



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:07 AM UTC

PDB ID : 2GMR / pdb_00002gmr
Title : Photosynthetic reaction center mutant from Rhodobacter sphaeroides with Asp L210 replaced with Asn
Authors : Stachnik, J.M.; Hermes, S.; Gerwert, K.; Hofmann, E.
Deposited on : 2006-04-07
Resolution : 2.50 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

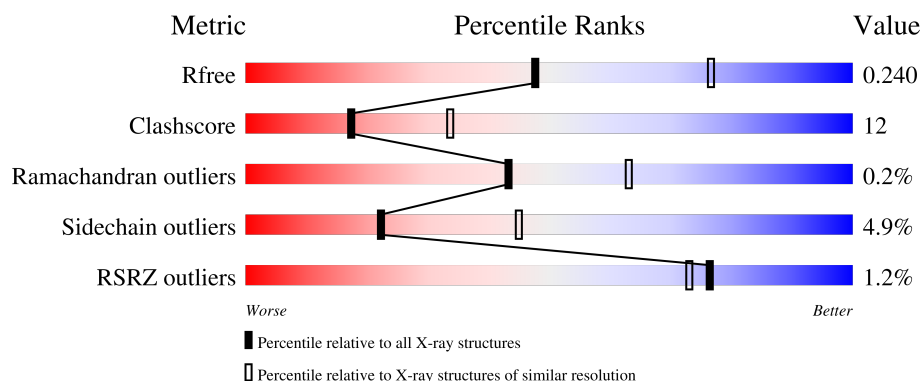
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

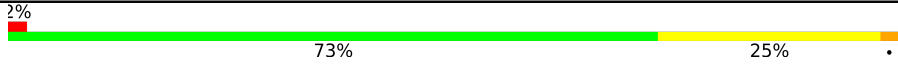
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	L	281	
2	M	307	
3	H	260	

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
4	BCL	L	301	X	-	-	-
5	BPH	L	305	X	-	-	-
5	BPH	M	310	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7286 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 Photosynthetic Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	280	Total	C	N	O	S	0	0	0
			2227	1505	355	359	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	210	ASN	ASP	engineered mutation	UNP Q3J1A5

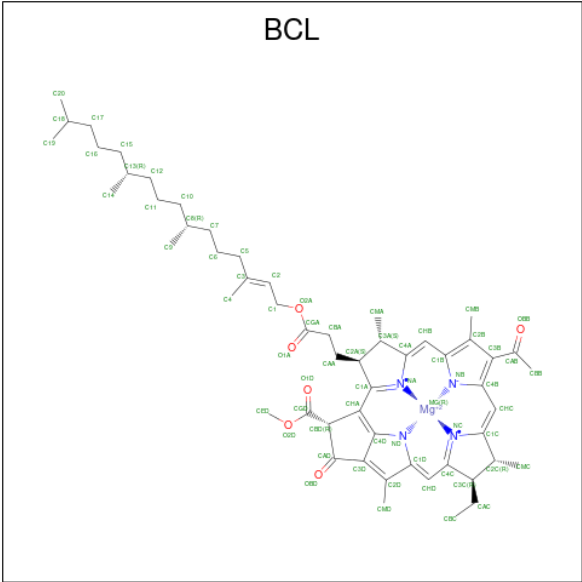
- Molecule 2 is a protein called Photosynthetic Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	297	Total	C	N	O	S	0	0	0
			2368	1582	387	389	10			

- Molecule 3 is a protein called Photosynthetic reaction center protein H chain.

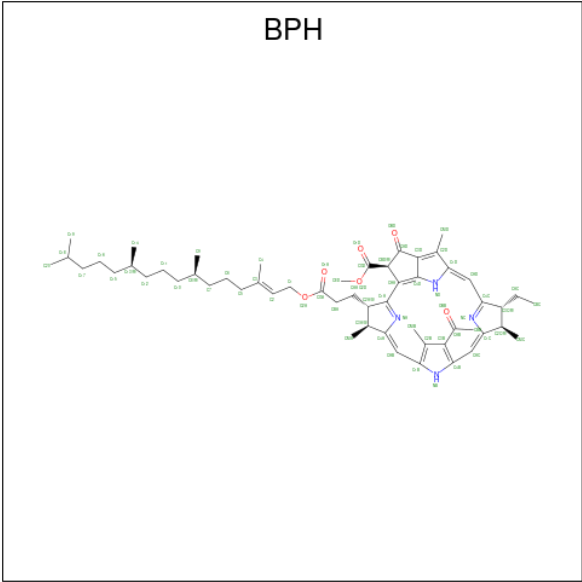
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



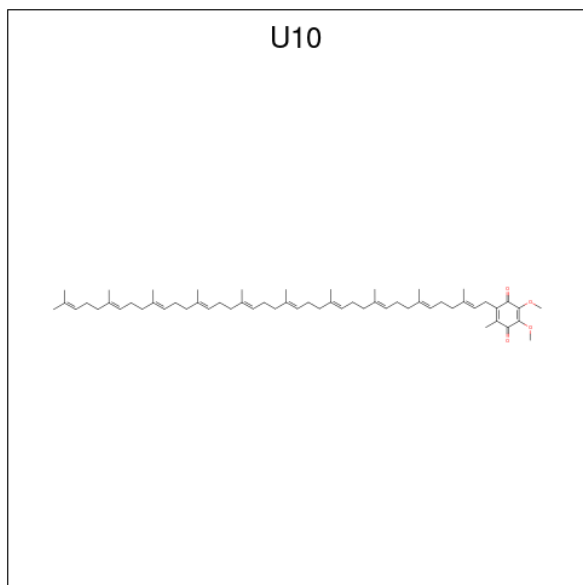
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



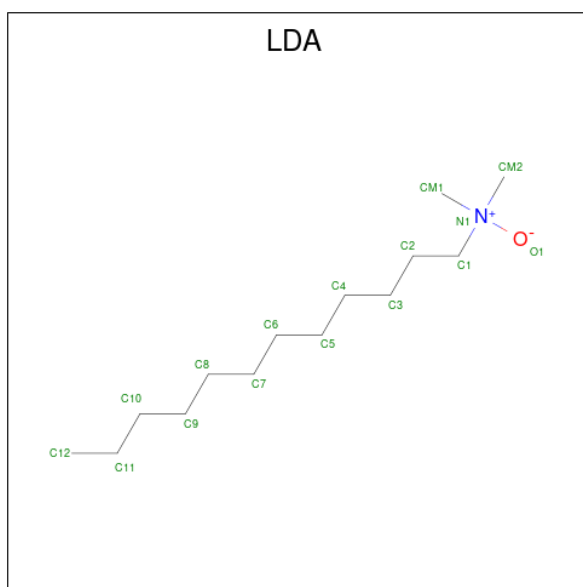
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	33	0
			63	59	4		
6	M	1	Total	C	O	16	0
			63	59	4		

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

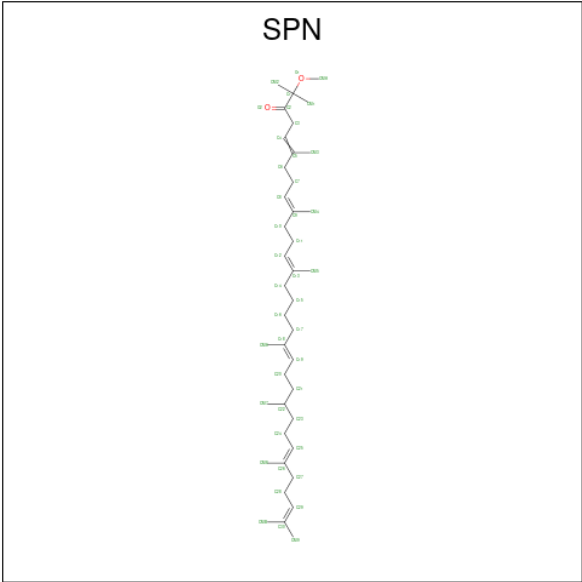


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂).



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

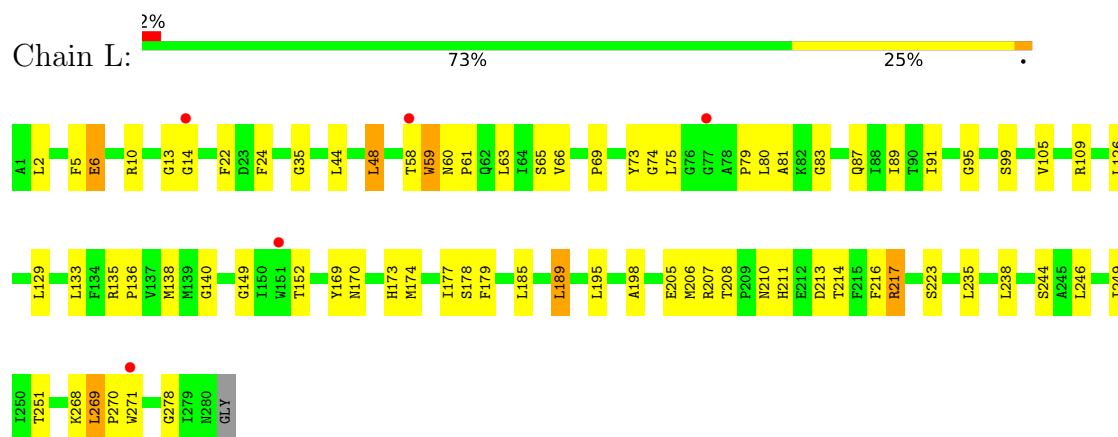
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	45	Total	O	0	0
			45	45		
10	M	65	Total	O	0	0
			65	65		
10	H	70	Total	O	0	0
			70	70		

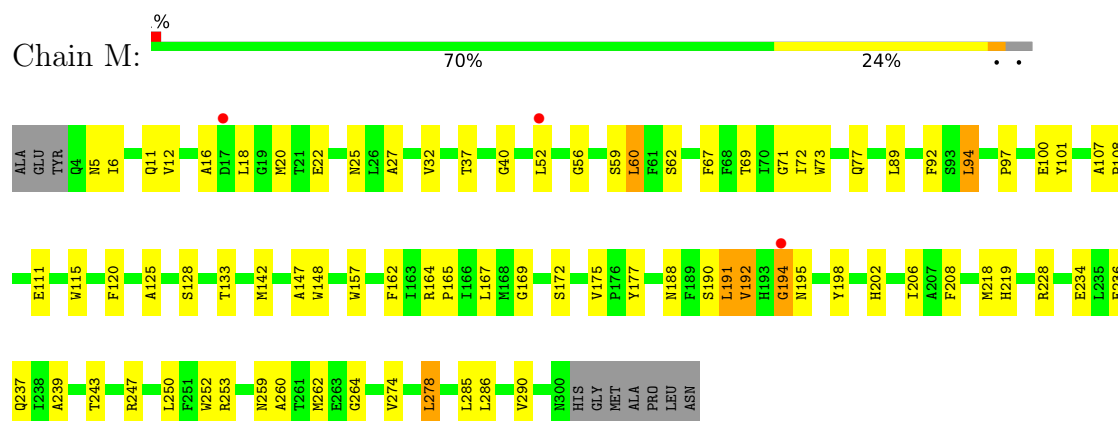
3 Residue-property plots

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.

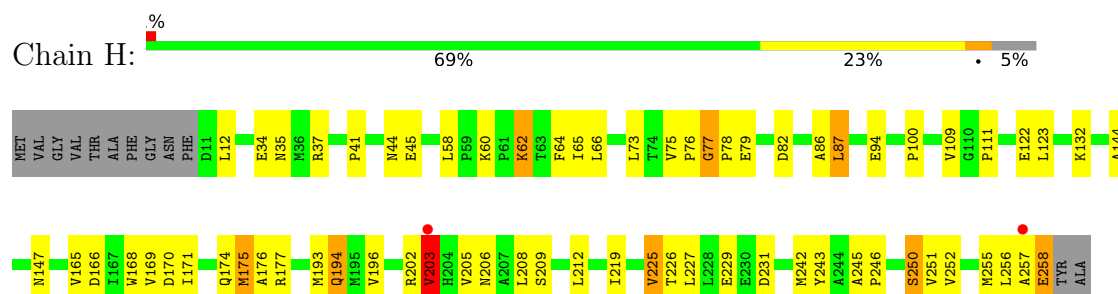
• Molecule 1: Photosynthetic Reaction center protein L chain



• Molecule 2: Photosynthetic Reaction center protein M chain



• Molecule 3: Photosynthetic reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 134.72Å 141.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.43 – 2.50 38.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.43-2.50) 97.4 (38.43-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.250 0.203 , 0.240	Depositor DCC
R_{free} test set	2514 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: U10, LDA, BCL, SPN, FE2, BPH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.41	0/2315	0.90	7/3170 (0.2%)
2	M	0.44	0/2458	0.92	5/3356 (0.1%)
3	H	0.44	0/1931	0.96	10/2627 (0.4%)
All	All	0.43	0/6704	0.93	22/9153 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	5	ASN	N-CA-C	-8.66	100.68	112.03
1	L	6	GLU	N-CA-C	7.36	120.74	111.69
3	H	203	VAL	N-CA-C	-6.72	95.94	107.24
3	H	77	GLY	CA-C-N	6.49	126.17	119.56
3	H	77	GLY	C-N-CA	6.49	126.17	119.56
1	L	35	GLY	N-CA-C	-6.24	104.78	112.77
3	H	250	SER	N-CA-C	6.09	117.91	110.41
3	H	44	ASN	N-CA-C	-5.97	102.49	110.55
1	L	269	LEU	CA-C-N	5.83	127.13	119.84
1	L	269	LEU	C-N-CA	5.83	127.13	119.84
2	M	234	GLU	N-CA-C	5.79	117.59	111.28
1	L	59	TRP	N-CA-C	-5.75	104.45	113.02
3	H	169	VAL	N-CA-C	5.70	117.21	108.71
1	L	271	TRP	N-CA-C	5.49	117.34	111.36
1	L	13	GLY	N-CA-C	5.48	118.96	112.33
3	H	170	ASP	N-CA-C	-5.27	99.92	108.41
2	M	194	GLY	N-CA-C	-5.25	101.42	112.45
3	H	147	ASN	CA-C-N	5.21	125.01	119.28
3	H	147	ASN	C-N-CA	5.21	125.01	119.28
2	M	169	GLY	N-CA-C	5.16	121.92	115.21
2	M	22	GLU	CB-CA-C	-5.14	110.62	116.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	206	ASN	N-CA-C	5.07	116.89	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2227	0	2186	50	0
2	M	2368	0	2288	61	0
3	H	1883	0	1895	54	0
4	L	198	0	222	15	0
4	M	66	0	74	5	0
5	L	65	0	76	2	0
5	M	65	0	76	7	0
6	L	63	0	90	5	0
6	M	63	0	90	2	0
7	H	16	0	31	2	0
7	L	16	0	31	0	0
7	M	32	0	62	5	0
8	M	1	0	0	0	0
9	M	43	0	69	8	0
10	H	70	0	0	6	0
10	L	45	0	0	1	0
10	M	65	0	0	3	0
All	All	7286	0	7190	177	0

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

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:THR:HG21	2:M:20:MET:H	1.16	1.06
7:M:314:LDA:H82	7:H:261:LDA:H122	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.58	0.83
1:L:210:ASN:O	1:L:214:THR:HG23	1.80	0.82
6:M:311:U10:H202	7:M:314:LDA:H122	1.62	0.80
2:M:71:GLY:HA2	9:M:312:SPN:HM32	1.65	0.78
2:M:77:GLN:HE21	2:M:92:PHE:HD2	1.33	0.77
3:H:175:MET:HG2	3:H:176:ALA:N	2.01	0.76
1:L:217:ARG:HD2	10:M:350:HOH:O	1.86	0.76
2:M:243:THR:O	2:M:247:ARG:HG3	1.87	0.75
1:L:105:VAL:O	1:L:109:ARG:HG3	1.89	0.72
2:M:69:THR:O	2:M:72:ILE:HG22	1.92	0.69
1:L:214:THR:HG21	2:M:20:MET:N	2.00	0.67
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.75	0.66
2:M:208:PHE:HE2	7:M:313:LDA:H101	1.58	0.66
3:H:37:ARG:O	3:H:75:VAL:HG22	1.95	0.66
3:H:87:LEU:HD13	3:H:109:VAL:HG21	1.78	0.65
4:L:301:BCL:H8	4:M:309:BCL:H202	1.78	0.64
3:H:209:SER:OG	3:H:212:LEU:HD23	1.98	0.64
2:M:190:SER:O	2:M:194:GLY:O	2.16	0.63
4:L:304:BCL:HBB2	4:L:304:BCL:HMB3	1.81	0.63
1:L:208:THR:H	1:L:211:HIS:CD2	2.17	0.63
5:L:305:BPH:HBB3	5:L:305:BPH:HMB3	1.82	0.61
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.00	0.61
3:H:242:MET:HE3	3:H:243:TYR:CZ	2.36	0.61
3:H:132:LYS:HE2	3:H:171:ILE:HD11	1.84	0.60
3:H:86:ALA:O	3:H:100:PRO:HA	2.01	0.60
2:M:56:GLY:O	2:M:60:LEU:HB2	2.03	0.59
3:H:257:ALA:O	3:H:258:GLU:HG2	2.03	0.58
1:L:14:GLY:O	1:L:109:ARG:HD3	2.03	0.58
2:M:52:LEU:HD12	2:M:52:LEU:O	2.04	0.58
3:H:257:ALA:C	3:H:258:GLU:HG2	2.28	0.58
1:L:178:SER:HB3	6:L:306:U10:H212	1.85	0.57
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.40	0.57
2:M:16:ALA:CB	2:M:32:VAL:HG21	2.31	0.56
3:H:34:GLU:O	3:H:37:ARG:HG3	2.05	0.56
4:L:301:BCL:H112	4:L:301:BCL:H162	1.89	0.55
2:M:162:PHE:CE1	9:M:312:SPN:HMB3	2.42	0.55
1:L:208:THR:H	1:L:211:HIS:HD2	1.54	0.55
4:L:302:BCL:HMB3	4:L:302:BCL:CBB	2.37	0.55
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.07	0.55
3:H:202:ARG:HD3	10:H:280:HOH:O	2.07	0.55
1:L:278:GLY:HA2	2:M:77:GLN:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.89	0.54
2:M:239:ALA:O	3:H:73:LEU:HD22	2.08	0.54
3:H:251:VAL:O	3:H:255:MET:HG3	2.08	0.54
1:L:170:ASN:O	1:L:173:HIS:HB3	2.07	0.54
3:H:75:VAL:HG22	3:H:76:PRO:HA	1.90	0.54
3:H:242:MET:HE3	3:H:243:TYR:CE1	2.43	0.54
4:M:309:BCL:HMB1	4:M:309:BCL:HBB3	1.90	0.54
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.89	0.53
2:M:18:LEU:HD22	10:M:378:HOH:O	2.07	0.53
3:H:87:LEU:CD1	3:H:109:VAL:HG21	2.38	0.53
3:H:37:ARG:NH2	3:H:62:LYS:HB3	2.24	0.53
3:H:250:SER:OG	3:H:252:VAL:HG22	2.08	0.53
2:M:94:LEU:HD22	2:M:115:TRP:HB2	1.90	0.52
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.09	0.52
1:L:44:LEU:O	1:L:48:LEU:HD13	2.10	0.52
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.44	0.52
2:M:60:LEU:HD22	5:M:310:BPH:H4C3	1.91	0.52
2:M:188:ASN:O	2:M:192:VAL:HG13	2.10	0.52
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.92	0.52
2:M:208:PHE:CE2	7:M:313:LDA:H101	2.42	0.52
1:L:213:ASP:O	1:L:217:ARG:HB2	2.10	0.51
1:L:198:ALA:HA	1:L:206:MET:HE3	1.91	0.51
5:L:305:BPH:HMB3	5:L:305:BPH:CBB	2.41	0.50
3:H:62:LYS:HD3	3:H:64:PHE:CZ	2.46	0.50
1:L:2:LEU:HB3	1:L:6:GLU:HB3	1.93	0.50
1:L:133:LEU:C	1:L:136:PRO:HD2	2.37	0.50
3:H:165:VAL:O	3:H:166:ASP:HB2	2.11	0.50
1:L:60:ASN:ND2	1:L:63:LEU:HG	2.27	0.49
3:H:242:MET:CE	3:H:243:TYR:CZ	2.94	0.49
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.93	0.49
3:H:252:VAL:O	3:H:256:LEU:HD13	2.13	0.49
1:L:69:PRO:HG3	1:L:83:GLY:HA3	1.93	0.49
1:L:189:LEU:HB3	6:L:306:U10:H4M3	1.93	0.49
1:L:179:PHE:CZ	6:L:306:U10:H203	2.48	0.48
2:M:177:TYR:HD1	9:M:312:SPN:H142	1.77	0.48
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.95	0.48
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.47	0.48
1:L:205:GLU:HG2	3:H:65:ILE:HG22	1.94	0.48
1:L:244:SER:OG	4:L:302:BCL:HMA2	2.13	0.48
2:M:101:TYR:CE2	2:M:107:ALA:HA	2.48	0.48
4:L:301:BCL:H152	4:L:301:BCL:H193	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:309:BCL:OBB	4:M:309:BCL:HHC	2.14	0.48
2:M:67:PHE:CE1	9:M:312:SPN:H61	2.49	0.48
3:H:132:LYS:HG2	10:H:305:HOH:O	2.14	0.48
2:M:290:VAL:HG21	3:H:12:LEU:HD12	1.95	0.47
3:H:245:ALA:N	3:H:246:PRO:CD	2.77	0.47
1:L:79:PRO:O	1:L:81:ALA:N	2.47	0.47
3:H:209:SER:HG	3:H:212:LEU:HD23	1.78	0.47
1:L:59:TRP:O	1:L:61:PRO:HD3	2.14	0.47
2:M:120:PHE:HD1	9:M:312:SPN:CM9	2.28	0.47
2:M:77:GLN:HG3	2:M:92:PHE:CD2	2.50	0.47
3:H:37:ARG:NH2	3:H:60:LYS:O	2.48	0.46
1:L:246:LEU:O	1:L:249:ILE:HG22	2.15	0.46
2:M:72:ILE:HG23	2:M:73:TRP:N	2.29	0.46
3:H:168:TRP:HZ3	3:H:225:VAL:HG22	1.79	0.46
1:L:216:PHE:CG	6:L:306:U10:H3M3	2.51	0.46
1:L:185:LEU:HD13	5:M:310:BPH:ND	2.30	0.46
3:H:78:PRO:O	3:H:79:GLU:C	2.56	0.46
1:L:60:ASN:HD22	1:L:63:LEU:CD1	2.28	0.46
1:L:87:GLN:O	1:L:91:ILE:HG12	2.16	0.46
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.98	0.46
5:M:310:BPH:HBC3	5:M:310:BPH:HHD	1.97	0.46
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.51	0.46
2:M:202:HIS:O	2:M:206:ILE:HG13	2.15	0.46
3:H:87:LEU:HD12	3:H:100:PRO:HA	1.97	0.46
4:M:309:BCL:HMB1	4:M:309:BCL:CBB	2.46	0.45
2:M:236:GLU:HB3	10:H:279:HOH:O	2.14	0.45
7:M:314:LDA:H82	7:H:261:LDA:C12	2.39	0.45
1:L:73:TYR:O	1:L:74:GLY:C	2.60	0.45
4:L:301:BCL:OBB	4:L:301:BCL:HHC	2.14	0.45
1:L:223:SER:HA	6:L:306:U10:H3M2	1.98	0.45
2:M:100:GLU:H	2:M:100:GLU:CD	2.24	0.45
3:H:132:LYS:HE3	10:H:263:HOH:O	2.15	0.45
4:L:301:BCL:HBB3	4:L:301:BCL:HMB1	1.99	0.45
3:H:75:VAL:HA	3:H:76:PRO:C	2.42	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.45
1:L:149:GLY:HA3	1:L:152:THR:OG1	2.16	0.45
1:L:5:PHE:C	1:L:5:PHE:CD1	2.95	0.45
1:L:95:GLY:O	1:L:99:SER:OG	2.22	0.45
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.99	0.45
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.99	0.45
4:L:302:BCL:HMB3	4:L:302:BCL:HBB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:217:ARG:NH1	10:L:338:HOH:O	2.48	0.44
2:M:97:PRO:O	2:M:172:SER:HB3	2.18	0.44
4:L:301:BCL:H192	9:M:312:SPN:HM43	2.00	0.44
3:H:37:ARG:O	3:H:75:VAL:CG2	2.63	0.44
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.99	0.43
1:L:79:PRO:C	1:L:81:ALA:N	2.75	0.43
2:M:60:LEU:HD22	5:M:310:BPH:C4	2.48	0.43
5:M:310:BPH:HBA2	5:M:310:BPH:H3A	1.79	0.43
3:H:41:PRO:HG3	3:H:58:LEU:HD11	1.99	0.43
2:M:60:LEU:HA	5:M:310:BPH:H4C2	2.00	0.43
2:M:72:ILE:CG2	2:M:73:TRP:N	2.82	0.43
2:M:228:ARG:HA	3:H:194:GLN:CG	2.48	0.43
2:M:253:ARG:HB2	2:M:259:ASN:HD22	1.83	0.43
2:M:191:LEU:HD12	2:M:191:LEU:HA	1.89	0.43
1:L:2:LEU:CD2	1:L:10:ARG:CZ	2.96	0.43
3:H:132:LYS:HE2	3:H:171:ILE:CD1	2.48	0.43
3:H:177:ARG:O	3:H:193:MET:HB2	2.19	0.43
4:L:302:BCL:OBB	4:L:302:BCL:HHC	2.19	0.43
2:M:219:HIS:HA	6:M:311:U10:H1M1	2.00	0.43
3:H:111:PRO:CG	3:H:242:MET:HE2	2.48	0.42
3:H:251:VAL:HG23	3:H:252:VAL:N	2.34	0.42
4:L:302:BCL:HBD	4:L:304:BCL:HAC1	2.02	0.42
2:M:278:LEU:HD12	2:M:278:LEU:HA	1.86	0.42
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.20	0.42
2:M:133:THR:HG21	2:M:147:ALA:HA	2.01	0.42
2:M:157:TRP:CE2	9:M:312:SPN:HM73	2.54	0.42
2:M:175:VAL:N	10:M:356:HOH:O	2.51	0.42
3:H:203:VAL:O	3:H:203:VAL:HG22	2.18	0.42
2:M:195:ASN:HB3	2:M:198:TYR:CD1	2.54	0.42
2:M:218:MET:HE3	2:M:252:TRP:CZ3	2.55	0.42
1:L:169:TYR:HA	1:L:174:MET:HE3	2.02	0.42
3:H:219:ILE:HG12	10:H:284:HOH:O	2.20	0.42
1:L:73:TYR:HE2	1:L:79:PRO:HD3	1.86	0.41
1:L:135:ARG:NH1	1:L:251:THR:O	2.53	0.41
1:L:268:LYS:HA	1:L:268:LYS:HD3	1.86	0.41
1:L:177:ILE:HD13	4:L:301:BCL:HMD2	2.02	0.41
3:H:111:PRO:HG3	3:H:242:MET:HE2	2.02	0.41
2:M:59:SER:HB2	2:M:128:SER:OG	2.20	0.41
4:M:309:BCL:HAA2	4:M:309:BCL:HBD	2.03	0.41
1:L:269:LEU:HA	1:L:270:PRO:HD2	1.86	0.41
1:L:138:MET:SD	1:L:249:ILE:HD11	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:CB	1:L:152:THR:HG21	2.51	0.41
1:L:66:VAL:HG11	1:L:89:ILE:HD12	2.02	0.41
4:L:301:BCL:H72	5:M:310:BPH:HMB3	2.03	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.21	0.41
3:H:77:GLY:HA2	3:H:78:PRO:HD3	1.89	0.41
2:M:11:GLN:OE1	2:M:40:GLY:HA3	2.21	0.41
4:L:301:BCL:C14	9:M:312:SPN:H101	2.51	0.40
2:M:62:SER:HB2	2:M:125:ALA:HB2	2.03	0.40
3:H:175:MET:HE3	3:H:177:ARG:HG3	2.04	0.40
1:L:6:GLU:HG3	2:M:250:LEU:CD2	2.51	0.40
3:H:202:ARG:CD	10:H:280:HOH:O	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	278/281 (99%)	262 (94%)	15 (5%)	1 (0%)	30	49
2	M	295/307 (96%)	280 (95%)	15 (5%)	0	100	100
3	H	246/260 (95%)	236 (96%)	9 (4%)	1 (0%)	30	49
All	All	819/848 (97%)	778 (95%)	39 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	80	LEU
3	H	82	ASP

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%)	211 (96%)	9 (4%)	27	53
2	M	233/240 (97%)	222 (95%)	11 (5%)	23	47
3	H	200/208 (96%)	188 (94%)	12 (6%)	17	36
All	All	653/668 (98%)	621 (95%)	32 (5%)	22	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	48	LEU
1	L	58	THR
1	L	126	LEU
1	L	129	LEU
1	L	189	LEU
1	L	195	LEU
1	L	217	ARG
1	L	235	LEU
1	L	238	LEU
2	M	6	ILE
2	M	12	VAL
2	M	37	THR
2	M	60	LEU
2	M	89	LEU
2	M	94	LEU
2	M	191	LEU
2	M	192	VAL
2	M	274	VAL
2	M	278	LEU
2	M	286	LEU
3	H	62	LYS
3	H	66	LEU
3	H	87	LEU
3	H	123	LEU
3	H	174	GLN
3	H	175	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	194	GLN
3	H	203	VAL
3	H	208	LEU
3	H	225	VAL
3	H	231	ASP
3	H	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	87	GLN
1	L	183	ASN
1	L	211	HIS
1	L	258	GLN
2	M	187	ASN
2	M	259	ASN
2	M	299	GLN
3	H	68	HIS
3	H	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
7	LDA	M	314	-	13,15,15	3.15	2 (15%)	14,17,17	0.68	0
9	SPN	M	312	-	42,42,42	2.84	19 (45%)	50,52,52	2.43	17 (34%)
4	BCL	L	301	2	69,74,74	1.28	8 (11%)	79,115,115	2.16	14 (17%)
5	BPH	M	310	-	59,70,70	1.88	12 (20%)	59,101,101	2.66	16 (27%)
6	U10	L	306	-	63,63,63	1.83	16 (25%)	78,79,79	1.58	17 (21%)
4	BCL	L	302	1	69,74,74	1.28	7 (10%)	79,115,115	1.90	11 (13%)
7	LDA	L	307	-	13,15,15	2.60	2 (15%)	14,17,17	0.55	0
7	LDA	H	261	-	13,15,15	2.42	2 (15%)	14,17,17	0.60	0
5	BPH	L	305	-	59,70,70	1.81	11 (18%)	59,101,101	2.55	13 (22%)
6	U10	M	311	-	63,63,63	1.73	17 (26%)	78,79,79	1.38	10 (12%)
4	BCL	M	309	2	69,74,74	1.26	8 (11%)	79,115,115	2.05	13 (16%)
4	BCL	L	304	1	69,74,74	1.26	6 (8%)	79,115,115	2.08	7 (8%)
7	LDA	M	313	-	13,15,15	2.37	2 (15%)	14,17,17	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	M	314	-	-	0/13/13/13	-
9	SPN	M	312	-	-	12/50/51/51	-
4	BCL	L	301	2	1/1/21/25	2/41/137/137	-
5	BPH	M	310	-	1/1/18/22	7/37/105/105	0/5/6/6
6	U10	L	306	-	-	16/63/87/87	0/1/1/1
4	BCL	L	302	1	-	2/41/137/137	-
7	LDA	L	307	-	-	1/13/13/13	-
7	LDA	H	261	-	-	0/13/13/13	-
5	BPH	L	305	-	1/1/18/22	9/37/105/105	0/5/6/6
6	U10	M	311	-	-	12/63/87/87	0/1/1/1
4	BCL	M	309	2	-	1/41/137/137	-
4	BCL	L	304	1	-	4/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	M	313	-	-	0/13/13/13	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	312	SPN	C4-C5	8.90	1.53	1.33
7	M	314	LDA	C1-N1	-8.21	1.43	1.51
7	M	313	LDA	O1-N1	-7.93	1.22	1.42
7	L	307	LDA	O1-N1	-7.92	1.22	1.42
7	M	314	LDA	O1-N1	-7.79	1.23	1.42
7	H	261	LDA	O1-N1	-7.29	1.24	1.42
5	M	310	BPH	C1D-C2D	5.98	1.46	1.39
5	L	305	BPH	O2D-CGD	5.96	1.47	1.33
5	M	310	BPH	O2D-CGD	5.65	1.47	1.33
9	M	312	SPN	C10-C9	-5.65	1.39	1.51
4	L	304	BCL	MG-NA	5.55	2.19	2.06
9	M	312	SPN	C17-C18	-5.53	1.39	1.51
5	M	310	BPH	C3A-C2A	-5.08	1.50	1.54
7	L	307	LDA	C1-N1	-4.95	1.46	1.51
4	M	309	BCL	MG-NA	4.92	2.17	2.06
7	H	261	LDA	C1-N1	-4.77	1.46	1.51
4	L	301	BCL	MG-NA	4.63	2.17	2.06
5	L	305	BPH	C1D-C2D	4.61	1.44	1.39
5	M	310	BPH	C1B-C2B	4.60	1.44	1.39
5	L	305	BPH	C3A-C2A	-4.50	1.50	1.54
4	L	302	BCL	MG-NA	4.48	2.16	2.06
5	L	305	BPH	C2C-C3C	-4.35	1.51	1.54
9	M	312	SPN	C10-C11	-4.35	1.39	1.53
6	L	306	U10	O3-C3M	-4.34	1.35	1.45
5	L	305	BPH	C1B-C2B	4.33	1.44	1.39
9	M	312	SPN	C21-C20	-4.31	1.39	1.53
5	M	310	BPH	O2A-CGA	4.25	1.45	1.33
4	L	302	BCL	O2D-CED	-4.19	1.36	1.45
4	L	302	BCL	O2D-CGD	4.16	1.43	1.33
4	L	301	BCL	O2D-CGD	4.05	1.43	1.33
4	L	304	BCL	O2D-CGD	4.03	1.43	1.33
6	M	311	U10	C7-C8	-3.82	1.44	1.50
5	M	310	BPH	C2C-C3C	-3.67	1.51	1.54
4	L	304	BCL	O2A-CGA	3.65	1.44	1.33
9	M	312	SPN	C20-C19	-3.65	1.39	1.50
9	M	312	SPN	C24-C25	-3.63	1.39	1.50
9	M	312	SPN	C28-C29	-3.63	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	312	SPN	C7-C8	-3.62	1.39	1.50
6	L	306	U10	C7-C6	3.62	1.58	1.51
9	M	312	SPN	C11-C12	-3.61	1.39	1.50
4	M	309	BCL	O2D-CGD	3.59	1.42	1.33
9	M	312	SPN	C16-C17	-3.51	1.39	1.52
5	L	305	BPH	C3B-C4B	3.50	1.47	1.41
4	L	301	BCL	MG-ND	-3.47	1.98	2.05
9	M	312	SPN	C15-C14	-3.45	1.39	1.52
5	L	305	BPH	O2D-CED	-3.32	1.37	1.45
4	M	309	BCL	C3B-C4B	3.29	1.47	1.41
6	L	306	U10	C7-C8	-3.27	1.45	1.50
6	L	306	U10	O4-C4M	-3.27	1.38	1.45
4	L	302	BCL	C3B-C4B	3.27	1.47	1.41
5	L	305	BPH	O2A-CGA	3.24	1.42	1.33
6	M	311	U10	O3-C3M	-3.24	1.38	1.45
4	L	304	BCL	C3B-C4B	3.22	1.47	1.41
4	M	309	BCL	O2A-CGA	2.98	1.42	1.33
4	L	301	BCL	C3B-C4B	2.95	1.46	1.41
6	L	306	U10	C8-C9	2.95	1.39	1.33
4	L	301	BCL	O2A-CGA	2.94	1.41	1.33
6	L	306	U10	C48-C49	2.90	1.39	1.33
5	M	310	BPH	C3B-C4B	2.89	1.46	1.41
6	L	306	U10	C13-C14	2.88	1.39	1.33
6	L	306	U10	C38-C39	2.87	1.39	1.33
5	L	305	BPH	C2-C3	2.87	1.39	1.33
6	L	306	U10	C28-C29	2.86	1.39	1.33
9	M	312	SPN	C12-C13	2.86	1.39	1.33
7	M	313	LDA	C1-N1	-2.86	1.48	1.51
4	M	309	BCL	MG-ND	-2.85	2.00	2.05
4	L	301	BCL	O2D-CED	-2.84	1.38	1.45
6	L	306	U10	C18-C19	2.84	1.39	1.33
5	M	310	BPH	C2-C3	2.84	1.39	1.33
6	L	306	U10	C33-C34	2.83	1.39	1.33
6	M	311	U10	C28-C29	2.83	1.39	1.33
6	M	311	U10	C48-C49	2.82	1.39	1.33
6	L	306	U10	C23-C24	2.82	1.39	1.33
6	M	311	U10	C23-C24	2.81	1.39	1.33
4	L	302	BCL	C2-C3	2.80	1.39	1.33
6	M	311	U10	C38-C39	2.80	1.39	1.33
6	M	311	U10	C43-C44	2.80	1.39	1.33
6	M	311	U10	C8-C9	2.80	1.39	1.33
9	M	312	SPN	C19-C18	2.80	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	312	SPN	C25-C26	2.79	1.39	1.33
6	L	306	U10	C43-C44	2.79	1.39	1.33
9	M	312	SPN	C8-C9	2.78	1.39	1.33
6	M	311	U10	C13-C14	2.78	1.39	1.33
6	M	311	U10	C27-C28	-2.78	1.42	1.50
4	M	309	BCL	C2-C3	2.77	1.39	1.33
6	M	311	U10	C17-C18	-2.72	1.42	1.50
6	M	311	U10	C33-C34	2.70	1.39	1.33
4	L	302	BCL	O2A-CGA	2.70	1.41	1.33
6	M	311	U10	C18-C19	2.69	1.39	1.33
5	M	310	BPH	O2D-CED	-2.68	1.39	1.45
6	L	306	U10	C6-C1	2.68	1.40	1.35
9	M	312	SPN	C21-C22	-2.66	1.39	1.52
4	L	302	BCL	C1-C2	-2.65	1.41	1.49
4	L	301	BCL	C2-C3	2.64	1.39	1.33
4	L	304	BCL	C2-C3	2.63	1.39	1.33
5	M	310	BPH	CHA-CBD	2.48	1.54	1.51
5	M	310	BPH	C3D-C4D	2.44	1.44	1.41
9	M	312	SPN	C16-C15	-2.43	1.39	1.51
9	M	312	SPN	C29-C30	2.38	1.39	1.32
4	M	309	BCL	O2D-CED	-2.38	1.40	1.45
4	M	309	BCL	C5-C3	2.37	1.56	1.51
6	L	306	U10	C53-C54	2.36	1.39	1.32
6	M	311	U10	C53-C54	2.35	1.39	1.32
4	L	304	BCL	O2D-CED	-2.27	1.40	1.45
5	L	305	BPH	C4-C3	2.25	1.56	1.50
6	M	311	U10	C42-C43	-2.14	1.44	1.50
6	L	306	U10	C51-C49	2.11	1.55	1.51
5	M	310	BPH	C3B-C2B	-2.10	1.36	1.39
5	L	305	BPH	C3B-C2B	-2.06	1.36	1.39
4	L	301	BCL	C1-C2	-2.06	1.43	1.49
6	M	311	U10	C22-C23	-2.05	1.44	1.50
6	M	311	U10	C10-C9	2.04	1.55	1.50

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	310	BPH	O2D-CGD-CBD	12.93	125.15	110.95
5	L	305	BPH	O2D-CGD-CBD	12.48	124.66	110.95
4	L	302	BCL	C1C-NC-C4C	10.08	111.28	106.68
4	L	301	BCL	C1C-NC-C4C	9.79	111.15	106.68
4	L	304	BCL	C1C-NC-C4C	9.66	111.08	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	309	BCL	C1C-NC-C4C	9.22	110.89	106.68
4	L	301	BCL	C4A-NA-C1A	8.94	110.76	106.68
4	L	304	BCL	C4A-NA-C1A	8.71	110.65	106.68
9	M	312	SPN	C3-C4-C5	-8.60	112.01	126.83
4	M	309	BCL	C4A-NA-C1A	8.56	110.58	106.68
4	L	304	BCL	O2D-CGD-CBD	7.79	124.84	111.23
5	M	310	BPH	O1D-CGD-CBD	-7.73	113.00	124.72
4	L	302	BCL	C4A-NA-C1A	7.67	110.18	106.68
5	L	305	BPH	O1D-CGD-CBD	-7.50	113.35	124.72
4	L	301	BCL	O2D-CGD-CBD	6.69	122.93	111.23
4	M	309	BCL	O2D-CGD-CBD	5.94	121.61	111.23
5	M	310	BPH	C4D-CHA-CBD	-5.78	105.68	108.45
5	L	305	BPH	C4D-CHA-CBD	-5.59	105.77	108.45
6	M	311	U10	C7-C8-C9	5.57	136.43	126.83
5	M	310	BPH	C1-C2-C3	5.49	135.19	126.20
4	L	304	BCL	O1D-CGD-CBD	-5.47	113.72	124.52
9	M	312	SPN	C6-C5-C4	-5.38	109.09	121.17
9	M	312	SPN	CM3-C5-C4	-4.86	111.14	123.63
4	L	301	BCL	O1D-CGD-CBD	-4.83	115.00	124.52
6	L	306	U10	C32-C33-C34	4.68	138.34	127.62
4	M	309	BCL	O1D-CGD-CBD	-4.46	115.73	124.52
9	M	312	SPN	CM2-C1-C2	4.39	118.59	109.43
4	M	309	BCL	C1-C2-C3	4.38	133.37	126.20
6	L	306	U10	C12-C13-C14	4.31	137.49	127.62
9	M	312	SPN	CM2-C1-CM1	4.27	120.10	110.73
9	M	312	SPN	O1-C1-C2	-4.01	100.69	108.90
5	L	305	BPH	O2A-CGA-CBA	3.96	123.89	111.83
4	L	302	BCL	O2D-CGD-CBD	3.88	118.02	111.23
5	M	310	BPH	O2A-CGA-CBA	3.74	123.24	111.83
5	M	310	BPH	OBB-CAB-C3B	3.70	126.17	119.99
6	M	311	U10	C27-C28-C29	3.67	136.03	127.62
9	M	312	SPN	C11-C10-C9	3.61	125.14	113.19
5	M	310	BPH	OBD-CAD-CBD	-3.50	120.69	125.82
5	L	305	BPH	O2A-CGA-O1A	-3.42	115.06	123.63
9	M	312	SPN	C16-C17-C18	3.40	121.75	113.47
5	L	305	BPH	OBD-CAD-CBD	-3.36	120.89	125.82
6	L	306	U10	C22-C23-C24	3.30	135.17	127.62
4	L	302	BCL	O2A-CGA-CBA	3.26	121.77	111.83
4	L	301	BCL	OBB-CAB-C3B	3.26	126.19	120.43
6	L	306	U10	C47-C48-C49	3.24	135.03	127.62
6	L	306	U10	C12-C11-C9	3.23	123.90	113.19
4	M	309	BCL	O2A-CGA-CBA	3.19	121.55	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	312	SPN	CM5-C13-C14	3.12	120.65	115.23
4	M	309	BCL	OBB-CAB-C3B	3.12	125.94	120.43
9	M	312	SPN	CM6-C18-C17	3.10	120.60	115.23
4	L	301	BCL	O2A-CGA-CBA	3.09	121.24	111.83
5	L	305	BPH	C2D-C1D-ND	3.02	111.61	109.43
5	L	305	BPH	C4D-ND-C1D	-3.02	105.26	108.87
5	L	305	BPH	OBB-CAB-C3B	2.96	124.94	119.99
6	L	306	U10	C42-C43-C44	2.91	134.29	127.62
5	M	310	BPH	O2A-CGA-O1A	-2.84	116.52	123.63
5	L	305	BPH	CMD-C2D-C3D	2.82	130.32	124.68
4	L	302	BCL	OBB-CAB-C3B	2.79	125.37	120.43
6	M	311	U10	C47-C48-C49	2.78	133.99	127.62
5	L	305	BPH	C1-C2-C3	2.77	130.74	126.20
6	M	311	U10	C7-C6-C1	-2.76	120.16	124.89
6	L	306	U10	C3M-O3-C3	2.76	126.16	116.47
5	M	310	BPH	C4D-ND-C1D	-2.74	105.59	108.87
9	M	312	SPN	CM8-C26-C27	2.73	119.97	115.23
6	L	306	U10	C52-C53-C54	2.67	136.54	127.64
5	M	310	BPH	C1C-C2C-C3C	2.65	105.36	102.84
4	L	302	BCL	O1D-CGD-CBD	-2.64	119.31	124.52
6	L	306	U10	C30-C29-C31	-2.61	110.69	115.23
4	L	301	BCL	C2A-C1A-CHA	2.60	128.38	123.87
4	L	302	BCL	C2C-C3C-C4C	2.58	105.21	101.34
4	L	301	BCL	CMB-C2B-C1B	-2.55	121.53	125.42
6	L	306	U10	C36-C34-C33	2.55	126.89	121.17
4	L	302	BCL	O2A-CGA-O1A	-2.53	117.29	123.63
4	L	301	BCL	CBB-CAB-C3B	-2.52	115.08	120.40
6	L	306	U10	C52-C51-C49	2.51	121.51	113.19
4	L	301	BCL	C2C-C3C-C4C	2.49	105.06	101.34
5	M	310	BPH	C3D-C4D-ND	2.47	110.87	107.71
4	L	301	BCL	CAB-C3B-C2B	2.47	132.87	127.74
6	L	306	U10	C20-C19-C21	-2.47	110.94	115.23
6	L	306	U10	C17-C18-C19	2.46	133.26	127.62
4	M	309	BCL	CAB-C3B-C2B	2.46	132.85	127.74
6	L	306	U10	C35-C34-C36	-2.46	110.96	115.23
9	M	312	SPN	CM7-C22-C21	2.44	119.98	111.27
9	M	312	SPN	CM4-C9-C10	2.44	119.46	115.23
9	M	312	SPN	CM7-C22-C23	2.44	119.96	111.27
4	M	309	BCL	C4D-CHA-C1A	2.44	124.15	121.24
5	L	305	BPH	C3D-C4D-ND	2.41	110.79	107.71
4	L	301	BCL	CED-O2D-CGD	-2.32	110.65	115.92
4	M	309	BCL	CBB-CAB-C3B	-2.31	115.54	120.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	C2C-C3C-C4C	2.30	104.79	101.34
4	L	301	BCL	O2A-CGA-O1A	-2.28	117.92	123.63
6	M	311	U10	C36-C37-C38	2.27	123.23	112.02
5	M	310	BPH	CMD-C2D-C3D	2.27	129.21	124.68
4	L	301	BCL	C6-C5-C3	-2.25	107.98	113.47
6	M	311	U10	C25-C24-C26	-2.25	111.33	115.23
4	L	304	BCL	CAB-C3B-C2B	2.25	132.41	127.74
4	M	309	BCL	C3A-C2A-C1A	2.23	104.68	101.34
6	L	306	U10	C31-C29-C28	2.23	126.17	121.17
4	L	302	BCL	CED-O2D-CGD	2.21	120.92	115.92
9	M	312	SPN	C20-C21-C22	2.20	126.28	114.56
4	M	309	BCL	C2C-C3C-C4C	2.20	104.63	101.34
4	L	302	BCL	CAB-C3B-C2B	2.19	132.30	127.74
5	M	310	BPH	OBD-CAD-C3D	2.16	131.27	127.89
5	L	305	BPH	CMA-C3A-C4A	-2.16	109.95	114.61
9	M	312	SPN	CM3-C5-C6	-2.14	111.51	115.23
5	M	310	BPH	C4C-C3C-C2C	2.14	104.88	102.84
4	L	304	BCL	OBB-CAB-C3B	2.12	124.18	120.43
9	M	312	SPN	CMB-C30-CM9	2.12	119.46	114.59
4	M	309	BCL	O2A-CGA-O1A	-2.11	118.35	123.63
6	L	306	U10	C7-C8-C9	2.10	130.44	126.83
4	L	302	BCL	C3C-C2C-C1C	2.09	105.25	101.87
6	M	311	U10	C6-C1-C2	2.07	120.81	119.17
6	M	311	U10	C41-C39-C38	2.06	125.80	121.17
6	L	306	U10	C50-C49-C51	-2.04	111.68	115.23
6	M	311	U10	C37-C36-C34	2.04	119.94	113.19
6	M	311	U10	C4M-O4-C4	2.04	123.62	116.47
5	M	310	BPH	CMC-C2C-C1C	-2.03	110.23	114.61
5	M	310	BPH	CMA-C3A-C4A	-2.03	110.24	114.61

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	301	BCL	C13
5	L	305	BPH	C13
5	M	310	BPH	C13

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	304	BCL	CHA-CBD-CGD-O2D
6	M	311	U10	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	312	SPN	C20-C21-C22-CM7
9	M	312	SPN	C3-C4-C5-CM3
5	M	310	BPH	O1A-CGA-O2A-C1
9	M	312	SPN	C14-C15-C16-C17
5	M	310	BPH	CBA-CGA-O2A-C1
5	M	310	BPH	C4-C3-C5-C6
6	L	306	U10	C12-C11-C9-C10
6	L	306	U10	C25-C24-C26-C27
9	M	312	SPN	C11-C10-C9-CM4
9	M	312	SPN	C16-C17-C18-CM6
6	L	306	U10	C12-C11-C9-C8
6	L	306	U10	C23-C24-C26-C27
9	M	312	SPN	C4-C5-C6-C7
9	M	312	SPN	C11-C10-C9-C8
9	M	312	SPN	C12-C13-C14-C15
9	M	312	SPN	C16-C17-C18-C19
9	M	312	SPN	CM5-C13-C14-C15
6	M	311	U10	C29-C31-C32-C33
5	M	310	BPH	C2-C3-C5-C6
5	L	305	BPH	C12-C13-C15-C16
6	M	311	U10	C38-C39-C41-C42
6	M	311	U10	C40-C39-C41-C42
9	M	312	SPN	C21-C22-C23-C24
5	L	305	BPH	C8-C10-C11-C12
5	L	305	BPH	O2A-C1-C2-C3
5	L	305	BPH	C11-C10-C8-C7
6	M	311	U10	C30-C29-C31-C32
6	M	311	U10	C35-C34-C36-C37
5	M	310	BPH	CBD-CGD-O2D-CED
6	M	311	U10	C28-C29-C31-C32
6	M	311	U10	C33-C34-C36-C37
6	L	306	U10	C1-C6-C7-C8
5	L	305	BPH	C4-C3-C5-C6
6	L	306	U10	C45-C44-C46-C47
5	L	305	BPH	C2-C3-C5-C6
6	L	306	U10	C48-C49-C51-C52
6	L	306	U10	C5-C6-C7-C8
6	L	306	U10	C15-C14-C16-C17
4	L	301	BCL	C15-C16-C17-C18
6	L	306	U10	C43-C44-C46-C47
5	M	310	BPH	O1D-CGD-O2D-CED
4	L	304	BCL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	309	BCL	CAA-CBA-CGA-O2A
6	L	306	U10	C30-C29-C31-C32
6	L	306	U10	C50-C49-C51-C52
7	L	307	LDA	C2-C3-C4-C5
6	L	306	U10	C28-C29-C31-C32
6	M	311	U10	C5-C4-O4-C4M
6	M	311	U10	C25-C24-C26-C27
6	L	306	U10	C13-C14-C16-C17
5	L	305	BPH	C16-C17-C18-C20
4	L	304	BCL	C13-C15-C16-C17
6	M	311	U10	C45-C44-C46-C47
6	M	311	U10	C23-C24-C26-C27
4	L	302	BCL	C2A-CAA-CBA-CGA
6	L	306	U10	C40-C39-C41-C42
5	L	305	BPH	C11-C10-C8-C9
5	L	305	BPH	C16-C17-C18-C19
4	L	302	BCL	C2-C1-O2A-CGA
9	M	312	SPN	C19-C20-C21-C22
4	L	304	BCL	C15-C16-C17-C18
5	M	310	BPH	C13-C15-C16-C17
6	L	306	U10	C38-C39-C41-C42
4	L	301	BCL	C2-C1-O2A-CGA

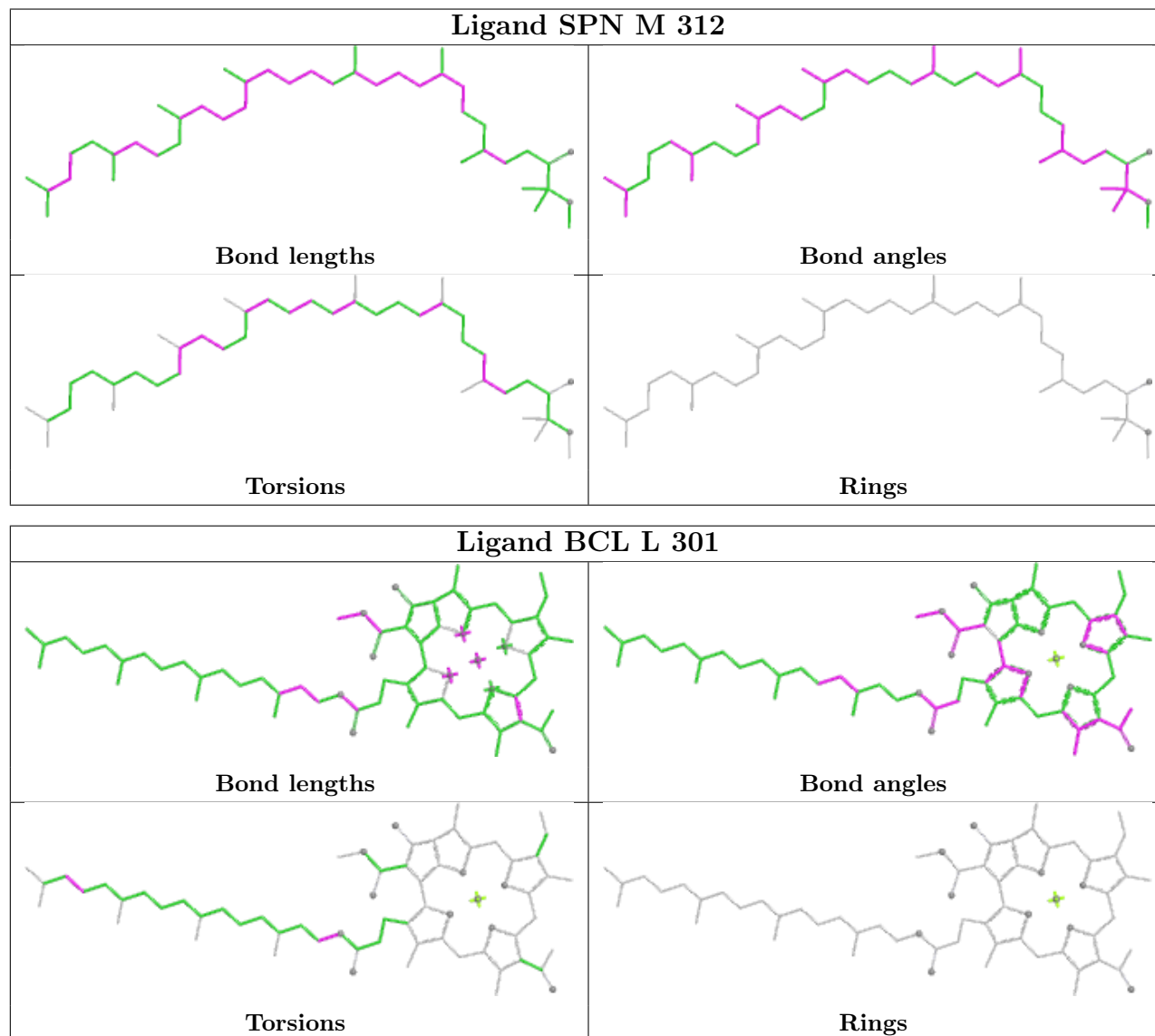
There are no ring outliers.

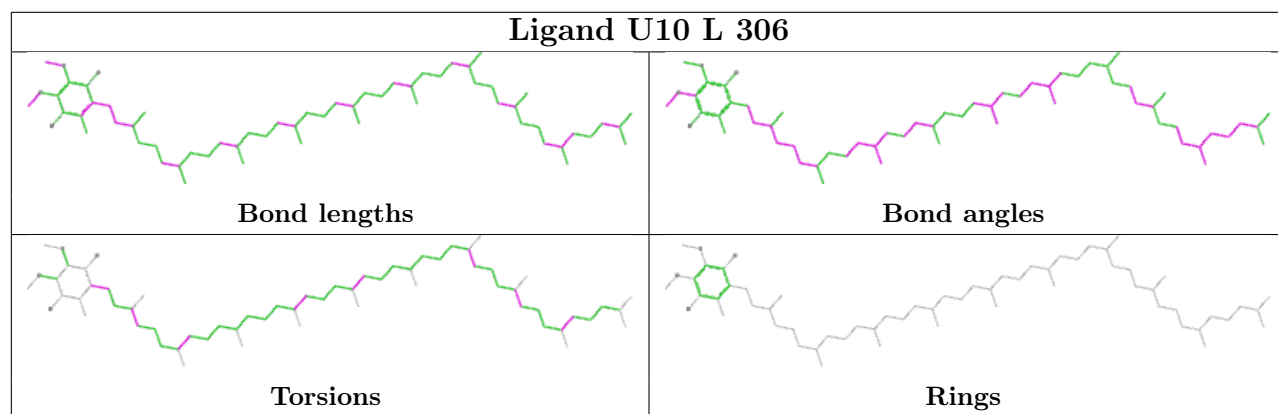
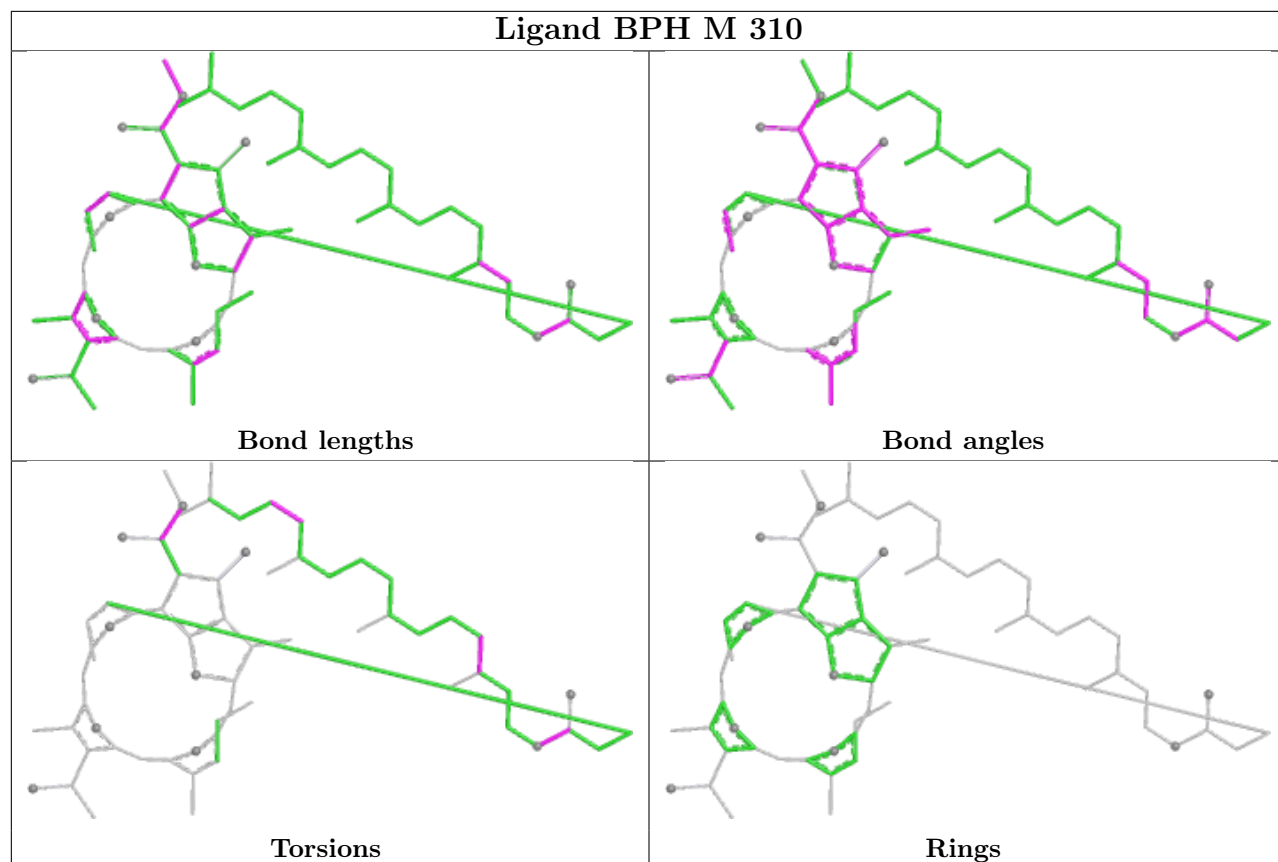
12 monomers are involved in 44 short contacts:

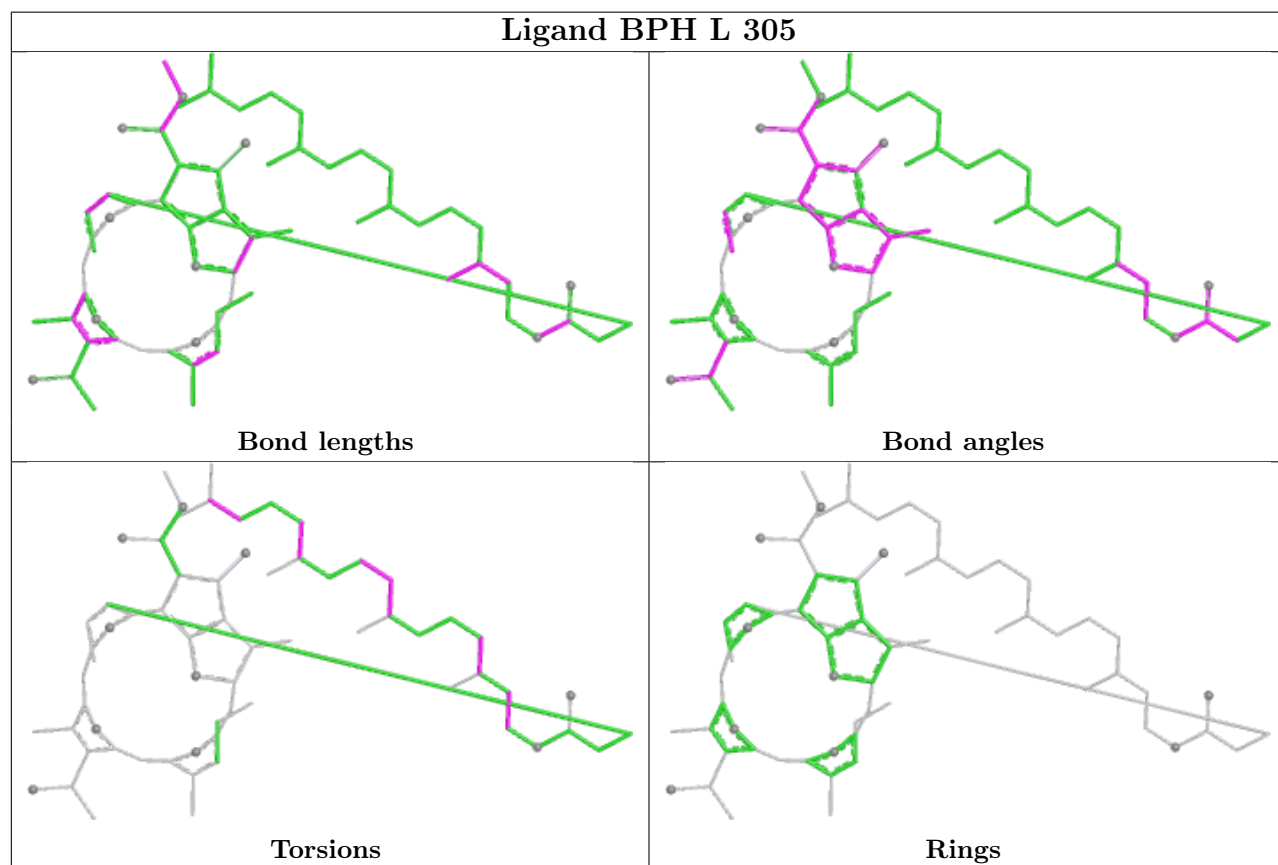
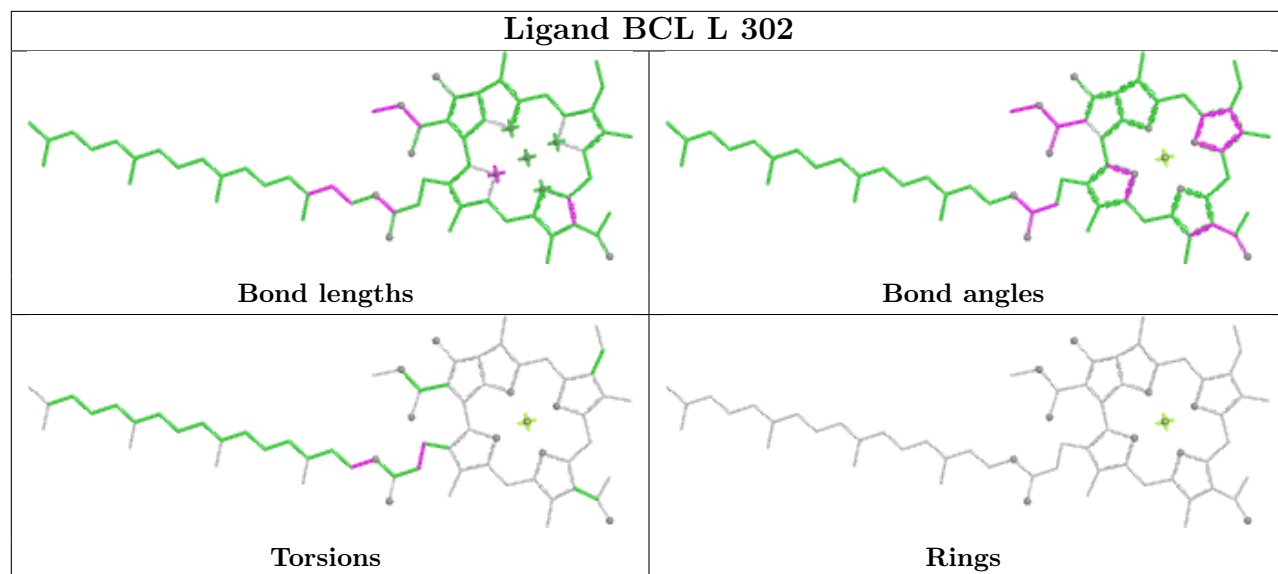
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	314	LDA	3	0
9	M	312	SPN	8	0
4	L	301	BCL	9	0
5	M	310	BPH	7	0
6	L	306	U10	5	0
4	L	302	BCL	5	0
7	H	261	LDA	2	0
5	L	305	BPH	2	0
6	M	311	U10	2	0
4	M	309	BCL	5	0
4	L	304	BCL	2	0
7	M	313	LDA	2	0

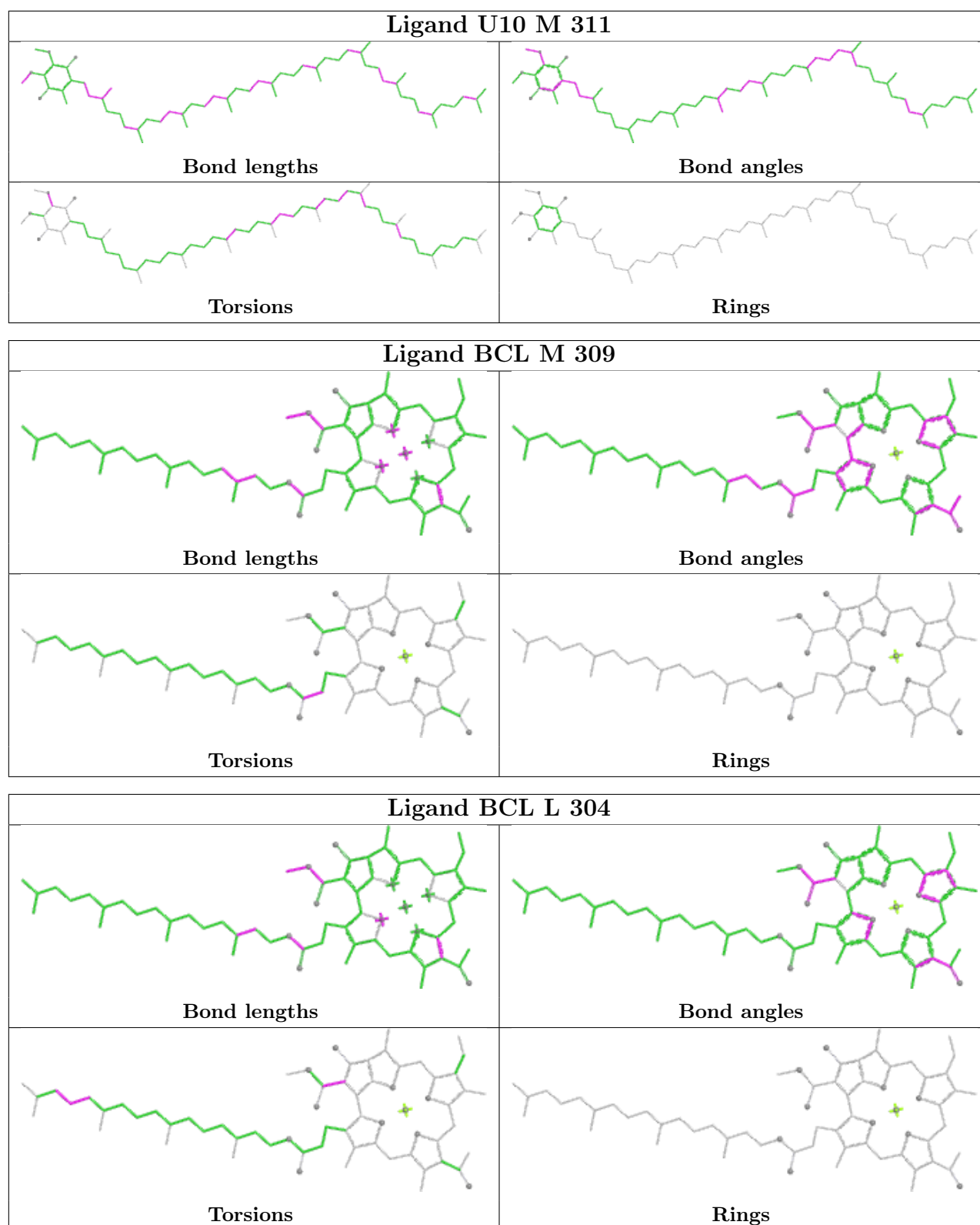
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

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	L	280/281 (99%)	0.10	5 (1%) 67 64	28, 46, 66, 78	0
2	M	297/307 (96%)	-0.09	3 (1%) 79 76	24, 43, 61, 71	0
3	H	248/260 (95%)	-0.01	2 (0%) 82 80	35, 47, 69, 89	0
All	All	825/848 (97%)	-0.00	10 (1%) 76 73	24, 45, 66, 89	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	271	TRP	3.2
2	M	52	LEU	3.0
3	H	257	ALA	2.5
2	M	17	ASP	2.3
1	L	58	THR	2.2
2	M	194	GLY	2.2
1	L	77	GLY	2.1
1	L	14	GLY	2.1
3	H	203	VAL	2.1
1	L	151	TRP	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 oligosaccharides in this entry.

6.4 Ligands

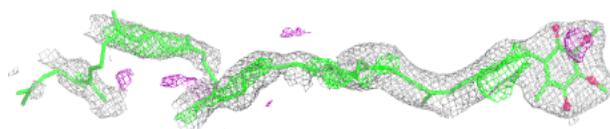
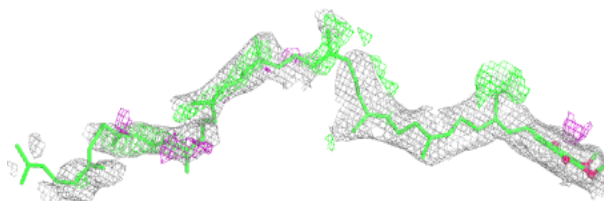
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	L	307	16/16	0.84	0.20	59,63,75,77	0
7	LDA	H	261	16/16	0.84	0.17	60,63,74,75	0
6	U10	L	306	63/63	0.85	0.17	51,79,90,90	33
7	LDA	M	313	16/16	0.89	0.12	39,48,58,60	0
7	LDA	M	314	16/16	0.91	0.13	41,46,59,60	0
9	SPN	M	312	43/43	0.92	0.12	38,46,68,70	0
5	BPH	M	310	65/65	0.93	0.11	26,35,77,78	0
6	U10	M	311	63/63	0.94	0.11	36,51,92,93	16
4	BCL	L	301	66/66	0.95	0.09	31,38,70,71	0
4	BCL	L	304	66/66	0.96	0.07	26,35,48,50	0
5	BPH	L	305	65/65	0.96	0.09	27,35,44,46	0
4	BCL	M	309	66/66	0.97	0.08	27,32,46,53	0
4	BCL	L	302	66/66	0.97	0.07	27,32,39,45	0
8	FE2	M	308	1/1	1.00	0.03	37,37,37,37	0

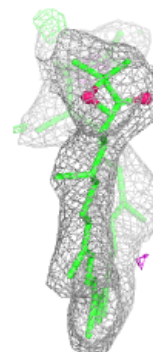
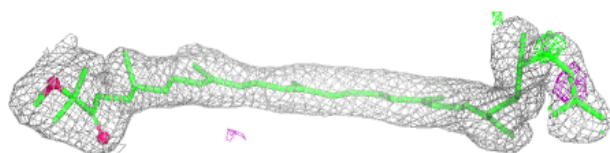
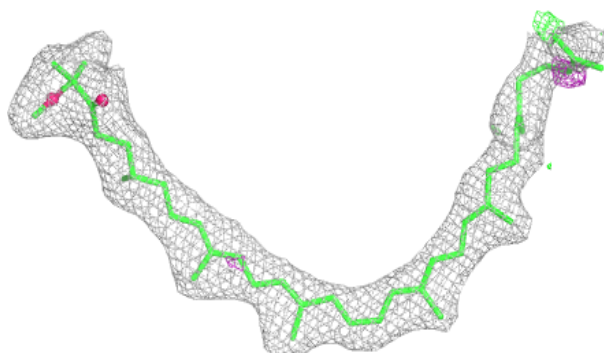
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 306:

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

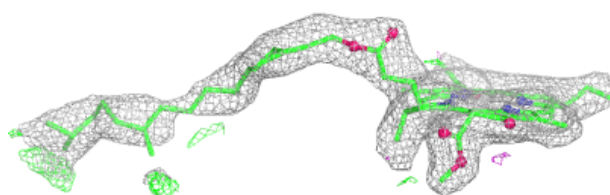
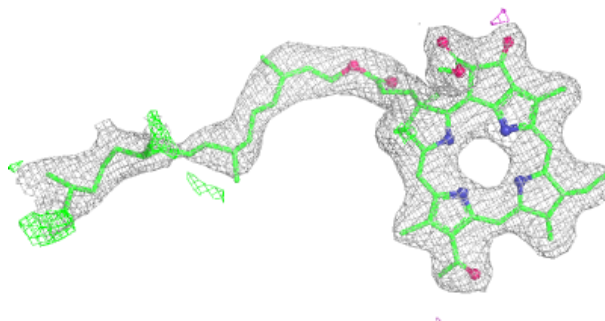
**Electron density around SPN M 312:**

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

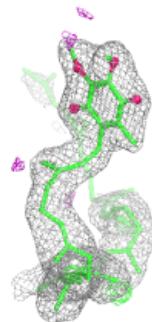
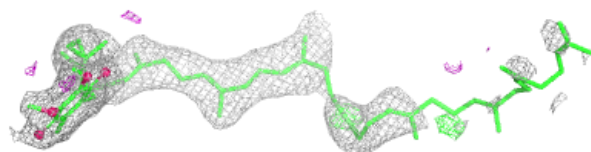
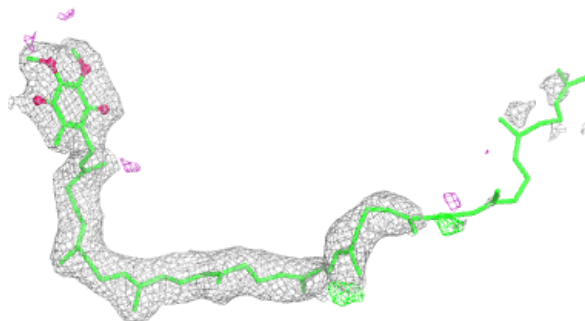


Electron density around BPH M 310:

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

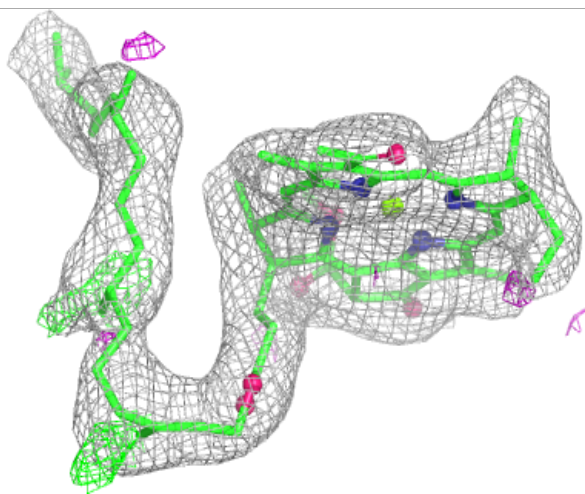
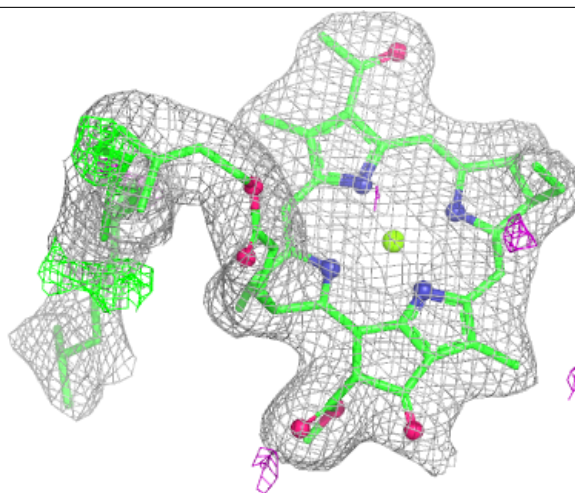
**Electron density around U10 M 311:**

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



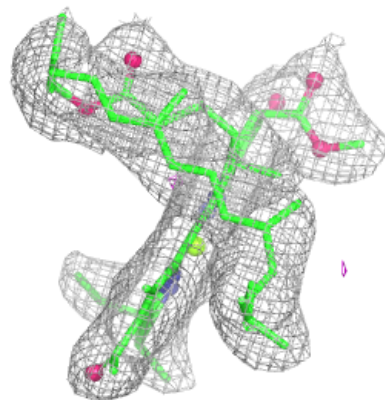
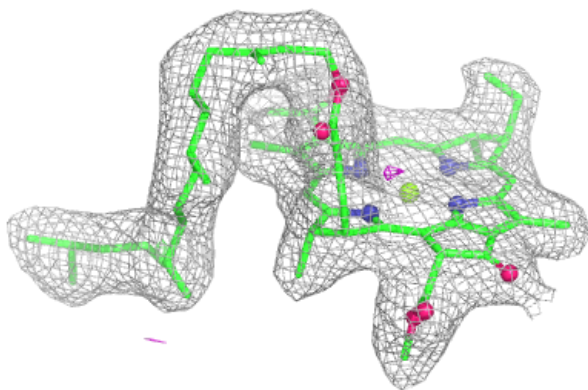
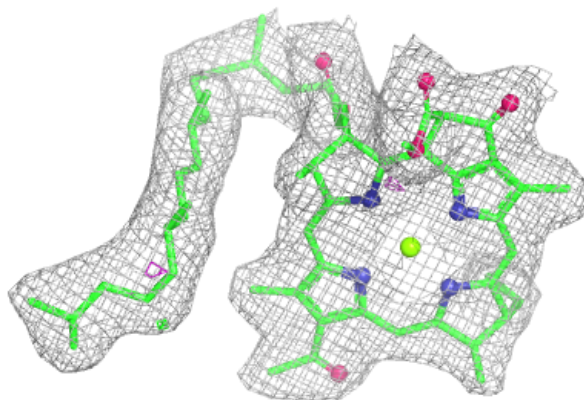
Electron density around BCL L 301:

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



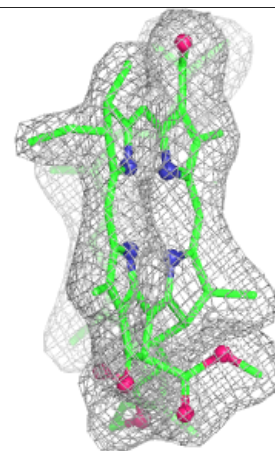
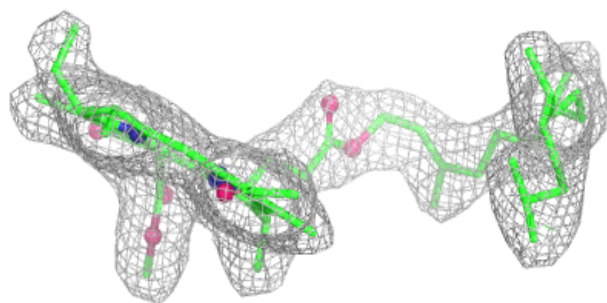
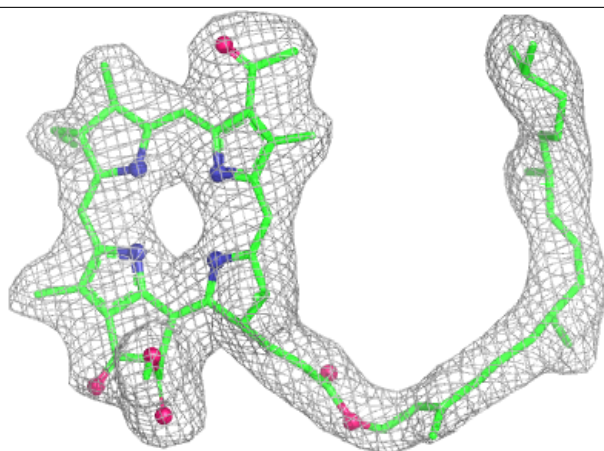
Electron density around BCL L 304:

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



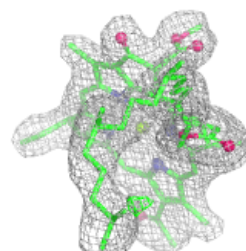
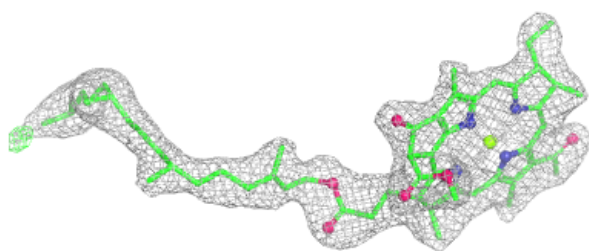
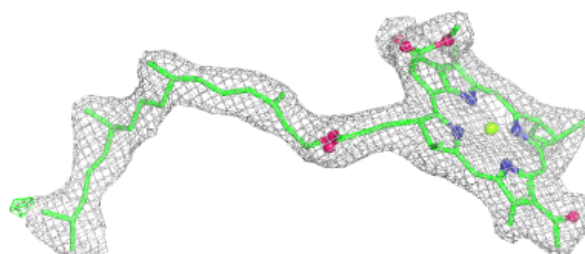
Electron density around BPH L 305:

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

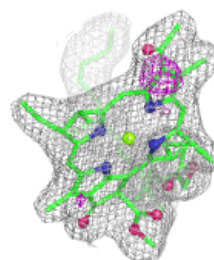
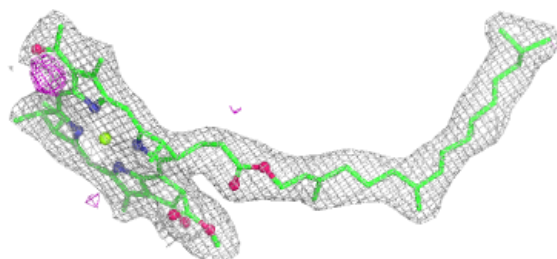


Electron density around BCL M 309:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.