



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 1RGN / pdb_00001rgn
Title : Structure of the reaction centre from Rhodobacter sphaeroides carotenoidless strain R-26.1 reconstituted with spheroidene
Authors : Roszak, A.W.; Frank, H.A.; McKendrick, K.; Mitchell, I.A.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2003-11-12
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

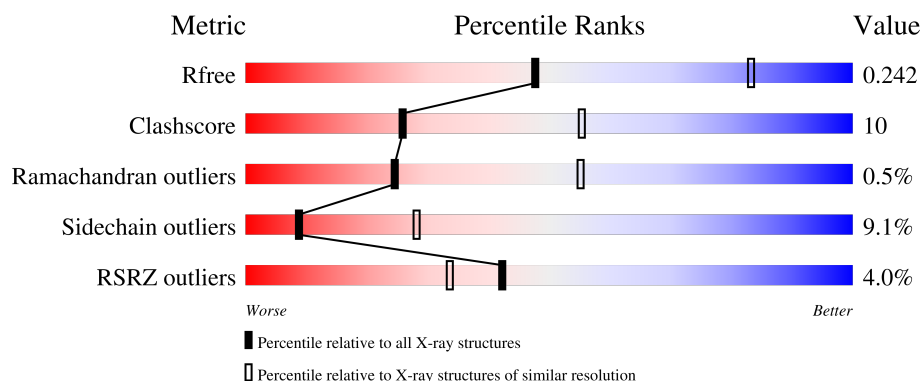
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	L	281	3% 79% 18% .
2	M	307	3% 75% 20% . .
3	H	260	7% 73% 15% . . 8%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7289 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

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

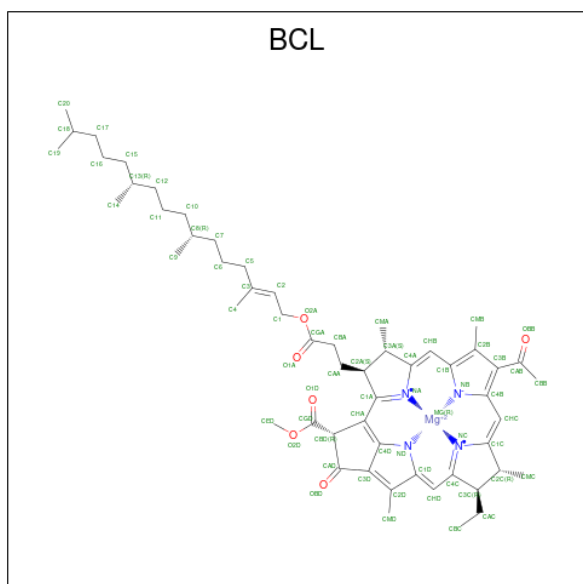
- Molecule 2 is a protein called Reaction center protein M chain.

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

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

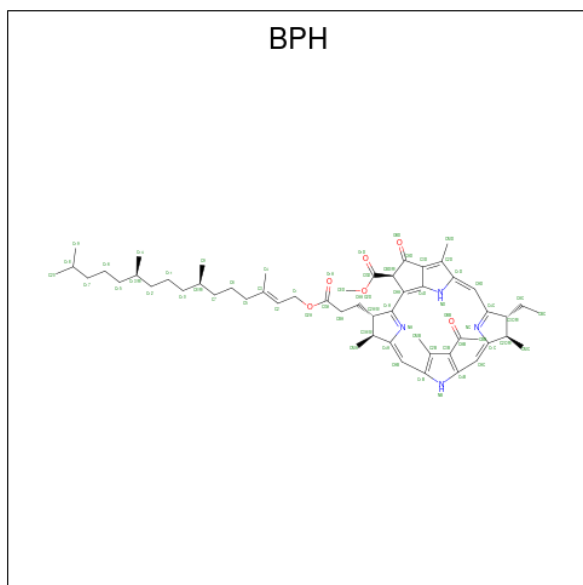
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	2	0
			1838	1173	318	338	9			

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



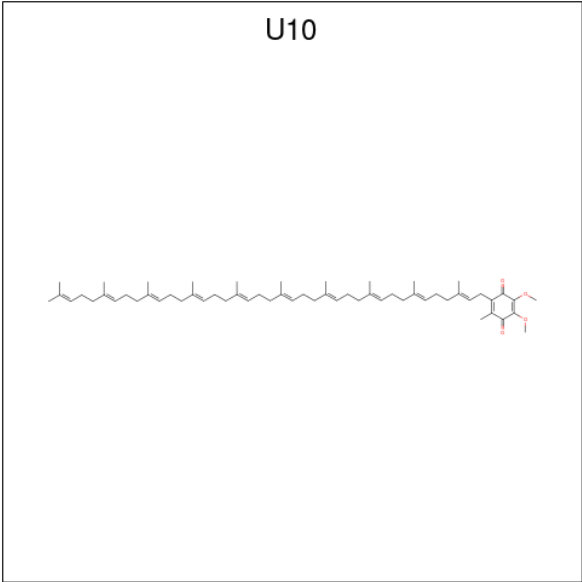
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



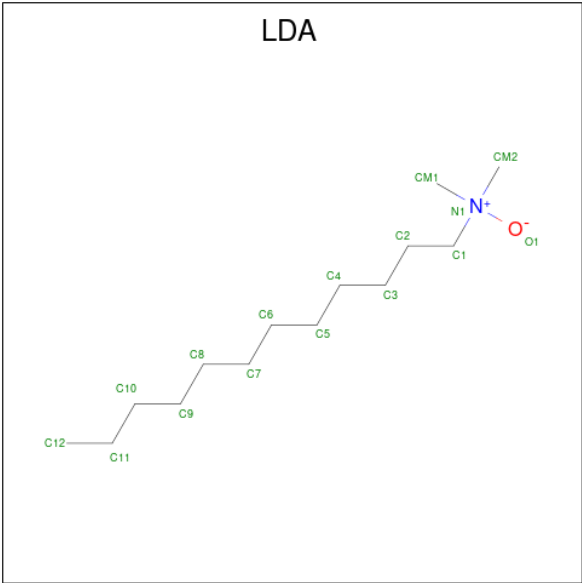
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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		

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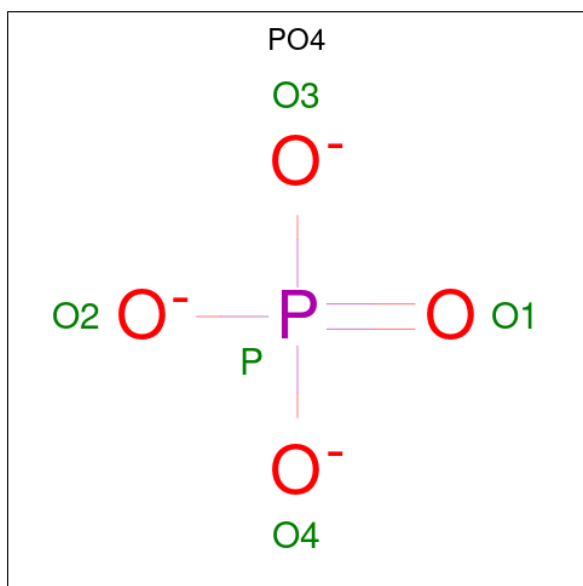
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

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

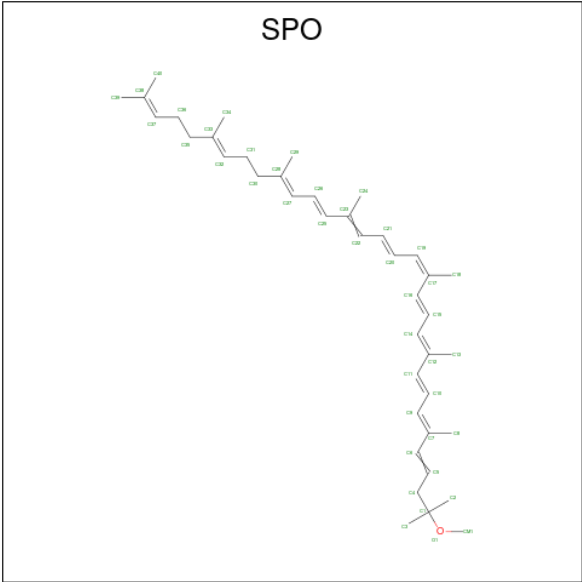
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

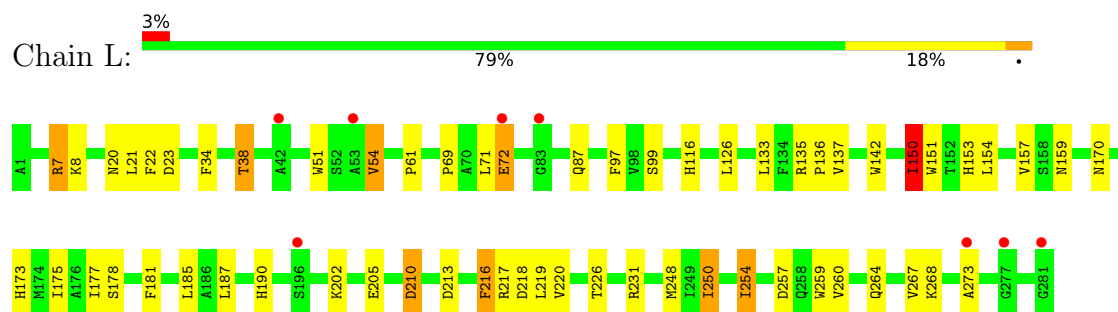
- Molecule 11 is water.

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

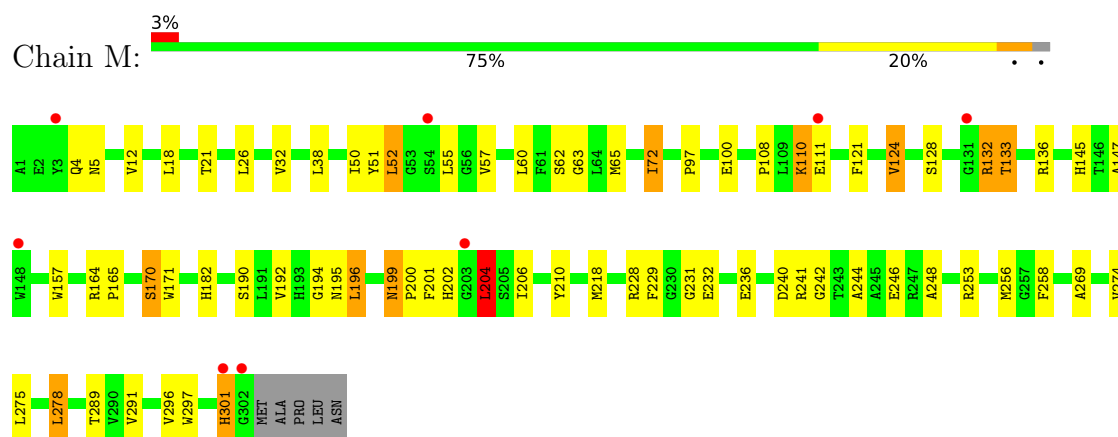
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

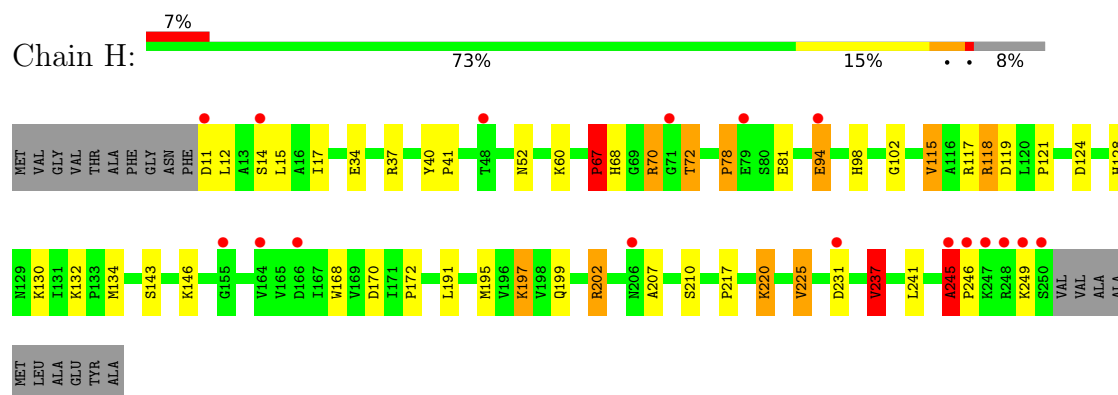
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.82Å 139.82Å 184.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.00 – 2.80 24.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (24.00-2.80) 88.0 (24.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.189 , 0.232 0.199 , 0.242	Depositor DCC
R_{free} test set	2277 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.09	1/2320 (0.0%)	1.12	3/3175 (0.1%)
2	M	1.13	5/2509 (0.2%)	1.14	7/3425 (0.2%)
3	H	1.19	4/1896 (0.2%)	1.16	1/2578 (0.0%)
All	All	1.13	10/6725 (0.1%)	1.14	11/9178 (0.1%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	237	VAL	CA-CB	6.77	1.63	1.54
2	M	57	VAL	CA-CB	6.18	1.62	1.54
3	H	245	ALA	CA-C	6.15	1.60	1.52
2	M	21	THR	N-CA	-6.07	1.39	1.46
2	M	21	THR	CA-C	-5.80	1.46	1.52
3	H	119	ASP	CA-C	5.68	1.60	1.52
1	L	97	PHE	C-O	-5.65	1.17	1.24
3	H	102	GLY	N-CA	5.65	1.49	1.44
2	M	248	ALA	C-O	5.54	1.30	1.24
2	M	72	ILE	CA-CB	5.08	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	217	PRO	CB-CA-C	-6.25	103.77	111.64
1	L	38	THR	N-CA-CB	5.90	118.80	110.12
2	M	145	HIS	N-CA-C	5.87	118.16	111.11
2	M	110	LYS	N-CA-C	-5.75	103.34	110.41
1	L	218	ASP	N-CA-C	-5.43	104.60	111.11
2	M	21	THR	CA-C-N	-5.36	111.30	121.54
2	M	21	THR	C-N-CA	-5.36	111.30	121.54
2	M	170	SER	N-CA-C	5.22	117.02	108.55
1	L	150	ILE	N-CA-C	5.13	115.75	110.36
2	M	231	GLY	N-CA-C	5.12	119.07	112.83
2	M	204	LEU	N-CA-C	-5.09	105.64	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	67	PRO	Peptide

5.2 Too-close contacts [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	2232	0	2187	46	0
2	M	2412	0	2323	48	0
3	H	1838	0	1847	33	0
4	L	132	0	148	6	0
4	M	132	0	148	5	0
5	L	65	0	75	4	0
5	M	65	0	76	8	0
6	L	48	0	63	7	0
6	M	48	0	63	1	0
7	H	16	0	31	2	0
7	L	16	0	31	0	0
7	M	64	0	124	6	0
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	1	0
11	H	80	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	41	0	0	3	0
11	M	52	0	0	2	0
All	All	7289	0	7176	136	0

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

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:401:BPH:H7C1	5:M:401:BPH:H4C1	1.60	0.84
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.64	0.79
1:L:7:ARG:HH11	3:H:98:HIS:CD2	2.02	0.77
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.70	0.73
2:M:199:ASN:HD22	2:M:199:ASN:C	1.96	0.72
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.73	0.70
1:L:21:LEU:HD23	1:L:22:PHE:CE1	2.28	0.68
1:L:216:PHE:CD2	6:L:502:U10:H102	2.28	0.68
2:M:51:TYR:O	2:M:132:ARG:NH2	2.26	0.67
3:H:220:LYS:HD2	11:H:935:HOH:O	1.93	0.67
1:L:175:ILE:HD11	6:L:502:U10:H402	1.77	0.67
1:L:34:PHE:O	1:L:38:THR:HG23	1.95	0.66
1:L:8:LYS:NZ	3:H:81:GLU:OE2	2.28	0.65
2:M:275:LEU:HD23	2:M:278:LEU:HD22	1.79	0.64
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.80	0.61
3:H:34:GLU:O	3:H:37:ARG:HG3	2.00	0.61
1:L:150:ILE:HG22	1:L:151:TRP:CD1	2.36	0.60
1:L:231:ARG:HD3	2:M:5:ASN:O	2.01	0.60
5:M:401:BPH:H4C1	5:M:401:BPH:C7	2.31	0.60
3:H:146:LYS:NZ	11:H:973:HOH:O	2.33	0.60
4:L:304:BCL:HBB3	5:L:402:BPH:H141	1.84	0.60
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.84	0.60
1:L:219:LEU:O	2:M:132:ARG:NH1	2.35	0.59
1:L:71:LEU:H	1:L:71:LEU:HD12	1.68	0.58
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.37	0.58
3:H:207:ALA:HB1	3:H:237:VAL:O	2.04	0.58
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.03	0.58
3:H:70:ARG:NH2	3:H:121:PRO:O	2.36	0.58
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.34	0.57
1:L:116:HIS:HE1	2:M:4:GLN:O	1.88	0.56
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:HIS:HA	6:L:502:U10:O2	2.04	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.87	0.56
1:L:259:TRP:O	1:L:260:VAL:C	2.48	0.56
2:M:157:TRP:CE2	10:M:600:SPO:H293	2.41	0.55
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.25	0.55
2:M:297:TRP:O	2:M:301:HIS:N	2.41	0.54
2:M:38:LEU:CD1	7:M:905:LDA:HM21	2.38	0.54
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.90	0.53
1:L:72:GLU:H	1:L:72:GLU:CD	2.16	0.53
5:M:401:BPH:H7C1	5:M:401:BPH:C4	2.35	0.53
1:L:250:ILE:HB	1:L:254:ILE:HD12	1.90	0.52
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.45	0.52
7:M:903:LDA:CM1	7:H:901:LDA:H31	2.40	0.52
3:H:14:SER:HA	3:H:17:ILE:HG22	1.91	0.52
4:L:304:BCL:HBA1	4:L:304:BCL:C4A	2.40	0.52
1:L:226:THR:HG22	6:L:502:U10:H3M2	1.92	0.51
2:M:289:THR:O	7:M:906:LDA:HM11	2.10	0.51
2:M:199:ASN:C	2:M:199:ASN:ND2	2.68	0.51
3:H:115:VAL:HG22	3:H:117:ARG:HG2	1.92	0.51
2:M:38:LEU:HD12	7:M:905:LDA:HM21	1.93	0.51
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.91	0.51
3:H:124:ASP:OD2	3:H:128:HIS:HB2	2.10	0.51
2:M:194:GLY:O	2:M:195:ASN:HB3	2.11	0.50
3:H:70:ARG:HG2	3:H:118[A]:ARG:NH1	2.26	0.50
3:H:197:LYS:HG2	3:H:199:GLN:HE21	1.76	0.50
4:L:302:BCL:CGA	4:L:304:BCL:HBC1	2.41	0.50
2:M:297:TRP:O	2:M:301:HIS:HA	2.11	0.50
4:M:908:BCL:H91	4:M:908:BCL:H122	1.93	0.50
1:L:154:LEU:HD21	4:L:304:BCL:HED2	1.94	0.49
3:H:98:HIS:HE1	11:H:909:HOH:O	1.96	0.49
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.46	0.49
3:H:37:ARG:NH2	3:H:60:LYS:O	2.45	0.49
2:M:232:GLU:CD	11:M:959:HOH:O	2.56	0.49
4:M:908:BCL:HMB3	4:M:908:BCL:HBB2	1.95	0.49
2:M:124:VAL:O	2:M:128:SER:OG	2.21	0.49
1:L:23:ASP:O	11:L:940:HOH:O	2.20	0.48
3:H:72:THR:HG22	11:H:939:HOH:O	2.13	0.48
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.96	0.48
1:L:38:THR:HG22	1:L:99:SER:CB	2.44	0.47
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.96	0.47
3:H:40:TYR:HA	3:H:41:PRO:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.77	0.47
2:M:63:GLY:HA3	5:M:401:BPH:H5C1	1.96	0.47
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.50	0.47
4:M:908:BCL:H91	4:M:908:BCL:C12	2.45	0.47
2:M:199:ASN:HD21	2:M:201:PHE:HB2	1.80	0.47
1:L:181:PHE:HB3	5:M:401:BPH:HBB2	1.97	0.46
1:L:268:LYS:O	1:L:273:ALA:HB2	2.15	0.46
2:M:199:ASN:HD22	2:M:200:PRO:N	2.13	0.46
1:L:153:HIS:O	1:L:157:VAL:HG23	2.15	0.46
1:L:210:ASP:OD1	1:L:210:ASP:N	2.48	0.46
2:M:65:MET:HE2	2:M:121:PHE:CZ	2.50	0.46
1:L:51:TRP:O	1:L:54:VAL:HG22	2.16	0.46
2:M:240:ASP:OD2	3:H:118[A]:ARG:HB2	2.16	0.45
3:H:220:LYS:CD	11:H:935:HOH:O	2.56	0.45
4:L:302:BCL:NA	4:M:909:BCL:HBB2	2.31	0.45
1:L:38:THR:HG22	1:L:99:SER:HB2	1.98	0.45
1:L:133:LEU:O	1:L:137:VAL:HG23	2.17	0.45
3:H:245:ALA:HB3	3:H:246:PRO:CD	2.47	0.45
2:M:110:LYS:C	2:M:111:GLU:HG3	2.41	0.45
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.99	0.45
3:H:94:GLU:HG2	11:H:965:HOH:O	2.17	0.44
2:M:199:ASN:ND2	2:M:201:PHE:N	2.65	0.44
3:H:72:THR:CG2	11:H:939:HOH:O	2.65	0.44
2:M:133:THR:CG2	2:M:147:ALA:HA	2.48	0.44
2:M:236:GLU:HB3	11:H:943:HOH:O	2.18	0.44
1:L:250:ILE:HB	1:L:254:ILE:CD1	2.48	0.43
6:L:502:U10:H202	7:M:905:LDA:H72	1.99	0.43
1:L:213:ASP:O	1:L:217:ARG:HG3	2.18	0.43
2:M:199:ASN:ND2	2:M:201:PHE:H	2.16	0.43
3:H:220:LYS:HE3	11:H:923:HOH:O	2.17	0.43
2:M:296:VAL:O	2:M:297:TRP:C	2.60	0.43
3:H:130:LYS:NZ	3:H:172:PRO:HG2	2.34	0.43
1:L:178:SER:HB3	6:L:502:U10:H272	1.99	0.43
2:M:108:PRO:O	2:M:110:LYS:O	2.37	0.43
1:L:216:PHE:HD2	6:L:502:U10:H102	1.80	0.43
1:L:257:ASP:HB3	11:L:936:HOH:O	2.18	0.43
4:L:302:BCL:OBB	4:L:302:BCL:HHC	2.19	0.43
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.54	0.43
2:M:133:THR:HG21	2:M:147:ALA:HA	2.01	0.43
3:H:130:LYS:HZ2	3:H:172:PRO:HG2	1.84	0.42
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:199:ASN:HD22	2:M:201:PHE:N	2.18	0.42
1:L:187:LEU:HD11	2:M:269:ALA:HB1	2.01	0.42
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.55	0.42
4:M:908:BCL:H62	4:M:909:BCL:H202	2.02	0.42
5:L:402:BPH:HH C	5:L:402:BPH:CBB	2.42	0.42
2:M:190:SER:HA	2:M:196:LEU:HD13	2.02	0.42
1:L:135:ARG:HD2	1:L:248:MET:O	2.20	0.41
2:M:204:LEU:HD13	7:M:902:LDA:H12	2.02	0.41
7:H:901:LDA:HM13	7:H:901:LDA:H21	1.89	0.41
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.50	0.41
2:M:291:VAL:HG13	2:M:297:TRP:HB2	2.01	0.41
3:H:195:MET:HE1	3:H:241:LEU:HD11	2.02	0.41
1:L:61:PRO:O	1:L:150:ILE:HD13	2.21	0.41
5:M:401:BPH:H3A	5:M:401:BPH:HBA2	1.85	0.41
1:L:226:THR:HB	11:M:952:HOH:O	2.21	0.41
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.21	0.41
2:M:218:MET:HE2	6:M:501:U10:H1M1	2.02	0.41
2:M:52:LEU:HD22	2:M:52:LEU:HA	1.98	0.41
1:L:170:ASN:HB2	1:L:259:TRP:CD1	2.56	0.40
3:H:132:LYS:NZ	11:H:929:HOH:O	2.52	0.40
1:L:159:ASN:ND2	11:L:931:HOH:O	2.54	0.40
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	279/281 (99%)	264 (95%)	15 (5%)	0	100	100
2	M	301/307 (98%)	283 (94%)	17 (6%)	1 (0%)	36	66
3	H	240/260 (92%)	221 (92%)	16 (7%)	3 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	820/848 (97%)	768 (94%)	48 (6%)	4 (0%)	24 55

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	220/220 (100%)	206 (94%)	14 (6%)	16 44
2	M	237/240 (99%)	213 (90%)	24 (10%)	7 23
3	H	197/208 (95%)	174 (88%)	23 (12%)	5 18
All	All	654/668 (98%)	593 (91%)	61 (9%)	9 27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	20	ASN
1	L	54	VAL
1	L	72	GLU
1	L	126	LEU
1	L	150	ILE
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU
1	L	210	ASP
1	L	216	PHE
1	L	220	VAL

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Mol	Chain	Res	Type
1	L	250	ILE
1	L	254	ILE
2	M	12	VAL
2	M	18	LEU
2	M	26	LEU
2	M	32	VAL
2	M	50	ILE
2	M	52	LEU
2	M	55	LEU
2	M	60	LEU
2	M	62	SER
2	M	72	ILE
2	M	100	GLU
2	M	124	VAL
2	M	132	ARG
2	M	133	THR
2	M	136	ARG
2	M	170	SER
2	M	182	HIS
2	M	192	VAL
2	M	196	LEU
2	M	199	ASN
2	M	204	LEU
2	M	253	ARG
2	M	274	VAL
2	M	278	LEU
3	H	11	ASP
3	H	12	LEU
3	H	15	LEU
3	H	52[A]	ASN
3	H	52[B]	ASN
3	H	70	ARG
3	H	72	THR
3	H	78	PRO
3	H	94	GLU
3	H	115	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	134	MET
3	H	143	SER
3	H	191	LEU
3	H	197	LYS

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Mol	Chain	Res	Type
3	H	202	ARG
3	H	210	SER
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL
3	H	249	LYS

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	116	HIS
1	L	159	ASN
1	L	183	ASN
1	L	258	GLN
2	M	199	ASN
2	M	259	ASN
3	H	32	GLN
3	H	44	ASN
3	H	68	HIS
3	H	98	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	BCL	L	302	1	69,74,74	1.40	4 (5%)	79,115,115	1.53	14 (17%)
4	BCL	L	304	1	69,74,74	1.30	7 (10%)	79,115,115	2.38	16 (20%)
5	BPH	L	402	-	59,70,70	1.39	7 (11%)	59,101,101	1.56	10 (16%)
6	U10	L	502	-	48,48,63	1.16	3 (6%)	60,61,79	1.48	11 (18%)
7	LDA	M	902	-	13,15,15	1.96	1 (7%)	14,17,17	0.74	1 (7%)
4	BCL	M	908	2	69,74,74	1.48	8 (11%)	79,115,115	1.49	15 (18%)
9	PO4	M	907	-	4,4,4	0.89	0	6,6,6	1.09	1 (16%)
5	BPH	M	401	-	59,70,70	1.24	6 (10%)	59,101,101	1.82	13 (22%)
10	SPO	M	600	-	41,41,41	1.05	1 (2%)	47,50,50	1.61	8 (17%)
7	LDA	L	904	-	13,15,15	1.85	1 (7%)	14,17,17	0.55	0
7	LDA	M	906	-	13,15,15	2.09	2 (15%)	14,17,17	0.72	1 (7%)
7	LDA	M	903	-	13,15,15	2.10	2 (15%)	14,17,17	0.60	0
4	BCL	M	909	2	69,74,74	1.37	6 (8%)	79,115,115	1.42	13 (16%)
7	LDA	H	901	-	13,15,15	1.74	2 (15%)	14,17,17	0.80	0
6	U10	M	501	-	48,48,63	1.14	4 (8%)	60,61,79	1.65	11 (18%)
7	LDA	M	905	-	13,15,15	1.93	1 (7%)	14,17,17	0.77	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	BCL	L	302	1	-	5/41/137/137	-
4	BCL	L	304	1	-	6/41/137/137	-
5	BPH	L	402	-	-	10/37/105/105	0/5/6/6
6	U10	L	502	-	-	16/45/69/87	0/1/1/1
7	LDA	M	902	-	-	6/13/13/13	-
4	BCL	M	908	2	-	5/41/137/137	-
5	BPH	M	401	-	-	7/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPO	M	600	-	-	9/47/47/47	-
7	LDA	L	904	-	-	8/13/13/13	-
7	LDA	M	906	-	-	9/13/13/13	-
7	LDA	M	903	-	-	8/13/13/13	-
4	BCL	M	909	2	-	6/41/137/137	-
7	LDA	H	901	-	-	10/13/13/13	-
6	U10	M	501	-	-	6/45/69/87	0/1/1/1
7	LDA	M	905	-	-	4/13/13/13	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	302	BCL	MG-NA	8.56	2.26	2.06
7	M	906	LDA	O1-N1	-7.09	1.24	1.42
7	M	903	LDA	O1-N1	-6.82	1.25	1.42
4	M	909	BCL	MG-NA	6.45	2.21	2.06
7	M	905	LDA	O1-N1	-6.35	1.26	1.42
7	M	902	LDA	O1-N1	-6.30	1.26	1.42
7	L	904	LDA	O1-N1	-6.26	1.26	1.42
4	M	908	BCL	MG-NA	6.23	2.21	2.06
5	M	401	BPH	C1D-C2D	5.99	1.46	1.39
7	H	901	LDA	O1-N1	-5.61	1.28	1.42
5	L	402	BPH	C1B-C2B	5.29	1.45	1.39
4	M	908	BCL	MG-NB	5.28	2.16	2.05
10	M	600	SPO	C21-C22	4.50	1.57	1.43
4	M	909	BCL	MG-NB	4.15	2.14	2.05
6	L	502	U10	O3-C3	4.10	1.46	1.36
4	L	304	BCL	MG-NB	4.08	2.13	2.05
6	M	501	U10	O3-C3	4.03	1.46	1.36
6	L	502	U10	O4-C4	3.78	1.45	1.36
4	M	908	BCL	C3B-C4B	3.65	1.48	1.41
4	L	304	BCL	C1D-C2D	-3.24	1.38	1.45
4	L	304	BCL	C3B-C4B	3.12	1.47	1.41
4	M	908	BCL	MG-NC	3.12	2.13	2.06
4	L	302	BCL	MG-NB	3.08	2.11	2.05
4	L	304	BCL	MG-NA	3.00	2.13	2.06
5	L	402	BPH	CBD-CGD	2.89	1.56	1.52
4	M	909	BCL	C3B-C4B	2.88	1.46	1.41
7	M	903	LDA	C1-N1	-2.87	1.48	1.51
4	L	304	BCL	MG-ND	-2.83	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	402	BPH	C2C-C3C	2.81	1.57	1.54
4	M	908	BCL	C1D-ND	2.74	1.41	1.37
5	L	402	BPH	C3A-C2A	-2.74	1.52	1.54
6	M	501	U10	O4-C4	2.71	1.43	1.36
5	L	402	BPH	C1B-NB	-2.69	1.33	1.38
4	L	302	BCL	C3B-C4B	2.63	1.46	1.41
4	M	909	BCL	C4B-NB	2.56	1.41	1.37
4	L	302	BCL	MG-ND	2.54	2.10	2.05
7	H	901	LDA	C1-N1	-2.42	1.49	1.51
5	M	401	BPH	C3B-C2B	-2.41	1.35	1.39
5	L	402	BPH	C1D-ND	2.38	1.42	1.38
4	M	908	BCL	CBA-CGA	-2.33	1.43	1.50
4	L	304	BCL	MG-NC	-2.32	2.00	2.06
4	M	909	BCL	CBA-CGA	-2.30	1.44	1.50
4	M	908	BCL	CHD-C1D	2.29	1.42	1.38
4	L	304	BCL	OBD-CAD	2.23	1.26	1.22
4	M	908	BCL	CHC-C1C	2.21	1.43	1.37
5	M	401	BPH	C3A-C2A	-2.21	1.52	1.54
7	M	906	LDA	C1-N1	-2.20	1.49	1.51
5	M	401	BPH	C1B-C2B	2.16	1.42	1.39
6	L	502	U10	C28-C29	2.16	1.38	1.33
6	M	501	U10	C31-C29	2.07	1.55	1.51
6	M	501	U10	C33-C34	2.06	1.37	1.33
5	L	402	BPH	C3B-C4B	2.03	1.44	1.41
5	M	401	BPH	C3B-C4B	2.02	1.44	1.41
5	M	401	BPH	C4D-ND	-2.01	1.35	1.38
4	M	909	BCL	C2C-C3C	-2.00	1.49	1.54

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	O2D-CGD-CBD	12.81	133.62	111.23
4	L	304	BCL	O1D-CGD-CBD	-8.74	107.28	124.52
4	L	304	BCL	CED-O2D-CGD	5.81	129.09	115.92
6	M	501	U10	C6-C1-C2	4.84	122.99	119.17
5	L	402	BPH	C1-C2-C3	-4.83	118.29	126.20
6	L	502	U10	C25-C24-C26	4.47	122.99	115.23
6	M	501	U10	C17-C18-C19	-4.44	117.46	127.62
5	M	401	BPH	C4D-CHA-CBD	-4.29	106.40	108.45
5	M	401	BPH	C2D-C1D-ND	-4.26	106.35	109.43
6	M	501	U10	C30-C29-C31	4.14	122.41	115.23
4	L	304	BCL	CAA-CBA-CGA	4.13	124.93	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	C11-C12-C13	-3.93	102.90	115.97
5	M	401	BPH	C2B-C1B-NB	-3.89	106.62	109.43
5	L	402	BPH	C2B-C1B-NB	-3.75	106.72	109.43
5	M	401	BPH	O2D-CGD-CBD	3.73	115.04	110.95
10	M	600	SPO	C20-C19-C17	-3.70	122.09	127.28
10	M	600	SPO	C4-C5-C6	-3.67	119.75	124.91
4	M	909	BCL	C4D-CHA-C1A	3.66	125.61	121.24
6	L	502	U10	C22-C23-C24	-3.66	119.25	127.62
5	M	401	BPH	C1-C2-C3	-3.62	120.27	126.20
4	M	909	BCL	C2B-C1B-NB	-3.56	106.64	110.33
4	M	909	BCL	CED-O2D-CGD	3.54	123.95	115.92
4	M	908	BCL	C2B-C1B-NB	-3.50	106.70	110.33
4	L	304	BCL	C2B-C1B-NB	-3.49	106.70	110.33
5	M	401	BPH	OBD-CAD-CBD	-3.48	120.72	125.82
4	L	302	BCL	O2A-CGA-O1A	-3.45	114.99	123.63
5	M	401	BPH	C1-O2A-CGA	3.45	125.01	116.65
4	M	908	BCL	C3B-C4B-NB	-3.42	105.24	109.76
4	L	304	BCL	OBB-CAB-CBB	-3.41	112.13	119.77
5	L	402	BPH	CMA-C3A-C4A	-3.39	107.31	114.61
4	L	302	BCL	CHD-C1D-ND	-3.34	120.09	124.80
10	M	600	SPO	C21-C22-C23	-3.34	122.59	127.28
6	M	501	U10	C15-C14-C16	3.31	120.97	115.23
4	L	302	BCL	C2B-C1B-NB	-3.22	106.99	110.33
4	M	908	BCL	C4D-CHA-C1A	3.13	124.98	121.24
4	M	908	BCL	C1D-ND-C4D	3.13	108.51	106.31
4	L	304	BCL	C4D-CHA-C1A	3.13	124.98	121.24
4	L	302	BCL	C4D-CHA-C1A	3.10	124.94	121.24
4	M	909	BCL	CHA-C1A-NA	-3.09	119.39	126.39
5	M	401	BPH	CAA-C2A-C3A	-3.08	104.67	113.00
5	M	401	BPH	C3B-C4B-NB	-3.06	103.60	108.05
4	L	304	BCL	C5-C3-C2	-3.05	114.32	121.17
4	M	908	BCL	CMA-C3A-C2A	-3.05	102.20	113.98
5	L	402	BPH	O2D-CGD-CBD	3.04	114.29	110.95
6	L	502	U10	C35-C34-C36	2.99	120.42	115.23
4	L	302	BCL	C3B-C4B-NB	-2.99	105.82	109.76
6	M	501	U10	C30-C29-C28	-2.97	115.99	123.63
4	M	908	BCL	C2D-C1D-ND	-2.93	107.23	110.13
4	M	908	BCL	CAA-C2A-C3A	-2.92	105.11	113.00
6	L	502	U10	C3M-O3-C3	2.91	126.70	116.47
4	L	302	BCL	CAA-C2A-C3A	-2.88	105.22	113.00
6	M	501	U10	C22-C23-C24	-2.87	121.06	127.62
10	M	600	SPO	C25-C23-C22	-2.86	114.51	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	OBD-CAD-C3D	2.85	132.33	127.89
4	M	909	BCL	OBB-CAB-CBB	-2.83	113.44	119.77
4	M	908	BCL	CHA-C1A-NA	-2.81	120.03	126.39
5	M	401	BPH	CMC-C2C-C1C	2.81	120.66	114.61
4	M	909	BCL	CHD-C1D-ND	-2.79	120.88	124.80
4	L	302	BCL	CHA-C1A-NA	-2.77	120.11	126.39
5	L	402	BPH	C2D-C1D-ND	-2.75	107.44	109.43
5	L	402	BPH	C1B-NB-C4B	2.74	112.81	108.82
4	L	302	BCL	CHD-C1D-C2D	2.72	131.14	125.49
5	L	402	BPH	C4D-CHA-CBD	-2.63	107.19	108.45
5	M	401	BPH	CMA-C3A-C4A	-2.62	108.96	114.61
4	M	908	BCL	CMB-C2B-C1B	-2.62	121.43	125.42
6	L	502	U10	O2-C2-C3	-2.62	115.48	121.03
4	M	909	BCL	C1-C2-C3	-2.61	121.92	126.20
4	L	304	BCL	CAA-C2A-C3A	-2.60	105.98	113.00
4	L	302	BCL	C4-C3-C5	2.56	119.68	115.23
4	M	908	BCL	O2A-C1-C2	2.56	117.95	108.11
6	M	501	U10	C7-C6-C5	-2.56	115.55	118.52
10	M	600	SPO	C34-C33-C35	2.53	119.63	115.23
4	L	304	BCL	C2D-C1D-ND	-2.51	107.64	110.13
4	M	908	BCL	O2D-CGD-CBD	2.50	115.60	111.23
4	M	908	BCL	CHD-C1D-C2D	2.49	130.68	125.49
4	M	909	BCL	C1D-ND-C4D	2.48	108.05	106.31
6	M	501	U10	C16-C14-C13	-2.47	115.62	121.17
4	L	304	BCL	OBB-CAB-C3B	2.47	124.80	120.43
4	L	304	BCL	O2D-CGD-O1D	-2.47	119.04	123.85
4	L	302	BCL	C5-C3-C2	-2.47	115.63	121.17
4	L	304	BCL	CHA-C1A-NA	-2.44	120.87	126.39
6	L	502	U10	C25-C24-C23	-2.43	117.38	123.63
4	L	304	BCL	C2A-C3A-C4A	2.41	105.76	101.87
4	M	909	BCL	CHD-C1D-C2D	2.40	130.48	125.49
4	L	302	BCL	O2A-CGA-CBA	2.40	119.15	111.83
6	M	501	U10	C1M-C1-C6	-2.39	120.52	124.45
5	M	401	BPH	C1B-NB-C4B	2.37	112.28	108.82
4	L	304	BCL	C2C-C3C-C4C	2.37	104.89	101.34
7	M	902	LDA	O1-N1-C1	2.34	115.02	109.27
4	M	909	BCL	CAC-C3C-C4C	-2.33	107.41	112.58
6	L	502	U10	C35-C34-C33	-2.32	117.68	123.63
10	M	600	SPO	C13-C12-C11	2.28	121.57	118.09
5	L	402	BPH	C3B-C4B-NB	-2.28	104.74	108.05
4	M	908	BCL	C2C-C3C-C4C	2.25	104.71	101.34
6	L	502	U10	C8-C7-C6	2.24	117.60	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	C1D-ND-C4D	2.22	107.87	106.31
6	L	502	U10	C7-C8-C9	-2.22	123.01	126.83
4	M	908	BCL	C6-C5-C3	-2.22	108.07	113.47
6	M	501	U10	C4M-O4-C4	2.21	124.25	116.47
10	M	600	SPO	C31-C32-C33	-2.20	122.60	127.62
10	M	600	SPO	C24-C23-C25	2.19	121.44	118.09
4	M	909	BCL	O2D-CGD-O1D	-2.19	119.59	123.85
6	M	501	U10	C20-C19-C18	-2.15	118.11	123.63
5	L	402	BPH	C7-C6-C5	-2.15	107.54	113.26
6	L	502	U10	C17-C18-C19	-2.11	122.79	127.62
5	L	402	BPH	CMA-C3A-C2A	-2.11	105.98	114.13
4	L	302	BCL	CMA-C3A-C4A	-2.08	106.17	111.77
4	M	909	BCL	CAB-C3B-C2B	2.08	132.06	127.74
9	M	907	PO4	O3-P-O2	2.08	114.37	107.91
7	M	906	LDA	CM2-N1-C1	2.06	114.57	110.23
4	L	302	BCL	OBB-CAB-C3B	2.06	124.08	120.43
4	M	909	BCL	C2C-C3C-C4C	2.04	104.39	101.34
4	M	908	BCL	CMA-C3A-C4A	-2.00	106.39	111.77
6	L	502	U10	C1M-C1-C6	-2.00	121.16	124.45

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O1D-CGD-O2D-CED
7	L	904	LDA	C2-C1-N1-CM1
7	L	904	LDA	C2-C1-N1-CM2
7	M	902	LDA	C2-C1-N1-CM1
7	M	906	LDA	C2-C1-N1-O1
7	M	906	LDA	C2-C1-N1-CM2
7	H	901	LDA	C2-C1-N1-CM1
7	H	901	LDA	C2-C1-N1-CM2
7	H	901	LDA	N1-C1-C2-C3
5	L	402	BPH	C3-C5-C6-C7
6	L	502	U10	C24-C26-C27-C28
4	M	908	BCL	C11-C10-C8-C9
5	L	402	BPH	C6-C7-C8-C9
10	M	600	SPO	C24-C23-C25-C26
7	M	903	LDA	C5-C6-C7-C8
6	M	501	U10	C24-C26-C27-C28
6	M	501	U10	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	M	906	LDA	C3-C4-C5-C6
7	M	905	LDA	C7-C8-C9-C10
4	M	908	BCL	C15-C16-C17-C18
5	L	402	BPH	C16-C17-C18-C20
6	L	502	U10	C15-C14-C16-C17
6	L	502	U10	C28-C29-C31-C32
6	L	502	U10	C33-C34-C36-C37
7	M	906	LDA	C2-C3-C4-C5
7	M	906	LDA	C11-C10-C9-C8
7	L	904	LDA	C5-C6-C7-C8
7	M	903	LDA	C7-C8-C9-C10
7	M	905	LDA	C5-C6-C7-C8
10	M	600	SPO	C22-C23-C25-C26
7	M	902	LDA	C1-C2-C3-C4
6	L	502	U10	C30-C29-C31-C32
7	M	903	LDA	C1-C2-C3-C4
7	L	904	LDA	C1-C2-C3-C4
5	L	402	BPH	C2C-C3C-CAC-CBC
7	H	901	LDA	C3-C4-C5-C6
7	H	901	LDA	C6-C7-C8-C9
7	M	902	LDA	C11-C10-C9-C8
4	M	909	BCL	C11-C12-C13-C15
5	L	402	BPH	C4-C3-C5-C6
6	L	502	U10	C35-C34-C36-C37
4	M	908	BCL	C10-C11-C12-C13
7	H	901	LDA	C1-C2-C3-C4
7	M	903	LDA	C4-C5-C6-C7
10	M	600	SPO	C4-C1-O1-CM1
5	L	402	BPH	C16-C17-C18-C19
5	L	402	BPH	C2-C3-C5-C6
6	L	502	U10	C13-C14-C16-C17
6	M	501	U10	C23-C24-C26-C27
10	M	600	SPO	C5-C6-C7-C9
5	L	402	BPH	O2A-C1-C2-C3
7	M	903	LDA	C9-C10-C11-C12
7	M	903	LDA	C3-C4-C5-C6
7	M	905	LDA	C6-C7-C8-C9
6	L	502	U10	C29-C31-C32-C33
7	L	904	LDA	C9-C10-C11-C12
10	M	600	SPO	C2-C1-O1-CM1
7	M	902	LDA	C3-C4-C5-C6
6	L	502	U10	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
7	M	906	LDA	C5-C6-C7-C8
4	L	302	BCL	C11-C12-C13-C14
4	M	909	BCL	C11-C12-C13-C14
5	M	401	BPH	C10-C11-C12-C13
4	L	302	BCL	C11-C12-C13-C15
5	L	402	BPH	C6-C7-C8-C10
7	H	901	LDA	C7-C8-C9-C10
10	M	600	SPO	C5-C6-C7-C8
7	M	903	LDA	C11-C10-C9-C8
6	M	501	U10	C25-C24-C26-C27
6	L	502	U10	C18-C19-C21-C22
7	H	901	LDA	C11-C10-C9-C8
7	M	903	LDA	C6-C7-C8-C9
4	M	909	BCL	C5-C6-C7-C8
4	M	909	BCL	C11-C10-C8-C7
7	L	904	LDA	C11-C10-C9-C8
5	M	401	BPH	C8-C10-C11-C12
7	M	902	LDA	C2-C1-N1-CM2
7	M	906	LDA	C2-C1-N1-CM1
5	M	401	BPH	C11-C10-C8-C7
4	M	909	BCL	C16-C17-C18-C19
4	M	909	BCL	C11-C10-C8-C9
7	L	904	LDA	C2-C1-N1-O1
7	H	901	LDA	C2-C1-N1-O1
5	L	402	BPH	C4C-C3C-CAC-CBC
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
6	L	502	U10	C31-C32-C33-C34
10	M	600	SPO	C12-C14-C15-C16
6	L	502	U10	C12-C11-C9-C10
4	L	304	BCL	C16-C17-C18-C19
7	L	904	LDA	C3-C4-C5-C6
7	M	906	LDA	C9-C10-C11-C12
10	M	600	SPO	C33-C35-C36-C37
10	M	600	SPO	C3-C1-O1-CM1
6	L	502	U10	C12-C11-C9-C8
4	L	302	BCL	C16-C17-C18-C19
7	M	902	LDA	C5-C6-C7-C8
6	M	501	U10	C26-C27-C28-C29
4	M	908	BCL	C8-C10-C11-C12
6	L	502	U10	C2-C3-O3-C3M
6	M	501	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
4	L	304	BCL	C16-C17-C18-C20
5	M	401	BPH	C14-C13-C15-C16
4	L	302	BCL	C2A-CAA-CBA-CGA
5	M	401	BPH	C12-C13-C15-C16
7	M	905	LDA	C1-C2-C3-C4
6	L	502	U10	C34-C36-C37-C38
6	L	502	U10	C5-C6-C7-C8
5	M	401	BPH	C11-C10-C8-C9
4	M	908	BCL	C11-C10-C8-C7
7	M	906	LDA	C4-C5-C6-C7
5	M	401	BPH	C11-C12-C13-C14
4	L	302	BCL	C4-C3-C5-C6
7	H	901	LDA	C9-C10-C11-C12

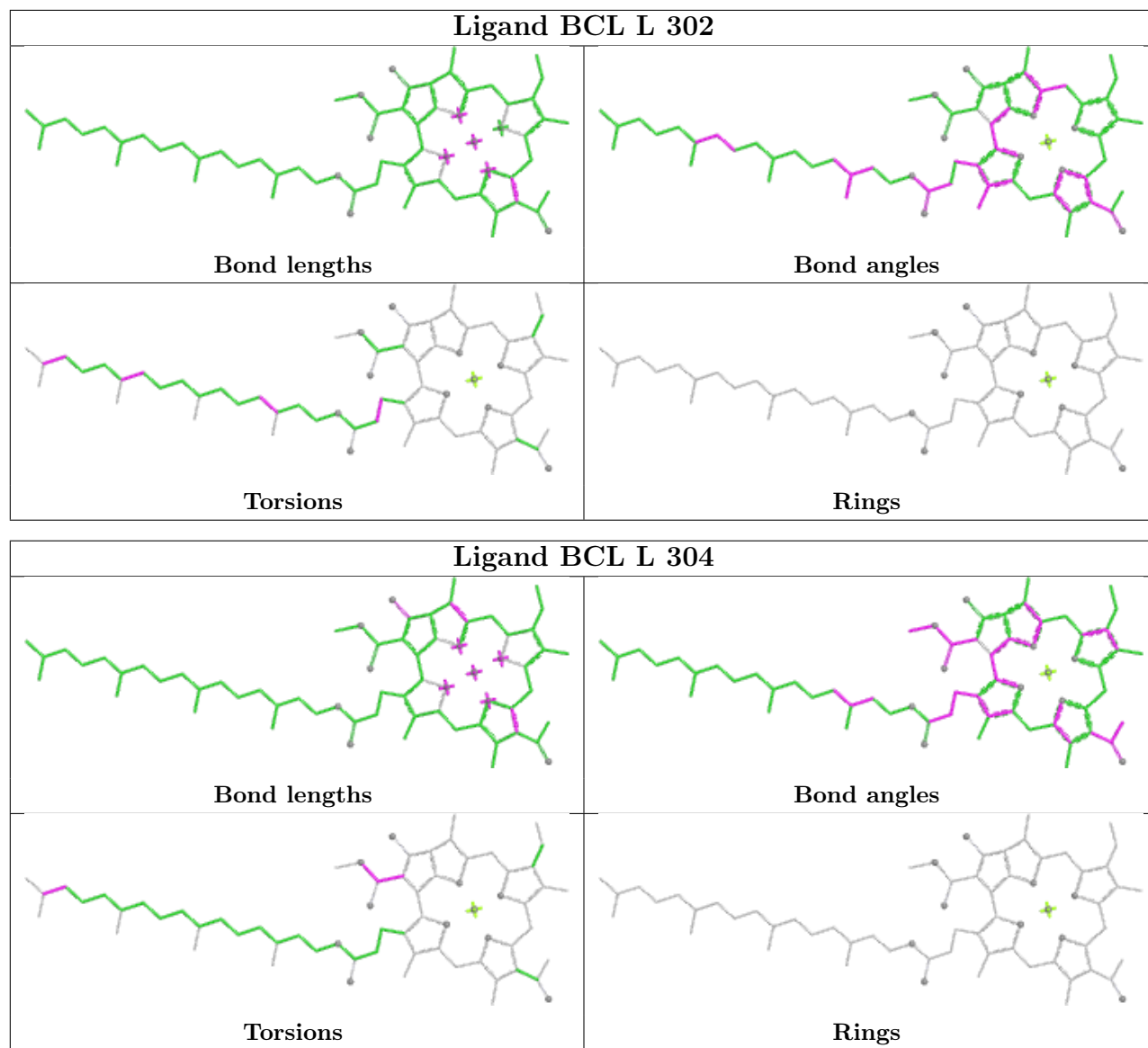
There are no ring outliers.

14 monomers are involved in 36 short contacts:

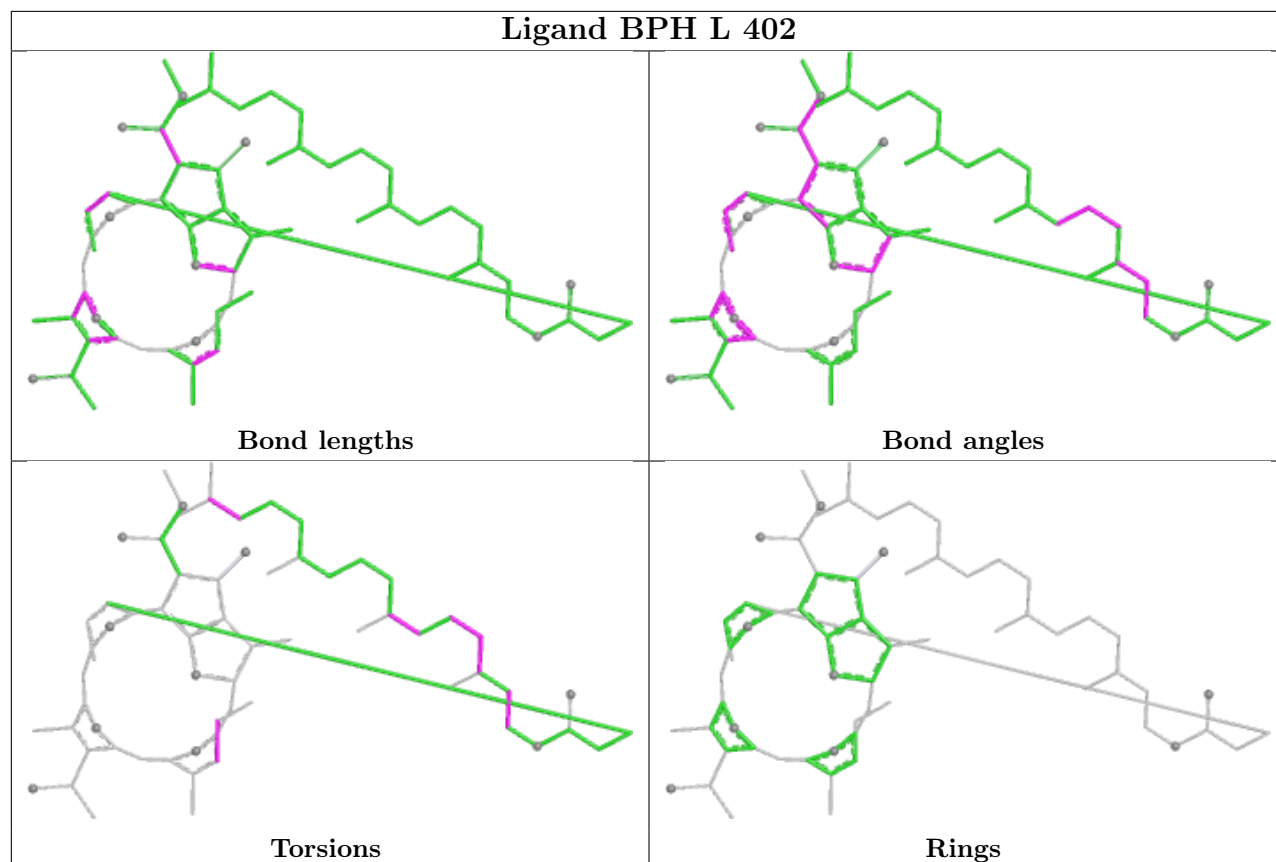
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	BCL	3	0
4	L	304	BCL	4	0
5	L	402	BPH	4	0
6	L	502	U10	7	0
7	M	902	LDA	1	0
4	M	908	BCL	4	0
5	M	401	BPH	8	0
10	M	600	SPO	1	0
7	M	906	LDA	1	0
7	M	903	LDA	1	0
4	M	909	BCL	2	0
7	H	901	LDA	2	0
6	M	501	U10	1	0
7	M	905	LDA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

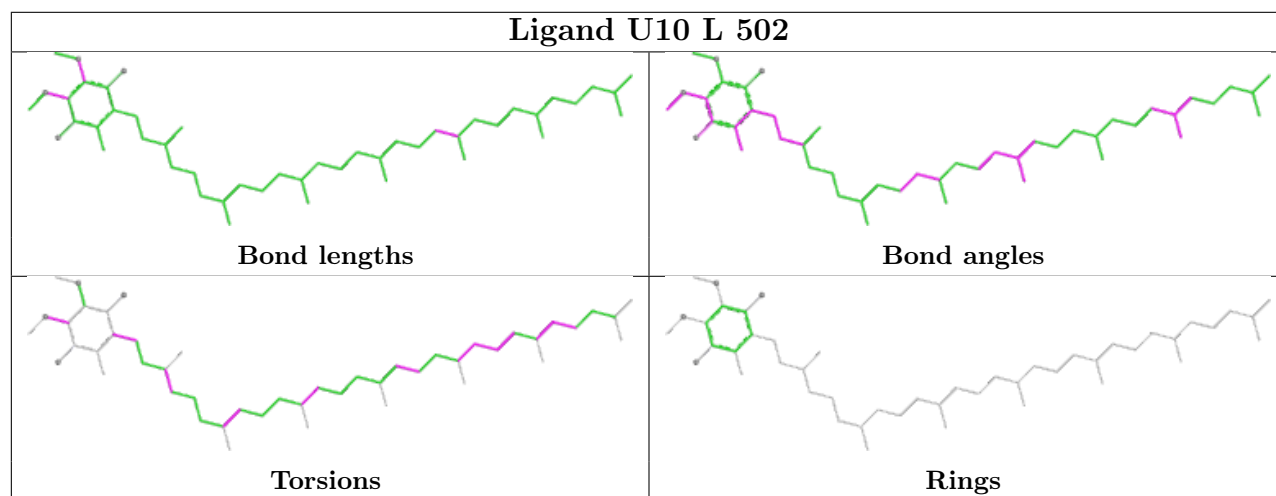
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

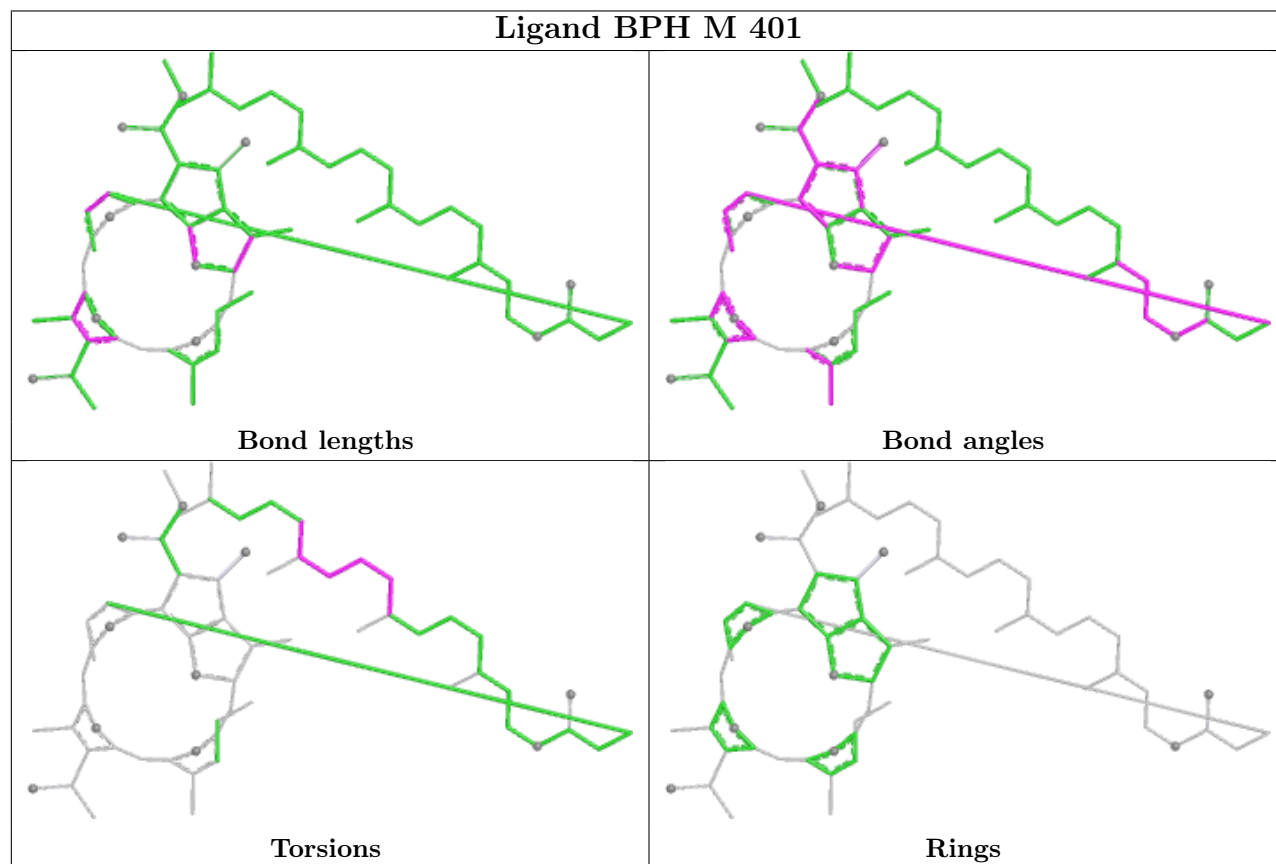
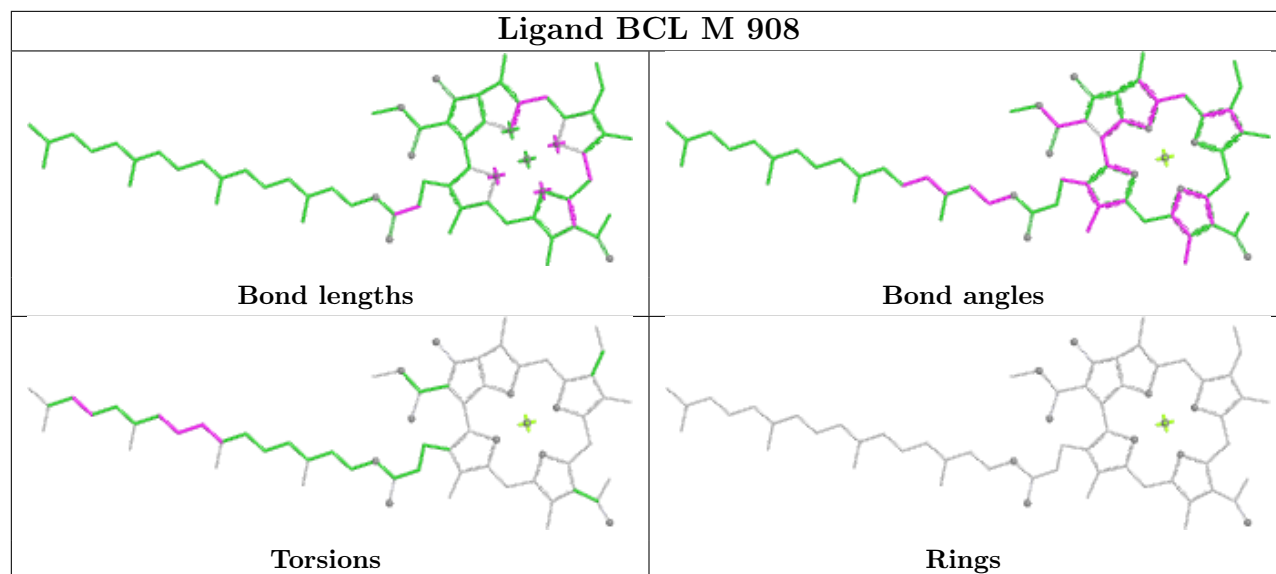


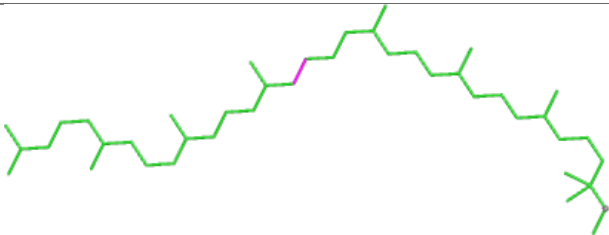
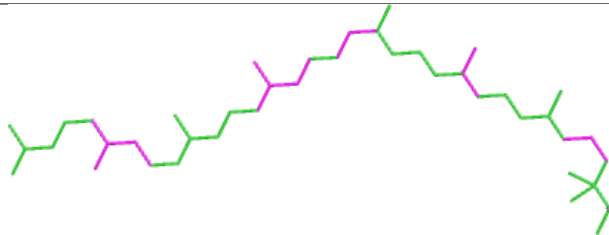
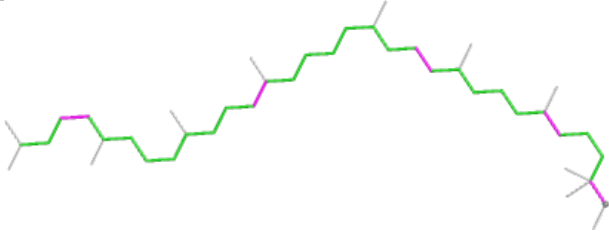
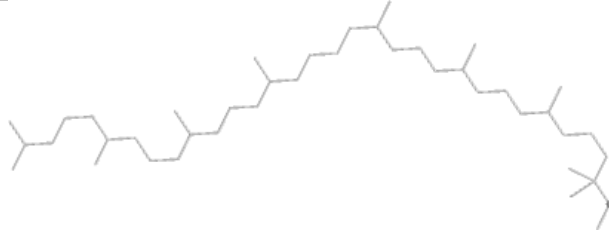
Ligand BPH L 402

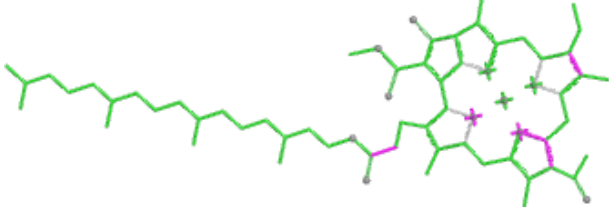
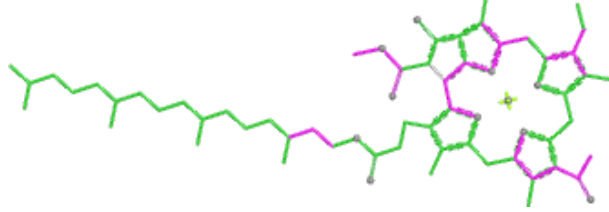
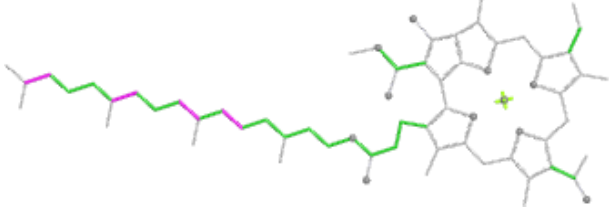
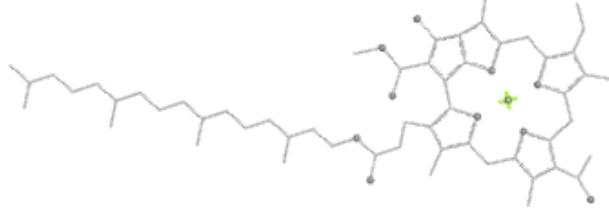


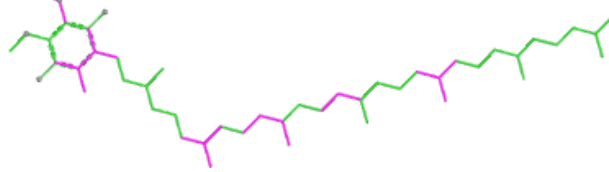
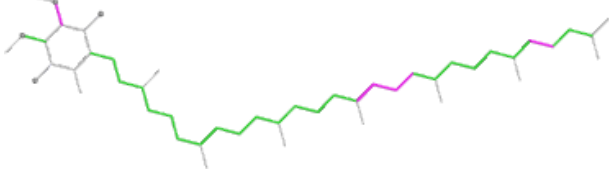
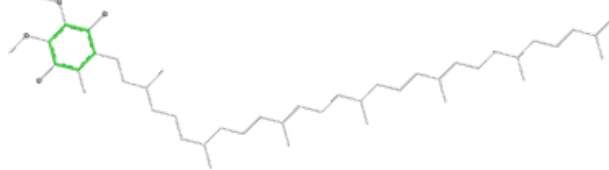
Ligand U10 L 502





Ligand SPO M 600	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL M 909	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 M 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.41	8 (2%) 55 45	62, 72, 79, 86	0
2	M	302/307 (98%)	0.42	8 (2%) 57 47	65, 73, 81, 102	1 (0%)
3	H	240/260 (92%)	0.75	17 (7%) 22 16	45, 72, 81, 121	2 (0%)
All	All	823/848 (97%)	0.51	33 (4%) 42 33	45, 72, 80, 121	3 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	6.6
3	H	246	PRO	4.9
3	H	245	ALA	4.7
1	L	281	GLY	4.5
3	H	249	LYS	4.0
3	H	14	SER	3.6
3	H	250	SER	3.6
1	L	53	ALA	3.5
3	H	247	LYS	3.5
2	M	3	TYR	3.5
3	H	231	ASP	3.4
3	H	94	GLU	3.3
3	H	248	ARG	3.2
3	H	79	GLU	3.2
3	H	206	ASN	3.1
1	L	42	ALA	3.1
2	M	54	SER	2.9
3	H	155	GLY	2.8
2	M	301	HIS	2.8
1	L	72	GLU	2.7
1	L	196	SER	2.6
1	L	83	GLY	2.5
1	L	277	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	111	GLU	2.5
2	M	148	TRP	2.2
3	H	11	ASP	2.2
3	H	48	THR	2.1
1	L	273	ALA	2.1
3	H	164	VAL	2.0
2	M	131	GLY	2.0
2	M	203	GLY	2.0
3	H	71	GLY	2.0
3	H	166	ASP	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	M	906	16/16	0.63	0.23	61,63,66,68	16
7	LDA	L	904	16/16	0.79	0.23	69,92,102,104	16
7	LDA	M	905	16/16	0.83	0.18	100,108,114,115	0
7	LDA	M	902	16/16	0.84	0.16	96,98,100,101	0
7	LDA	M	903	16/16	0.84	0.18	107,112,113,113	0
6	U10	L	502	48/63	0.89	0.19	62,65,73,74	48
7	LDA	H	901	16/16	0.89	0.15	98,103,115,115	0
9	PO4	M	907	5/5	0.90	0.19	95,101,101,102	0
4	BCL	M	908	66/66	0.91	0.13	64,71,94,96	0
4	BCL	L	302	66/66	0.92	0.14	64,72,89,95	0
5	BPH	M	401	65/65	0.92	0.11	68,77,104,105	0
6	U10	M	501	48/63	0.93	0.12	68,78,90,91	0
4	BCL	L	304	66/66	0.94	0.10	54,62,82,86	0

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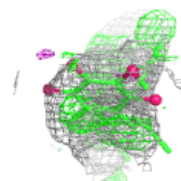
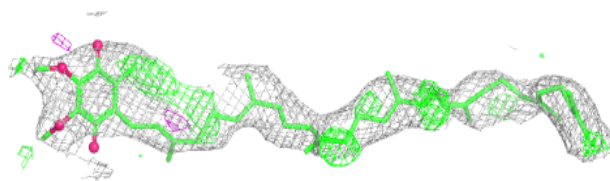
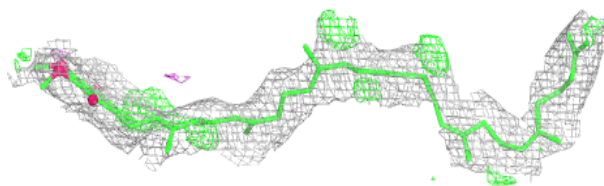
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BCL	M	909	66/66	0.94	0.13	66,70,83,89	0
10	SPO	M	600	42/42	0.94	0.11	69,77,82,84	0
5	BPH	L	402	65/65	0.96	0.10	62,69,79,85	0
8	FE	M	500	1/1	1.00	0.04	71,71,71,71	0

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

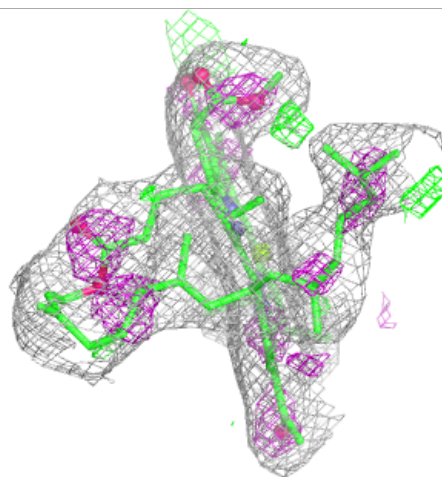
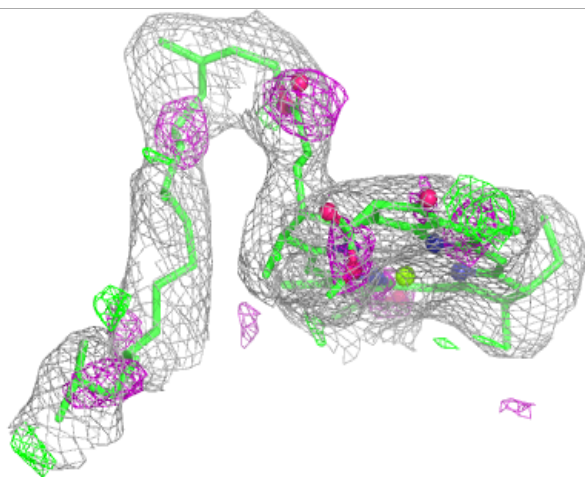
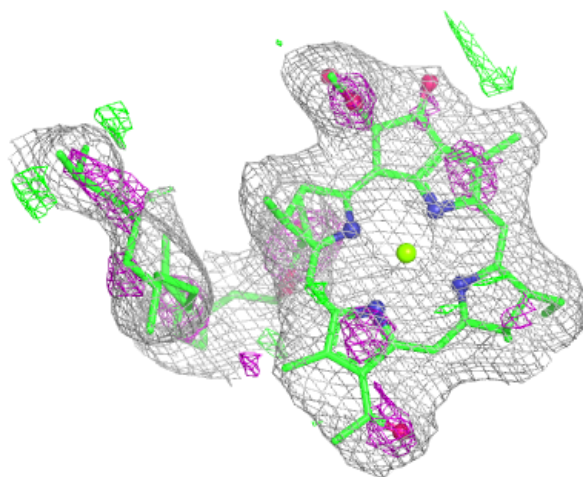
Electron density around U10 L 502:

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



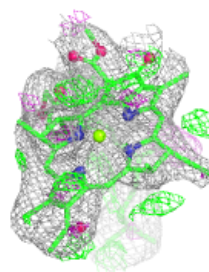
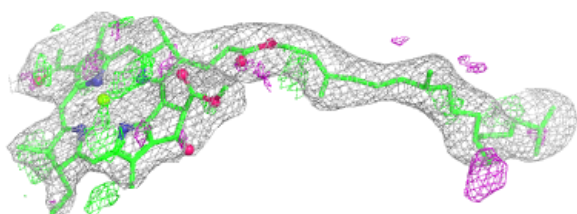
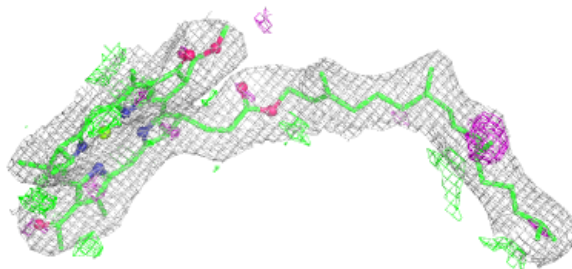
Electron density around BCL M 908:

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

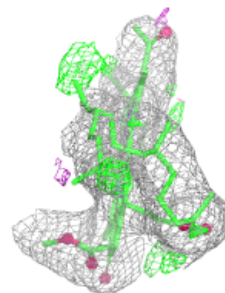
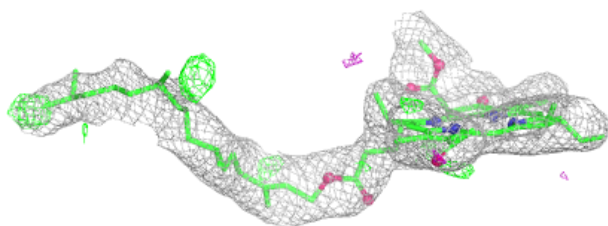
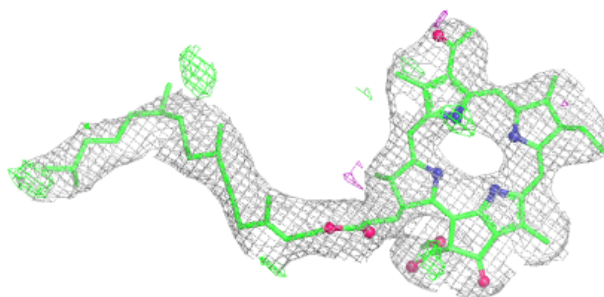


Electron density around BCL L 302:

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

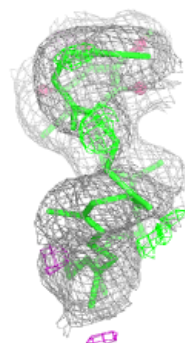
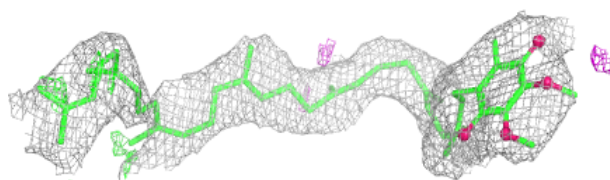
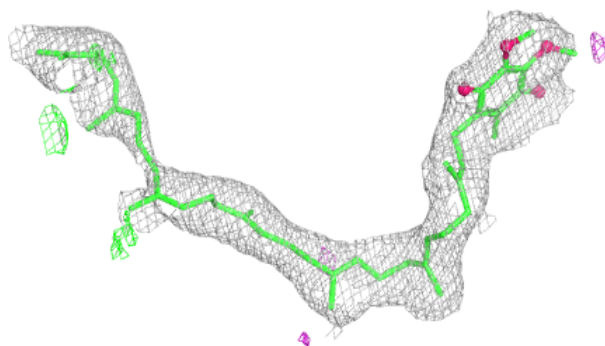
**Electron density around BPH M 401:**

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



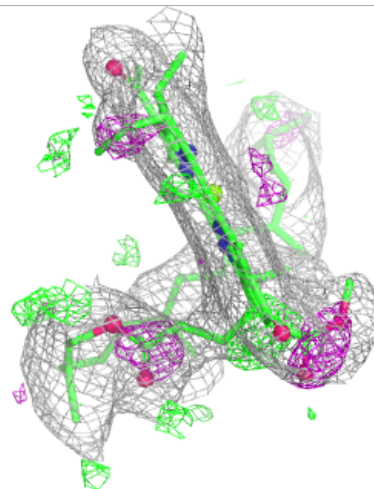
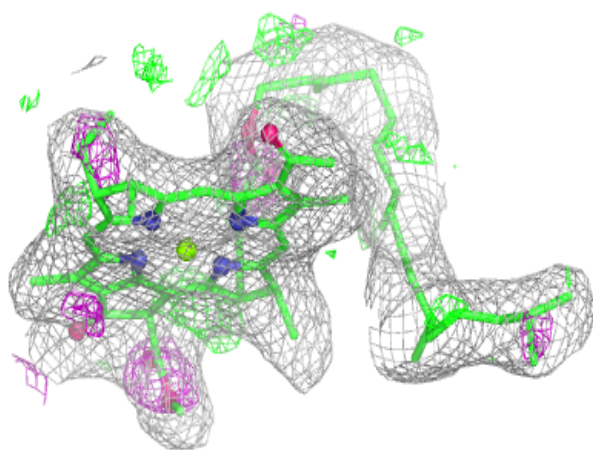
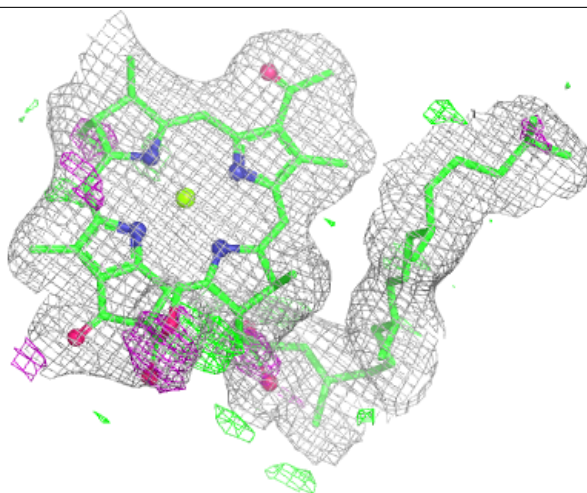
Electron density around U10 M 501:

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



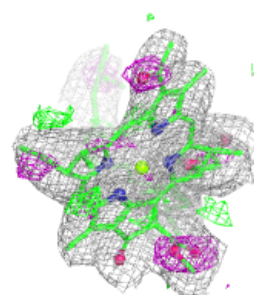
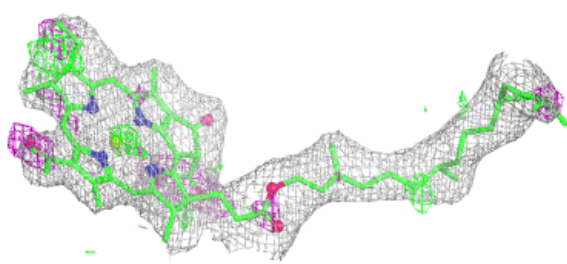
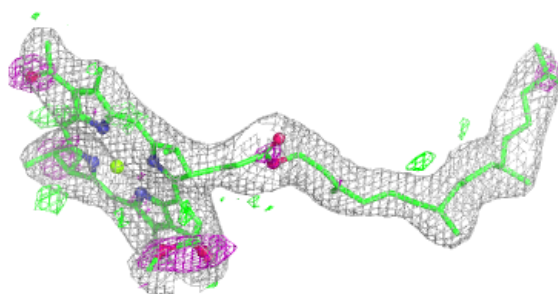
Electron density around BCL L 304:

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

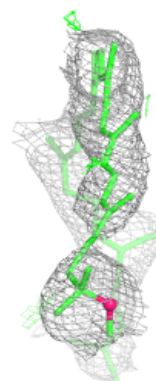
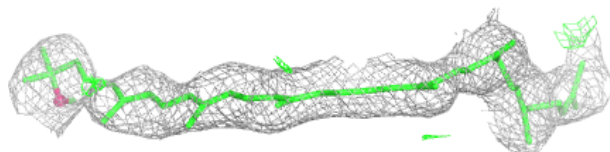
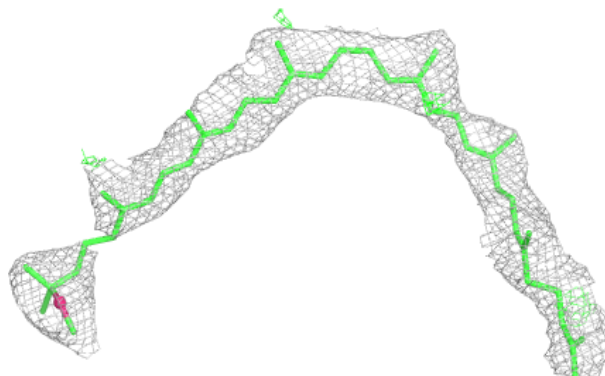


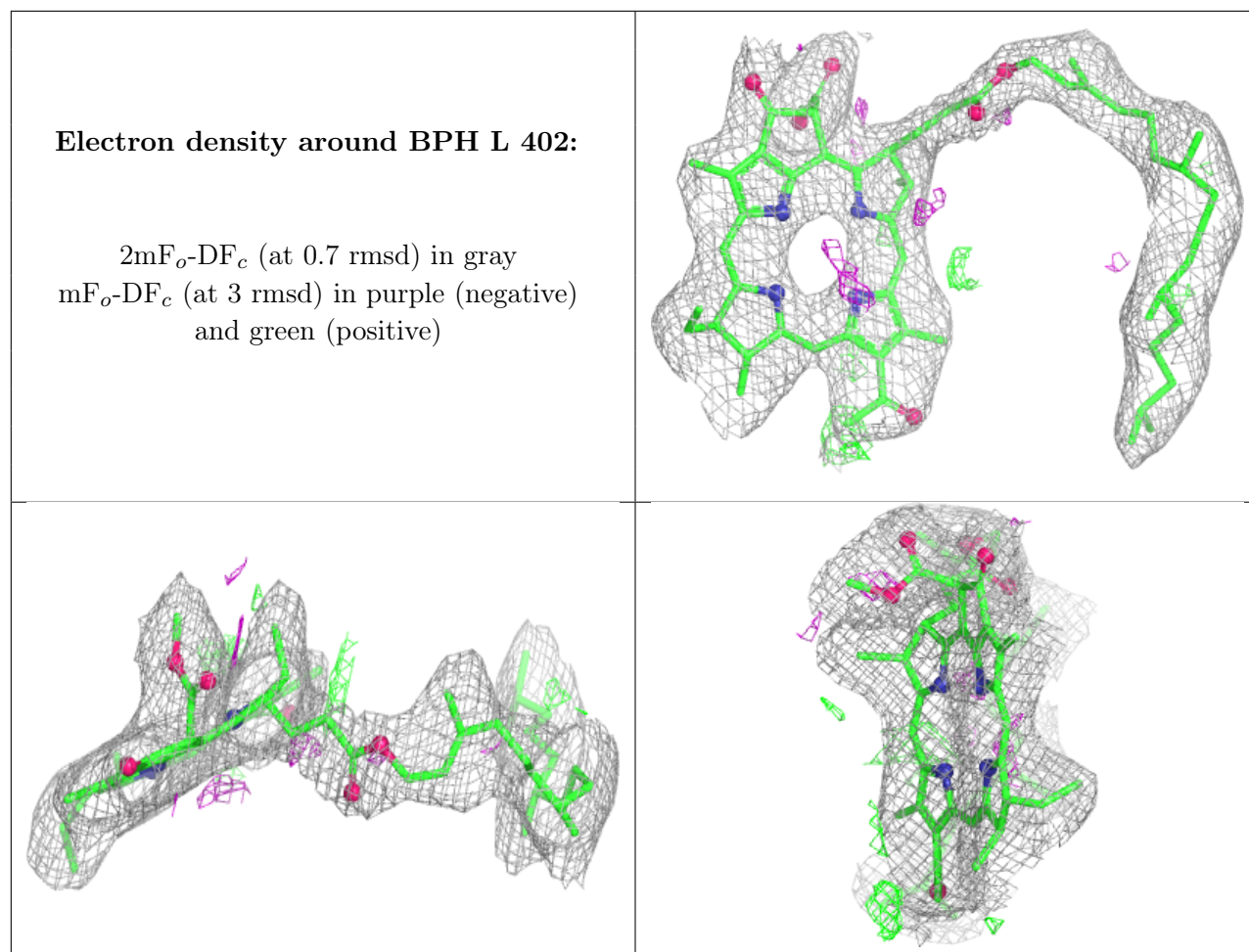
Electron density around BCL M 909:

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

**Electron density around SPO M 600:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.