10-C8-C7
6	L	402	BPH	C11-C10-C8-C9
4	M	703	LDA	N1-C1-C2-C3
4	H	704	LDA	C1-C2-C3-C4
7	M	501	U10	C28-C29-C31-C32
6	L	402	BPH	O2A-C1-C2-C3
7	M	501	U10	C25-C24-C26-C27
4	H	709	LDA	C5-C6-C7-C8
5	L	302	BCL	C11-C10-C8-C9
5	M	303	BCL	C10-C11-C12-C13
5	L	302	BCL	O1D-CGD-O2D-CED
7	L	502	U10	C20-C19-C21-C22
7	M	501	U10	C30-C29-C31-C32
7	M	501	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
7	L	502	U10	C25-C24-C26-C27
4	M	705	LDA	C2-C3-C4-C5
5	M	303	BCL	C4-C3-C5-C6
5	M	304	BCL	C3A-C2A-CAA-CBA
5	L	302	BCL	CAD-CBD-CGD-O2D
6	L	402	BPH	C16-C17-C18-C19
7	M	501	U10	C23-C24-C26-C27
5	M	303	BCL	C2-C3-C5-C6
7	L	502	U10	C2-C3-O3-C3M
6	M	401	BPH	CHA-CBD-CGD-O1D
6	M	401	BPH	CHA-CBD-CGD-O2D
10	M	600	SPN	C21-C22-C23-C24
7	M	501	U10	C3-C4-O4-C4M
7	L	502	U10	C36-C37-C38-C39
7	M	501	U10	C16-C17-C18-C19
7	L	502	U10	C23-C24-C26-C27
5	M	304	BCL	C1A-C2A-CAA-CBA
4	H	702	LDA	C5-C6-C7-C8
5	L	302	BCL	C2A-CAA-CBA-CGA
7	L	502	U10	C30-C29-C31-C32
6	L	402	BPH	C5-C6-C7-C8
10	M	600	SPN	CM1-C1-C2-O2
4	M	701	LDA	C11-C10-C9-C8
10	M	600	SPN	C25-C26-C27-C28
10	M	600	SPN	C9-C10-C11-C12
5	M	303	BCL	C8-C10-C11-C12

There are no ring outliers.

15 monomers are involved in 42 short contacts:

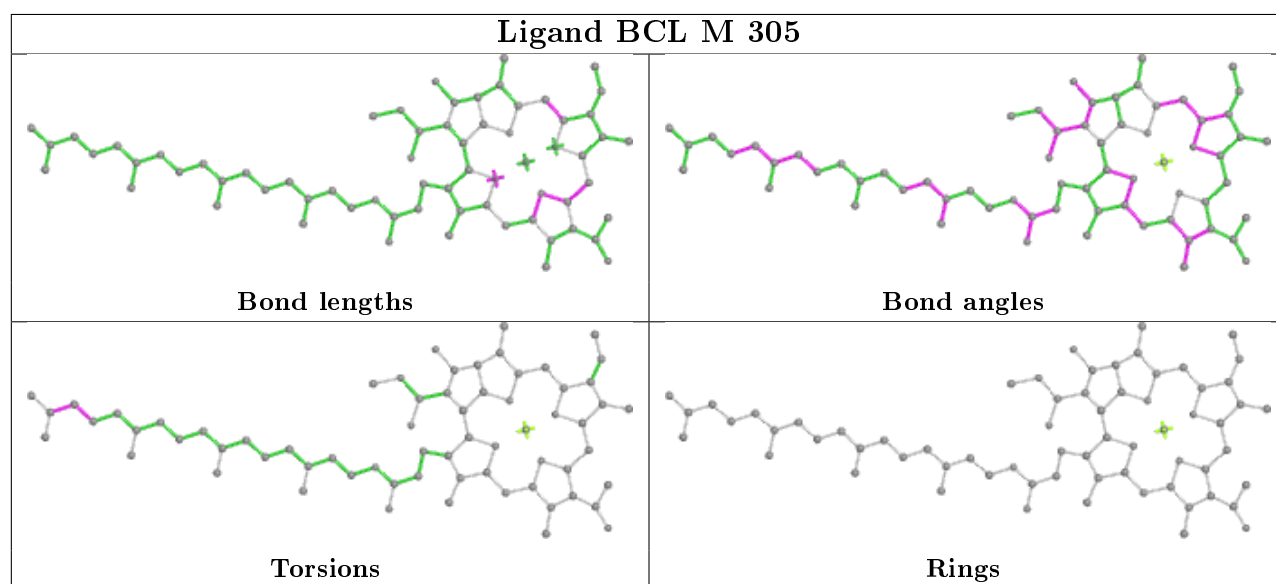
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	305	BCL	2	0
4	H	702	LDA	3	0
8	L	900	DIO	2	0
4	M	701	LDA	1	0
4	H	704	LDA	2	0
7	L	502	U10	5	0
4	M	705	LDA	1	0
6	M	401	BPH	5	0
10	M	600	SPN	6	0
5	L	302	BCL	4	0
7	M	501	U10	1	0

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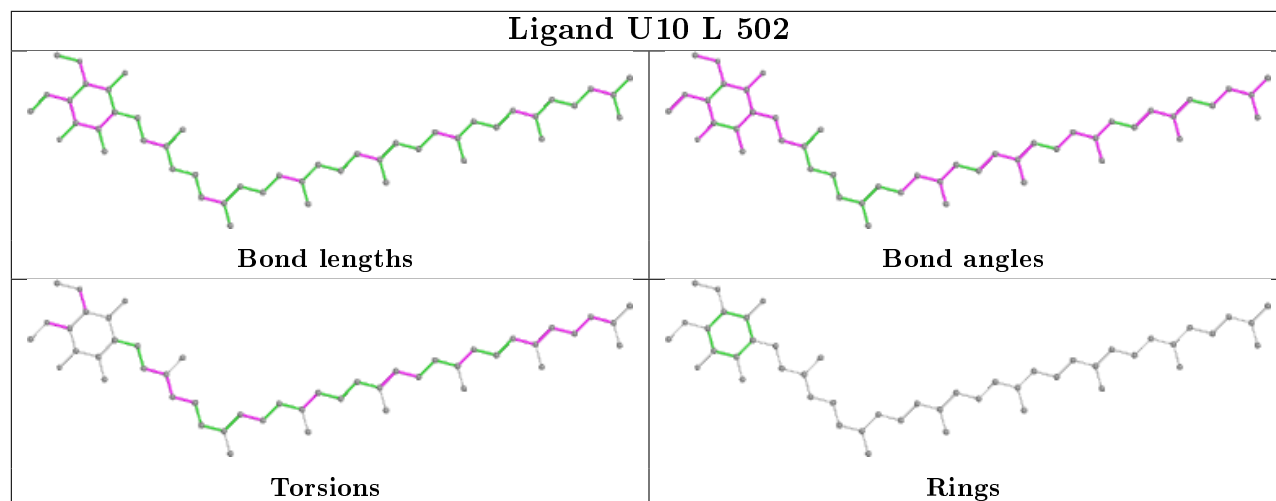
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	304	BCL	5	0
5	M	303	BCL	7	0
6	L	402	BPH	6	0
4	M	703	LDA	1	0

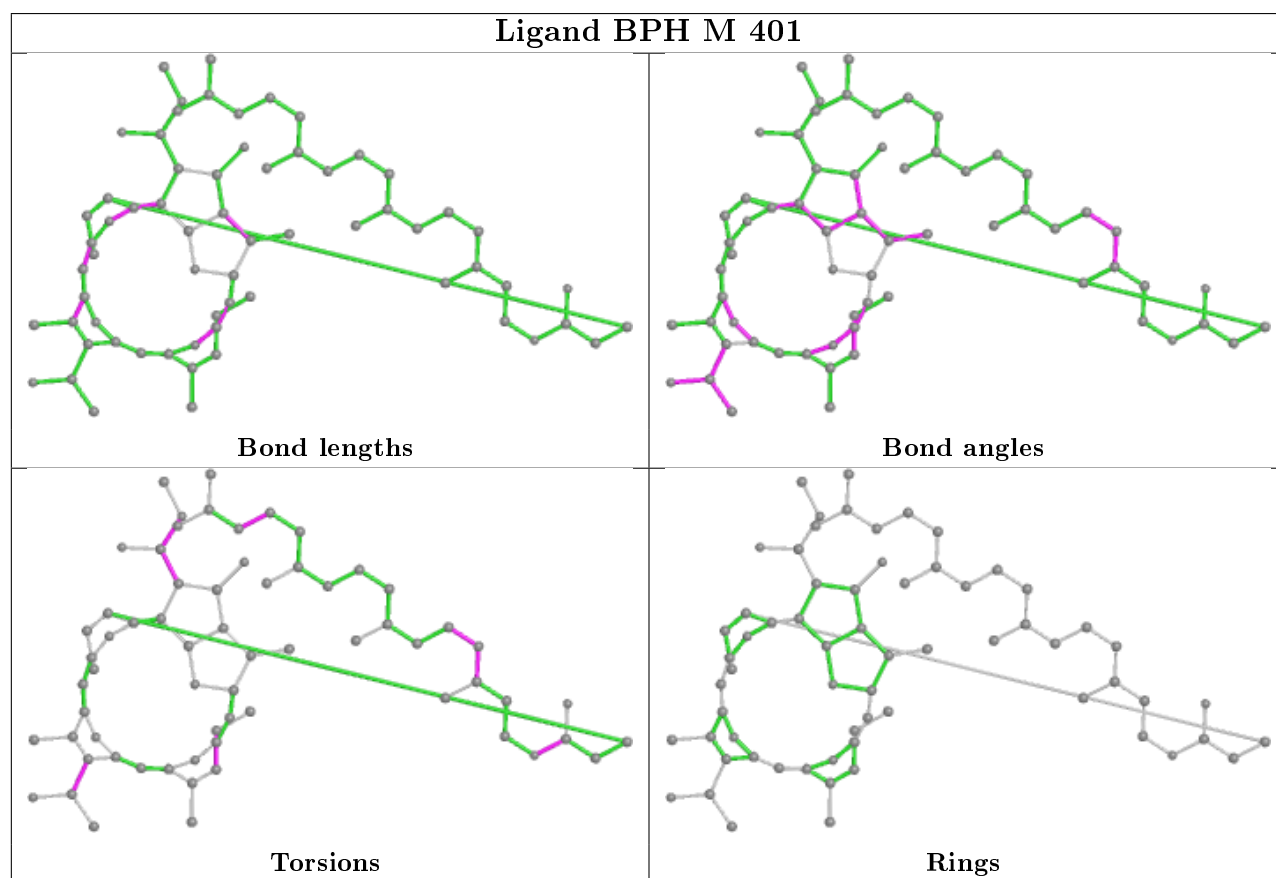
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

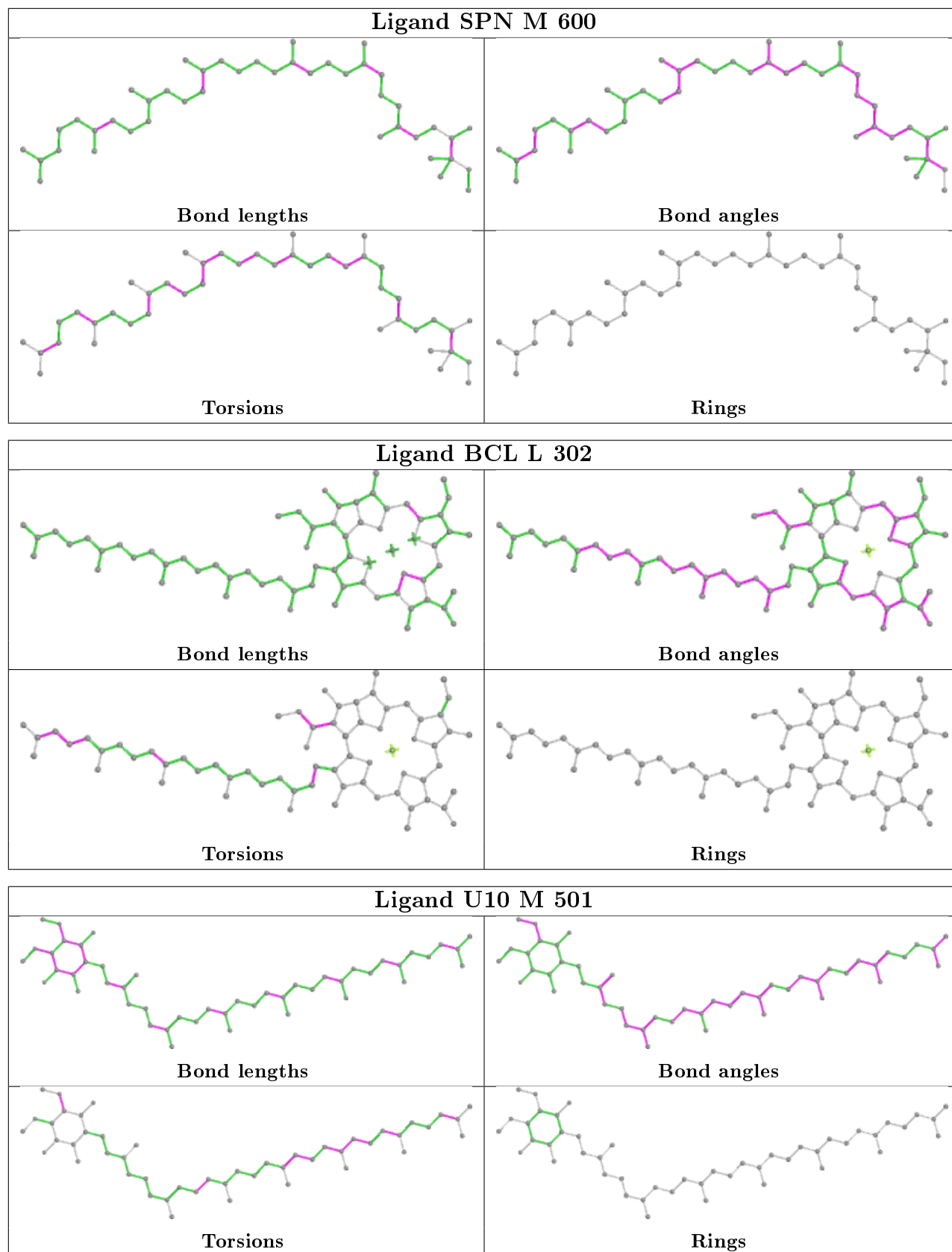


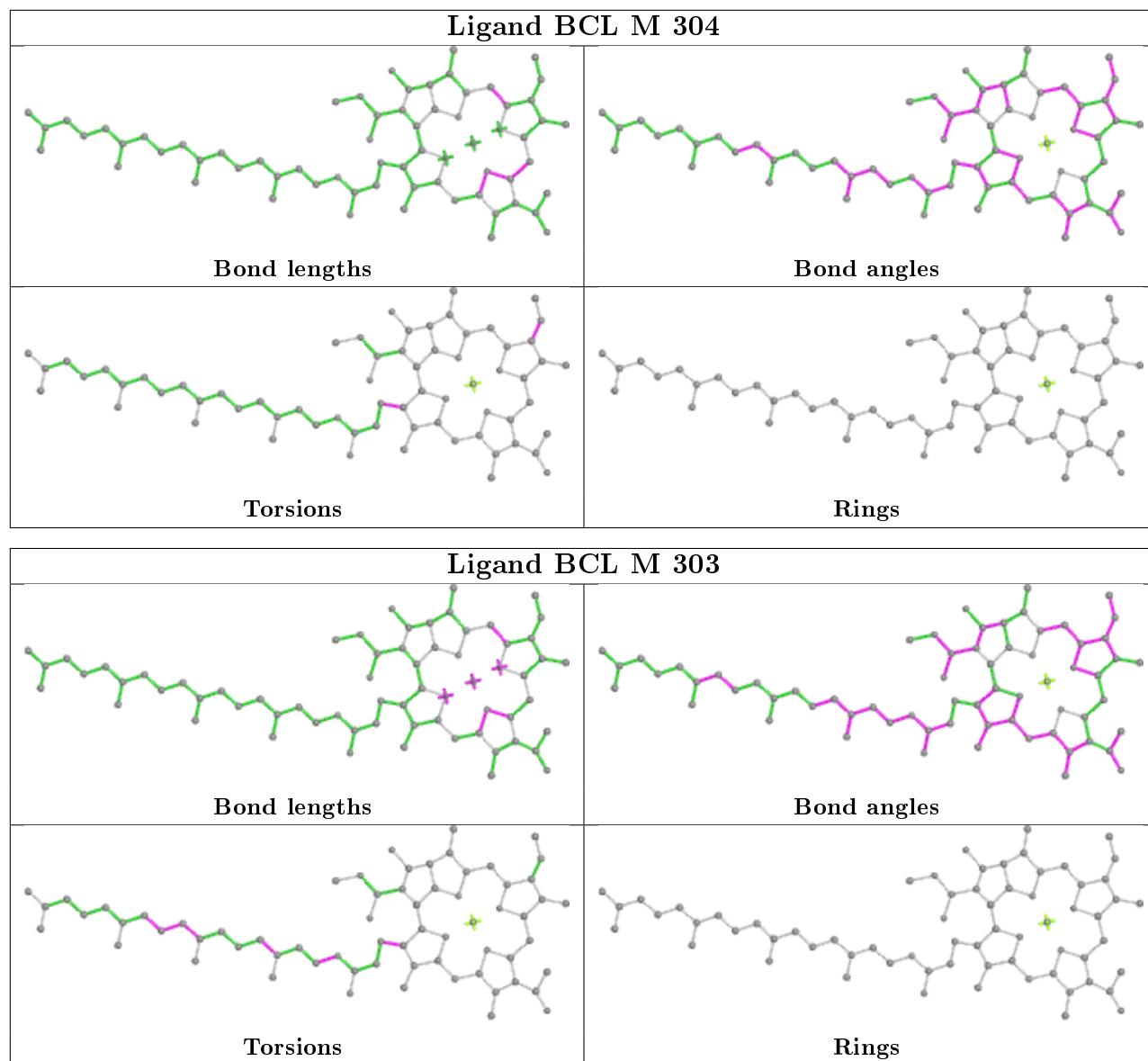
Ligand U10 L 502

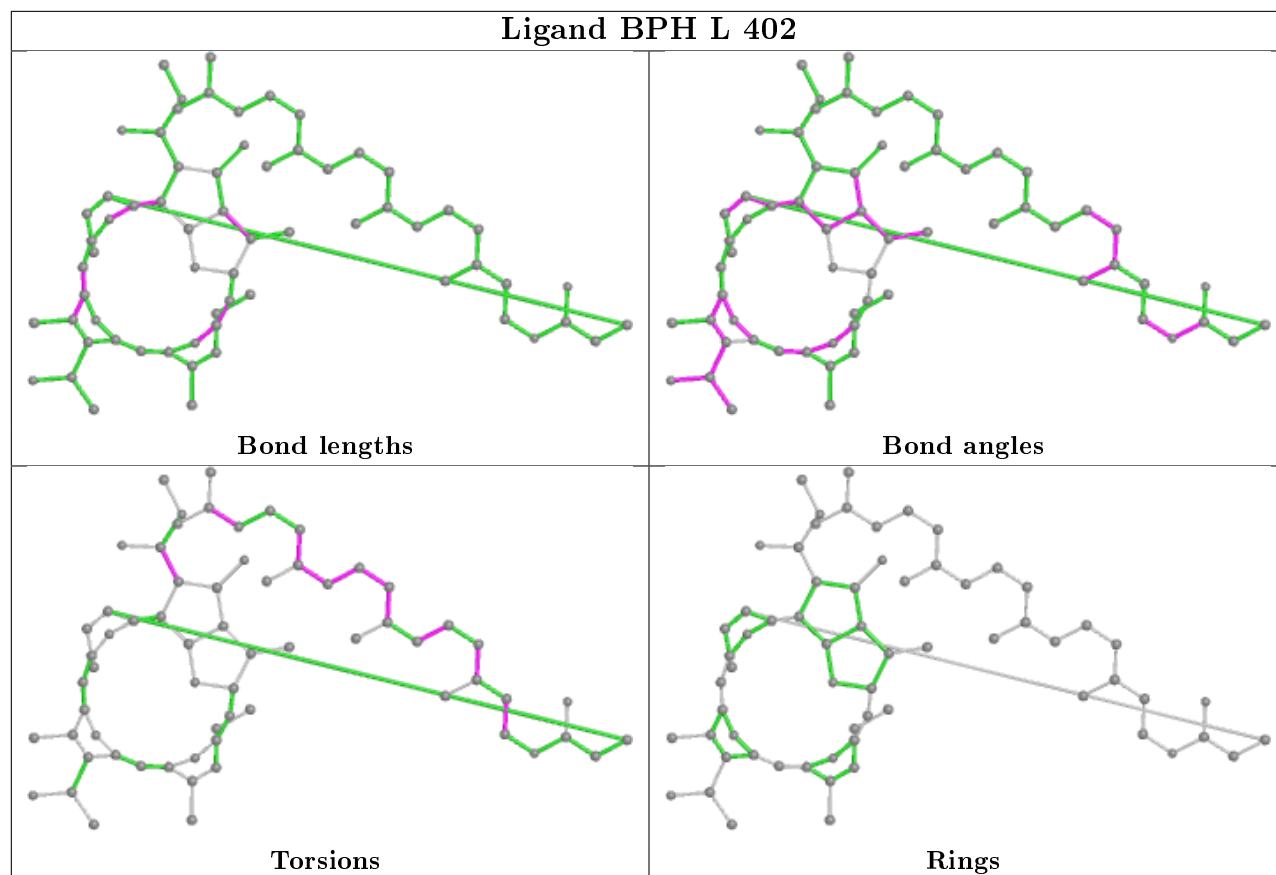


Ligand BPH M 401









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	241/241 (100%)	-0.45	4 (1%) 70 63	19, 35, 54, 102	0
2	L	281/281 (100%)	-0.46	2 (0%) 87 84	20, 36, 70, 94	0
3	M	302/302 (100%)	-0.64	0 100 100	21, 39, 65, 82	0
All	All	824/824 (100%)	-0.52	6 (0%) 87 84	19, 36, 65, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.3
1	H	10	PHE	3.8
2	L	59	TRP	3.1
1	H	245	ALA	2.6
1	H	246	PRO	2.3
2	L	281	GLY	2.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

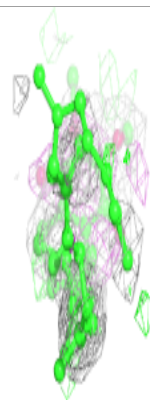
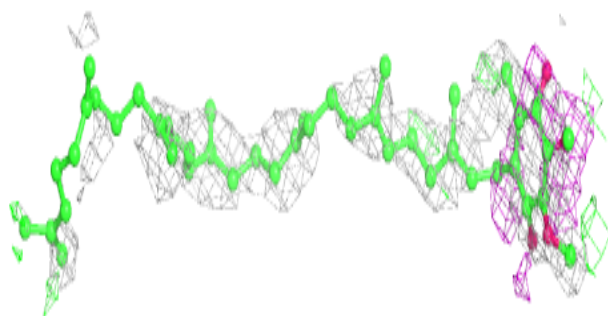
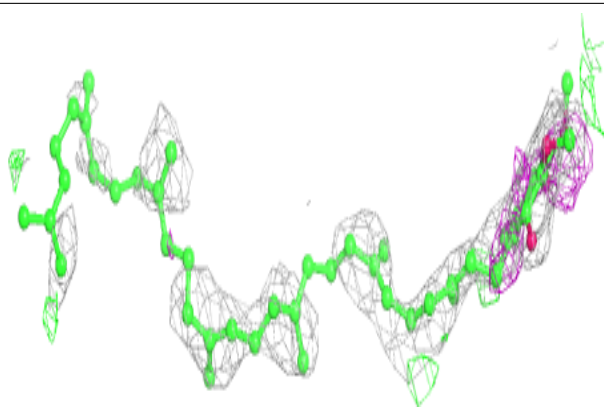
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LDA	M	707	16/16	0.73	0.29	42,59,91,96	0
11	PO4	M	801	5/5	0.73	0.28	54,68,85,101	0
7	U10	L	502	48/63	0.74	0.48	31,64,107,115	0
4	LDA	M	708	16/16	0.76	0.32	35,64,90,93	0
4	LDA	H	704	16/16	0.83	0.36	40,50,73,75	0
4	LDA	M	705	16/16	0.85	0.41	36,50,81,81	0
8	DIO	M	902	6/6	0.85	0.56	45,53,62,68	0
4	LDA	H	709	16/16	0.87	0.37	32,57,87,89	0
4	LDA	M	703	16/16	0.87	0.29	38,49,69,73	0
4	LDA	M	701	16/16	0.88	0.21	21,41,51,55	0
10	SPN	M	600	43/43	0.90	0.21	29,49,77,87	0
4	LDA	H	702	16/16	0.90	0.22	46,59,70,73	0
8	DIO	L	901	6/6	0.90	0.26	46,48,53,58	0
8	DIO	L	900	6/6	0.91	0.33	51,55,63,70	0
6	BPH	M	401	65/65	0.92	0.17	23,32,93,104	0
11	PO4	M	803	5/5	0.94	0.14	66,72,79,87	0
5	BCL	M	303	66/66	0.94	0.17	20,29,53,63	0
7	U10	M	501	48/63	0.94	0.17	19,30,50,61	0
5	BCL	L	302	66/66	0.94	0.16	21,29,38,55	0
5	BCL	M	305	66/66	0.95	0.13	21,26,38,52	0
12	CL	M	306	1/1	0.95	0.09	50,50,50,50	0
5	BCL	M	304	66/66	0.96	0.14	22,30,43,60	0
6	BPH	L	402	65/65	0.96	0.15	14,28,39,42	0
11	PO4	M	800	5/5	0.98	0.07	24,33,44,47	0
9	FE	M	500	1/1	0.99	0.11	24,24,24,24	0

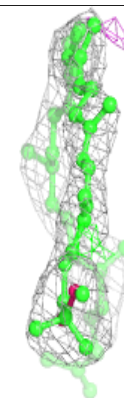
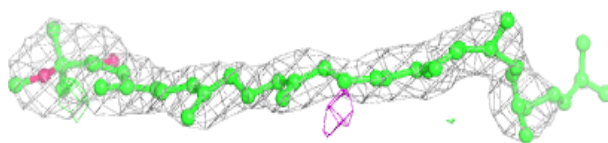
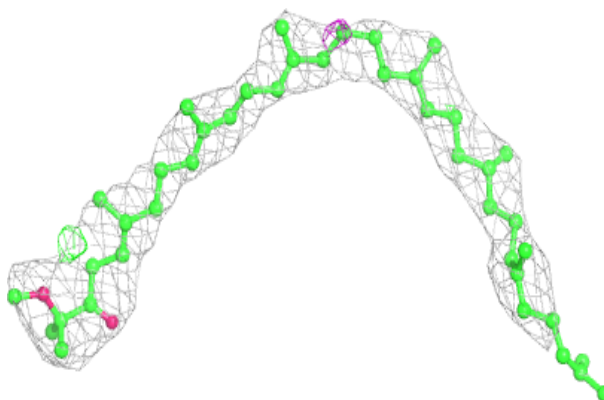
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U10 L 502:

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

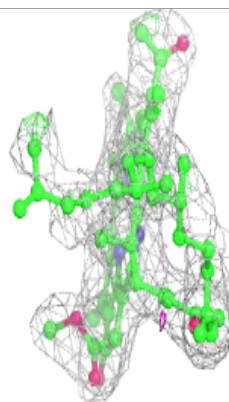
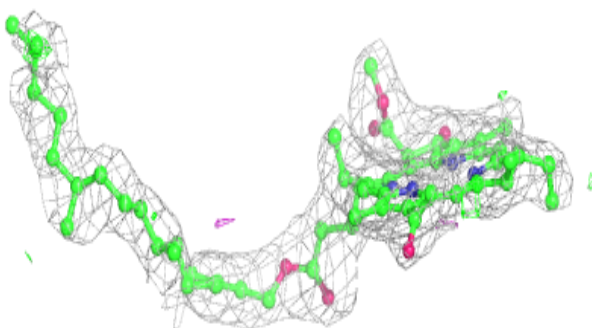
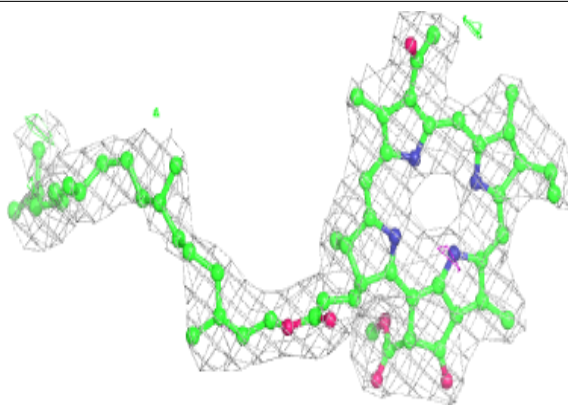
**Electron density around SPN M 600:**

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

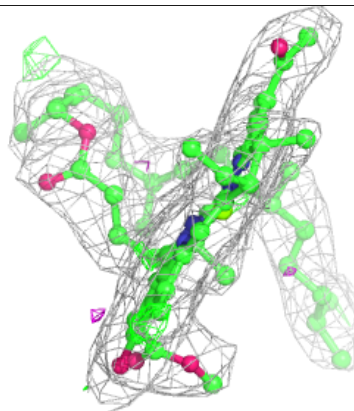
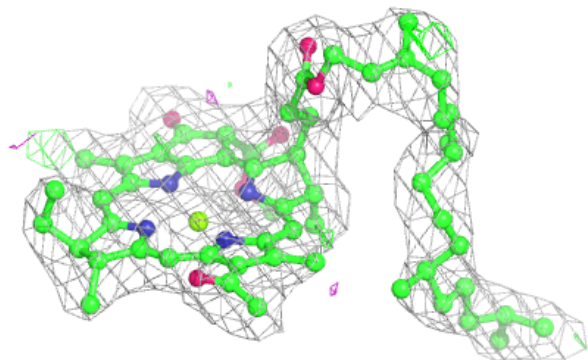
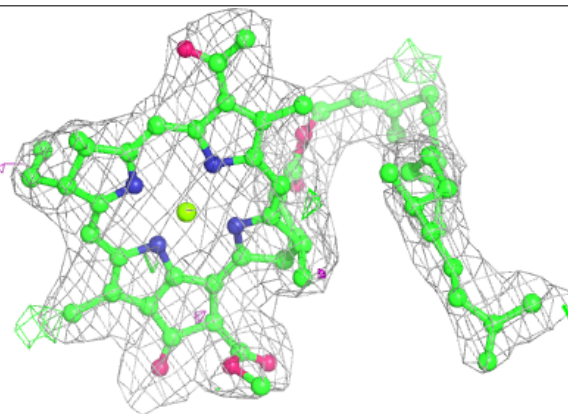


Electron density around BPH M 401:

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

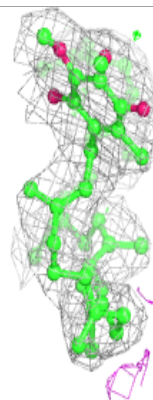
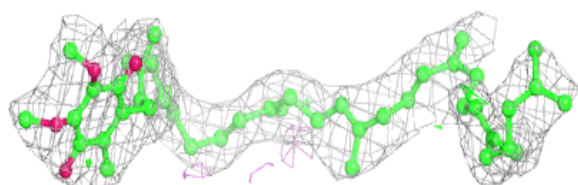
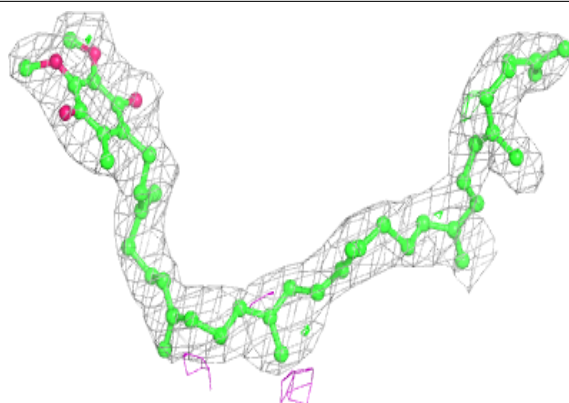
**Electron density around BCL M 303:**

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

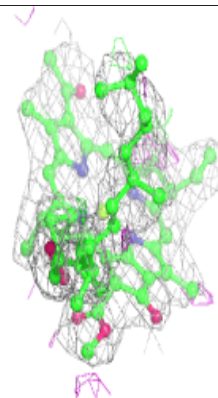
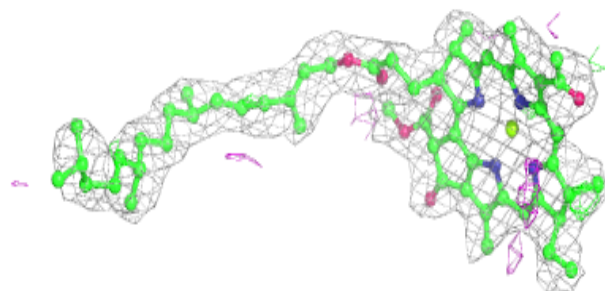
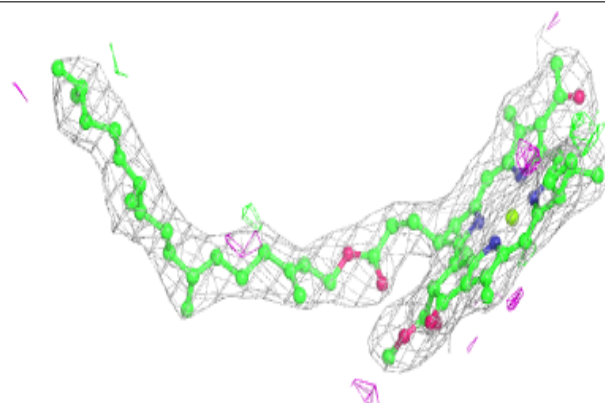


Electron density around U10 M 501:

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

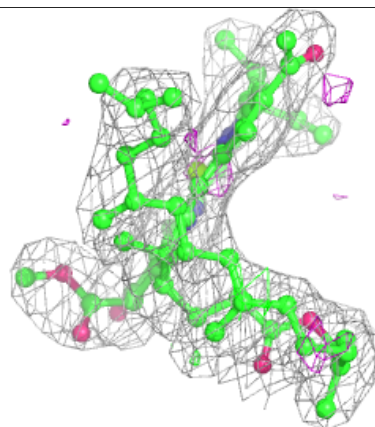
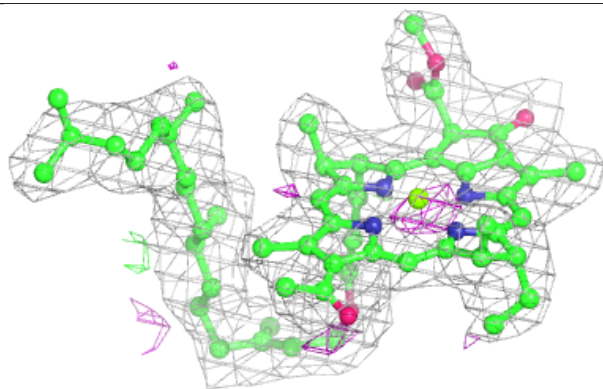
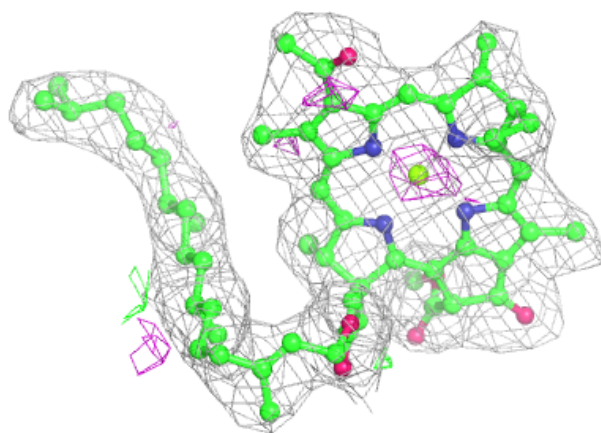
**Electron density around BCL L 302:**

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

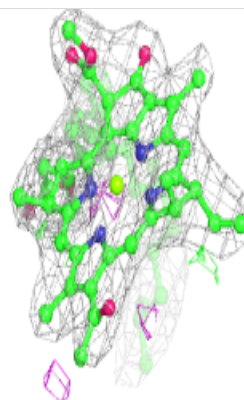
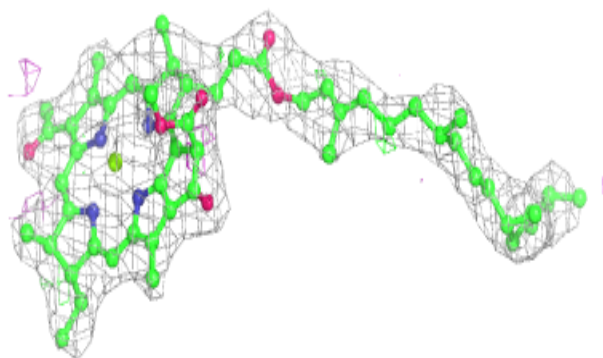
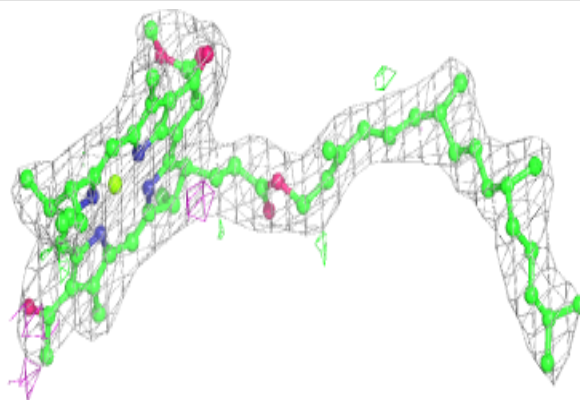


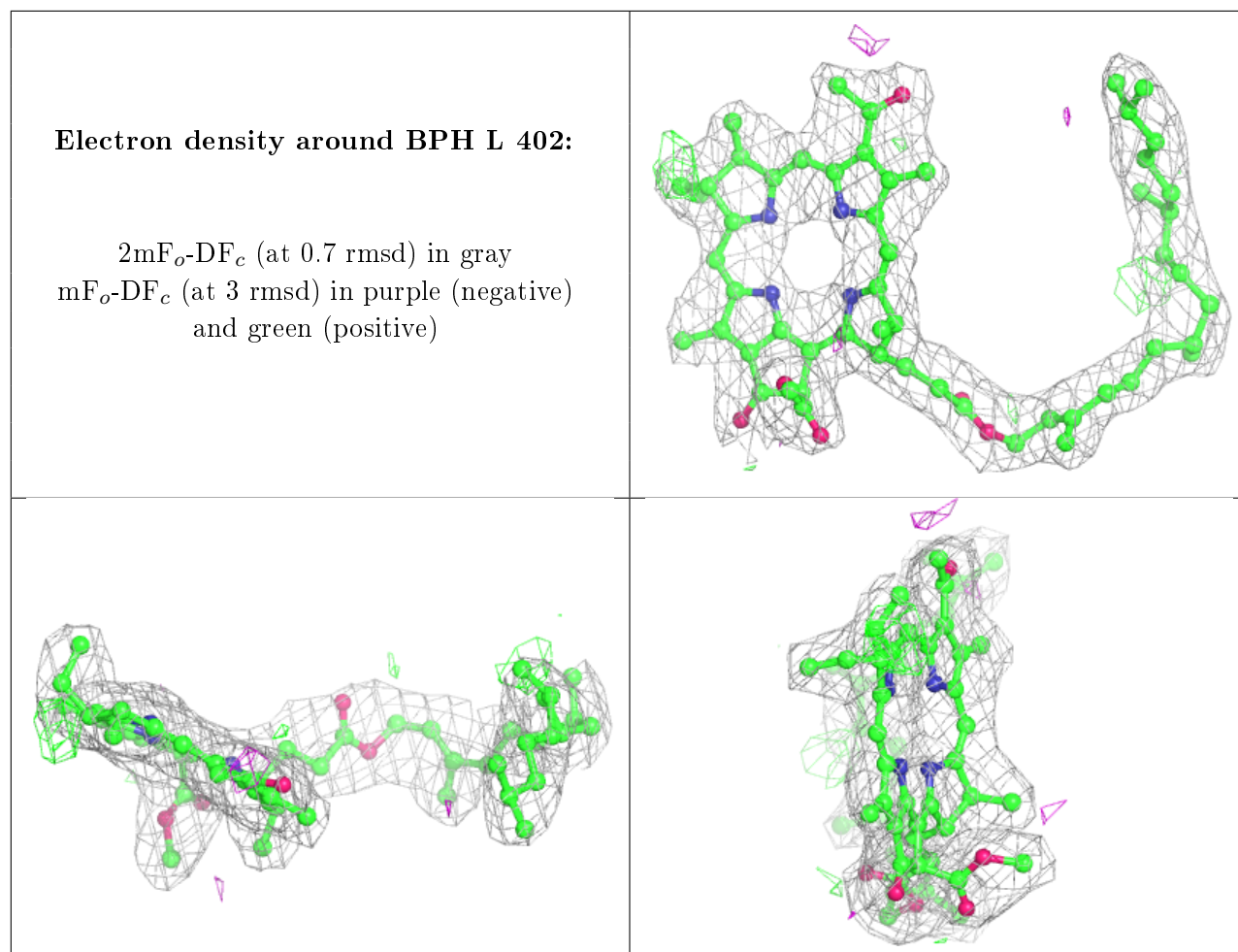
Electron density around BCL M 305:

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

**Electron density around BCL M 304:**

$2mF_o-DF_c$ (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.