



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:28 AM EDT

PDB ID : 3V3Y / pdb_00003v3y
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

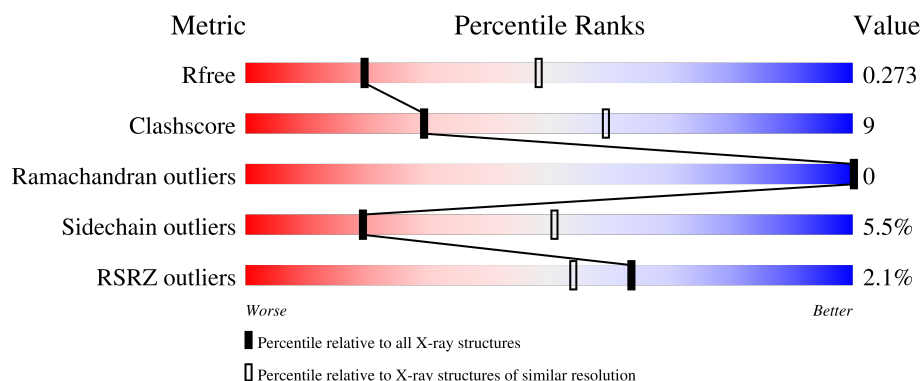
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 80% 19% .
2	L	281	4% 74% 24% .
3	M	302	% 80% 18% .

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	-	-	-

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

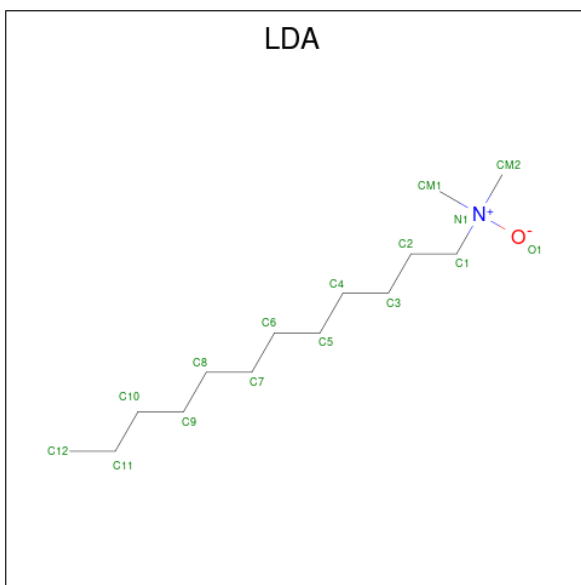
- Molecule 3 is a protein called Reaction center protein M chain.

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:

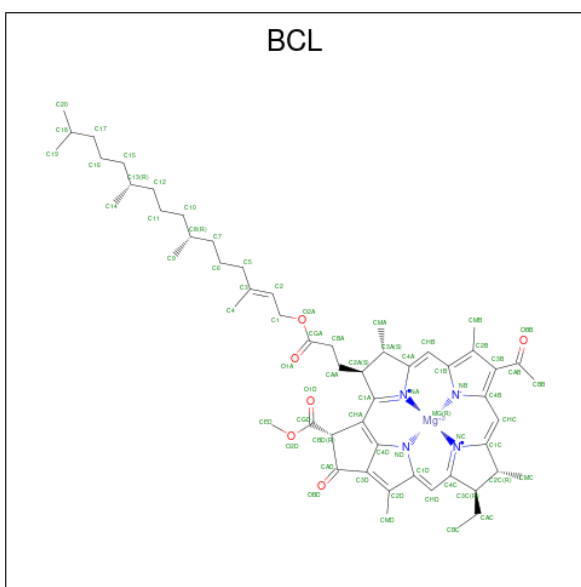
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



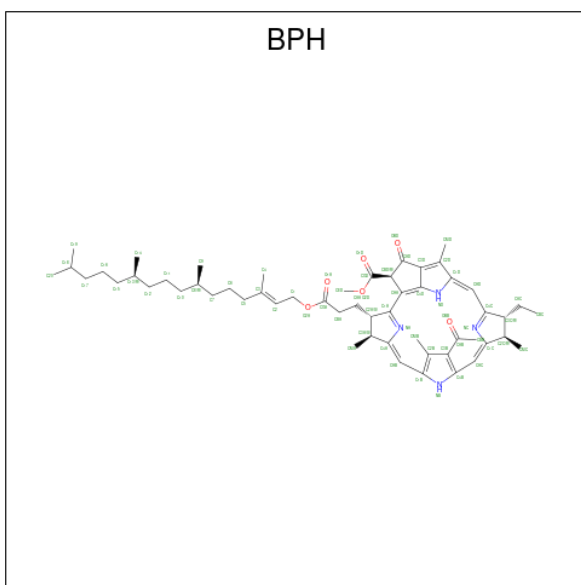
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



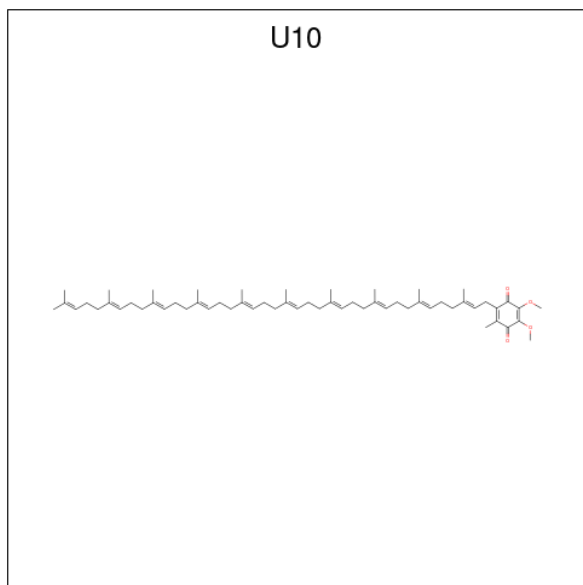
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



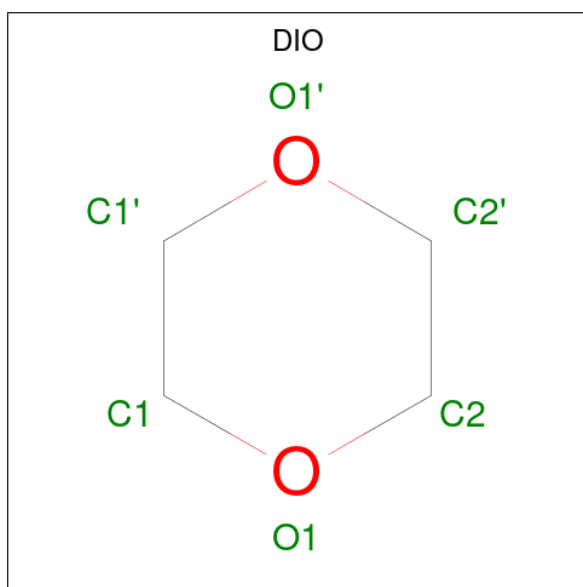
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (CCD ID: 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 (CCD ID: DIO) (formula: $C_4H_8O_2$).

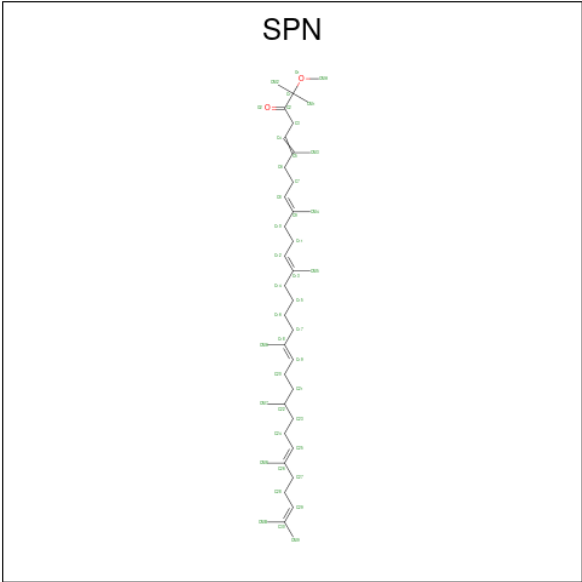


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			6	4	2		
8	L	1	Total	C	O	0	0
			6	4	2		
8	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is FE (III) ION (CCD ID: FE) (formula: Fe).

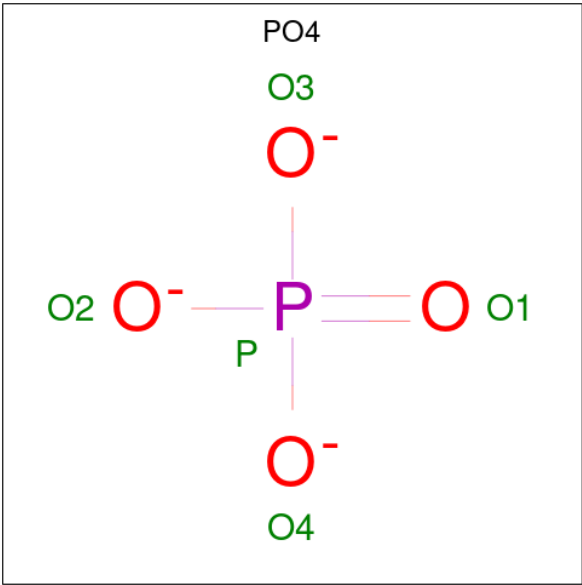
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPEROIDENONE (CCD ID: 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 (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: CL) (formula: Cl).

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

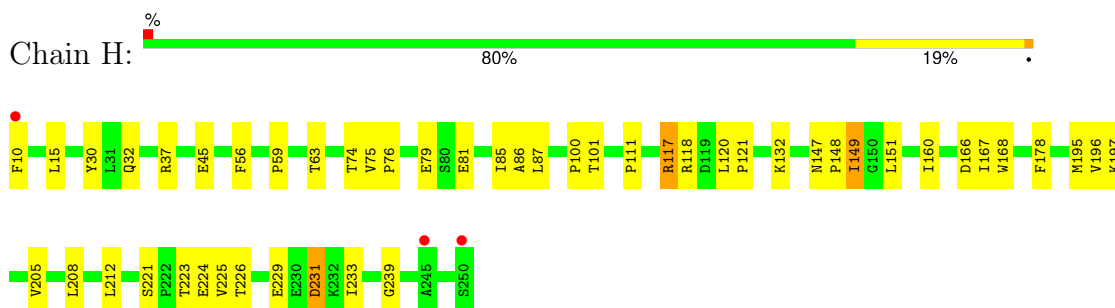
- Molecule 13 is water.

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		

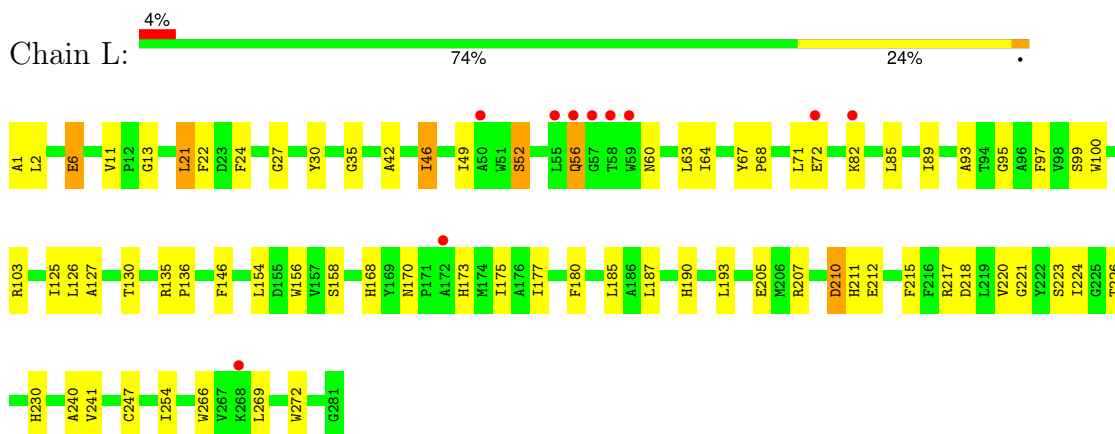
3 Residue-property plots [i](#)

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

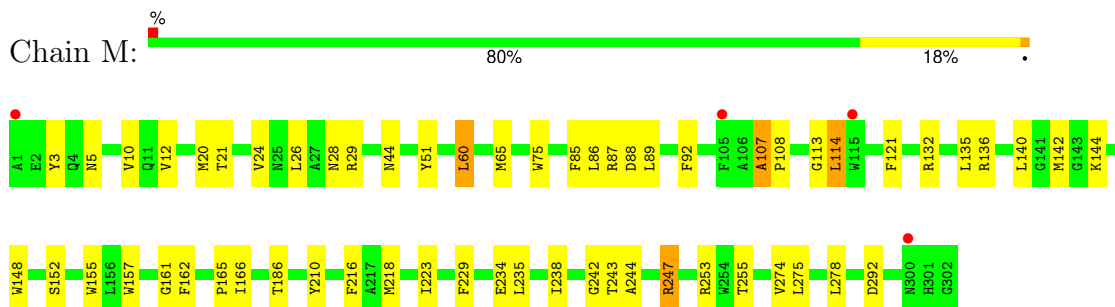
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

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 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.94-2.80) 98.9 (19.94-2.80)	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 0.240 , 0.273	Depositor DCC
R_{free} test set	2645 reflections (5.07%)	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)	0.28 , 28.9	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPN, PO4, BPH, U10, LDA, BCL, FE, DIO, CL

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	0.60	0/1889	1.01	7/2569 (0.3%)
2	L	0.60	0/2321	0.92	8/3177 (0.3%)
3	M	0.60	0/2501	0.91	4/3415 (0.1%)
All	All	0.60	0/6711	0.94	19/9161 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	147	ASN	CA-C-N	6.38	125.95	119.19
1	H	147	ASN	C-N-CA	6.38	125.95	119.19
2	L	269	LEU	CA-C-N	6.01	126.17	119.32
2	L	269	LEU	C-N-CA	6.01	126.17	119.32
2	L	6	GLU	N-CA-C	5.93	117.83	111.36
3	M	107	ALA	CA-C-N	5.89	126.23	119.92
3	M	107	ALA	C-N-CA	5.89	126.23	119.92
2	L	11	VAL	N-CA-C	-5.86	104.38	109.19
1	H	132	LYS	CA-C-N	-5.60	114.02	119.78
1	H	132	LYS	C-N-CA	-5.60	114.02	119.78
3	M	113	GLY	N-CA-C	-5.53	105.95	113.37
3	M	89	LEU	N-CA-C	5.40	117.87	111.33
1	H	117	ARG	N-CA-C	-5.32	102.14	110.17
1	H	167	ILE	CB-CA-C	-5.28	103.28	110.77
2	L	13	GLY	N-CA-C	5.25	116.94	111.95
2	L	35	GLY	N-CA-C	-5.23	106.16	112.49
2	L	27	GLY	CA-C-N	5.08	124.58	119.19
2	L	27	GLY	C-N-CA	5.08	124.58	119.19
1	H	195	MET	N-CA-C	5.01	119.08	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1840	0	1845	26	0
2	L	2233	0	2189	42	0
3	M	2409	0	2323	44	0
4	H	48	0	93	5	0
4	M	80	0	155	3	0
5	L	66	0	74	3	0
5	M	198	0	222	13	0
6	L	65	0	76	6	0
6	M	65	0	76	6	0
7	L	48	0	63	5	0
7	M	48	0	63	2	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	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (124) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:TYR:O	2:L:103:ARG:NH2	2.26	0.69
6:L:402:BPH:HHC	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
3:M:140:LEU:HB2	3:M:142:MET:HE2	1.83	0.60
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.82	0.60
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
6:M:401:BPH:HBB3	6:M:401:BPH:HHC	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:N	2:L:210:ASP:OD1	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:1:ALA:C	2:L:2:LEU:HD23	2.37	0.50
2:L:266:TRP:CD2	8:L:900:DIO:H21	2.47	0.50
3:M:218:MET:HE2	7:M:501:U10:H1M1	1.94	0.50
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.47	0.49
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:H142	5:M:303:BCL:H111	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:ARG:NH1	3:M:255:THR:O	2.42	0.46
2:L:175:ILE:HG12	7:L:502:U10:H261	1.97	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:135:ARG:HB3	2:L:136:PRO:HD3	1.98	0.45
3:M:60:LEU:HA	6:M:401:BPH:H4C2	1.98	0.45
3:M:162:PHE:C	3:M:165:PRO:HD2	2.42	0.45
5:M:303:BCL:H2	6:M:401:BPH:CMB	2.46	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
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: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
7:L:502:U10:H72	7:L:502:U10:H1M3	1.82	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
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:93:ALA:HB2	6:L:402:BPH:H122	2.01	0.43
2:L:95:GLY:O	2:L:99:SER:OG	2.36	0.43
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.19	0.43
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.54	0.43
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:304:BCL:OBB	5:M:304:BCL:HHC	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
1:H:75:VAL:HA	1:H:76:PRO:C	2.45	0.42
4:M:705:LDA:H21	4:M:705:LDA:HM13	1.73	0.42
1:H:212:LEU:HA	1:H:212:LEU:HD23	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:H61	5:M:303:BCL:H102	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
1:H:231:ASP:CG	3:M:243:THR:HG22	2.46	0.41
2:L:67:TYR:HA	2:L:68:PRO:HD3	1.93	0.41
5:M:303:BCL:H2	6:M:401:BPH:HMB3	2.02	0.41
6:M:401:BPH:HBA2	6:M:401:BPH:H3A	1.82	0.41
3:M:140:LEU:HD23	3:M:140:LEU:HA	1.95	0.41
1:H:208:LEU:HD23	1:H:208:LEU:HA	1.88	0.41
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
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.56	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: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:H7C2	6:L:402:BPH:H112	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

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	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%)	186 (95%)	10 (5%)	21	54
2	L	220/220 (100%)	203 (92%)	17 (8%)	12	36
3	M	236/236 (100%)	227 (96%)	9 (4%)	29	64
All	All	652/652 (100%)	616 (94%)	36 (6%)	19	51

All (36) 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	79	GLU
1	H	149	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	197	LYS
1	H	221	SER
1	H	223	THR
1	H	224	GLU
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	82	LYS
2	L	85	LEU
2	L	126	LEU
2	L	154	LEU
2	L	158	SER
2	L	185	LEU
2	L	210	ASP
2	L	220	VAL
2	L	226	THR
2	L	247	CYS
2	L	254	ILE
3	M	10	VAL
3	M	12	VAL
3	M	60	LEU
3	M	114	LEU
3	M	144	LYS
3	M	148	TRP
3	M	247	ARG
3	M	274	VAL
3	M	292	ASP

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

Mol	Chain	Res	Type
1	H	129	ASN
2	L	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
4	LDA	M	707	-	13,15,15	2.15	2 (15%)	14,17,17	0.43	0
8	DIO	M	902	-	6,6,6	0.76	0	6,6,6	0.97	0
5	BCL	M	305	2	69,74,74	1.22	6 (8%)	79,115,115	2.35	21 (26%)
8	DIO	L	900	-	6,6,6	0.83	0	6,6,6	0.85	0
6	BPH	L	402	-	59,70,70	1.41	4 (6%)	59,101,101	2.17	16 (27%)
5	BCL	M	303	3	69,74,74	1.31	8 (11%)	79,115,115	2.27	22 (27%)
8	DIO	L	901	-	6,6,6	0.77	0	6,6,6	1.03	0
6	BPH	M	401	-	59,70,70	1.56	7 (11%)	59,101,101	1.85	13 (22%)
5	BCL	L	302	2	69,74,74	1.25	5 (7%)	79,115,115	1.99	22 (27%)
11	PO4	M	803	-	4,4,4	0.81	0	6,6,6	0.61	0
4	LDA	M	705	-	13,15,15	2.31	2 (15%)	14,17,17	0.48	0
5	BCL	M	304	3	69,74,74	1.24	6 (8%)	79,115,115	2.02	19 (24%)
7	U10	L	502	-	48,48,63	2.83	13 (27%)	60,61,79	1.74	20 (33%)
4	LDA	H	702	-	13,15,15	2.11	2 (15%)	14,17,17	0.58	0
10	SPN	M	600	-	42,42,42	1.27	7 (16%)	50,52,52	1.69	12 (24%)
4	LDA	M	701	-	13,15,15	2.08	2 (15%)	14,17,17	0.43	0
4	LDA	H	704	-	13,15,15	2.16	2 (15%)	14,17,17	0.46	0
4	LDA	M	708	-	13,15,15	2.24	2 (15%)	14,17,17	0.49	0
4	LDA	H	709	-	13,15,15	2.13	2 (15%)	14,17,17	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	U10	M	501	-	48,48,63	2.73	14 (29%)	60,61,79	1.66	14 (23%)
4	LDA	M	703	-	13,15,15	2.10	2 (15%)	14,17,17	0.46	0
11	PO4	M	801	-	4,4,4	0.58	0	6,6,6	0.82	0
11	PO4	M	800	-	4,4,4	1.17	0	6,6,6	0.55	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
4	LDA	M	707	-	-	8/13/13/13	-
8	DIO	M	902	-	-	-	0/1/1/1
5	BCL	M	305	2	-	3/41/137/137	-
8	DIO	L	900	-	-	-	0/1/1/1
6	BPH	L	402	-	2/2/18/22	12/37/105/105	0/5/6/6
5	BCL	M	303	3	-	9/41/137/137	-
8	DIO	L	901	-	-	-	0/1/1/1
6	BPH	M	401	-	2/2/18/22	9/37/105/105	0/5/6/6
5	BCL	L	302	2	-	7/41/137/137	-
4	LDA	M	705	-	-	4/13/13/13	-
5	BCL	M	304	3	-	3/41/137/137	-
7	U10	L	502	-	-	22/45/69/87	0/1/1/1
4	LDA	H	702	-	-	7/13/13/13	-
10	SPN	M	600	-	-	17/50/51/51	-
4	LDA	M	701	-	-	8/13/13/13	-
4	LDA	H	704	-	-	5/13/13/13	-
4	LDA	M	708	-	-	4/13/13/13	-
4	LDA	H	709	-	-	8/13/13/13	-
7	U10	M	501	-	-	14/45/69/87	0/1/1/1
4	LDA	M	703	-	-	9/13/13/13	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	BPH	C1D-C2D	8.80	1.49	1.39
6	L	402	BPH	C1D-C2D	7.71	1.48	1.39
7	L	502	U10	C13-C14	7.11	1.49	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	502	U10	C8-C9	7.01	1.49	1.33
7	M	501	U10	C13-C14	6.93	1.49	1.33
4	M	708	LDA	O1-N1	-6.70	1.25	1.42
7	L	502	U10	C18-C19	6.67	1.48	1.33
7	M	501	U10	C33-C34	6.64	1.48	1.33
4	M	705	LDA	O1-N1	-6.64	1.25	1.42
7	L	502	U10	C28-C29	6.62	1.48	1.33
4	M	701	LDA	O1-N1	-6.55	1.26	1.42
7	L	502	U10	C23-C24	6.53	1.48	1.33
7	L	502	U10	C33-C34	6.51	1.48	1.33
4	H	709	LDA	O1-N1	-6.44	1.26	1.42
7	M	501	U10	C18-C19	6.43	1.47	1.33
4	H	702	LDA	O1-N1	-6.42	1.26	1.42
4	M	707	LDA	O1-N1	-6.40	1.26	1.42
4	H	704	LDA	O1-N1	-6.38	1.26	1.42
4	M	703	LDA	O1-N1	-6.31	1.26	1.42
7	M	501	U10	C8-C9	6.08	1.47	1.33
7	M	501	U10	C28-C29	6.06	1.47	1.33
7	M	501	U10	C23-C24	5.73	1.46	1.33
5	L	302	BCL	MG-ND	-5.46	1.95	2.05
5	M	303	BCL	MG-ND	-5.32	1.95	2.05
7	L	502	U10	C38-C39	5.32	1.48	1.32
7	M	501	U10	C38-C39	5.27	1.48	1.32
5	M	304	BCL	MG-ND	-5.12	1.95	2.05
7	M	501	U10	O3-C3	-5.03	1.24	1.36
4	M	705	LDA	C1-N1	-4.93	1.46	1.51
7	L	502	U10	O3-C3	-4.83	1.25	1.36
5	M	305	BCL	MG-ND	-4.79	1.96	2.05
5	M	303	BCL	MG-NB	-4.76	1.96	2.05
5	M	305	BCL	MG-NB	-4.75	1.96	2.05
7	M	501	U10	O4-C4	-4.54	1.25	1.36
5	M	304	BCL	MG-NB	-4.44	1.97	2.05
4	M	708	LDA	C1-N1	-4.30	1.47	1.51
4	H	704	LDA	C1-N1	-4.27	1.47	1.51
5	L	302	BCL	MG-NB	-4.26	1.97	2.05
7	L	502	U10	O4-C4	-4.20	1.26	1.36
4	M	707	LDA	C1-N1	-4.18	1.47	1.51
6	L	402	BPH	C4D-CHA	-4.10	1.33	1.39
4	H	709	LDA	C1-N1	-4.03	1.47	1.51
4	M	703	LDA	C1-N1	-3.96	1.47	1.51
4	H	702	LDA	C1-N1	-3.93	1.47	1.51
5	M	305	BCL	C1D-C2D	-3.66	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	BCL	C1D-C2D	-3.53	1.38	1.45
5	M	303	BCL	C1D-C2D	-3.45	1.38	1.45
5	M	304	BCL	C1D-C2D	-3.33	1.38	1.45
4	M	701	LDA	C1-N1	-3.30	1.48	1.51
10	M	600	SPN	C1-C2	-3.20	1.50	1.53
6	M	401	BPH	C4D-CHA	-3.07	1.35	1.39
10	M	600	SPN	C25-C26	3.07	1.40	1.33
10	M	600	SPN	C8-C9	2.85	1.39	1.33
7	L	502	U10	C3-C2	-2.81	1.40	1.48
7	M	501	U10	C4-C5	-2.74	1.40	1.48
6	L	402	BPH	C3D-C2D	-2.71	1.35	1.39
10	M	600	SPN	C19-C18	2.69	1.39	1.33
7	L	502	U10	C6-C1	2.68	1.40	1.35
7	M	501	U10	C3-C2	-2.66	1.41	1.48
5	M	305	BCL	C4B-NB	2.64	1.41	1.37
5	L	302	BCL	C4B-NB	2.62	1.41	1.37
5	M	305	BCL	MG-NA	-2.61	2.00	2.06
7	L	502	U10	C4-C5	-2.60	1.41	1.48
7	M	501	U10	C1-C2	-2.55	1.38	1.47
5	M	303	BCL	C1B-NB	2.53	1.41	1.37
5	M	304	BCL	C1B-C2B	-2.53	1.37	1.43
6	M	401	BPH	CBD-CGD	-2.52	1.49	1.52
6	M	401	BPH	C4D-ND	-2.49	1.34	1.38
5	M	303	BCL	MG-NA	-2.49	2.00	2.06
10	M	600	SPN	C3-C2	-2.45	1.50	1.52
7	M	501	U10	C6-C1	2.42	1.39	1.35
6	M	401	BPH	C3D-C2D	-2.41	1.35	1.39
5	M	303	BCL	C1B-C2B	-2.39	1.37	1.43
5	M	304	BCL	C4B-NB	2.39	1.41	1.37
7	M	501	U10	C6-C5	-2.31	1.40	1.46
6	M	401	BPH	C3D-C4D	2.30	1.44	1.41
5	L	302	BCL	C1B-C2B	-2.29	1.37	1.43
10	M	600	SPN	C12-C13	2.25	1.38	1.33
5	M	303	BCL	C4B-NB	2.25	1.40	1.37
5	M	304	BCL	C1B-NB	2.24	1.40	1.37
6	L	402	BPH	C4D-ND	-2.20	1.35	1.38
7	L	502	U10	C1-C2	-2.17	1.39	1.47
5	M	303	BCL	MG-NC	-2.09	2.01	2.06
10	M	600	SPN	C4-C5	2.06	1.37	1.33
6	M	401	BPH	CMB-C2B	-2.03	1.47	1.51
5	M	305	BCL	C1B-C2B	-2.03	1.38	1.43

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	BCL	C1D-ND-C4D	-11.63	98.15	106.31
5	M	305	BCL	C1D-ND-C4D	-11.31	98.38	106.31
5	M	304	BCL	C1D-ND-C4D	-9.13	99.91	106.31
5	L	302	BCL	C1D-ND-C4D	-8.93	100.05	106.31
6	L	402	BPH	C4D-CHA-CBD	8.90	112.72	108.45
5	M	305	BCL	O2D-CGD-CBD	7.70	124.68	111.23
6	M	401	BPH	C2D-C1D-ND	-6.47	104.75	109.43
5	M	303	BCL	C2D-C1D-ND	5.87	115.93	110.13
6	M	401	BPH	C4D-CHA-CBD	5.77	111.22	108.45
6	L	402	BPH	C2D-C1D-ND	-5.48	105.47	109.43
5	M	305	BCL	C2D-C1D-ND	5.23	115.30	110.13
5	M	303	BCL	C1C-NC-C4C	5.17	109.04	106.68
10	M	600	SPN	C3-C4-C5	-5.12	118.00	126.83
5	M	304	BCL	O2D-CGD-CBD	5.12	120.18	111.23
6	L	402	BPH	C1A-C2A-C3A	-5.12	97.97	102.84
6	L	402	BPH	C2B-C1B-NB	-4.75	106.00	109.43
5	M	305	BCL	C1C-NC-C4C	4.71	108.83	106.68
5	M	305	BCL	C4A-NA-C1A	4.52	108.74	106.68
7	M	501	U10	C32-C33-C34	-4.26	117.86	127.62
6	L	402	BPH	C4C-C3C-C2C	-4.23	98.81	102.84
7	L	502	U10	C7-C6-C1	-4.03	117.98	124.89
5	L	302	BCL	CHD-C1D-ND	-4.00	119.18	124.80
7	M	501	U10	C22-C23-C24	-4.00	118.48	127.62
5	L	302	BCL	C1C-NC-C4C	3.98	108.49	106.68
5	M	303	BCL	C3D-C4D-ND	3.97	116.44	109.99
5	M	304	BCL	C1C-NC-C4C	3.94	108.47	106.68
5	M	303	BCL	O2D-CGD-CBD	3.89	118.03	111.23
5	M	303	BCL	C4-C3-C5	3.84	121.90	115.23
5	M	304	BCL	C2D-C1D-ND	3.75	113.83	110.13
7	L	502	U10	O5-C5-C4	-3.74	113.10	121.03
5	M	305	BCL	O2D-CGD-O1D	-3.73	116.58	123.85
6	L	402	BPH	OBB-CAB-C3B	3.71	126.18	119.99
5	M	305	BCL	C3D-C4D-ND	3.70	116.00	109.99
5	M	303	BCL	C3A-C2A-C1A	-3.65	95.87	101.34
5	L	302	BCL	C2D-C1D-ND	3.65	113.74	110.13
5	M	303	BCL	CHD-C1D-ND	-3.61	119.73	124.80
5	M	304	BCL	CHD-C1D-ND	-3.52	119.85	124.80
7	M	501	U10	C30-C29-C31	3.48	121.27	115.23
6	M	401	BPH	C2B-C1B-NB	-3.47	106.92	109.43
7	M	501	U10	C35-C34-C36	3.45	121.21	115.23
6	M	401	BPH	C6-C5-C3	3.45	121.86	113.47
5	M	304	BCL	CHB-C4A-NA	3.40	129.31	124.40
5	M	305	BCL	CHD-C1D-ND	-3.40	120.02	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	502	U10	C7-C6-C5	3.39	122.45	118.52
10	M	600	SPN	C7-C8-C9	-3.36	119.94	127.62
5	M	304	BCL	O2D-CGD-O1D	-3.33	117.37	123.85
5	M	304	BCL	C3D-C4D-ND	3.32	115.39	109.99
5	L	302	BCL	CED-O2D-CGD	3.28	123.36	115.92
5	M	304	BCL	C1-C2-C3	-3.27	120.84	126.20
5	M	305	BCL	O2A-CGA-CBA	3.21	121.61	111.83
5	M	303	BCL	O1D-CGD-CBD	-3.18	118.24	124.52
7	M	501	U10	C17-C18-C19	-3.18	120.34	127.62
6	M	401	BPH	OBB-CAB-C3B	3.17	125.29	119.99
10	M	600	SPN	CM3-C5-C6	3.15	120.70	115.23
5	L	302	BCL	C4-C3-C5	3.14	120.69	115.23
6	M	401	BPH	C4D-ND-C1D	3.11	112.60	108.87
5	L	302	BCL	CHC-C4B-NB	-3.05	119.47	124.05
10	M	600	SPN	C24-C25-C26	-3.03	120.70	127.62
6	L	402	BPH	CMC-C2C-C1C	-3.01	108.13	114.61
7	M	501	U10	C25-C24-C26	3.01	120.45	115.23
6	M	401	BPH	C1A-C2A-C3A	-3.00	99.98	102.84
5	L	302	BCL	C3D-C4D-ND	3.00	114.86	109.99
7	L	502	U10	C22-C23-C24	-2.99	120.77	127.62
5	M	305	BCL	O1D-CGD-CBD	-2.94	118.72	124.52
6	M	401	BPH	CMD-C2D-C3D	2.93	130.54	124.68
7	M	501	U10	C12-C13-C14	-2.92	120.93	127.62
5	M	304	BCL	CAA-C2A-C3A	-2.90	105.15	113.00
6	M	401	BPH	C1C-C2C-C3C	-2.90	100.08	102.84
6	L	402	BPH	C6-C5-C3	2.89	120.52	113.47
5	M	305	BCL	CHB-C4A-NA	2.88	128.56	124.40
5	M	303	BCL	CHB-C4A-NA	2.87	128.55	124.40
6	L	402	BPH	OBB-CAB-CBB	-2.86	114.09	120.19
7	L	502	U10	C17-C18-C19	-2.85	121.10	127.62
7	L	502	U10	C32-C33-C34	-2.84	121.11	127.62
5	M	304	BCL	C4A-NA-C1A	2.82	107.97	106.68
5	M	305	BCL	CHB-C1B-NB	-2.82	119.82	124.05
5	M	303	BCL	C6-C5-C3	-2.81	106.62	113.47
5	L	302	BCL	CMD-C2D-C1D	2.81	129.67	124.73
5	M	304	BCL	O2A-CGA-CBA	2.80	120.36	111.83
5	L	302	BCL	O2D-CGD-CBD	2.79	116.11	111.23
10	M	600	SPN	C20-C19-C18	-2.78	121.25	127.62
5	M	303	BCL	CBB-CAB-C3B	2.78	126.26	120.40
5	L	302	BCL	O2A-CGA-CBA	2.77	120.28	111.83
5	M	305	BCL	C3C-C4C-CHD	-2.74	117.62	123.39
10	M	600	SPN	CM6-C18-C17	2.71	119.93	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	304	BCL	CGD-CBD-CAD	-2.70	102.11	110.85
5	L	302	BCL	C1-C2-C3	-2.70	121.78	126.20
5	M	303	BCL	O2A-CGA-CBA	2.60	119.76	111.83
7	L	502	U10	C20-C19-C21	2.60	119.73	115.23
5	M	305	BCL	C11-C12-C13	-2.57	107.42	115.97
5	M	304	BCL	C4-C3-C5	2.55	119.66	115.23
6	M	401	BPH	OBB-CAB-CBB	-2.54	114.77	120.19
7	L	502	U10	C27-C28-C29	-2.53	121.82	127.62
5	L	302	BCL	C7-C6-C5	-2.51	106.58	113.26
7	M	501	U10	C15-C14-C16	2.49	119.55	115.23
7	L	502	U10	C35-C34-C36	2.48	119.54	115.23
7	M	501	U10	C27-C28-C29	-2.48	121.95	127.62
6	L	402	BPH	C1C-C2C-C3C	-2.48	100.48	102.84
6	L	402	BPH	C1-O2A-CGA	-2.48	110.65	116.65
7	L	502	U10	C4M-O4-C4	2.47	125.16	116.47
7	L	502	U10	C25-C24-C26	2.46	119.49	115.23
10	M	600	SPN	C11-C12-C13	-2.44	122.03	127.62
5	M	305	BCL	C6-C5-C3	-2.44	107.53	113.47
5	M	304	BCL	CHC-C4B-NB	-2.43	120.41	124.05
7	L	502	U10	C1M-C1-C6	-2.42	120.47	124.45
7	L	502	U10	C3M-O3-C3	2.41	124.94	116.47
5	M	303	BCL	C1-C2-C3	-2.41	122.25	126.20
5	M	303	BCL	C3C-C4C-CHD	-2.39	118.34	123.39
5	M	305	BCL	O2A-CGA-O1A	-2.39	117.65	123.63
5	M	303	BCL	CBC-CAC-C3C	-2.38	108.36	113.41
5	M	305	BCL	C4D-CHA-C1A	-2.38	118.41	121.24
7	L	502	U10	C30-C29-C31	2.38	119.35	115.23
10	M	600	SPN	CMA-O1-C1	2.38	126.25	114.23
5	M	303	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
7	M	501	U10	C4M-O4-C4	2.37	124.79	116.47
6	M	401	BPH	CMA-C3A-C4A	-2.34	109.58	114.61
7	L	502	U10	O2-C2-C3	-2.32	116.12	121.03
7	M	501	U10	C22-C21-C19	-2.31	105.53	113.19
5	M	305	BCL	C4-C3-C5	2.31	119.24	115.23
5	M	304	BCL	CBC-CAC-C3C	-2.31	108.52	113.41
7	L	502	U10	O5-C5-C6	-2.30	117.33	121.79
6	M	401	BPH	C4C-C3C-C2C	-2.30	100.65	102.84
6	L	402	BPH	CMD-C2D-C3D	2.30	129.27	124.68
5	L	302	BCL	C11-C10-C8	-2.29	108.35	115.97
5	L	302	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
10	M	600	SPN	C7-C6-C5	2.27	120.71	113.19
5	M	305	BCL	C16-C15-C13	-2.26	108.46	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	BCL	OBB-CAB-CBB	-2.25	114.73	119.77
5	L	302	BCL	C11-C12-C13	-2.23	108.55	115.97
6	L	402	BPH	CMA-C3A-C4A	-2.23	109.81	114.61
5	L	302	BCL	CMD-C2D-C3D	-2.22	122.59	127.69
5	M	303	BCL	O2A-CGA-O1A	-2.22	118.08	123.63
5	L	302	BCL	C1-O2A-CGA	2.20	121.98	116.65
5	L	302	BCL	C3C-C4C-CHD	-2.19	118.78	123.39
7	L	502	U10	C8-C7-C6	2.18	117.45	112.08
7	M	501	U10	C25-C24-C23	-2.16	118.07	123.63
5	L	302	BCL	CHB-C4A-NA	2.16	127.52	124.40
5	M	303	BCL	CHC-C4B-NB	-2.16	120.80	124.05
5	M	304	BCL	C2B-C1B-NB	2.16	112.57	110.33
10	M	600	SPN	CM5-C13-C14	2.16	118.97	115.23
6	L	402	BPH	C4-C3-C5	-2.16	111.48	115.23
5	M	305	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
6	M	401	BPH	O1D-CGD-CBD	-2.14	121.48	124.72
10	M	600	SPN	O1-C1-C2	-2.13	104.54	108.90
10	M	600	SPN	C28-C29-C30	-2.13	120.53	127.64
7	L	502	U10	C41-C39-C40	2.12	119.48	114.59
5	M	303	BCL	C11-C12-C13	-2.12	108.92	115.97
5	M	304	BCL	C11-C10-C8	-2.10	109.00	115.97
5	L	302	BCL	O2A-CGA-O1A	-2.10	118.39	123.63
5	L	302	BCL	CBB-CAB-C3B	2.08	124.79	120.40
6	L	402	BPH	C4D-ND-C1D	2.08	111.36	108.87
7	L	502	U10	C37-C38-C39	-2.06	120.76	127.64
7	M	501	U10	C10-C9-C11	2.06	118.81	115.23
6	L	402	BPH	O2D-CGD-CBD	2.05	113.20	110.95
5	M	305	BCL	C1-C2-C3	-2.05	122.84	126.20
7	L	502	U10	C7-C8-C9	-2.05	123.30	126.83
5	M	304	BCL	C1D-CHD-C4C	-2.04	121.70	126.62
7	M	501	U10	C41-C39-C40	2.03	119.27	114.59
5	M	303	BCL	CMA-C3A-C4A	-2.01	106.36	111.77

All (4) chirality outliers are listed below:

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

All (149) 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	H	709	LDA	C2-C1-N1-O1
4	H	709	LDA	C2-C1-N1-CM1
4	H	709	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	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
4	M	707	LDA	C2-C1-N1-O1
4	M	707	LDA	C2-C1-N1-CM1
4	M	707	LDA	C2-C1-N1-CM2
4	M	708	LDA	C2-C1-N1-CM1
6	L	402	BPH	C14-C13-C15-C16
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	M	501	U10	C27-C28-C29-C30
7	M	501	U10	C32-C33-C34-C35
7	M	501	U10	C32-C33-C34-C36
10	M	600	SPN	CM1-C1-C2-C3
10	M	600	SPN	C28-C29-C30-CMB
6	M	401	BPH	C4-C3-C5-C6
10	M	600	SPN	CM5-C13-C14-C15
10	M	600	SPN	C4-C5-C6-C7
10	M	600	SPN	C11-C10-C9-C8
10	M	600	SPN	C12-C13-C14-C15
7	M	501	U10	C27-C28-C29-C31
4	M	703	LDA	C1-C2-C3-C4
7	M	501	U10	C37-C38-C39-C40
10	M	600	SPN	CM3-C5-C6-C7
10	M	600	SPN	C11-C10-C9-CM4
6	M	401	BPH	C2-C3-C5-C6
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	L	502	U10	C34-C36-C37-C38
7	M	501	U10	C29-C31-C32-C33
10	M	600	SPN	CM6-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	502	U10	C12-C11-C9-C10
10	M	600	SPN	C16-C17-C18-CM6
7	L	502	U10	C12-C11-C9-C8
10	M	600	SPN	C14-C15-C16-C17
7	M	501	U10	C37-C38-C39-C41
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	H	704	LDA	C4-C5-C6-C7
5	L	302	BCL	C15-C16-C17-C18
4	M	705	LDA	C3-C4-C5-C6
4	M	705	LDA	C5-C6-C7-C8
4	H	704	LDA	C2-C3-C4-C5
4	H	709	LDA	C4-C5-C6-C7
4	M	707	LDA	C7-C8-C9-C10
6	L	402	BPH	C11-C10-C8-C7
6	L	402	BPH	C11-C12-C13-C15
6	M	401	BPH	C3-C5-C6-C7
4	M	701	LDA	C1-C2-C3-C4
6	M	401	BPH	CBA-CGA-O2A-C1
4	M	703	LDA	C11-C10-C9-C8
4	M	707	LDA	C1-C2-C3-C4
4	M	707	LDA	C4-C5-C6-C7
4	M	703	LDA	C7-C8-C9-C10
7	L	502	U10	C37-C38-C39-C41
4	H	704	LDA	C7-C8-C9-C10
4	H	704	LDA	C5-C6-C7-C8
4	M	708	LDA	C5-C6-C7-C8
4	H	702	LDA	C7-C8-C9-C10
6	M	401	BPH	O1A-CGA-O2A-C1
5	M	304	BCL	C2C-C3C-CAC-CBC
4	M	708	LDA	C1-C2-C3-C4
6	M	401	BPH	CBD-CGD-O2D-CED
6	L	402	BPH	C4-C3-C5-C6
5	M	303	BCL	C11-C10-C8-C9
6	L	402	BPH	C2-C3-C5-C6
4	M	707	LDA	C5-C6-C7-C8
7	L	502	U10	C35-C34-C36-C37
5	M	303	BCL	C11-C10-C8-C7
4	M	703	LDA	C6-C7-C8-C9
4	M	703	LDA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	M	305	BCL	C16-C17-C18-C19
7	L	502	U10	C33-C34-C36-C37
5	M	305	BCL	C16-C17-C18-C20
4	H	702	LDA	C9-C10-C11-C12
10	M	600	SPN	C28-C29-C30-CM9
4	H	709	LDA	C3-C4-C5-C6
4	M	705	LDA	C1-C2-C3-C4
7	M	501	U10	C24-C26-C27-C28
4	M	707	LDA	C9-C10-C11-C12
5	L	302	BCL	C13-C15-C16-C17
6	L	402	BPH	C12-C13-C15-C16
4	M	703	LDA	C3-C4-C5-C6
4	H	709	LDA	C9-C10-C11-C12
6	M	401	BPH	C15-C16-C17-C18
5	L	302	BCL	CBD-CGD-O2D-CED
5	M	303	BCL	C1A-C2A-CAA-CBA
6	M	401	BPH	O1D-CGD-O2D-CED
7	L	502	U10	C5-C4-O4-C4M
5	L	302	BCL	C16-C17-C18-C19
6	L	402	BPH	C8-C10-C11-C12
5	L	302	BCL	C16-C17-C18-C20
4	M	701	LDA	C9-C10-C11-C12
10	M	600	SPN	C19-C20-C21-C22
4	H	702	LDA	C2-C3-C4-C5
4	M	708	LDA	N1-C1-C2-C3
4	M	701	LDA	C6-C7-C8-C9
4	H	709	LDA	C1-C2-C3-C4
7	L	502	U10	C14-C16-C17-C18
6	L	402	BPH	C11-C10-C8-C9
7	M	501	U10	C25-C24-C26-C27
4	H	704	LDA	C1-C2-C3-C4
7	L	502	U10	C20-C19-C21-C22
7	L	502	U10	C25-C24-C26-C27
5	M	303	BCL	C2-C3-C5-C6
7	M	501	U10	C23-C24-C26-C27
5	M	303	BCL	C10-C11-C12-C13
5	M	303	BCL	C4-C3-C5-C6
4	H	709	LDA	C5-C6-C7-C8
7	M	501	U10	C5-C4-O4-C4M
5	M	304	BCL	C3A-C2A-CAA-CBA
7	L	502	U10	C23-C24-C26-C27
5	L	302	BCL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

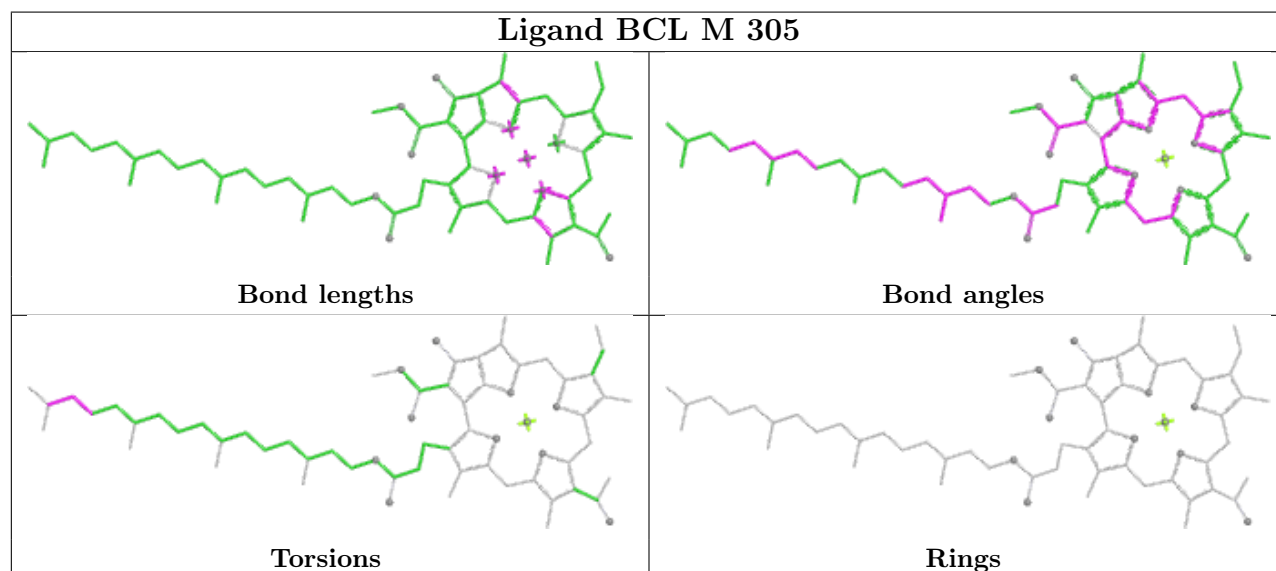
Mol	Chain	Res	Type	Atoms
6	L	402	BPH	O2A-C1-C2-C3
4	M	705	LDA	C2-C3-C4-C5
6	L	402	BPH	C16-C17-C18-C19
7	M	501	U10	C3-C4-O4-C4M
10	M	600	SPN	C21-C22-C23-C24
5	M	303	BCL	C2-C1-O2A-CGA
7	M	501	U10	C28-C29-C31-C32
10	M	600	SPN	C25-C26-C27-C28
7	L	502	U10	C30-C29-C31-C32
5	M	304	BCL	C1A-C2A-CAA-CBA
7	L	502	U10	C2-C3-O3-C3M
7	L	502	U10	C18-C19-C21-C22
5	M	303	BCL	C6-C7-C8-C10
4	H	702	LDA	C5-C6-C7-C8
5	L	302	BCL	C2A-CAA-CBA-CGA
7	L	502	U10	C36-C37-C38-C39
7	M	501	U10	C16-C17-C18-C19
6	L	402	BPH	C5-C6-C7-C8
10	M	600	SPN	CM1-C1-C2-O2
5	M	303	BCL	C8-C10-C11-C12
4	M	701	LDA	C11-C10-C9-C8
6	M	401	BPH	C5-C6-C7-C8

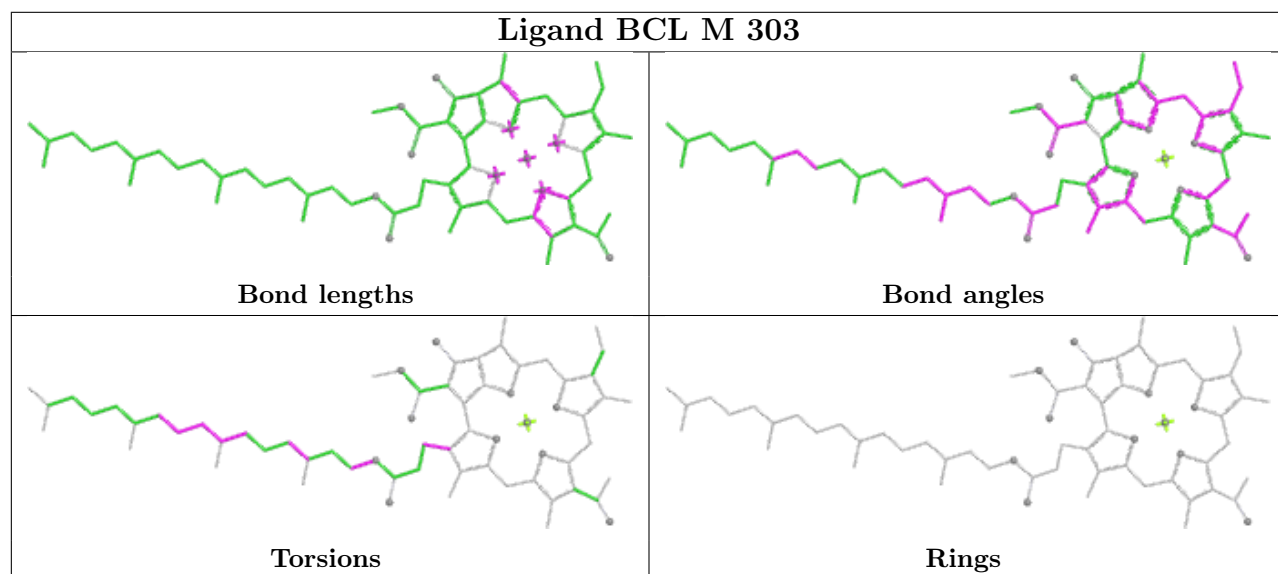
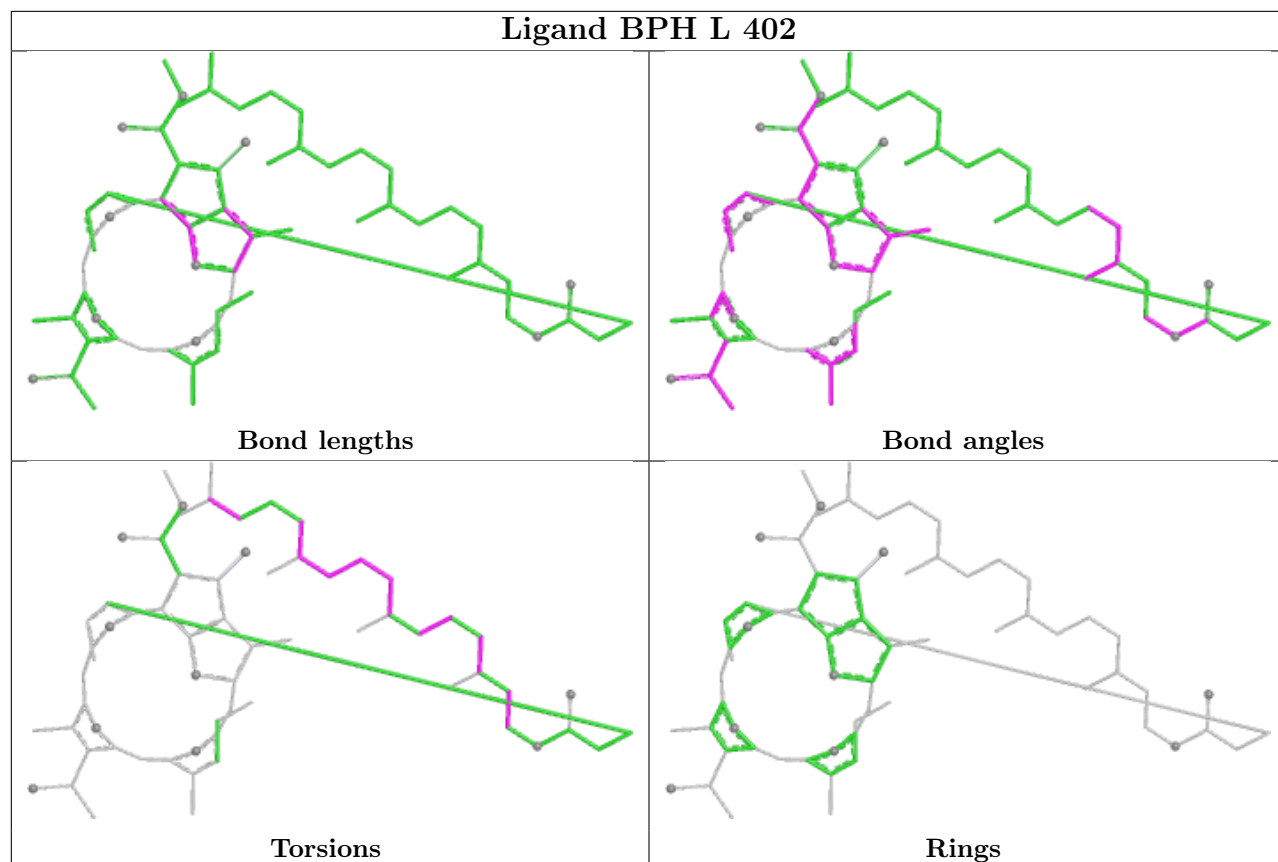
There are no ring outliers.

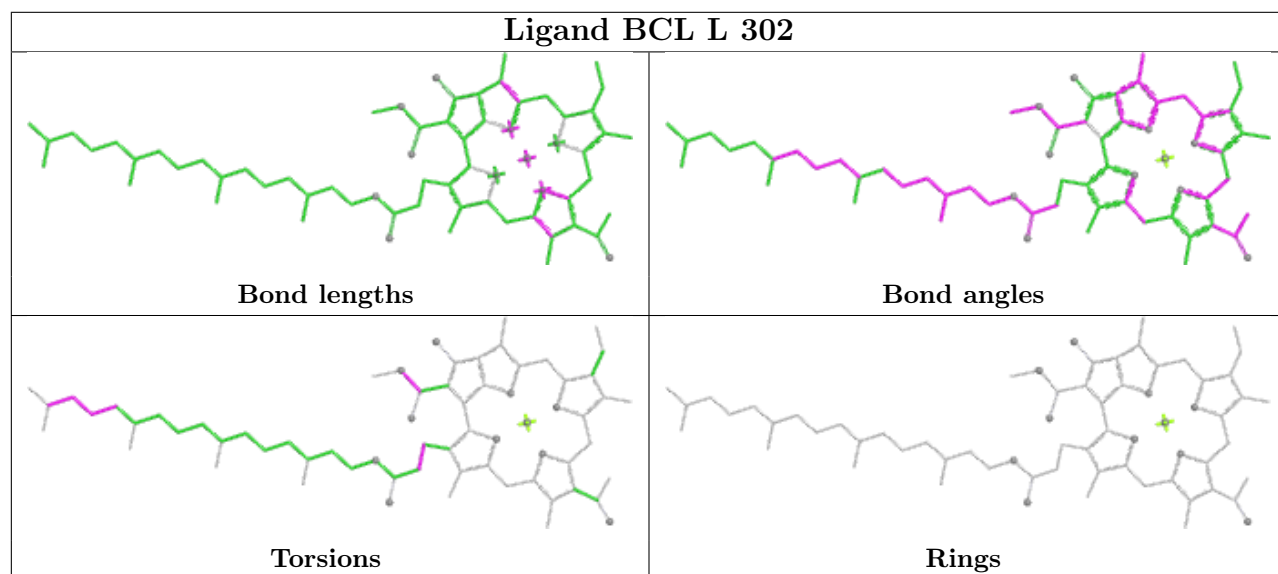
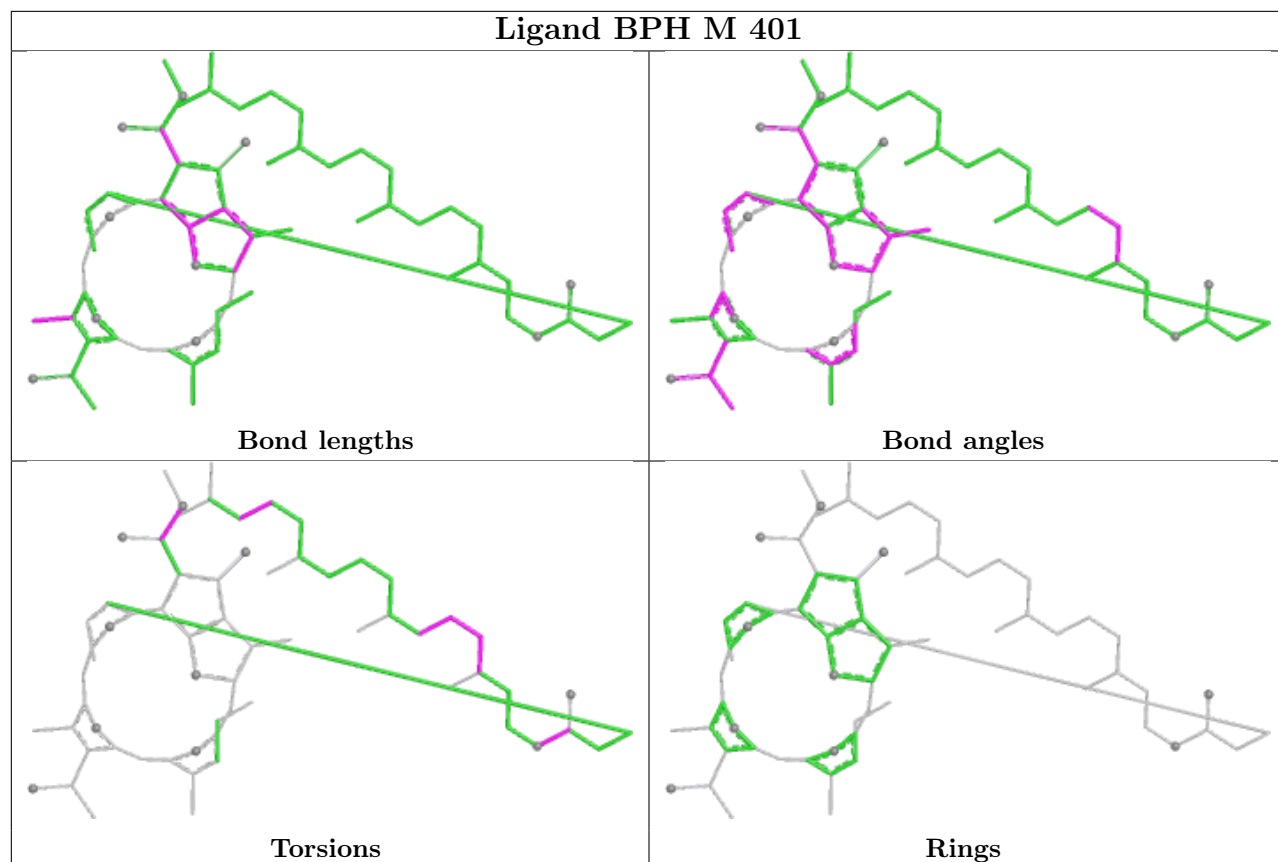
15 monomers are involved in 42 short contacts:

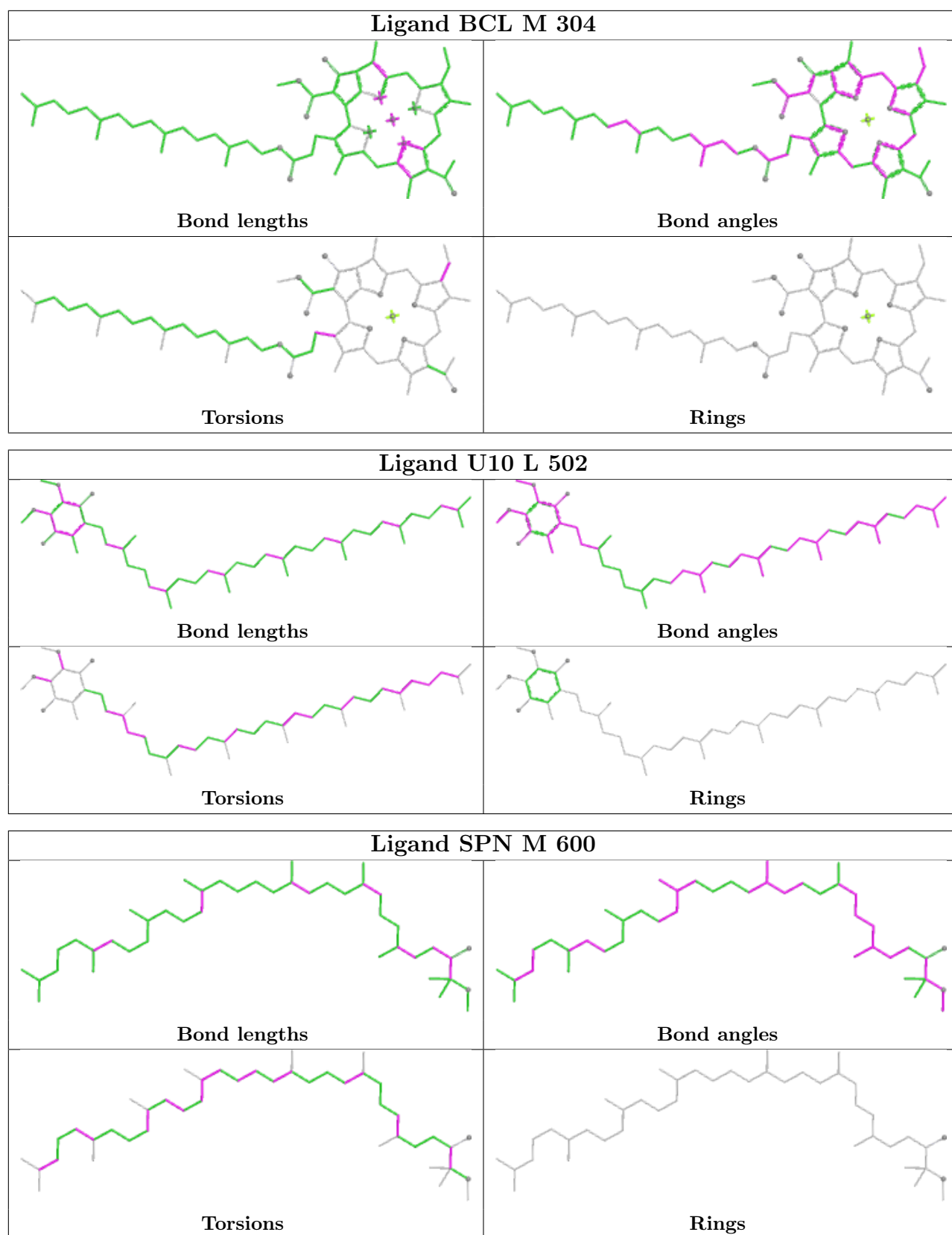
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	305	BCL	1	0
8	L	900	DIO	2	0
6	L	402	BPH	6	0
5	M	303	BCL	8	0
6	M	401	BPH	6	0
5	L	302	BCL	3	0
4	M	705	LDA	1	0
5	M	304	BCL	5	0
7	L	502	U10	5	0
4	H	702	LDA	3	0
10	M	600	SPN	6	0
4	M	701	LDA	1	0
4	H	704	LDA	2	0
7	M	501	U10	2	0
4	M	703	LDA	1	0

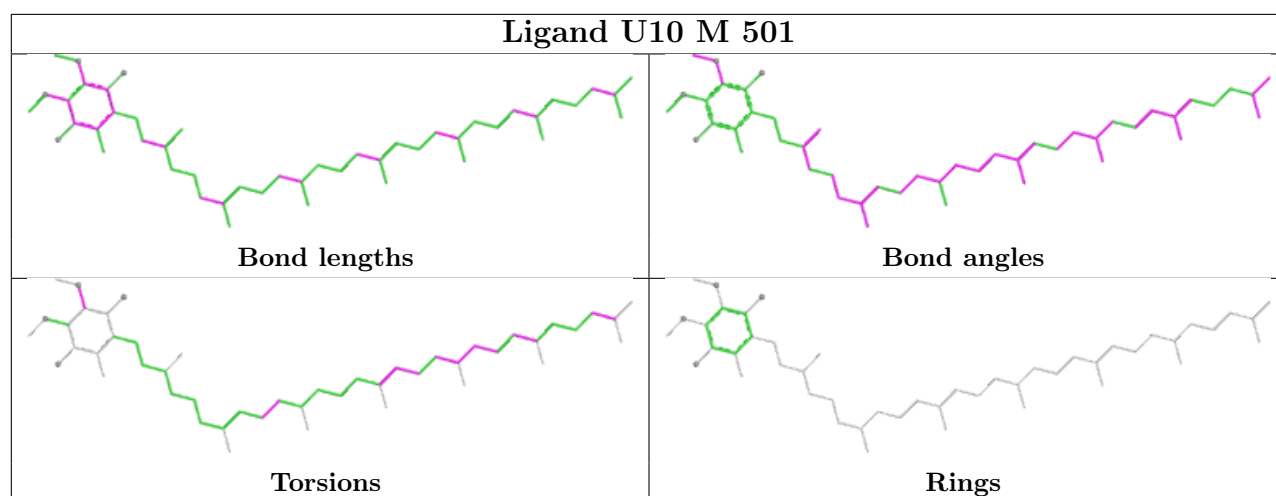
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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%)	-0.06	3 (1%) 76 68	19, 35, 54, 102	0
2	L	281/281 (100%)	0.23	10 (3%) 46 37	20, 36, 70, 94	0
3	M	302/302 (100%)	0.08	4 (1%) 75 66	21, 39, 65, 82	0
All	All	824/824 (100%)	0.09	17 (2%) 63 54	19, 36, 65, 102	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	4.9
2	L	56	GLN	4.2
1	H	250	SER	3.8
2	L	57	GLY	3.6
1	H	10	PHE	3.3
2	L	82	LYS	3.3
2	L	58	THR	3.3
2	L	55	LEU	3.1
2	L	50	ALA	2.9
3	M	115	TRP	2.7
1	H	245	ALA	2.6
2	L	172	ALA	2.5
3	M	1	ALA	2.4
2	L	72	GLU	2.2
3	M	300	ASN	2.2
3	M	105	PHE	2.1
2	L	268	LYS	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

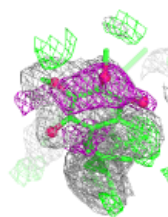
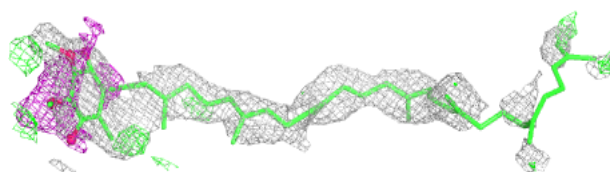
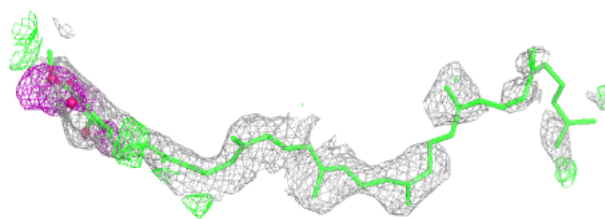
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	PO4	M	801	5/5	0.56	0.24	54,68,85,101	0
7	U10	L	502	48/63	0.61	0.28	31,64,107,115	0
4	LDA	M	708	16/16	0.65	0.23	35,64,90,93	0
4	LDA	M	707	16/16	0.73	0.19	42,59,91,96	0
4	LDA	M	705	16/16	0.75	0.21	36,50,81,81	0
4	LDA	M	703	16/16	0.78	0.20	38,49,69,73	0
4	LDA	H	704	16/16	0.78	0.22	40,50,73,75	0
8	DIO	L	901	6/6	0.80	0.19	46,48,53,58	0
8	DIO	M	902	6/6	0.81	0.30	45,53,62,68	0
4	LDA	H	702	16/16	0.83	0.18	46,59,70,73	0
4	LDA	H	709	16/16	0.84	0.15	32,57,87,89	0
11	PO4	M	803	5/5	0.84	0.08	66,72,79,87	0
4	LDA	M	701	16/16	0.85	0.17	21,41,51,55	0
8	DIO	L	900	6/6	0.87	0.17	51,55,63,70	0
10	SPN	M	600	43/43	0.90	0.15	29,49,77,87	0
7	U10	M	501	48/63	0.91	0.12	19,30,50,61	0
12	CL	M	306	1/1	0.91	0.09	50,50,50,50	0
6	BPH	M	401	65/65	0.92	0.12	23,32,93,104	0
5	BCL	M	303	66/66	0.92	0.11	20,29,53,63	0
5	BCL	M	304	66/66	0.93	0.11	22,30,43,60	0
5	BCL	M	305	66/66	0.93	0.09	21,26,38,52	0
5	BCL	L	302	66/66	0.93	0.10	21,29,38,55	0
6	BPH	L	402	65/65	0.94	0.10	14,28,39,42	0
11	PO4	M	800	5/5	0.97	0.06	24,33,44,47	0
9	FE	M	500	1/1	0.99	0.04	24,24,24,24	0

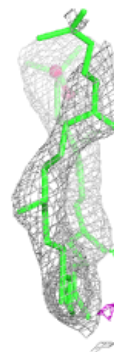
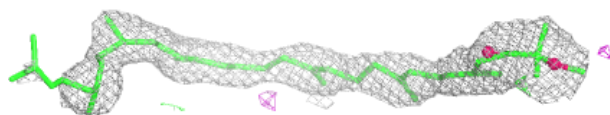
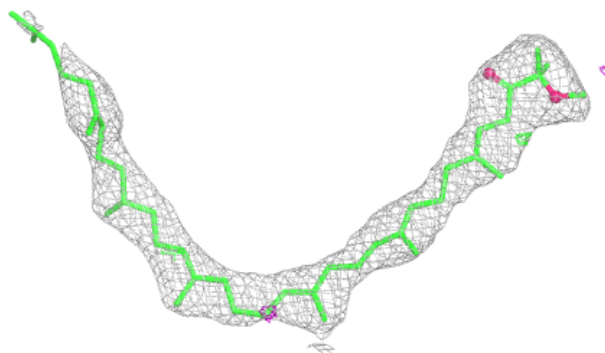
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

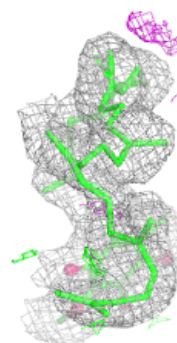
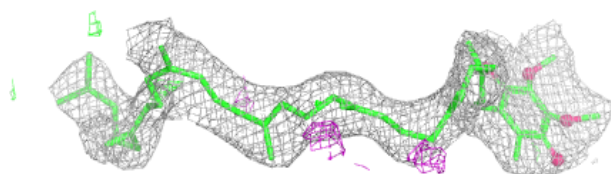
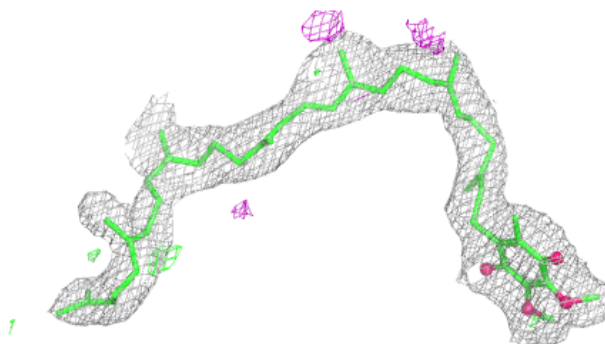
**Electron density around SPN M 600:**

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

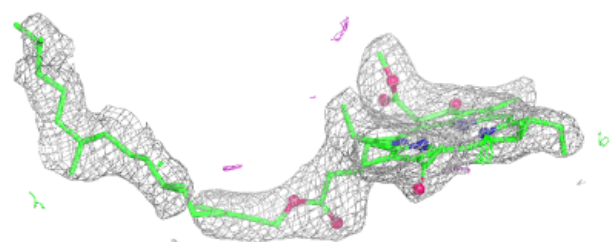
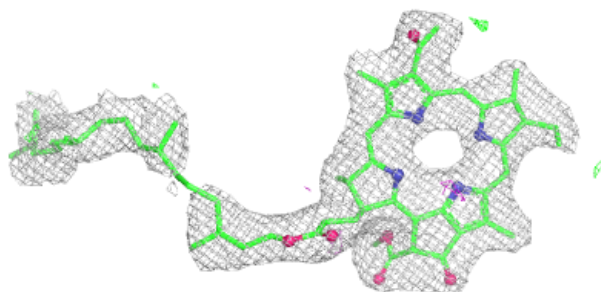


Electron density around U10 M 501:

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

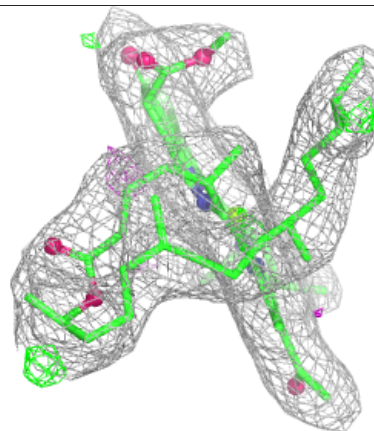
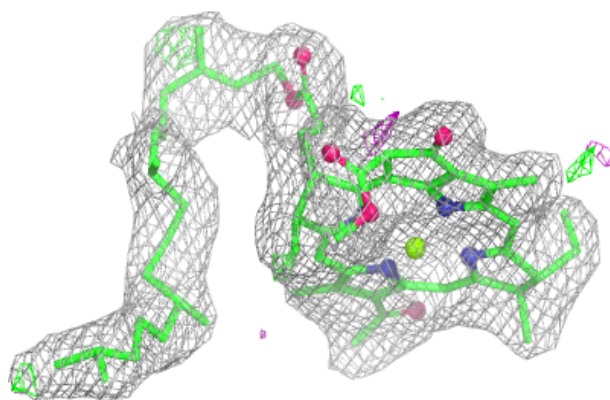
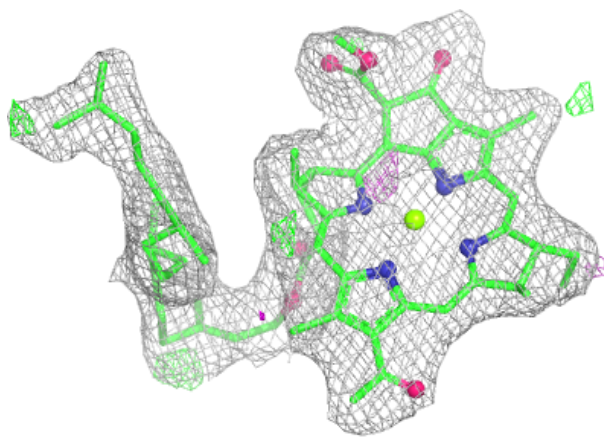
**Electron density around BPH M 401:**

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



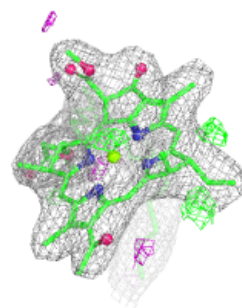
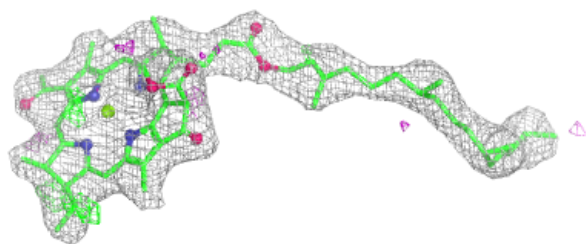
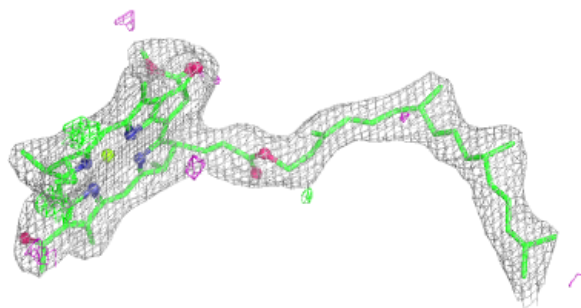
Electron density around BCL M 303:

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

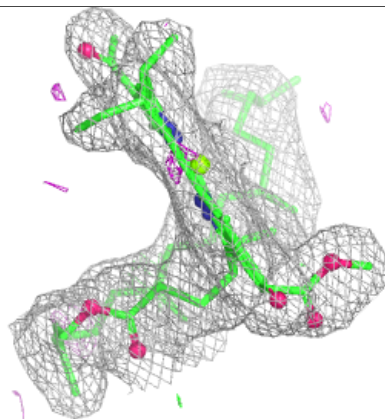
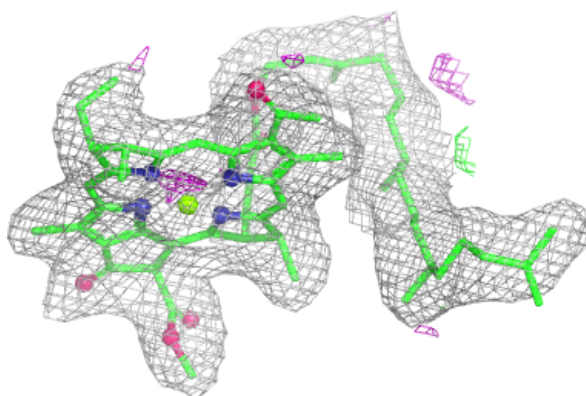
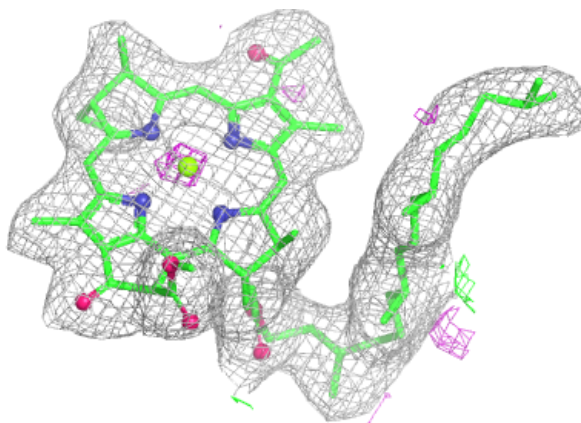


Electron density around BCL M 304:

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

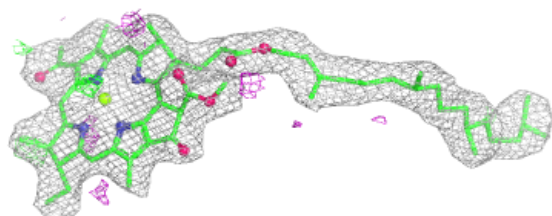
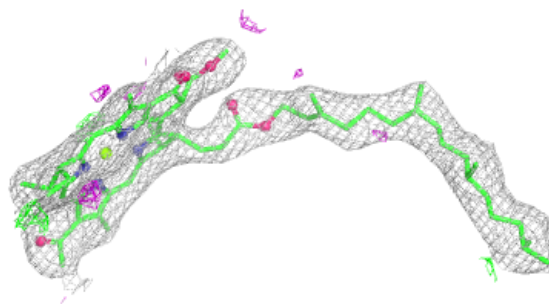
**Electron density around BCL M 305:**

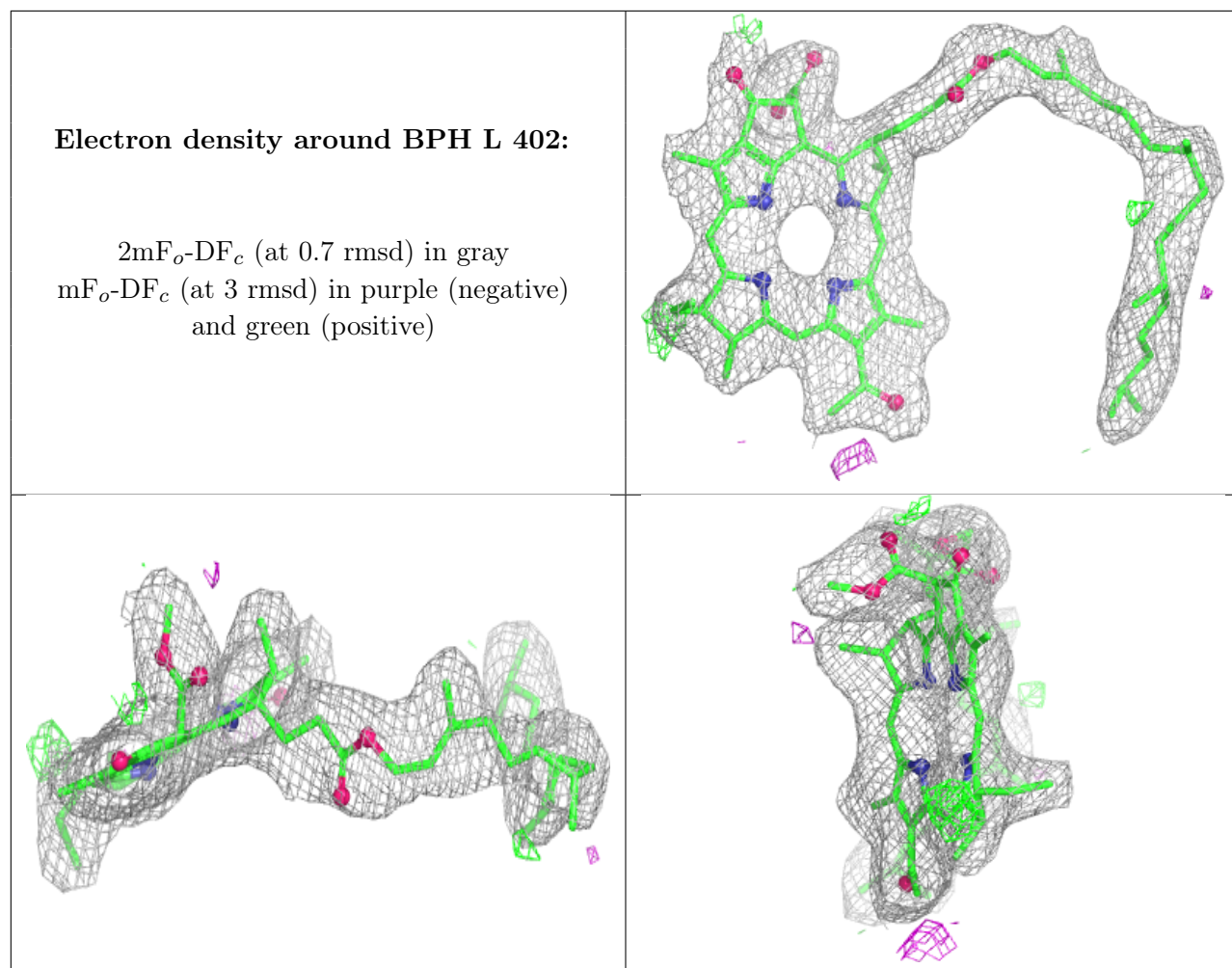
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL L 302:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.