



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:41 am BST

PDB ID : 1RGN
Title : Structure of the reaction centre from Rhodobacter sphaeroides carotenoidless strain R-26.1 reconstituted with spheroidene
Authors : Roszak, A.W.; Frank, H.A.; McKendrick, K.; Mitchell, I.A.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2003-11-12
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

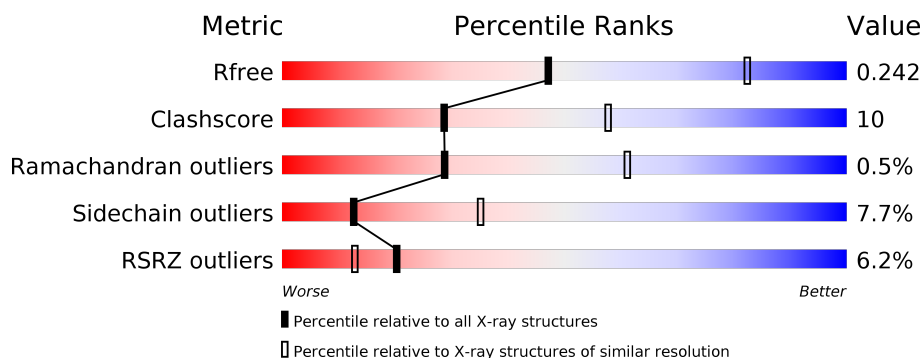
1 Overall quality at a glance

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	L	281	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
2	M	307	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>.</div> </div> </div>
3	H	260	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>5%</div> <div>8%</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	U10	L	502	-	-	-	X
7	LDA	L	904	-	-	-	X
7	LDA	M	906	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7289 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 L chain.

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

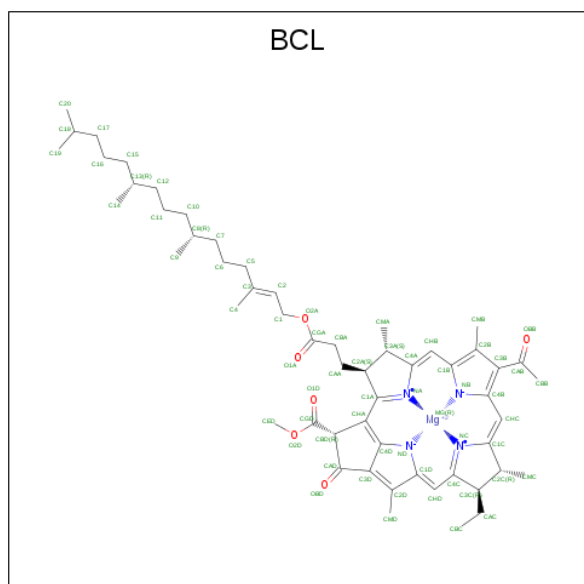
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	1	0
			2412	1609	394	399	10			

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

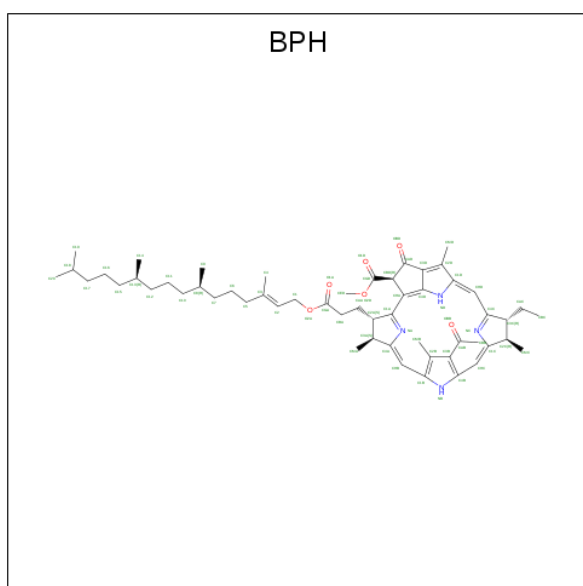
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	2	0
			1838	1173	318	338	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



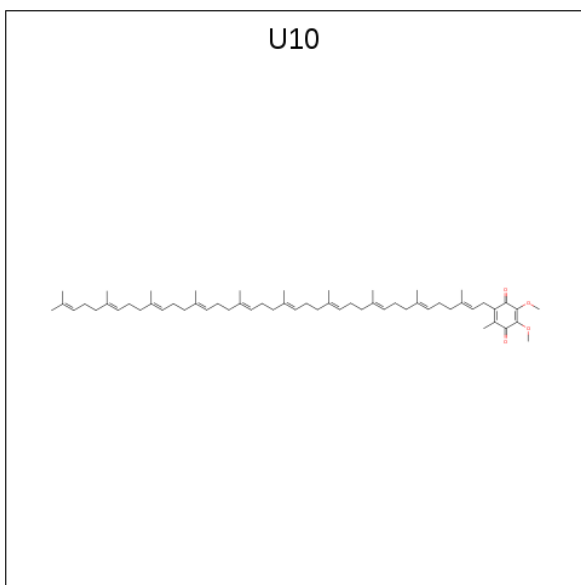
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



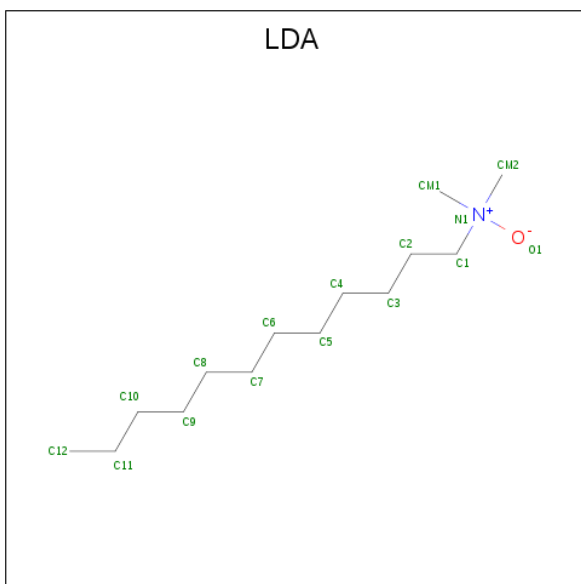
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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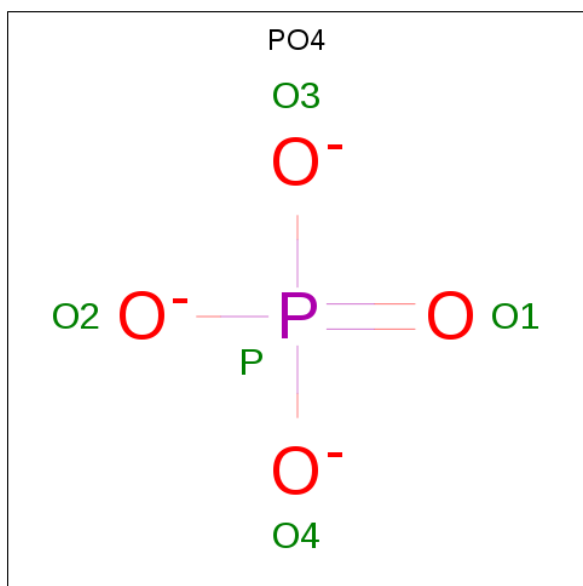
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

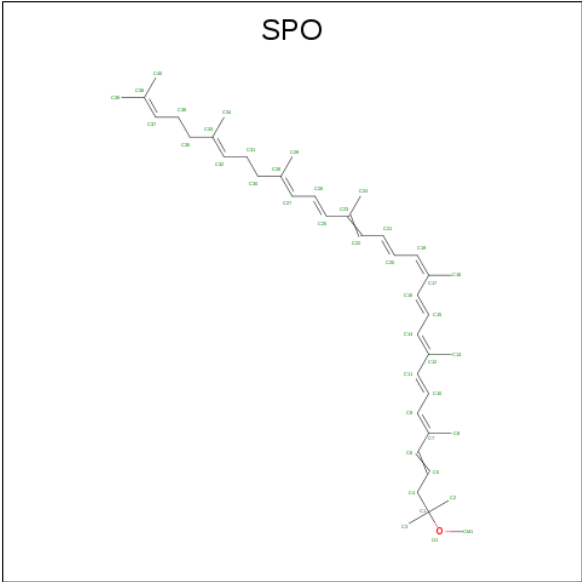
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



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

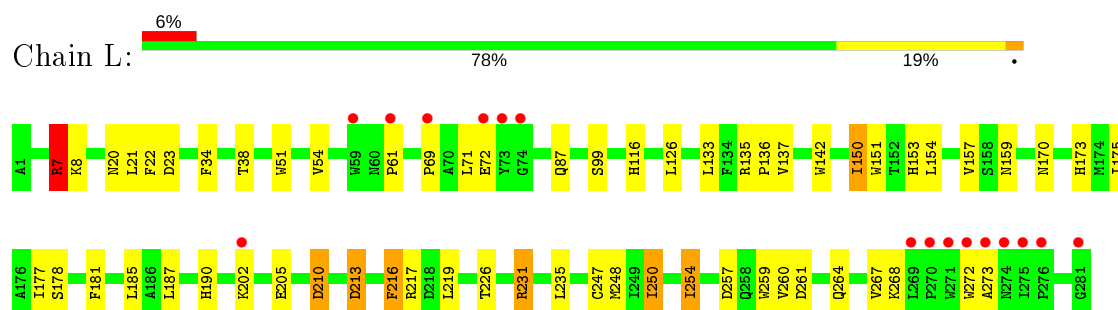
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	41	Total	O	0	0
			41	41		
11	M	52	Total	O	0	0
			52	52		
11	H	80	Total	O	0	0
			80	80		

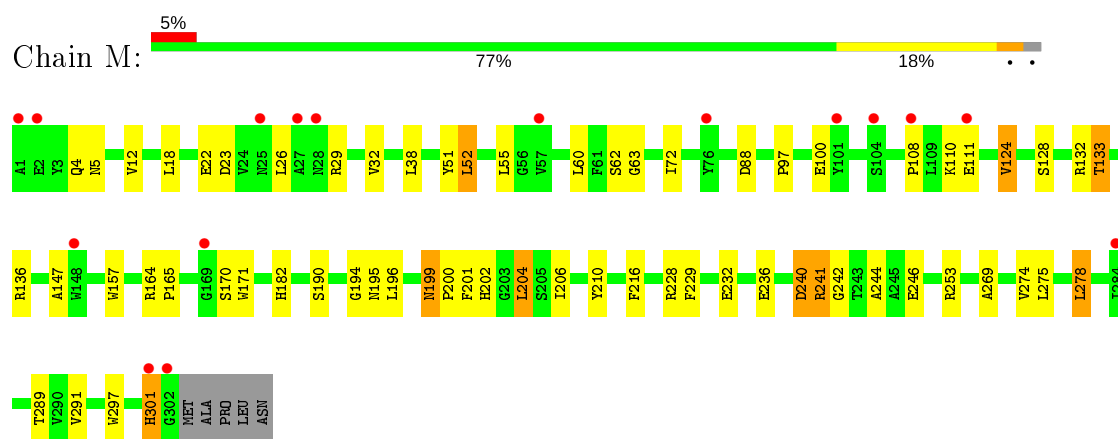
3 Residue-property plots [i](#)

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.

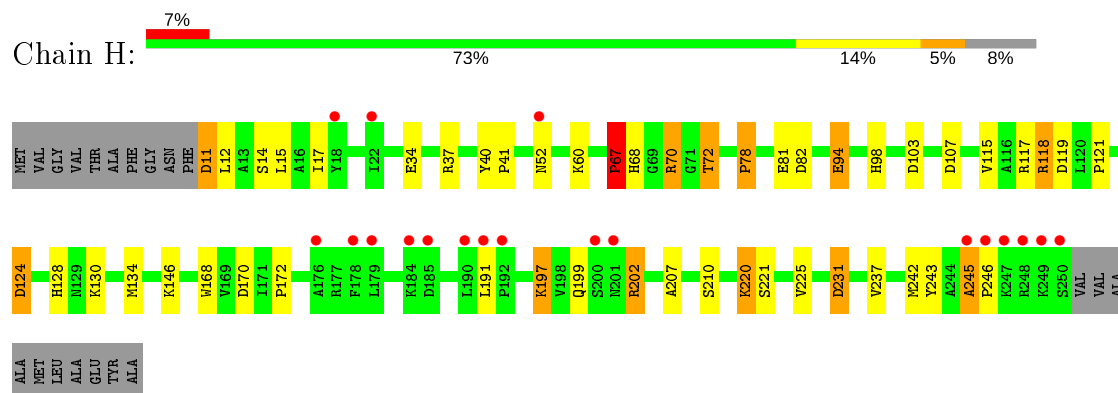
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.82Å 139.82Å 184.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.00 – 2.80 24.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (24.00-2.80) 88.2 (24.01-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.189 , 0.232 0.199 , 0.242	Depositor DCC
R_{free} test set	2277 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, BPH, PO4, FE, SPO, 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	L	0.84	0/2320	0.87	7/3175 (0.2%)
2	M	0.87	1/2509 (0.0%)	0.89	5/3425 (0.1%)
3	H	0.91	0/1896	1.00	8/2578 (0.3%)
All	All	0.87	1/6725 (0.0%)	0.91	20/9178 (0.2%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	22	GLU	CB-CG	5.43	1.62	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	231	ASP	CB-CG-OD2	9.22	126.60	118.30
1	L	213	ASP	CB-CG-OD2	8.26	125.73	118.30
1	L	7	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	M	240	ASP	CB-CG-OD1	6.69	124.32	118.30
2	M	29	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	M	23	ASP	CB-CG-OD2	6.51	124.16	118.30
3	H	82	ASP	CB-CG-OD2	6.51	124.16	118.30
3	H	103	ASP	CB-CG-OD1	6.51	124.16	118.30
2	M	241	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	231	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	M	88	ASP	CB-CG-OD2	5.57	123.31	118.30
3	H	119	ASP	CB-CG-OD2	5.42	123.18	118.30
3	H	124	ASP	CB-CG-OD1	5.31	123.08	118.30
1	L	231	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	L	7	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	H	202	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	L	261	ASP	CB-CG-OD2	5.14	122.92	118.30
3	H	107	ASP	CB-CG-OD2	5.08	122.87	118.30
1	L	235	LEU	CB-CG-CD1	-5.07	102.37	111.00
3	H	11	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	67	PRO	Peptide

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	L	2232	0	2187	45	0
2	M	2412	0	2323	45	0
3	H	1838	0	1847	32	0
4	L	132	0	148	9	0
4	M	132	0	148	7	0
5	L	65	0	75	4	0
5	M	65	0	76	8	0
6	L	48	0	63	10	0
6	M	48	0	63	0	0
7	H	16	0	31	2	0
7	L	16	0	31	0	0
7	M	64	0	124	6	0
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	80	0	0	9	0
11	L	41	0	0	3	0
11	M	52	0	0	2	0
All	All	7289	0	7176	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (138) 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:401:BPH:H4C1	5:M:401:BPH:H7C1	1.60	0.84
5:L:402:BPH:HH C	5:L:402:BPH:HBB3	1.64	0.79
1:L:7:ARG:HH11	3:H:98:HIS:CD2	2.02	0.77
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.70	0.73
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.73	0.70
1:L:21:LEU:HD23	1:L:22:PHE:CE1	2.28	0.68
1:L:216:PHE:CD2	6:L:502:U10:H102	2.28	0.68
2:M:199:ASN:HD22	2:M:199:ASN:C	1.96	0.68
2:M:51:TYR:O	2:M:132:ARG:NH2	2.26	0.67
3:H:220:LYS:HD2	11:H:935:HOH:O	1.93	0.67
1:L:175:ILE:HD11	6:L:502:U10:H402	1.77	0.67
1:L:34:PHE:O	1:L:38:THR:HG23	1.95	0.66
1:L:8:LYS:NZ	3:H:81:GLU:OE2	2.28	0.65
2:M:275:LEU:HD23	2:M:278:LEU:HD22	1.79	0.64
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.80	0.61
3:H:34:GLU:O	3:H:37:ARG:HG3	2.00	0.61
3:H:146:LYS:NZ	11:H:973:HOH:O	2.33	0.60
1:L:150:ILE:HG22	1:L:151:TRP:CD1	2.36	0.60
5:M:401:BPH:H4C1	5:M:401:BPH:C7	2.31	0.60
1:L:231:ARG:HD3	2:M:5:ASN:O	2.01	0.60
4:M:908:BCL:HMB1	4:M:908:BCL:HBB2	1.82	0.60
4:L:304:BCL:HBB3	5:L:402:BPH:H141	1.84	0.60
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.84	0.60
1:L:219:LEU:O	2:M:132:ARG:NH1	2.35	0.59
1:L:71:LEU:H	1:L:71:LEU:HD12	1.68	0.58
3:H:207:ALA:HB1	3:H:237:VAL:O	2.04	0.58
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.03	0.58
3:H:70:ARG:NH2	3:H:121:PRO:O	2.36	0.58
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.34	0.57
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:HIS:HA	6:L:502:U10:O2	2.04	0.56
1:L:116:HIS:HE1	2:M:4:GLN:O	1.88	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.87	0.56
2:M:157:TRP:CE2	10:M:600:SPO:H293	2.41	0.55
4:L:302:BCL:HMB1	4:L:302:BCL:HBB3	1.89	0.55
2:M:297:TRP:O	2:M:301:HIS:N	2.41	0.54
2:M:38:LEU:CD1	7:M:905:LDA:HM21	2.38	0.54
6:L:502:U10:H351	6:L:502:U10:H38	1.89	0.54
5:M:401:BPH:HHC	5:M:401:BPH:HBB3	1.90	0.53
5:M:401:BPH:C4	5:M:401:BPH:H7C1	2.35	0.53
1:L:250:ILE:HB	1:L:254:ILE:HD12	1.90	0.52
4:L:304:BCL:HMB1	4:L:304:BCL:HBB2	1.92	0.52
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.45	0.52
3:H:14:SER:HA	3:H:17:ILE:HG22	1.91	0.52
7:M:903:LDA:CM1	7:H:901:LDA:H31	2.40	0.52
4:L:304:BCL:HBA1	4:L:304:BCL:C4A	2.40	0.52
1:L:259:TRP:O	1:L:260:VAL:C	2.48	0.51
1:L:226:THR:HG22	6:L:502:U10:H3M2	1.92	0.51
2:M:289:THR:O	7:M:906:LDA:HM11	2.10	0.51
3:H:115:VAL:HG22	3:H:117:ARG:HG2	1.92	0.51
2:M:38:LEU:HD12	7:M:905:LDA:HM21	1.93	0.51
3:H:124:ASP:OD2	3:H:128:HIS:HB2	2.10	0.51
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.91	0.51
2:M:194:GLY:O	2:M:195:ASN:HB3	2.11	0.50
3:H:197:LYS:HG2	3:H:199:GLN:HE21	1.76	0.50
3:H:70:ARG:HG2	3:H:118[A]:ARG:NH1	2.26	0.50
4:M:908:BCL:CBB	4:M:908:BCL:HMB1	2.41	0.50
4:L:302:BCL:CBB	4:L:302:BCL:HMB1	2.42	0.50
4:L:302:BCL:CGA	4:L:304:BCL:HBC1	2.41	0.50
2:M:297:TRP:O	2:M:301:HIS:HA	2.11	0.50
4:M:908:BCL:H122	4:M:908:BCL:H91	1.93	0.50
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.46	0.49
3:H:98:HIS:HE1	11:H:909:HOH:O	1.96	0.49
1:L:154:LEU:HD21	4:L:304:BCL:HED2	1.94	0.49
3:H:37:ARG:NH2	3:H:60:LYS:O	2.45	0.49
1:L:72:GLU:H	1:L:72:GLU:CD	2.16	0.49
2:M:124:VAL:O	2:M:128:SER:OG	2.21	0.49
1:L:23:ASP:O	11:L:940:HOH:O	2.20	0.48
3:H:72:THR:HG22	11:H:939:HOH:O	2.13	0.48
3:H:242:MET:HE2	3:H:243:TYR:CZ	2.49	0.48
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:THR:HG22	1:L:99:SER:CB	2.44	0.47
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.96	0.47
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.77	0.47
2:M:63:GLY:HA3	5:M:401:BPH:H5C1	1.96	0.47
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.50	0.47
4:M:908:BCL:C12	4:M:908:BCL:H91	2.45	0.47
2:M:199:ASN:HD21	2:M:201:PHE:HB2	1.80	0.47
1:L:181:PHE:HB3	5:M:401:BPH:HBB2	1.97	0.46
1:L:268:LYS:O	1:L:273:ALA:HB2	2.15	0.46
2:M:199:ASN:HD22	2:M:200:PRO:N	2.13	0.46
1:L:153:HIS:O	1:L:157:VAL:HG23	2.15	0.46
1:L:210:ASP:OD1	1:L:210:ASP:N	2.48	0.46
1:L:51:TRP:O	1:L:54:VAL:HG22	2.16	0.46
2:M:240:ASP:OD2	3:H:118[A]:ARG:HB2	2.16	0.45
3:H:220:LYS:CD	11:H:935:HOH:O	2.56	0.45
4:L:302:BCL:NA	4:M:909:BCL:HBB2	2.31	0.45
1:L:38:THR:HG22	1:L:99:SER:HB2	1.98	0.45
3:H:245:ALA:HB3	3:H:246:PRO:CD	2.47	0.45
1:L:133:LEU:O	1:L:137:VAL:HG23	2.17	0.45
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.99	0.45
3:H:94:GLU:HG2	11:H:965:HOH:O	2.17	0.44
3:H:72:THR:CG2	11:H:939:HOH:O	2.65	0.44
2:M:199:ASN:ND2	2:M:201:PHE:N	2.65	0.44
2:M:232:GLU:CD	11:M:959:HOH:O	2.56	0.44
2:M:133:THR:CG2	2:M:147:ALA:HA	2.48	0.44
2:M:206:ILE:HG12	4:M:909:BCL:HMB3	1.99	0.44
2:M:236:GLU:HB3	11:H:943:HOH:O	2.18	0.44
1:L:250:ILE:HB	1:L:254:ILE:CD1	2.48	0.43
6:L:502:U10:H202	7:M:905:LDA:H72	1.99	0.43
3:H:220:LYS:HE3	11:H:923:HOH:O	2.17	0.43
1:L:213:ASP:O	1:L:217:ARG:HG3	2.18	0.43
2:M:199:ASN:ND2	2:M:201:PHE:H	2.16	0.43
3:H:130:LYS:NZ	3:H:172:PRO:HG2	2.34	0.43
1:L:178:SER:HB3	6:L:502:U10:H272	1.99	0.43
2:M:108:PRO:O	2:M:110:LYS:O	2.37	0.43
1:L:257:ASP:HB3	11:L:936:HOH:O	2.18	0.43
1:L:216:PHE:HD2	6:L:502:U10:H102	1.80	0.43
3:H:40:TYR:HA	3:H:41:PRO:C	2.39	0.43
4:L:302:BCL:HHC	4:L:302:BCL:OBB	2.19	0.43
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.54	0.43
2:M:133:THR:HG21	2:M:147:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:199:ASN:ND2	2:M:199:ASN:C	2.68	0.42
3:H:130:LYS:HZ2	3:H:172:PRO:HG2	1.84	0.42
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.87	0.42
2:M:199:ASN:HD22	2:M:201:PHE:N	2.18	0.42
1:L:187:LEU:HD11	2:M:269:ALA:HB1	2.01	0.42
6:L:502:U10:H351	6:L:502:U10:C38	2.50	0.42
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.55	0.42
4:M:908:BCL:H62	4:M:909:BCL:H202	2.02	0.42
5:L:402:BPH:HH C	5:L:402:BPH:CBB	2.42	0.42
2:M:190:SER:HA	2:M:196:LEU:HD13	2.02	0.42
1:L:135:ARG:HD2	1:L:248:MET:O	2.20	0.41
7:H:901:LDA:HM13	7:H:901:LDA:H21	1.89	0.41
2:M:204:LEU:HD13	7:M:902:LDA:H12	2.02	0.41
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.50	0.41
2:M:291:VAL:HG13	2:M:297:TRP:HB2	2.01	0.41
1:L:61:PRO:O	1:L:150:ILE:HD13	2.21	0.41
5:M:401:BPH:H3A	5:M:401:BPH:HBA2	1.85	0.41
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.21	0.41
1:L:226:THR:HB	11:M:952:HOH:O	2.21	0.41
2:M:52:LEU:HD22	2:M:52:LEU:HA	1.98	0.41
6:L:502:U10:C33	6:L:502:U10:H301	2.50	0.41
1:L:170:ASN:HB2	1:L:259:TRP:CD1	2.56	0.40
2:M:110:LYS:C	2:M:111:GLU:HG3	2.41	0.40
1:L:159:ASN:ND2	11:L:931:HOH:O	2.54	0.40
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	L	279/281 (99%)	264 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	301/307 (98%)	283 (94%)	17 (6%)	1 (0%)	41	72
3	H	240/260 (92%)	221 (92%)	16 (7%)	3 (1%)	12	36
All	All	820/848 (97%)	768 (94%)	48 (6%)	4 (0%)	29	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	301	HIS
3	H	67	PRO
3	H	78	PRO

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	L	220/220 (100%)	207 (94%)	13 (6%)	19	49
2	M	237/240 (99%)	216 (91%)	21 (9%)	9	28
3	H	197/208 (95%)	179 (91%)	18 (9%)	9	27
All	All	654/668 (98%)	602 (92%)	52 (8%)	13	34

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

Mol	Chain	Res	Type
1	L	7	ARG
1	L	20	ASN
1	L	126	LEU
1	L	150	ILE
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS

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Mol	Chain	Res	Type
1	L	250	ILE
1	L	254	ILE
1	L	272	TRP
2	M	12	VAL
2	M	18	LEU
2	M	26	LEU
2	M	32	VAL
2	M	52	LEU
2	M	55	LEU
2	M	60	LEU
2	M	62	SER
2	M	72	ILE
2	M	100	GLU
2	M	124	VAL
2	M	133	THR
2	M	136	ARG
2	M	170	SER
2	M	182	HIS
2	M	199	ASN
2	M	204	LEU
2	M	216	PHE
2	M	253	ARG
2	M	274	VAL
2	M	278	LEU
3	H	11	ASP
3	H	12	LEU
3	H	15	LEU
3	H	52[A]	ASN
3	H	52[B]	ASN
3	H	70	ARG
3	H	72	THR
3	H	78	PRO
3	H	94	GLU
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	134	MET
3	H	191	LEU
3	H	197	LYS
3	H	210	SER
3	H	220	LYS
3	H	221	SER
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	116	HIS
1	L	159	ASN
2	M	199	ASN
3	H	68	HIS
3	H	98	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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$
4	BCL	M	908	2	58,74,74	1.50	5 (8%)	69,115,115	1.54	15 (21%)
7	LDA	H	901	-	12,15,15	1.74	1 (8%)	14,17,17	0.82	0
6	U10	L	502	-	48,48,63	1.13	3 (6%)	58,61,79	1.51	10 (17%)
7	LDA	M	905	-	12,15,15	2.02	1 (8%)	14,17,17	0.77	0
4	BCL	M	909	2	58,74,74	1.49	3 (5%)	69,115,115	1.44	11 (15%)
6	U10	M	501	-	48,48,63	1.12	4 (8%)	58,61,79	1.70	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PO4	M	907	-	4,4,4	0.84	0	6,6,6	1.04	0
7	LDA	M	902	-	12,15,15	2.04	1 (8%)	14,17,17	0.73	1 (7%)
7	LDA	L	904	-	12,15,15	1.96	1 (8%)	14,17,17	0.56	0
7	LDA	M	903	-	12,15,15	2.11	1 (8%)	14,17,17	0.60	0
7	LDA	M	906	-	12,15,15	2.18	1 (8%)	14,17,17	0.73	1 (7%)
4	BCL	L	304	1	58,74,74	1.17	5 (8%)	69,115,115	2.53	18 (26%)
10	SPO	M	600	-	40,41,41	1.09	1 (2%)	47,50,50	1.56	9 (19%)
5	BPH	L	402	-	64,70,70	0.98	4 (6%)	76,101,101	1.36	8 (10%)
5	BPH	M	401	-	64,70,70	0.81	1 (1%)	76,101,101	1.49	12 (15%)
4	BCL	L	302	1	58,74,74	1.56	3 (5%)	69,115,115	1.56	14 (20%)

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
4	BCL	M	908	2	-	6/37/137/137	-
7	LDA	H	901	-	-	10/13/13/13	-
6	U10	L	502	-	-	15/45/69/87	0/1/1/1
7	LDA	M	905	-	-	4/13/13/13	-
4	BCL	M	909	2	-	8/37/137/137	-
6	U10	M	501	-	-	6/45/69/87	0/1/1/1
7	LDA	M	902	-	-	6/13/13/13	-
7	LDA	L	904	-	-	9/13/13/13	-
7	LDA	M	903	-	-	9/13/13/13	-
7	LDA	M	906	-	-	9/13/13/13	-
4	BCL	L	304	1	-	6/37/137/137	-
10	SPO	M	600	-	-	9/47/47/47	-
5	BPH	L	402	-	-	12/54/105/105	0/5/6/6
5	BPH	M	401	-	-	10/54/105/105	0/5/6/6
4	BCL	L	302	1	-	7/37/137/137	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	302	BCL	MG-NA	8.56	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	906	LDA	O1-N1	-7.43	1.24	1.42
7	M	903	LDA	O1-N1	-7.15	1.25	1.42
4	M	909	BCL	C4B-NB	6.75	1.41	1.35
7	M	905	LDA	O1-N1	-6.66	1.26	1.42
7	M	902	LDA	O1-N1	-6.61	1.26	1.42
7	L	904	LDA	O1-N1	-6.57	1.26	1.42
4	M	909	BCL	MG-NA	6.45	2.21	2.06
4	M	908	BCL	MG-NA	6.23	2.21	2.06
7	H	901	LDA	O1-N1	-5.89	1.28	1.42
4	L	302	BCL	C1B-NB	5.30	1.39	1.35
4	M	908	BCL	C1B-NB	5.03	1.39	1.35
4	M	908	BCL	C4B-NB	4.72	1.39	1.35
10	M	600	SPO	C21-C22	4.42	1.57	1.43
6	L	502	U10	O3-C3	4.00	1.46	1.36
6	M	501	U10	O3-C3	3.94	1.46	1.36
6	L	502	U10	O4-C4	3.69	1.45	1.36
4	L	302	BCL	C4B-NB	3.28	1.38	1.35
4	L	304	BCL	C1B-NB	3.23	1.38	1.35
4	M	908	BCL	MG-NC	3.12	2.13	2.06
4	L	304	BCL	MG-NA	3.00	2.13	2.06
4	L	304	BCL	OBD-CAD	2.88	1.26	1.22
5	M	401	BPH	CHC-C1C	2.88	1.42	1.36
6	M	501	U10	O4-C4	2.64	1.43	1.36
5	L	402	BPH	C4C-NC	2.52	1.42	1.37
5	L	402	BPH	C3C-C4C	2.38	1.54	1.50
4	L	304	BCL	C3D-C2D	-2.36	1.35	1.39
4	M	908	BCL	CBA-CGA	-2.32	1.43	1.50
4	L	304	BCL	MG-NC	-2.32	2.00	2.06
4	M	909	BCL	CBA-CGA	-2.28	1.44	1.50
5	L	402	BPH	C1B-NB	-2.24	1.33	1.38
6	L	502	U10	C28-C29	2.11	1.38	1.33
6	M	501	U10	C31-C29	2.05	1.55	1.51
5	L	402	BPH	O1D-CGD	2.02	1.26	1.21
6	M	501	U10	C33-C34	2.01	1.37	1.33

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	O2D-CGD-CBD	12.58	133.62	111.27
4	L	304	BCL	O1D-CGD-CBD	-8.41	107.28	124.48
4	L	304	BCL	CED-O2D-CGD	5.82	129.09	115.94
6	M	501	U10	C6-C1-C2	4.82	122.99	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	U10	C25-C24-C26	4.59	122.99	115.27
4	M	908	BCL	CMB-C2B-C1B	-4.58	121.43	128.46
5	M	401	BPH	CAC-C3C-C2C	-4.53	102.93	114.26
5	L	402	BPH	C1-C2-C3	-4.49	118.29	126.04
6	M	501	U10	C30-C29-C31	4.24	122.41	115.27
6	M	501	U10	C17-C18-C19	-4.24	117.46	127.66
4	L	302	BCL	C11-C12-C13	-4.03	102.90	115.92
4	M	909	BCL	CAC-C3C-C2C	-4.00	104.25	114.26
4	L	304	BCL	CAA-CBA-CGA	3.99	124.93	113.25
4	M	909	BCL	CMB-C2B-C1B	-3.72	122.74	128.46
4	L	304	BCL	CAC-C3C-C2C	-3.72	104.97	114.26
10	M	600	SPO	C20-C19-C17	-3.66	122.09	127.31
5	M	401	BPH	OBD-CAD-CBD	-3.62	120.72	125.89
4	L	304	BCL	OBB-CAB-CBB	-3.57	112.13	120.17
4	L	304	BCL	C3D-CAD-CBD	-3.57	102.91	107.61
4	M	908	BCL	O2A-C1-C2	3.55	117.95	108.64
4	M	909	BCL	CED-O2D-CGD	3.54	123.95	115.94
6	L	502	U10	C22-C23-C24	-3.49	119.25	127.66
5	L	402	BPH	CHD-C4C-NC	-3.47	121.08	125.20
4	L	302	BCL	C4B-C3B-CAB	-3.46	120.45	127.13
4	L	302	BCL	O2A-CGA-O1A	-3.41	114.99	123.59
6	M	501	U10	C15-C14-C16	3.39	120.97	115.27
4	L	304	BCL	C5-C3-C2	-3.36	114.32	121.12
4	L	304	BCL	CMB-C2B-C1B	-3.36	123.30	128.46
5	L	402	BPH	C1B-NB-C4B	3.34	112.81	106.51
5	M	401	BPH	C1-C2-C3	-3.34	120.27	126.04
10	M	600	SPO	C21-C22-C23	-3.31	122.59	127.31
5	M	401	BPH	C1-O2A-CGA	3.27	125.01	116.44
4	M	908	BCL	OBD-CAD-CBD	-3.27	121.23	125.89
4	L	302	BCL	CMB-C2B-C1B	-3.23	123.50	128.46
5	L	402	BPH	C1C-NC-C4C	-3.22	107.71	110.54
5	L	402	BPH	CAC-C3C-C4C	3.11	120.66	112.67
5	M	401	BPH	CMC-C2C-C1C	3.06	120.66	112.09
6	L	502	U10	C35-C34-C36	3.06	120.42	115.27
4	M	909	BCL	CHA-C1A-NA	-3.06	119.39	126.40
5	M	401	BPH	C1B-NB-C4B	3.06	112.28	106.51
5	M	401	BPH	O2A-C1-C2	-3.04	100.65	108.64
6	M	501	U10	C30-C29-C28	-3.00	115.99	123.68
4	M	909	BCL	OBB-CAB-CBB	-2.99	113.44	120.17
5	M	401	BPH	CAA-C2A-C3A	-2.96	104.67	112.78
4	M	908	BCL	C4D-C3D-CAD	-2.96	106.82	108.47
10	M	600	SPO	C25-C23-C22	-2.89	114.51	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	U10	C3M-O3-C3	2.89	126.70	116.47
4	M	908	BCL	CMA-C3A-C2A	-2.88	102.20	113.83
4	M	908	BCL	CAA-C2A-C3A	-2.80	105.11	112.78
4	M	908	BCL	CHA-C1A-NA	-2.78	120.03	126.40
4	L	302	BCL	CAA-C2A-C3A	-2.76	105.22	112.78
4	L	302	BCL	CHA-C1A-NA	-2.74	120.11	126.40
6	M	501	U10	C22-C23-C24	-2.74	121.06	127.66
6	M	501	U10	C16-C14-C13	-2.72	115.62	121.12
4	L	302	BCL	C5-C3-C2	-2.71	115.63	121.12
4	L	304	BCL	OBB-CAB-C3B	2.71	124.80	119.99
4	M	908	BCL	CMB-C2B-C3B	2.69	129.71	124.68
5	M	401	BPH	OBD-CAD-C3D	2.62	132.33	127.98
4	L	302	BCL	C4-C3-C5	2.62	119.68	115.27
4	L	304	BCL	O2A-C1-C2	2.60	115.46	108.64
10	M	600	SPO	C34-C33-C35	2.59	119.63	115.27
6	L	502	U10	O2-C2-C3	-2.57	115.48	120.93
5	M	401	BPH	CAC-C3C-C4C	2.51	119.12	112.67
4	L	304	BCL	CAA-C2A-C3A	-2.48	105.98	112.78
4	L	302	BCL	CMB-C2B-C3B	2.48	129.32	124.68
6	L	502	U10	C25-C24-C23	-2.45	117.38	123.68
4	L	304	BCL	O2D-CGD-O1D	-2.45	119.04	123.84
10	M	600	SPO	C2-C1-C4	-2.44	107.11	110.86
4	M	908	BCL	O2D-CGD-CBD	2.44	115.60	111.27
6	M	501	U10	C7-C6-C5	-2.44	115.55	118.48
4	L	304	BCL	CHA-C1A-NA	-2.41	120.87	126.40
4	L	304	BCL	C2A-C3A-C4A	2.41	105.76	101.87
4	L	302	BCL	C4B-CHC-C1C	-2.40	125.37	130.12
4	M	909	BCL	C1-C2-C3	-2.39	121.92	126.04
6	M	501	U10	C1M-C1-C6	-2.38	120.52	124.40
4	L	302	BCL	CAC-C3C-C2C	-2.37	108.33	114.26
4	L	304	BCL	C2C-C3C-C4C	2.37	104.89	101.34
7	M	902	LDA	O1-N1-C1	2.34	115.02	109.27
4	M	908	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
6	L	502	U10	C35-C34-C33	-2.34	117.68	123.68
4	M	909	BCL	CAC-C3C-C4C	-2.33	107.41	112.58
4	M	909	BCL	C4D-C3D-CAD	-2.32	107.18	108.47
4	L	302	BCL	O2A-CGA-CBA	2.31	119.15	111.91
4	L	302	BCL	OBB-CAB-C3B	2.30	124.08	119.99
6	L	502	U10	C7-C8-C9	-2.27	123.01	126.79
4	M	908	BCL	C2C-C3C-C4C	2.25	104.71	101.34
10	M	600	SPO	C13-C12-C11	2.22	121.57	118.08
4	M	909	BCL	C4B-C3B-CAB	-2.21	122.86	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	501	U10	C4M-O4-C4	2.20	124.25	116.47
6	M	501	U10	C20-C19-C18	-2.17	118.11	123.68
4	M	909	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
5	L	402	BPH	C7-C6-C5	-2.14	107.54	113.36
4	M	908	BCL	CAC-C3C-C2C	-2.14	108.91	114.26
10	M	600	SPO	C24-C23-C25	2.13	121.44	118.08
5	M	401	BPH	O2D-CGD-CBD	2.12	115.04	111.27
4	M	908	BCL	OBb-CAB-C3B	2.12	123.75	119.99
4	L	304	BCL	OBD-CAD-C3D	2.12	131.49	127.98
5	M	401	BPH	C2B-C1B-NB	-2.10	106.62	109.79
10	M	600	SPO	C31-C32-C33	-2.10	122.60	127.66
5	L	402	BPH	CMD-C2D-C3D	2.09	128.59	124.68
4	L	302	BCL	CMA-C3A-C4A	-2.08	106.17	111.77
7	M	906	LDA	CM2-N1-C1	2.06	114.57	110.23
6	L	502	U10	C8-C7-C6	2.06	117.60	112.05
4	M	908	BCL	C6-C5-C3	-2.05	108.07	113.45
6	M	501	U10	C26-C24-C23	2.05	125.27	121.12
6	M	501	U10	C31-C32-C33	2.05	118.62	111.88
4	L	304	BCL	CMB-C2B-C3B	2.05	128.51	124.68
5	L	402	BPH	C2B-C1B-NB	-2.04	106.72	109.79
4	M	909	BCL	C2C-C3C-C4C	2.04	104.39	101.34
10	M	600	SPO	C40-C38-C39	2.03	119.08	114.60
6	L	502	U10	C17-C18-C19	-2.02	122.79	127.66
4	M	908	BCL	CMA-C3A-C4A	-2.00	106.39	111.77

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	901	LDA	C2-C1-N1-CM1
7	H	901	LDA	C2-C1-N1-CM2
7	H	901	LDA	N1-C1-C2-C3
6	L	502	U10	C24-C26-C27-C28
7	M	902	LDA	C2-C1-N1-CM1
7	L	904	LDA	C2-C1-N1-CM1
7	L	904	LDA	C2-C1-N1-CM2
7	M	906	LDA	C2-C1-N1-O1
7	M	906	LDA	C2-C1-N1-CM2
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O1D-CGD-O2D-CED
10	M	600	SPO	C24-C23-C25-C26
5	L	402	BPH	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	L	402	BPH	C2C-C3C-CAC-CBC
5	L	402	BPH	O2A-C1-C2-C3
5	M	401	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C4B-C3B-CAB-OB
5	L	402	BPH	C3-C5-C6-C7
7	M	903	LDA	C5-C6-C7-C8
4	M	908	BCL	C11-C10-C8-C9
5	L	402	BPH	C6-C7-C8-C9
5	M	401	BPH	C12-C13-C15-C16
6	M	501	U10	C24-C26-C27-C28
6	M	501	U10	C34-C36-C37-C38
6	L	502	U10	C15-C14-C16-C17
7	M	906	LDA	C3-C4-C5-C6
7	M	905	LDA	C7-C8-C9-C10
7	M	906	LDA	C11-C10-C9-C8
7	M	905	LDA	C5-C6-C7-C8
7	M	906	LDA	C2-C3-C4-C5
4	M	908	BCL	C15-C16-C17-C18
5	L	402	BPH	C16-C17-C18-C20
7	L	904	LDA	C5-C6-C7-C8
7	M	903	LDA	C1-C2-C3-C4
7	M	903	LDA	C7-C8-C9-C10
7	H	901	LDA	C3-C4-C5-C6
7	M	902	LDA	C11-C10-C9-C8
7	L	904	LDA	C1-C2-C3-C4
5	L	402	BPH	C4-C3-C5-C6
6	L	502	U10	C13-C14-C16-C17
6	M	501	U10	C23-C24-C26-C27
5	L	402	BPH	C2-C3-C5-C6
7	M	902	LDA	C1-C2-C3-C4
7	M	903	LDA	C4-C5-C6-C7
6	L	502	U10	C29-C31-C32-C33
6	L	502	U10	C30-C29-C31-C32
6	M	501	U10	C25-C24-C26-C27
6	L	502	U10	C28-C29-C31-C32
6	L	502	U10	C33-C34-C36-C37
5	M	401	BPH	C14-C13-C15-C16
7	H	901	LDA	C6-C7-C8-C9
10	M	600	SPO	C5-C6-C7-C8
10	M	600	SPO	C22-C23-C25-C26
7	H	901	LDA	C1-C2-C3-C4
4	M	908	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	M	905	LDA	C6-C7-C8-C9
7	M	903	LDA	C9-C10-C11-C12
7	L	904	LDA	C9-C10-C11-C12
10	M	600	SPO	C4-C1-O1-CM1
7	M	902	LDA	C3-C4-C5-C6
6	L	502	U10	C20-C19-C21-C22
6	L	502	U10	C35-C34-C36-C37
7	M	906	LDA	C5-C6-C7-C8
7	M	903	LDA	C3-C4-C5-C6
5	L	402	BPH	C16-C17-C18-C19
5	M	401	BPH	C10-C11-C12-C13
10	M	600	SPO	C2-C1-O1-CM1
6	L	502	U10	C18-C19-C21-C22
4	M	909	BCL	C11-C12-C13-C15
5	M	401	BPH	C11-C12-C13-C14
10	M	600	SPO	C5-C6-C7-C9
7	M	903	LDA	N1-C1-C2-C3
7	M	903	LDA	C11-C10-C9-C8
7	H	901	LDA	C7-C8-C9-C10
7	H	901	LDA	C11-C10-C9-C8
7	M	903	LDA	C6-C7-C8-C9
4	M	909	BCL	C5-C6-C7-C8
4	M	909	BCL	C11-C12-C13-C14
4	L	302	BCL	C11-C12-C13-C14
4	M	909	BCL	C11-C10-C8-C7
5	L	402	BPH	C6-C7-C8-C10
4	L	302	BCL	C11-C12-C13-C15
7	L	904	LDA	C11-C10-C9-C8
7	M	902	LDA	C2-C1-N1-CM2
7	M	906	LDA	C2-C1-N1-CM1
4	M	909	BCL	C16-C17-C18-C19
5	M	401	BPH	C8-C10-C11-C12
7	H	901	LDA	C2-C1-N1-O1
7	L	904	LDA	C2-C1-N1-O1
5	M	401	BPH	C11-C10-C8-C7
4	M	909	BCL	C11-C10-C8-C9
10	M	600	SPO	C33-C35-C36-C37
7	L	904	LDA	C3-C4-C5-C6
7	M	906	LDA	C9-C10-C11-C12
4	L	304	BCL	C16-C17-C18-C19
6	L	502	U10	C31-C32-C33-C34
10	M	600	SPO	C3-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
6	L	502	U10	C12-C11-C9-C10
7	M	902	LDA	C5-C6-C7-C8
10	M	600	SPO	C12-C14-C15-C16
4	L	302	BCL	C16-C17-C18-C19
6	M	501	U10	C26-C27-C28-C29
6	L	502	U10	C2-C3-O3-C3M
4	M	908	BCL	C8-C10-C11-C12
4	M	909	BCL	C6-C7-C8-C10
6	L	502	U10	C12-C11-C9-C8
4	L	302	BCL	C2A-CAA-CBA-CGA
6	L	502	U10	C34-C36-C37-C38
4	M	909	BCL	C6-C7-C8-C9
4	L	302	BCL	C11-C10-C8-C9
7	M	905	LDA	C1-C2-C3-C4
4	L	304	BCL	C16-C17-C18-C20
6	M	501	U10	C5-C4-O4-C4M
5	M	401	BPH	C11-C12-C13-C15
5	L	402	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C11-C10-C8-C9
4	M	908	BCL	CAD-CBD-CGD-O2D
5	L	402	BPH	CAD-CBD-CGD-O2D
4	L	302	BCL	CAD-CBD-CGD-O2D
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
7	L	904	LDA	N1-C1-C2-C3
7	M	906	LDA	C4-C5-C6-C7
7	H	901	LDA	C9-C10-C11-C12
4	M	908	BCL	C11-C10-C8-C7
4	L	302	BCL	C11-C10-C8-C7

There are no ring outliers.

13 monomers are involved in 43 short contacts:

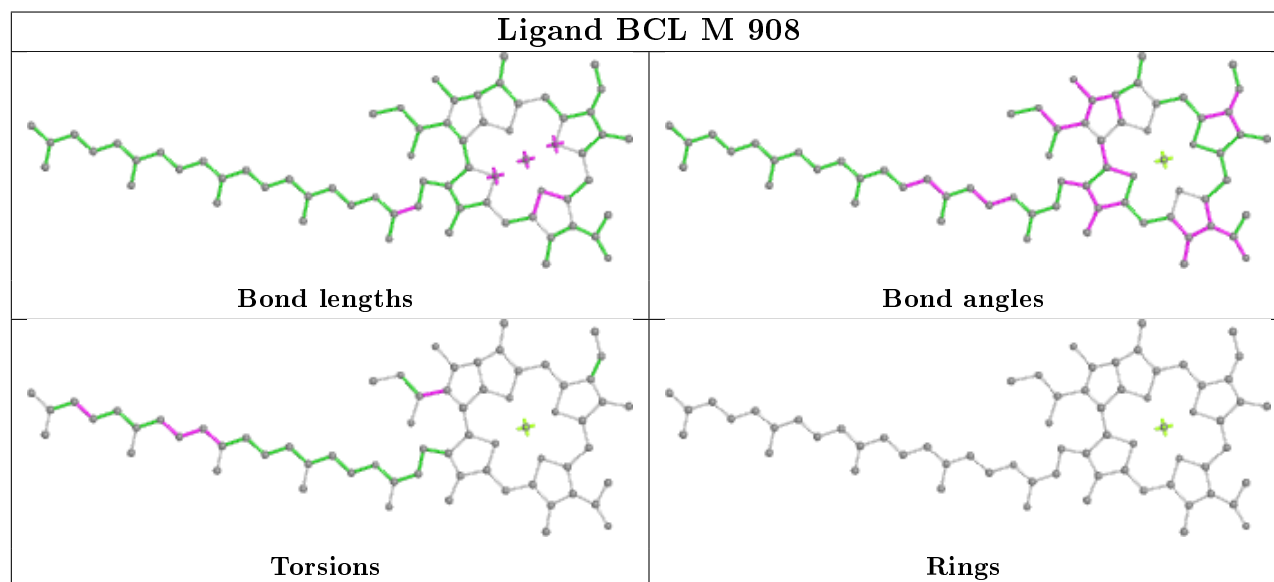
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	908	BCL	5	0
7	H	901	LDA	2	0
6	L	502	U10	10	0
7	M	905	LDA	3	0
4	M	909	BCL	3	0
7	M	902	LDA	1	0
7	M	903	LDA	1	0
7	M	906	LDA	1	0

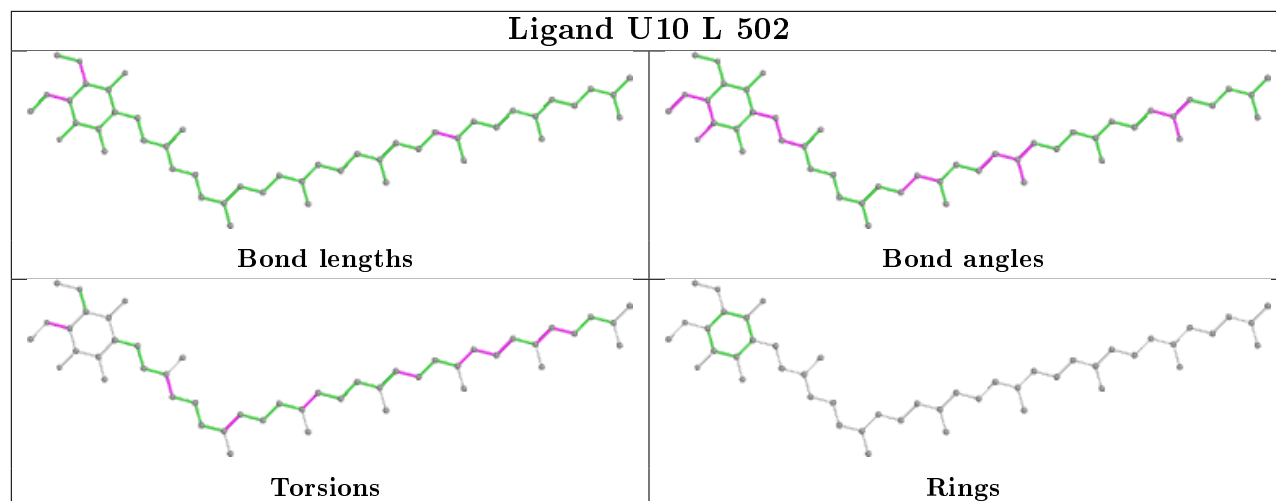
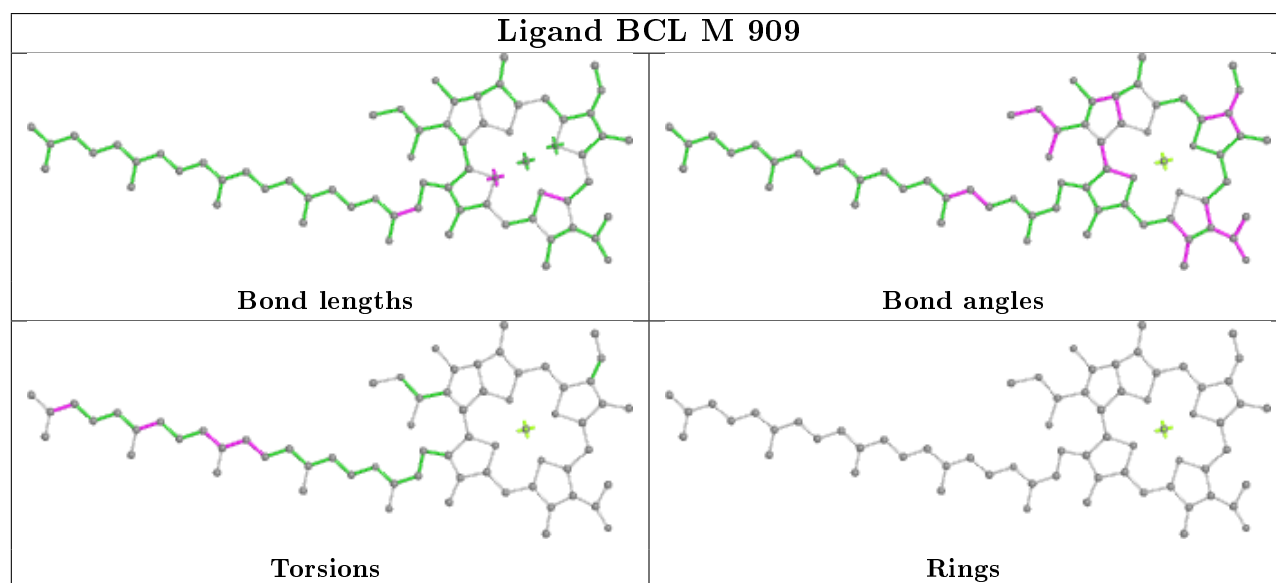
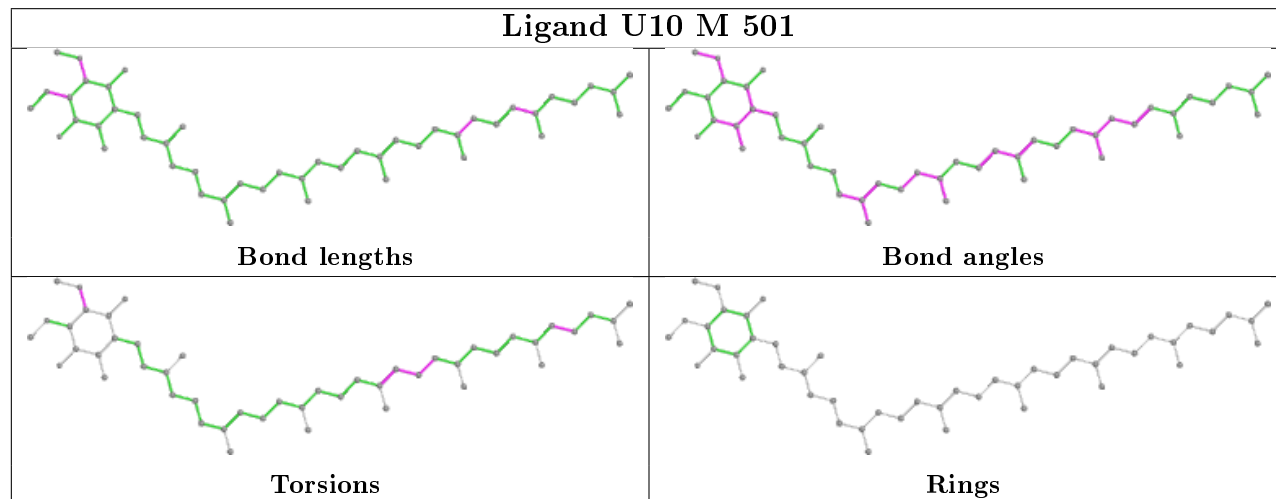
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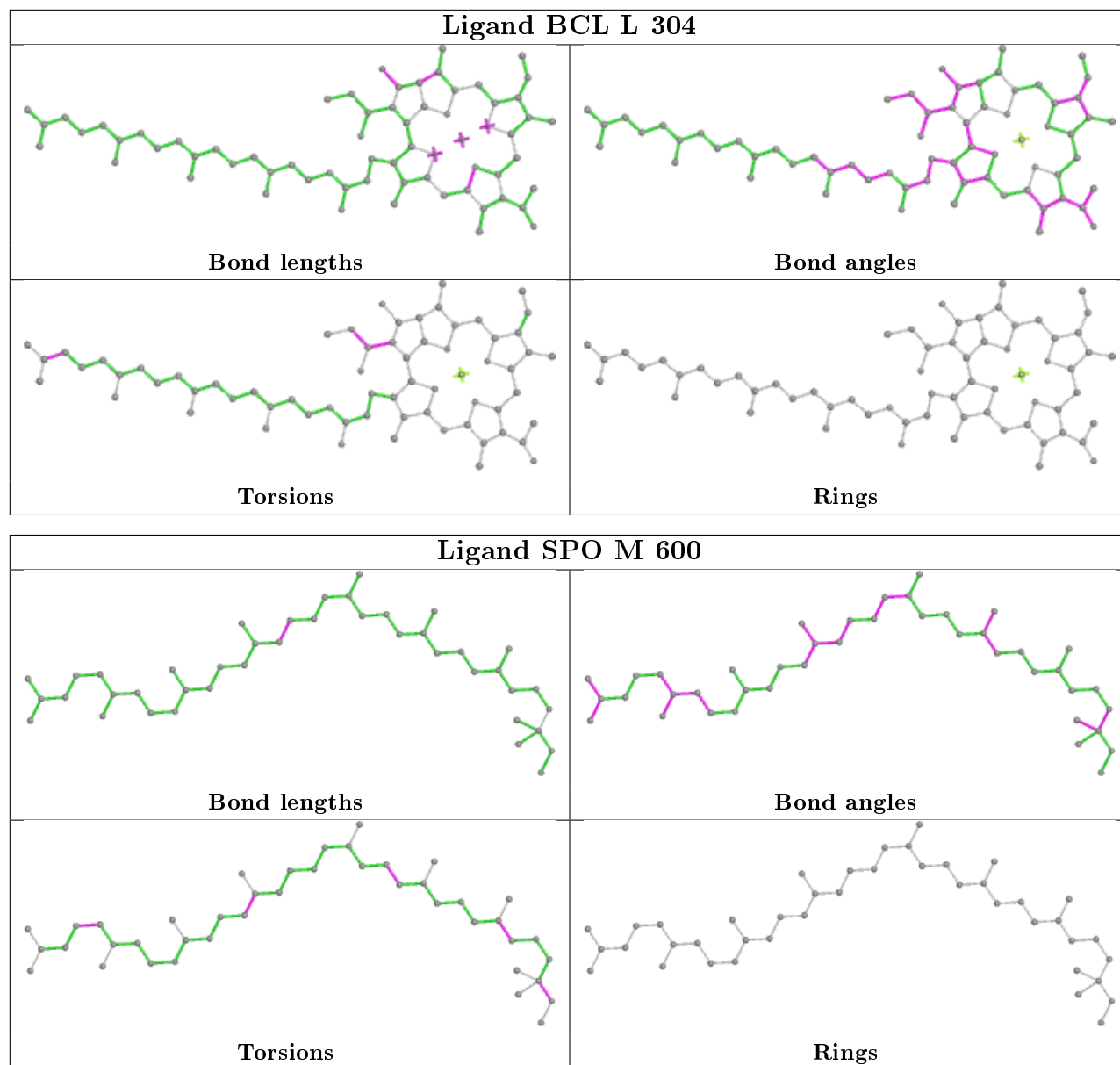
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	304	BCL	5	0
10	M	600	SPO	1	0
5	L	402	BPH	4	0
5	M	401	BPH	8	0
4	L	302	BCL	5	0

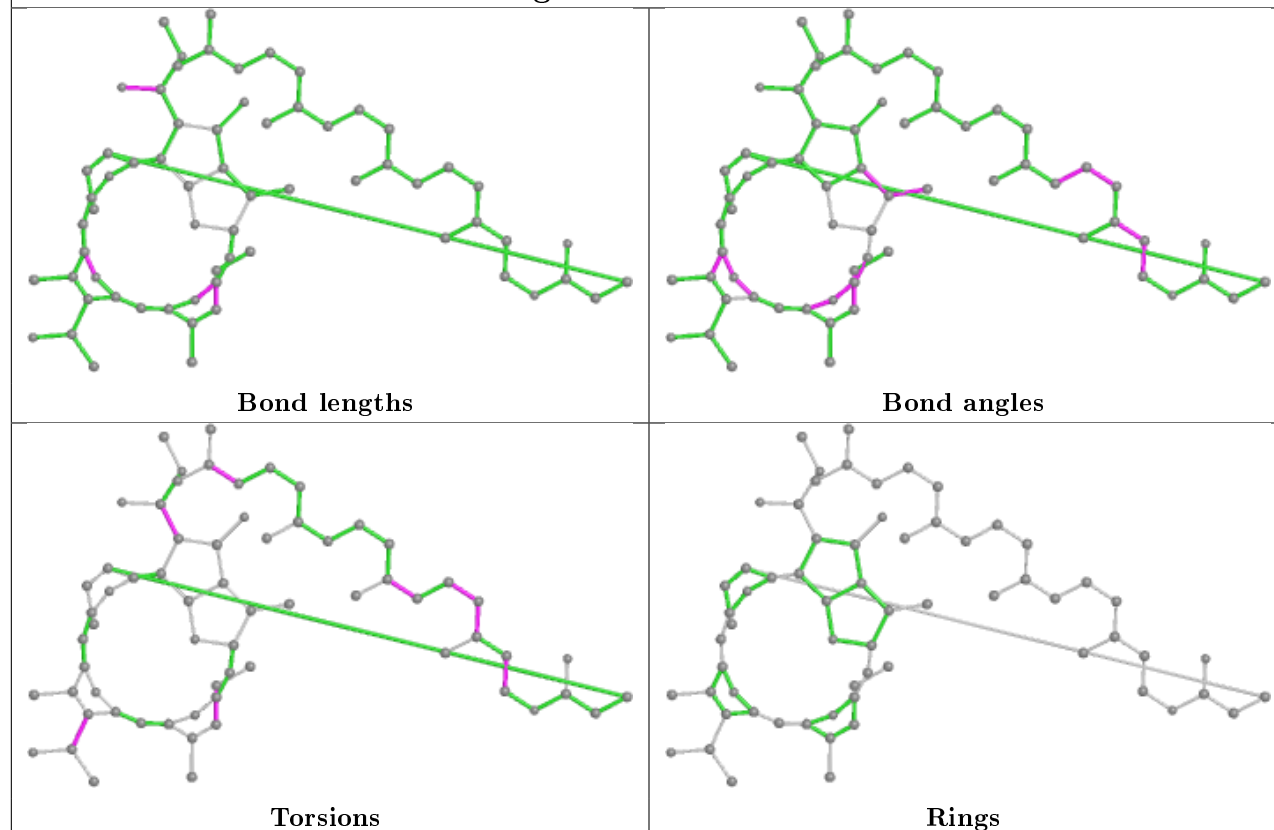
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



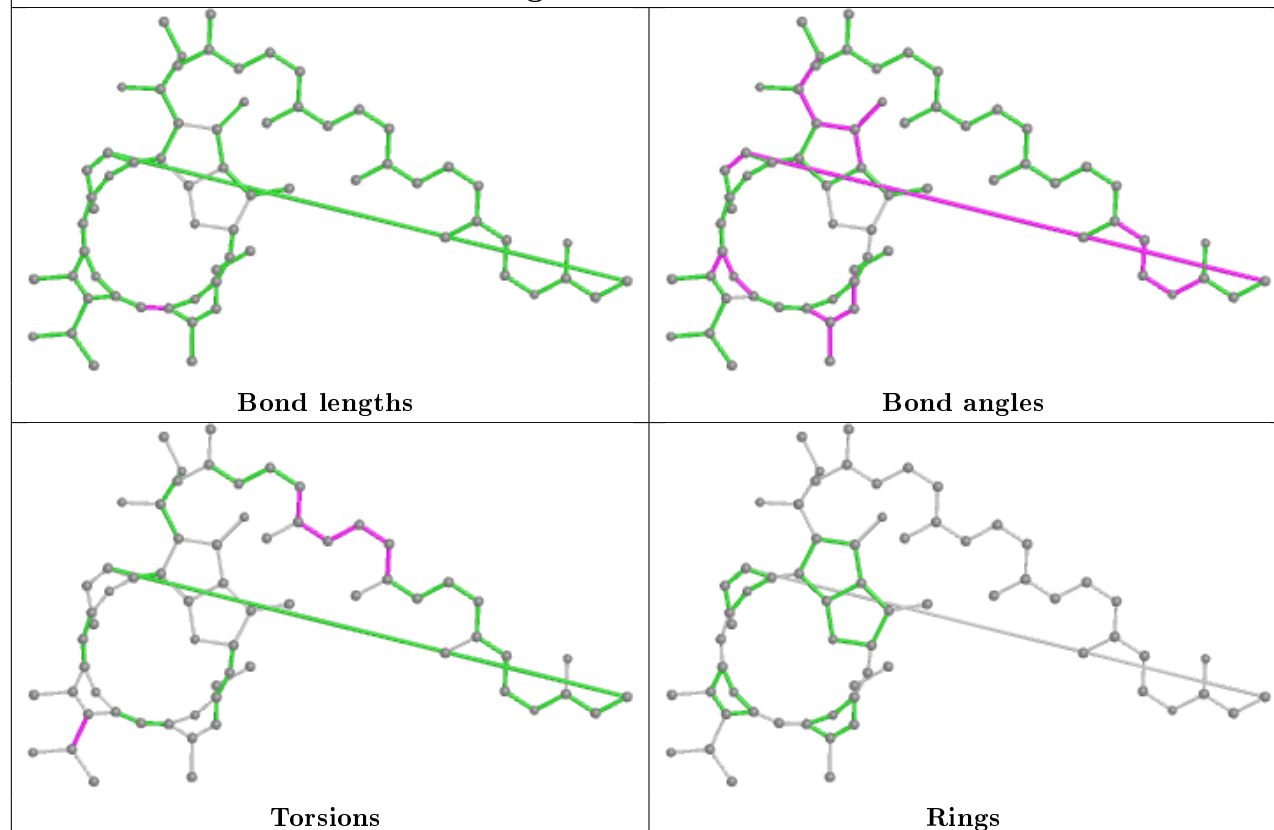
Ligand U10 L 502**Ligand BCL M 909****Ligand U10 M 501**

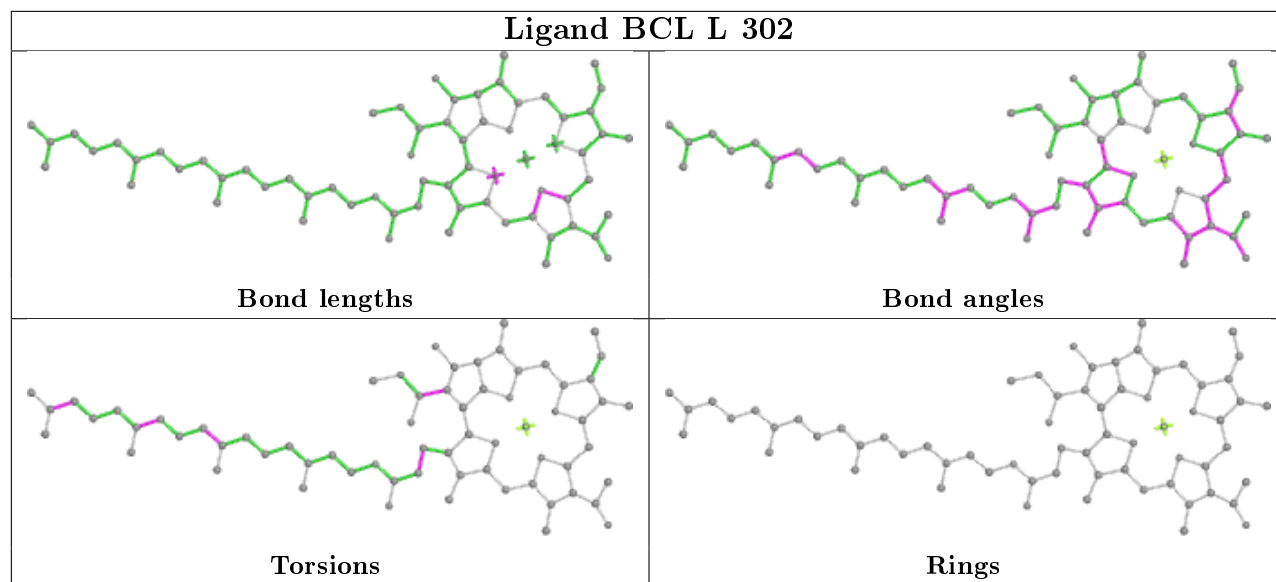


Ligand BPH L 402



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.11	16 (5%)	23 15	62, 72, 79, 86	0
2	M	302/307 (98%)	0.22	16 (5%)	26 17	65, 73, 82, 102	0
3	H	240/260 (92%)	0.33	19 (7%)	12 7	65, 72, 81, 121	0
All	All	823/848 (97%)	0.21	51 (6%)	20 13	62, 72, 81, 121	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	8.5
3	H	245	ALA	5.7
3	H	249	LYS	5.7
3	H	247	LYS	5.3
3	H	246	PRO	5.2
3	H	191	LEU	4.7
1	L	270	PRO	4.5
2	M	302	GLY	4.4
1	L	281	GLY	4.2
2	M	28	ASN	3.6
2	M	111	GLU	3.6
2	M	27	ALA	3.1
3	H	22	ILE	3.1
3	H	248	ARG	3.1
2	M	1	ALA	2.9
1	L	73	TYR	2.9
2	M	104	SER	2.7
1	L	271	TRP	2.7
3	H	200	SER	2.7
2	M	148	TRP	2.6
1	L	269	LEU	2.6
3	H	179	LEU	2.6
2	M	301	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	190	LEU	2.6
1	L	72	GLU	2.5
2	M	169	GLY	2.5
2	M	76	TYR	2.4
1	L	59	TRP	2.4
3	H	18	TYR	2.3
2	M	25	ASN	2.3
1	L	61	PRO	2.3
1	L	202	LYS	2.3
2	M	57	VAL	2.3
3	H	176	ALA	2.3
3	H	201	ASN	2.3
2	M	101	TYR	2.3
1	L	275	ILE	2.2
1	L	274	ASN	2.2
1	L	272	TRP	2.2
3	H	192	PRO	2.2
1	L	69	PRO	2.2
3	H	185	ASP	2.2
2	M	108	PRO	2.2
1	L	74	GLY	2.2
2	M	2[A]	GLU	2.2
1	L	273	ALA	2.1
2	M	284	ILE	2.1
3	H	52[A]	ASN	2.1
1	L	276	PRO	2.1
3	H	184	LYS	2.1
3	H	178	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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,

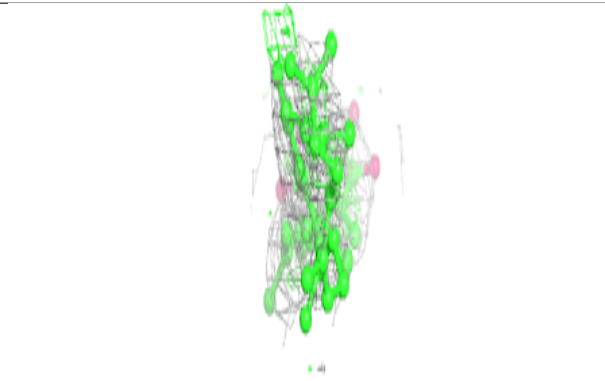
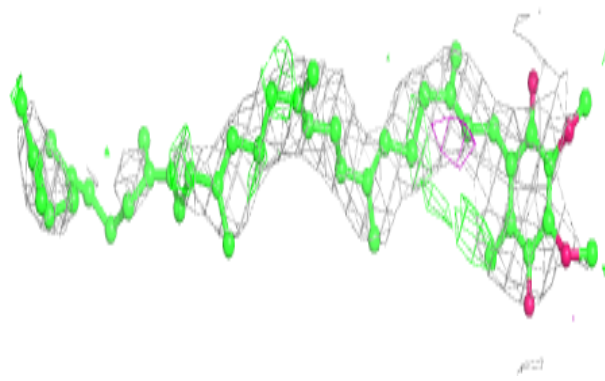
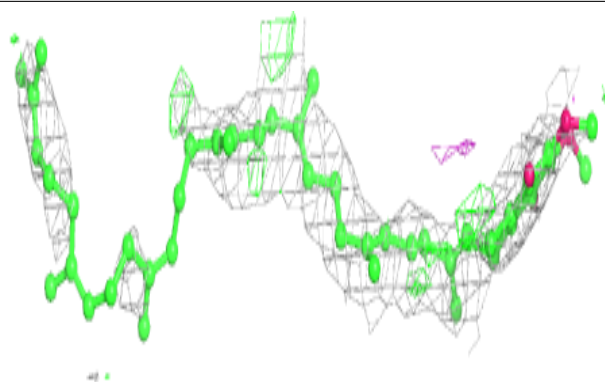
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	L	904	16/16	0.38	0.49	69,92,102,104	16
7	LDA	M	906	16/16	0.54	0.45	61,63,66,68	16
6	U10	L	502	48/63	0.59	0.57	62,65,73,74	48
7	LDA	M	905	16/16	0.74	0.40	100,108,114,115	0
10	SPO	M	600	42/42	0.76	0.36	69,77,82,84	0
5	BPH	M	401	65/65	0.82	0.25	68,77,104,105	0
7	LDA	M	903	16/16	0.84	0.27	107,112,113,113	0
7	LDA	H	901	16/16	0.85	0.21	98,103,115,115	0
7	LDA	M	902	16/16	0.88	0.22	96,98,100,101	0
4	BCL	M	908	66/66	0.92	0.15	64,71,94,96	0
6	U10	M	501	48/63	0.93	0.24	68,78,90,91	0
5	BPH	L	402	65/65	0.94	0.25	62,69,79,85	0
9	PO4	M	907	5/5	0.94	0.16	95,101,101,102	0
4	BCL	L	302	66/66	0.94	0.22	64,72,89,95	0
4	BCL	M	909	66/66	0.95	0.19	66,70,83,89	0
4	BCL	L	304	66/66	0.95	0.14	54,62,82,86	0
8	FE	M	500	1/1	0.98	0.14	71,71,71,71	0

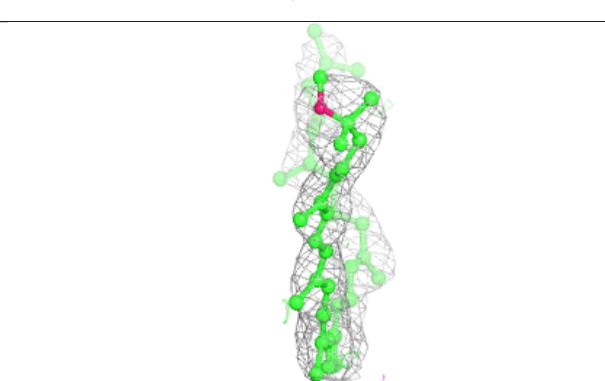
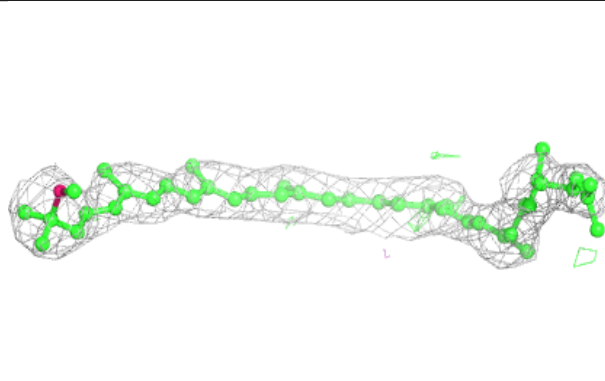
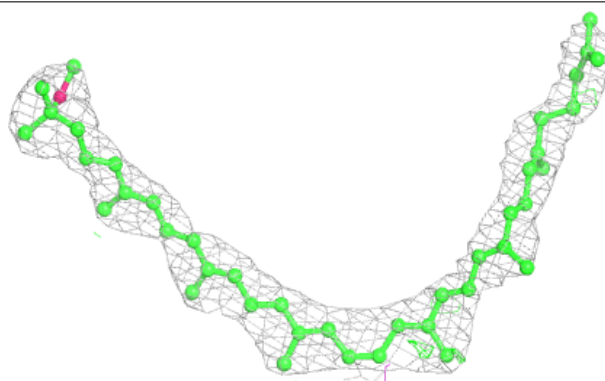
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

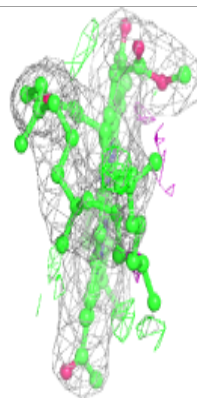
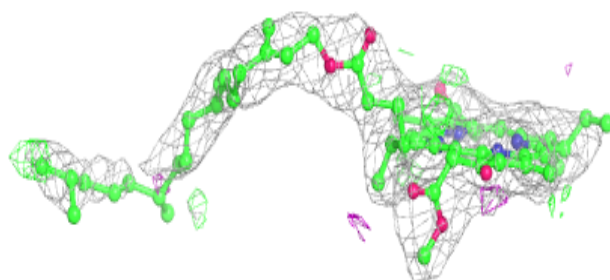
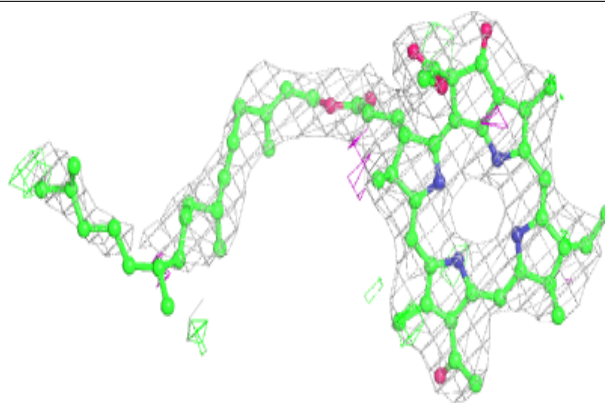
**Electron density around SPO M 600:**

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



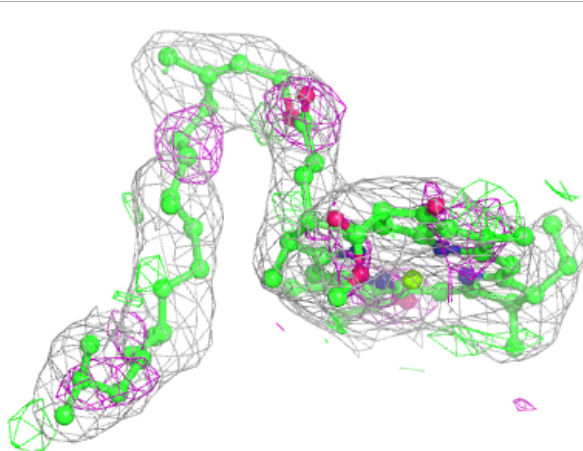
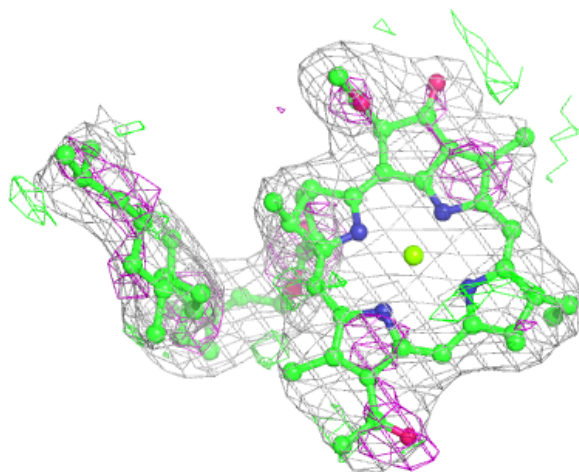
Electron density around BPH M 401:

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



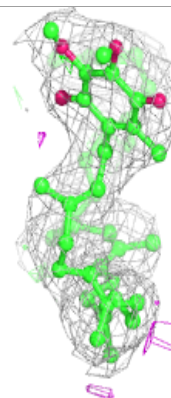
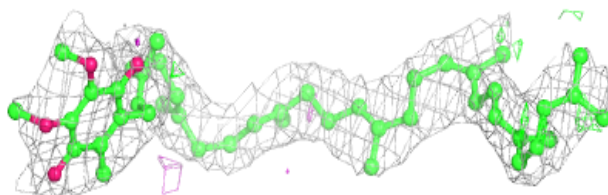
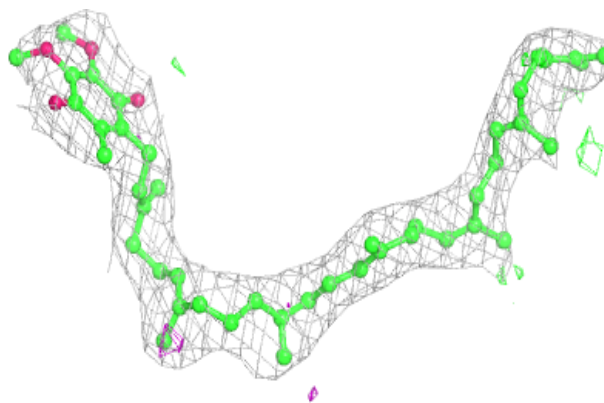
Electron density around BCL M 908:

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

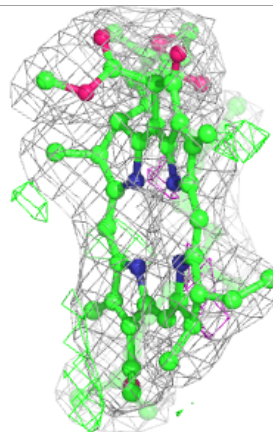
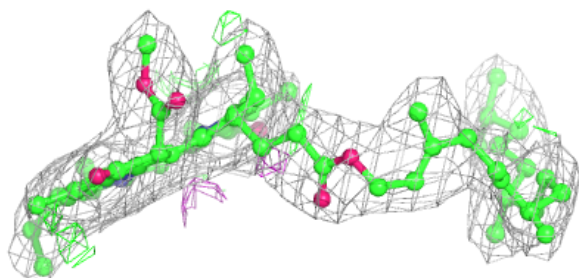
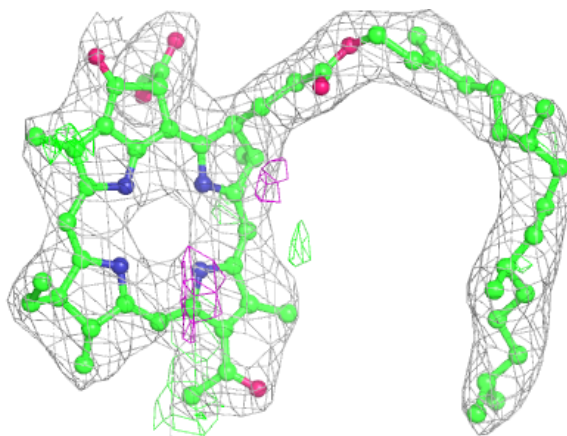


Electron density around U10 M 501:

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

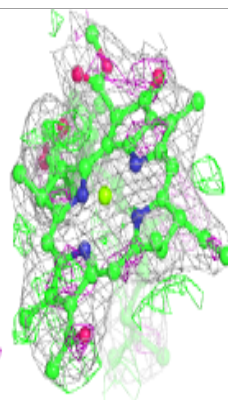
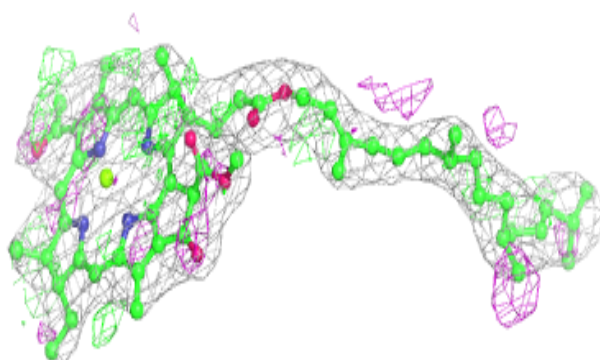
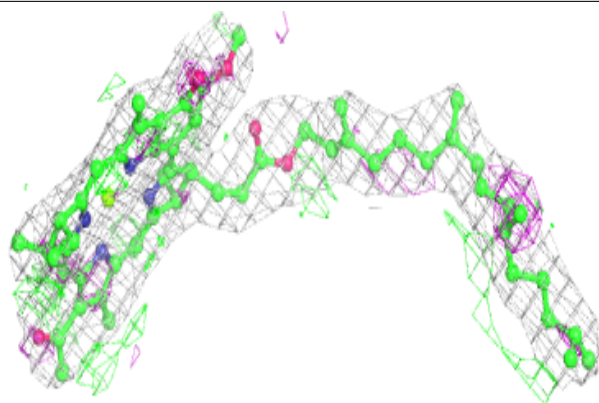
**Electron density around BPH L 402:**

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

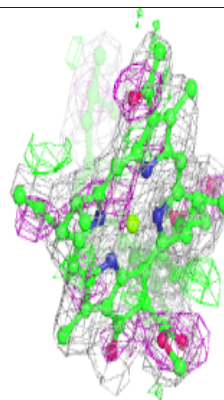
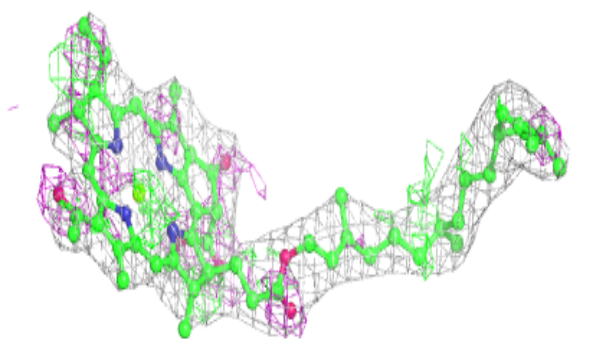
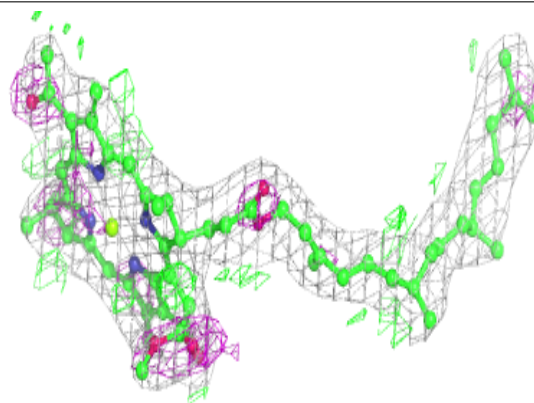


Electron density around BCL L 302:

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

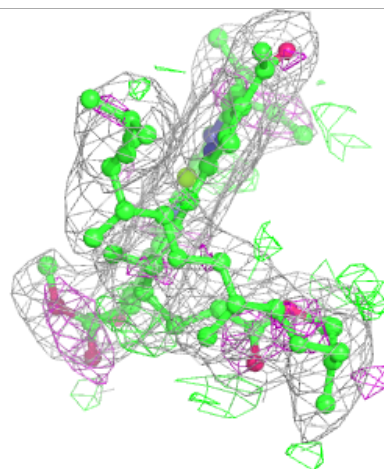
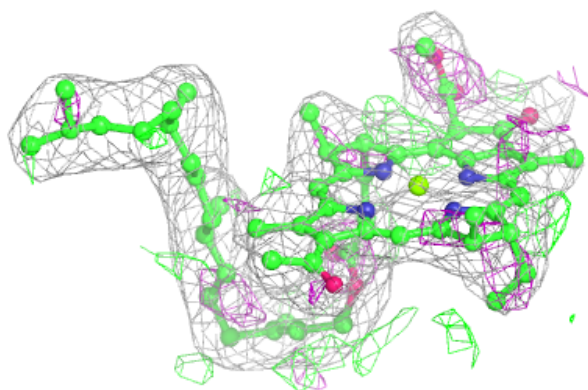
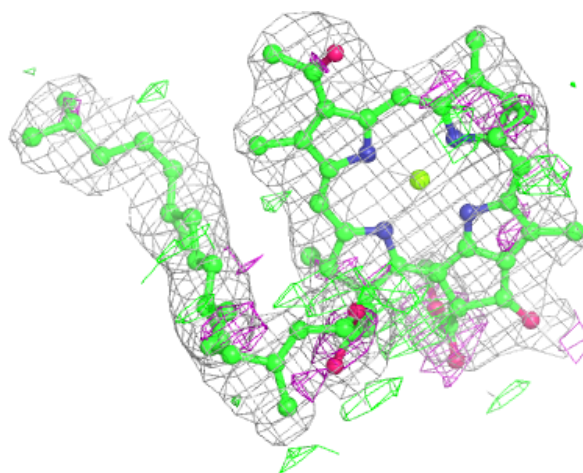
**Electron density around BCL M 909:**

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



Electron density around BCL L 304:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.