



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 11:54 AM EDT

PDB ID : 8C7C / pdb_00008c7c
Title : Double mutant V(M84)C/A(L278)C structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors : Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.; Uhimchuk, D.
Deposited on : 2023-01-14
Resolution : 2.60 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

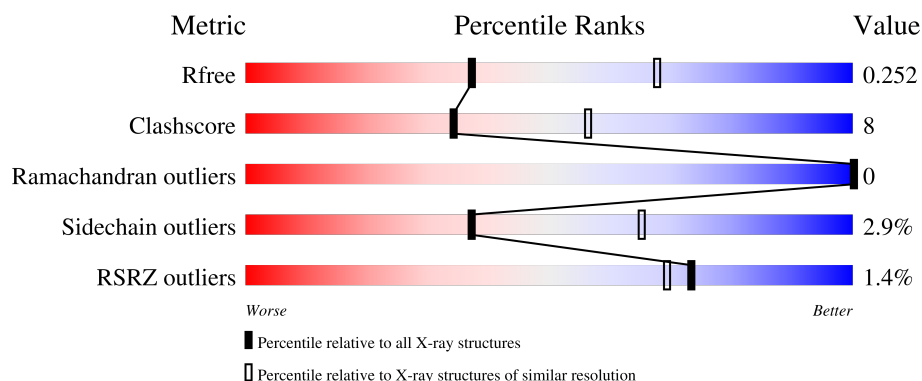
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	251	85% 14%
2	L	281	3% 85% 13% .
3	M	303	% 82% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	L	309	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	250	Total	C	N	O	S	0	2	0
			1913	1226	327	350	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2246	1517	356	364	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	conflict	UNP P0C0Y8
L	278	CYS	GLY	engineered mutation	UNP P0C0Y8

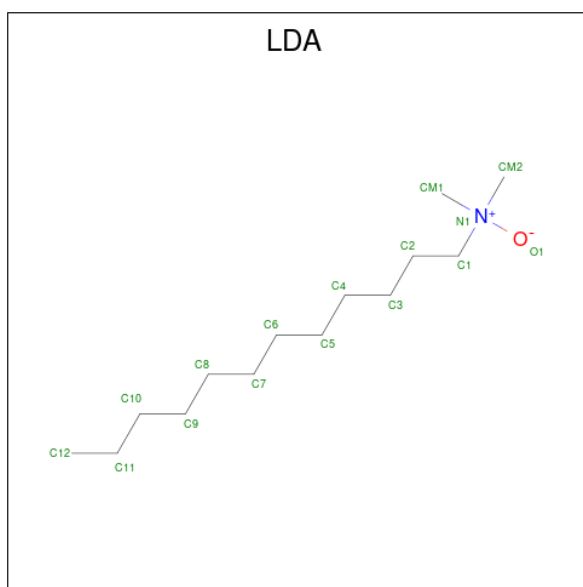
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2421	1616	397	397	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9
M	84	CYS	VAL	engineered mutation	UNP P0C0Y9

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

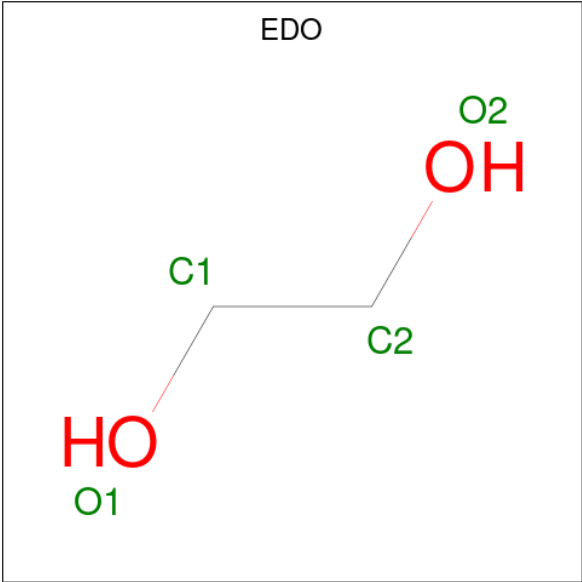


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	16	0
			16	14	1	1		

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

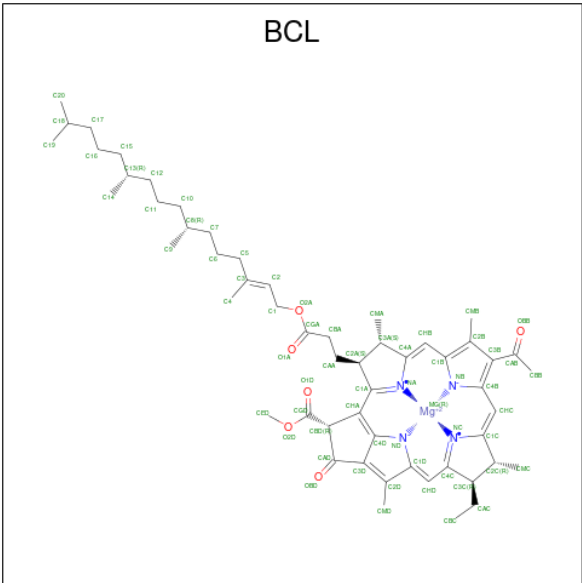
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	C	0	0
			27	27		
5	L	3	Total	C	0	0
			37	37		
5	M	3	Total	C	0	0
			39	39		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



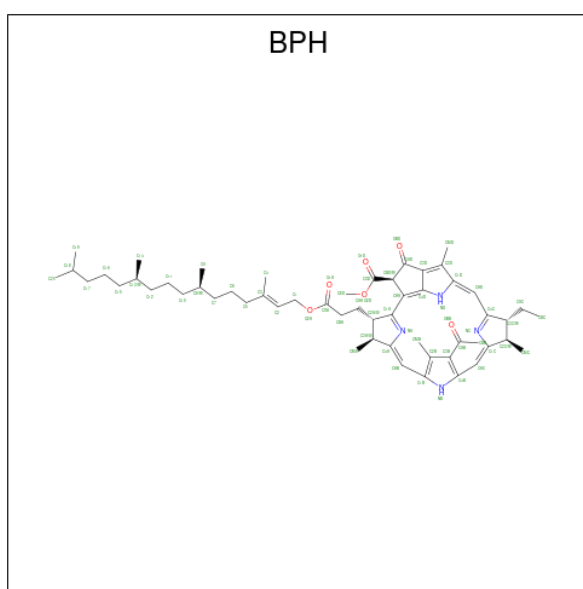
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	4	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



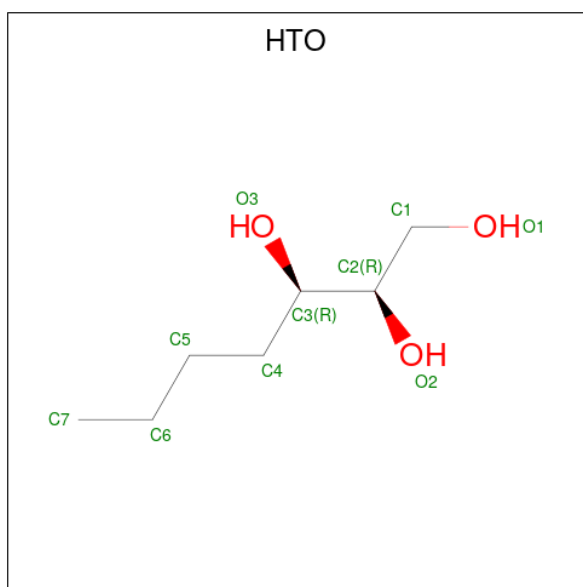
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



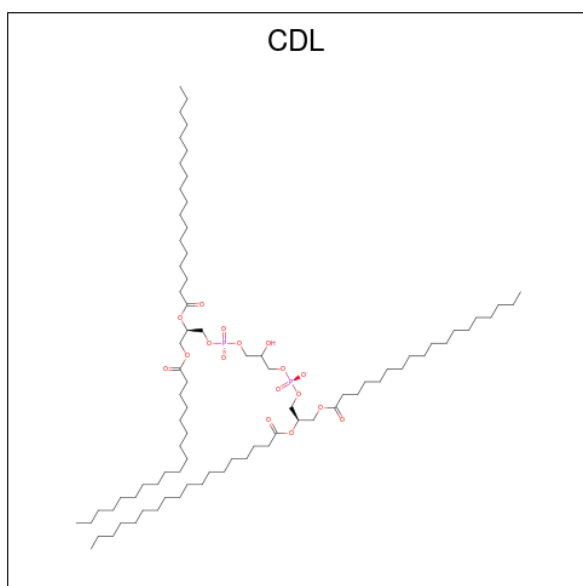
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

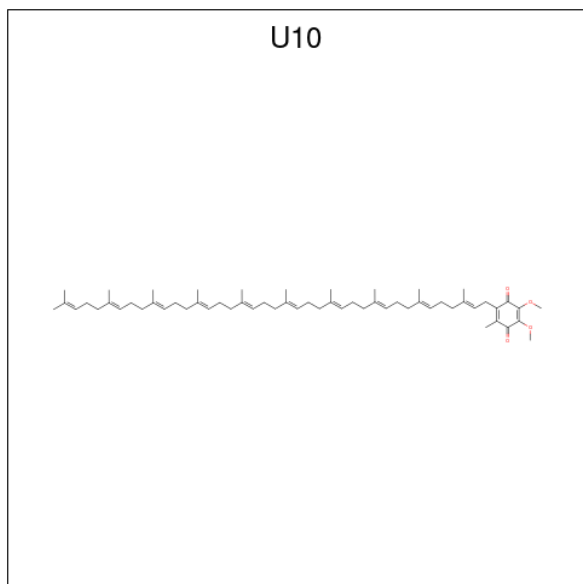


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

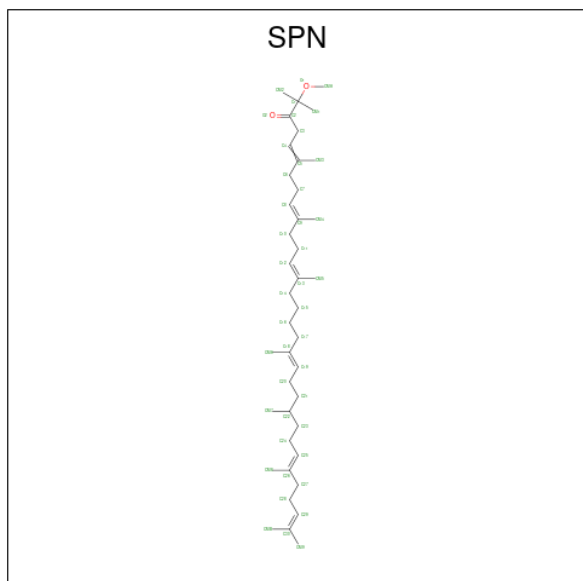
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



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

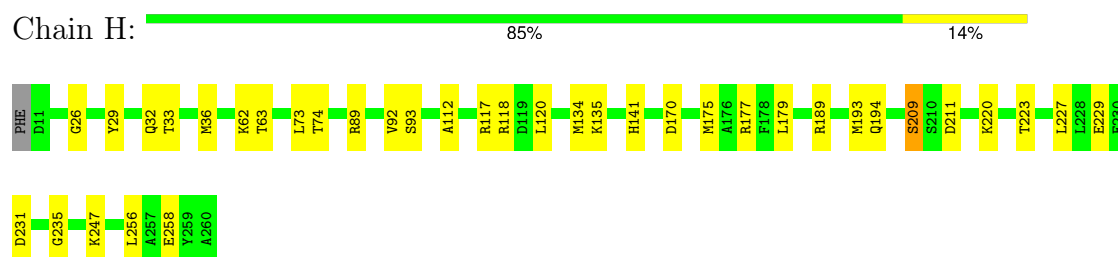
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	7	Total	O	0	0
			7	7		
14	L	7	Total	O	0	0
			7	7		
14	M	7	Total	O	0	0
			7	7		

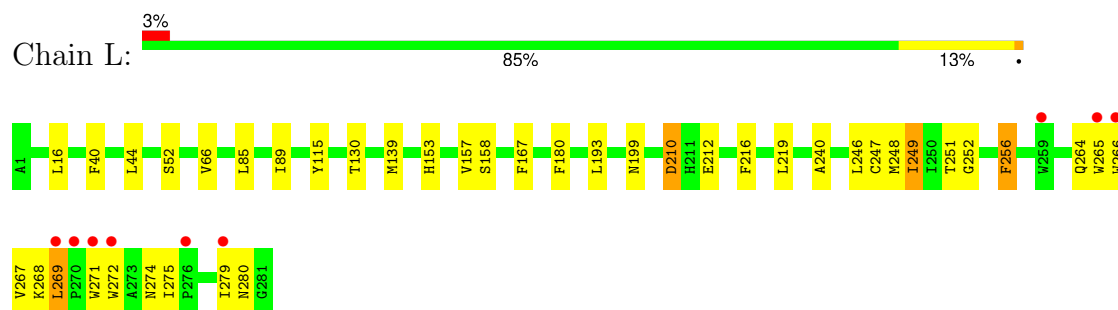
3 Residue-property plots [i](#)

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

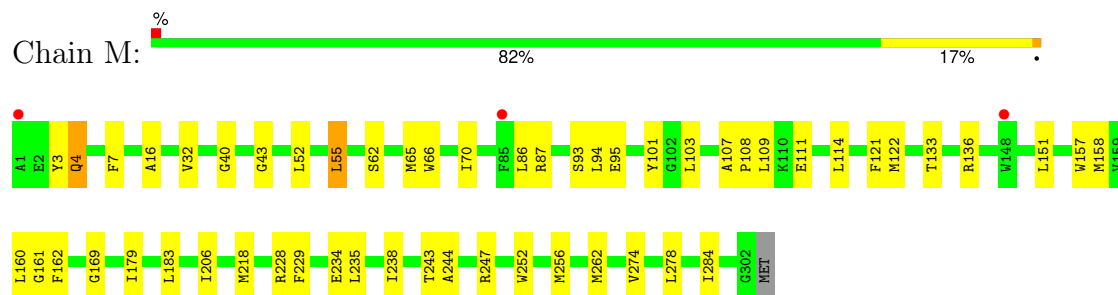
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	253.13Å 75.98Å 65.85Å 90.00° 95.58° 90.00°	Depositor
Resolution (Å)	41.99 – 2.60 41.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.99-2.60) 98.7 (41.99-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.249 0.200 , 0.252	Depositor DCC
R_{free} test set	1608 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: FE, U10, UNL, SPN, HTO, BCL, CDL, LDA, EDO, 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	H	0.38	0/1968	0.57	0/2677
2	L	0.36	0/2337	0.54	0/3199
3	M	0.37	0/2519	0.58	0/3438
All	All	0.37	0/6824	0.56	0/9314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1913	0	1933	25	0
2	L	2246	0	2205	32	0
3	M	2421	0	2342	47	0
4	H	16	0	31	2	0
4	L	16	0	31	0	0
4	M	48	0	93	1	0
5	H	27	0	0	0	0
5	L	37	0	0	0	0
5	M	39	0	0	0	0
6	H	8	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	8	0	12	5	0
7	L	132	0	148	4	0
7	M	132	0	148	3	0
8	L	65	0	76	2	0
8	M	65	0	76	1	0
9	L	10	0	16	0	0
10	M	81	0	106	6	0
11	M	1	0	0	0	0
12	M	48	0	63	2	0
13	M	43	0	70	10	0
14	H	7	0	0	0	0
14	L	7	0	0	0	0
14	M	7	0	0	1	0
All	All	7377	0	7362	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (112) 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)
6:L:309:EDO:H22	3:M:228:ARG:HH22	1.41	0.85
1:H:177:ARG:HE	6:H:304:EDO:H21	1.42	0.84
2:L:265:TRP:CD1	2:L:266:TRP:H	1.98	0.80
2:L:275:ILE:HB	3:M:87:ARG:HH12	1.52	0.75
1:H:170:ASP:HB2	1:H:177:ARG:HD2	1.70	0.73
1:H:118[A]:ARG:HD3	1:H:120:LEU:HD12	1.73	0.70
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.72	0.70
1:H:179:LEU:HG	1:H:193:MET:HE1	1.76	0.68
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.77	0.67
2:L:267:VAL:HA	3:M:87:ARG:HD2	1.77	0.66
3:M:122:MET:HE1	13:M:407:SPN:H19	1.79	0.65
8:M:404:BPH:HBC3	8:M:404:BPH:HHD	1.79	0.63
1:H:26:GLY:HA3	10:M:401:CDL:H191	1.80	0.62
1:H:29:TYR:O	1:H:33:THR:HG23	2.00	0.61
3:M:122:MET:HE3	13:M:407:SPN:HM72	1.81	0.61
3:M:161:GLY:HA3	13:M:407:SPN:H201	1.82	0.61
2:L:280:ASN:O	3:M:87:ARG:NH2	2.34	0.60
3:M:162:PHE:HB2	13:M:407:SPN:H241	1.83	0.60
6:L:309:EDO:H22	3:M:228:ARG:NH2	2.13	0.60
3:M:234:GLU:O	3:M:238:ILE:HG13	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:TRP:O	3:M:70:ILE:HD12	2.03	0.59
2:L:269:LEU:HB3	2:L:271:TRP:CD1	2.38	0.57
3:M:278:LEU:HD11	10:M:401:CDL:H362	1.87	0.57
1:H:134:MET:HE3	1:H:141:HIS:HA	1.88	0.56
3:M:101:TYR:CE2	3:M:107:ALA:HA	2.40	0.56
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.89	0.55
10:M:401:CDL:H332	10:M:401:CDL:H542	1.89	0.54
3:M:122:MET:HE1	13:M:407:SPN:C19	2.37	0.54
3:M:162:PHE:CD1	13:M:407:SPN:H241	2.43	0.53
1:H:220:LYS:HG2	1:H:229:GLU:OE2	2.08	0.53
6:L:309:EDO:C2	3:M:228:ARG:HH22	2.20	0.52
1:H:117:ARG:NH1	1:H:227:LEU:HD22	2.24	0.52
4:H:301:LDA:H121	4:M:408:LDA:H91	1.92	0.52
2:L:40:PHE:CE1	2:L:44:LEU:HD12	2.45	0.52
2:L:275:ILE:HB	3:M:87:ARG:NH1	2.24	0.52
7:M:402:BCL:CAB	13:M:407:SPN:H162	2.41	0.51
1:H:179:LEU:CD2	1:H:193:MET:HE1	2.41	0.51
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.46	0.51
1:H:33:THR:HA	1:H:36:MET:HE2	1.93	0.51
2:L:265:TRP:CD1	2:L:266:TRP:N	2.73	0.50
10:M:401:CDL:H522	10:M:401:CDL:H312	1.93	0.50
1:H:179:LEU:CG	1:H:193:MET:HE1	2.41	0.50
3:M:93:SER:OG	3:M:95:GLU:OE2	2.26	0.50
3:M:160:LEU:HD13	3:M:284:ILE:HG21	1.94	0.49
2:L:115:TYR:CZ	6:L:309:EDO:H12	2.48	0.49
3:M:122:MET:CE	3:M:157:TRP:HE1	2.26	0.48
2:L:66:VAL:HG11	2:L:89:ILE:HD12	1.95	0.48
3:M:4:GLN:NE2	3:M:4:GLN:HA	2.29	0.47
3:M:40:GLY:HA2	3:M:43:GLY:O	2.14	0.47
2:L:210:ASP:N	2:L:210:ASP:OD1	2.48	0.47
3:M:122:MET:CE	13:M:407:SPN:HM72	2.43	0.47
3:M:234:GLU:HG2	3:M:262:MET:SD	2.55	0.47
10:M:401:CDL:H562	10:M:401:CDL:H781	1.97	0.46
1:H:89:ARG:NH2	1:H:92:VAL:O	2.49	0.46
1:H:112:ALA:HA	1:H:235:GLY:O	2.15	0.46
2:L:153:HIS:O	2:L:157:VAL:HG23	2.16	0.46
4:H:301:LDA:H22	4:H:301:LDA:HM11	1.59	0.45
3:M:256:MET:CE	12:M:406:U10:H102	2.46	0.45
2:L:249:ILE:HD12	2:L:249:ILE:HA	1.86	0.45
1:H:62:LYS:O	1:H:74:THR:HA	2.17	0.45
3:M:65:MET:HE3	3:M:65:MET:HB3	1.77	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:SER:HB2	1:H:211:ASP:OD1	2.16	0.44
2:L:193:LEU:HG	2:L:212:GLU:HG2	1.99	0.44
1:H:92:VAL:HG23	1:H:93:SER:H	1.82	0.44
7:L:302:BCL:H2	8:L:303:BPH:HMB2	2.00	0.44
2:L:167:PHE:CZ	2:L:251:THR:HG21	2.51	0.44
3:M:243:THR:O	3:M:247:ARG:HG3	2.18	0.44
3:M:55:LEU:HD12	3:M:55:LEU:HA	1.80	0.44
3:M:70:ILE:HA	3:M:94:LEU:HD12	1.99	0.44
1:H:256:LEU:HD23	1:H:256:LEU:HA	1.67	0.44
2:L:272:TRP:O	2:L:274:ASN:N	2.50	0.44
3:M:108:PRO:HB2	3:M:111:GLU:HG3	2.00	0.44
1:H:189:ARG:HG2	1:H:189:ARG:HH11	1.83	0.44
1:H:211:ASP:OD2	1:H:247:LYS:NZ	2.26	0.44
3:M:206:ILE:HG12	7:M:403:BCL:CHB	2.48	0.44
3:M:218:MET:HE3	3:M:252:TRP:CH2	2.53	0.43
2:L:139:MET:HE3	2:L:252:GLY:HA3	1.99	0.43
3:M:3:TYR:OH	3:M:7:PHE:O	2.32	0.43
3:M:122:MET:HE3	3:M:157:TRP:HE1	1.82	0.43
2:L:246:LEU:HD12	2:L:246:LEU:O	2.19	0.43
1:H:194:GLN:H	1:H:194:GLN:CD	2.27	0.43
3:M:179:ILE:O	3:M:183:LEU:HD23	2.19	0.43
2:L:167:PHE:HZ	2:L:251:THR:HG21	1.83	0.42
3:M:109:LEU:HG	3:M:114:LEU:HG	2.01	0.42
2:L:264:GLN:OE1	2:L:268:LYS:NZ	2.53	0.42
1:H:227:LEU:HD23	1:H:227:LEU:HA	1.78	0.42
1:H:135:LYS:HE2	1:H:135:LYS:HB3	1.90	0.42
3:M:162:PHE:HB2	13:M:407:SPN:H232	2.02	0.42
2:L:158:SER:HA	7:L:301:BCL:HBC1	2.01	0.42
2:L:274:ASN:O	2:L:275:ILE:C	2.63	0.42
2:L:248:MET:HE3	2:L:248:MET:HB3	1.65	0.41
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.92	0.41
2:L:199:ASN:HB3	10:M:401:CDL:H1	2.01	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.02	0.41
7:L:301:BCL:H162	7:L:301:BCL:H141	1.82	0.41
3:M:218:MET:HE3	3:M:252:TRP:CZ3	2.56	0.41
1:H:32:GLN:O	1:H:36:MET:HG3	2.20	0.41
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.56	0.41
8:L:303:BPH:OBB	8:L:303:BPH:HHC	2.21	0.41
3:M:103:LEU:HG	3:M:169:GLY:O	2.21	0.41
7:L:301:BCL:HAA2	7:L:302:BCL:HAC2	2.03	0.41
7:M:402:BCL:H193	13:M:407:SPN:H72	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:TYR:CE2	6:L:309:EDO:H12	2.56	0.41
2:L:16:LEU:HD23	2:L:16:LEU:HA	1.78	0.40
2:L:256:PHE:CD1	2:L:256:PHE:N	2.88	0.40
12:M:406:U10:H33	12:M:406:U10:H372	1.82	0.40
2:L:266:TRP:CD1	2:L:271:TRP:HZ2	2.39	0.40
3:M:65:MET:HB3	3:M:121:PHE:CE2	2.56	0.40
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.56	0.40
3:M:136:ARG:HD3	14:M:501:HOH:O	2.20	0.40
1:H:63:THR:HA	1:H:73:LEU:O	2.22	0.40
2:L:130:THR:HG23	2:L:249:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	250/251 (100%)	245 (98%)	5 (2%)	0	100	100
2	L	281/281 (100%)	267 (95%)	14 (5%)	0	100	100
3	M	302/303 (100%)	290 (96%)	12 (4%)	0	100	100
All	All	833/835 (100%)	802 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	203/202 (100%)	198 (98%)	5 (2%)	42	69
2	L	223/221 (101%)	216 (97%)	7 (3%)	35	63
3	M	238/237 (100%)	230 (97%)	8 (3%)	32	60
All	All	664/660 (101%)	644 (97%)	20 (3%)	37	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	175	MET
1	H	209	SER
1	H	223	THR
1	H	231	ASP
1	H	258	GLU
2	L	210	ASP
2	L	216	PHE
2	L	247	CYS
2	L	249	ILE
2	L	256	PHE
2	L	269	LEU
2	L	279	ILE
3	M	4	GLN
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	55	LEU
3	M	62	SER
3	M	86	LEU
3	M	151	LEU
3	M	274	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 8 are unknown and 1 is monoatomic - leaving 19 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	$\# Z > 2$
9	HTO	L	310	-	9,9,9	0.44	0	10,10,10	0.72	0
7	BCL	M	402	-	69,74,74	1.31	6 (8%)	79,115,115	1.71	14 (17%)
4	LDA	L	304	-	13,15,15	2.32	2 (15%)	14,17,17	0.52	0
4	LDA	M	413	-	13,15,15	2.39	2 (15%)	14,17,17	0.55	0
6	EDO	H	305	-	3,3,3	0.56	0	2,2,2	0.33	0
10	CDL	M	401	-	80,80,99	0.45	1 (1%)	86,92,111	0.38	0
4	LDA	H	301	-	13,15,15	2.30	2 (15%)	14,17,17	0.37	0
4	LDA	M	409	-	13,15,15	2.01	2 (15%)	14,17,17	0.75	0
7	BCL	L	301	-	69,74,74	1.40	8 (11%)	79,115,115	1.38	9 (11%)
13	SPN	M	407	-	42,42,42	0.36	0	50,52,52	1.01	3 (6%)
6	EDO	H	304	-	3,3,3	0.59	0	2,2,2	0.21	0
6	EDO	L	309	-	3,3,3	0.45	0	2,2,2	0.18	0
7	BCL	L	302	-	69,74,74	1.36	8 (11%)	79,115,115	1.43	9 (11%)
7	BCL	M	403	-	69,74,74	1.29	6 (8%)	79,115,115	1.38	10 (12%)
4	LDA	M	408	-	13,15,15	2.17	2 (15%)	14,17,17	0.41	0
6	EDO	L	308	-	3,3,3	0.42	0	2,2,2	0.37	0
8	BPH	L	303	-	59,70,70	1.37	8 (13%)	59,101,101	2.01	10 (16%)
8	BPH	M	404	-	59,70,70	1.40	9 (15%)	59,101,101	2.24	13 (22%)
12	U10	M	406	-	48,48,63	2.73	14 (29%)	60,61,79	1.57	12 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	L	310	-	-	3/10/10/10	-
7	BCL	M	402	-	-	8/41/137/137	-
4	LDA	L	304	-	-	2/13/13/13	-
4	LDA	M	413	-	-	8/13/13/13	-
6	EDO	H	305	-	-	0/1/1/1	-
10	CDL	M	401	-	-	42/91/91/110	-
4	LDA	H	301	-	-	4/13/13/13	-
4	LDA	M	409	-	-	7/13/13/13	-
7	BCL	L	301	-	-	0/41/137/137	-
13	SPN	M	407	-	-	20/50/51/51	-
6	EDO	H	304	-	-	0/1/1/1	-
6	EDO	L	309	-	-	1/1/1/1	-
7	BCL	L	302	-	-	2/41/137/137	-
7	BCL	M	403	-	-	2/41/137/137	-
4	LDA	M	408	-	-	5/13/13/13	-
6	EDO	L	308	-	-	0/1/1/1	-
8	BPH	L	303	-	-	4/37/105/105	0/5/6/6
8	BPH	M	404	-	-	6/37/105/105	0/5/6/6
12	U10	M	406	-	-	6/45/69/87	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	406	U10	C8-C9	6.88	1.48	1.33
4	M	413	LDA	O1-N1	-6.80	1.25	1.42
4	L	304	LDA	O1-N1	-6.58	1.26	1.42
4	M	408	LDA	O1-N1	-6.55	1.26	1.42
4	H	301	LDA	O1-N1	-6.52	1.26	1.42
12	M	406	U10	C28-C29	6.44	1.47	1.33
12	M	406	U10	C18-C19	6.27	1.47	1.33
12	M	406	U10	C13-C14	6.17	1.47	1.33
4	M	409	LDA	O1-N1	-6.08	1.27	1.42
12	M	406	U10	C33-C34	5.96	1.46	1.33
12	M	406	U10	C23-C24	5.92	1.46	1.33
7	L	301	BCL	MG-NA	5.50	2.19	2.06
12	M	406	U10	C38-C39	5.27	1.48	1.32
4	M	413	LDA	C1-N1	-5.22	1.46	1.51
7	M	403	BCL	MG-NA	5.14	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	404	BPH	OBD-CAD	5.13	1.29	1.22
7	L	302	BCL	MG-NA	5.05	2.18	2.06
4	L	304	LDA	C1-N1	-5.02	1.46	1.51
7	M	402	BCL	MG-NA	5.00	2.18	2.06
4	H	301	LDA	C1-N1	-4.97	1.46	1.51
12	M	406	U10	O3-C3	-4.91	1.24	1.36
12	M	406	U10	O4-C4	-4.65	1.25	1.36
8	L	303	BPH	C1D-C2D	4.40	1.44	1.39
7	L	301	BCL	MG-NC	4.40	2.16	2.06
7	M	403	BCL	MG-NC	4.24	2.16	2.06
8	L	303	BPH	CBD-CGD	-4.03	1.47	1.52
4	M	408	LDA	C1-N1	-3.86	1.47	1.51
7	L	302	BCL	MG-NC	3.85	2.15	2.06
7	M	402	BCL	C3B-C4B	3.77	1.48	1.41
4	M	409	LDA	C1-N1	-3.71	1.47	1.51
7	L	302	BCL	OBD-CAD	3.60	1.28	1.22
8	L	303	BPH	C3B-C4B	3.40	1.47	1.41
7	M	402	BCL	MG-NC	3.36	2.14	2.06
7	L	301	BCL	C3B-C4B	3.36	1.47	1.41
12	M	406	U10	C6-C1	3.30	1.41	1.35
7	M	403	BCL	C3B-C4B	3.27	1.47	1.41
8	M	404	BPH	CHA-CBD	3.24	1.55	1.51
7	L	301	BCL	O1A-CGA	-3.14	1.13	1.22
7	L	301	BCL	C1D-ND	3.11	1.41	1.37
7	L	302	BCL	CHD-C1D	3.09	1.44	1.38
8	M	404	BPH	CBD-CGD	-2.96	1.48	1.52
7	M	402	BCL	CHD-C1D	2.92	1.44	1.38
7	L	302	BCL	C1D-ND	2.84	1.41	1.37
8	L	303	BPH	C3D-CAD	-2.78	1.42	1.47
8	M	404	BPH	C3D-C2D	2.78	1.44	1.39
7	L	302	BCL	C5-C3	2.69	1.56	1.51
7	M	403	BCL	C1D-ND	2.59	1.41	1.37
7	L	302	BCL	CBD-CGD	-2.54	1.44	1.52
7	L	302	BCL	C3B-C4B	2.52	1.46	1.41
12	M	406	U10	C3-C2	-2.49	1.41	1.48
8	L	303	BPH	CAC-C3C	2.47	1.59	1.53
8	M	404	BPH	C3B-C4B	2.44	1.45	1.41
7	M	403	BCL	C1-C2	2.36	1.55	1.49
7	M	402	BCL	C1D-ND	2.32	1.40	1.37
12	M	406	U10	C6-C5	-2.32	1.40	1.46
7	M	403	BCL	CHD-C1D	2.30	1.42	1.38
8	M	404	BPH	C4D-CHA	2.28	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	406	U10	C1-C2	-2.24	1.39	1.47
12	M	406	U10	C4-C5	-2.21	1.42	1.48
7	L	301	BCL	CHD-C1D	2.18	1.42	1.38
8	L	303	BPH	C2C-C3C	-2.15	1.52	1.54
8	M	404	BPH	C1-C2	2.15	1.55	1.49
7	L	301	BCL	CHC-C1C	2.13	1.43	1.37
10	M	401	CDL	OA8-CA6	2.12	1.49	1.45
8	L	303	BPH	OBD-CAD	2.12	1.25	1.22
8	L	303	BPH	CHA-CBD	2.10	1.54	1.51
8	M	404	BPH	C5-C3	2.06	1.55	1.51
7	M	402	BCL	CMD-C2D	2.01	1.54	1.50
8	M	404	BPH	C1D-C2D	2.01	1.41	1.39
7	L	301	BCL	C4-C3	2.00	1.55	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	404	BPH	C4D-CHA-CBD	-11.15	103.11	108.45
8	L	303	BPH	C4D-CHA-CBD	-9.73	103.79	108.45
7	M	402	BCL	C1-O2A-CGA	5.69	130.42	116.65
7	L	302	BCL	C4D-CHA-C1A	5.35	127.63	121.24
7	M	402	BCL	C4D-CHA-C1A	5.26	127.52	121.24
8	M	404	BPH	C1-C2-C3	-4.80	118.33	126.20
7	M	403	BCL	C4D-CHA-C1A	4.54	126.66	121.24
7	L	302	BCL	C1D-ND-C4D	-4.47	103.17	106.31
8	M	404	BPH	C1-O2A-CGA	4.47	127.46	116.65
7	L	301	BCL	C4D-CHA-C1A	4.34	126.42	121.24
7	M	402	BCL	CHD-C1D-ND	-4.22	118.86	124.80
7	M	403	BCL	C1D-ND-C4D	-4.19	103.37	106.31
8	L	303	BPH	C11-C10-C8	-4.04	102.54	115.97
7	M	402	BCL	C1-C2-C3	-3.99	119.66	126.20
8	L	303	BPH	C4D-ND-C1D	-3.98	104.11	108.87
7	L	302	BCL	CHD-C1D-ND	-3.97	119.21	124.80
7	M	402	BCL	C16-C15-C13	3.96	129.14	115.97
12	M	406	U10	C32-C33-C34	-3.94	118.60	127.62
7	L	301	BCL	CHD-C1D-ND	-3.93	119.27	124.80
8	L	303	BPH	C3D-C4D-ND	3.92	112.73	107.71
7	M	402	BCL	C1D-ND-C4D	-3.82	103.63	106.31
8	M	404	BPH	C3D-C4D-ND	3.60	112.32	107.71
7	L	301	BCL	C1D-ND-C4D	-3.56	103.81	106.31
8	M	404	BPH	C11-C10-C8	3.56	127.80	115.97
7	M	403	BCL	CHD-C1D-ND	-3.54	119.83	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	303	BPH	OBD-CAD-CBD	-3.49	120.70	125.82
8	M	404	BPH	C4D-ND-C1D	-3.46	104.73	108.87
8	M	404	BPH	OBD-CAD-CBD	-3.36	120.89	125.82
12	M	406	U10	C30-C29-C31	3.29	120.94	115.23
13	M	407	SPN	C23-C24-C25	3.24	120.67	112.16
7	M	402	BCL	C6-C7-C8	3.21	126.63	115.97
12	M	406	U10	C27-C28-C29	-3.18	120.34	127.62
12	M	406	U10	C35-C34-C36	3.17	120.73	115.23
7	M	403	BCL	C4A-NA-C1A	3.07	108.08	106.68
7	M	403	BCL	CHA-C1A-NA	-2.98	119.65	126.39
8	M	404	BPH	O2D-CGD-CBD	2.89	114.12	110.95
7	L	302	BCL	CHA-C1A-NA	-2.89	119.84	126.39
12	M	406	U10	C15-C14-C16	2.84	120.16	115.23
8	M	404	BPH	CMD-C2D-C3D	2.81	130.30	124.68
8	L	303	BPH	CMB-C2B-C3B	2.76	130.21	124.68
12	M	406	U10	C25-C24-C26	2.76	120.02	115.23
7	M	402	BCL	CHA-C1A-NA	-2.76	120.14	126.39
8	M	404	BPH	CMB-C2B-C3B	2.74	130.15	124.68
7	L	302	BCL	C17-C16-C15	-2.73	101.03	113.28
8	M	404	BPH	C2D-C1D-ND	2.73	111.40	109.43
7	L	301	BCL	CHA-C1A-NA	-2.65	120.39	126.39
12	M	406	U10	O5-C5-C6	-2.65	116.67	121.79
7	M	402	BCL	OBB-CAB-CBB	-2.63	113.89	119.77
7	L	302	BCL	C2A-C1A-CHA	2.61	128.39	123.87
7	L	301	BCL	C2A-C1A-CHA	2.61	128.39	123.87
8	L	303	BPH	CMA-C3A-C4A	-2.59	109.03	114.61
7	M	402	BCL	C1C-NC-C4C	2.56	107.85	106.68
7	L	302	BCL	C6-C5-C3	2.55	119.67	113.47
7	M	402	BCL	C4A-NA-C1A	2.53	107.83	106.68
7	M	403	BCL	C2A-C1A-CHA	2.52	128.25	123.87
13	M	407	SPN	C24-C25-C26	2.48	133.31	127.62
12	M	406	U10	C12-C13-C14	-2.47	121.97	127.62
8	L	303	BPH	CBC-CAC-C3C	2.45	118.60	113.78
12	M	406	U10	C4M-O4-C4	2.45	125.08	116.47
12	M	406	U10	C10-C9-C11	2.45	119.48	115.23
7	L	302	BCL	CED-O2D-CGD	2.43	121.44	115.92
7	M	402	BCL	C2A-C1A-CHA	2.38	128.00	123.87
12	M	406	U10	C17-C18-C19	-2.34	122.28	127.62
7	M	402	BCL	C11-C10-C8	-2.33	108.21	115.97
7	M	403	BCL	O2A-CGA-O1A	-2.33	117.81	123.63
8	M	404	BPH	OBD-CAD-C3D	2.31	131.50	127.89
7	L	301	BCL	CMB-C2B-C1B	-2.27	121.97	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	CAA-CBA-CGA	2.26	119.64	113.21
12	M	406	U10	C20-C19-C21	2.24	119.11	115.23
7	L	302	BCL	C4A-NA-C1A	2.20	107.68	106.68
7	M	403	BCL	CED-O2D-CGD	2.16	120.82	115.92
7	L	301	BCL	OBB-CAB-CBB	-2.14	114.98	119.77
13	M	407	SPN	C3-C4-C5	2.09	130.44	126.83
8	M	404	BPH	C6-C5-C3	2.08	118.54	113.47
7	M	402	BCL	CHD-C1D-C2D	2.08	129.82	125.49
7	M	403	BCL	CAB-C3B-C2B	2.08	132.06	127.74
7	M	403	BCL	CMB-C2B-C1B	-2.03	122.32	125.42
8	L	303	BPH	C2D-C1D-ND	2.02	110.89	109.43
8	L	303	BPH	CED-O2D-CGD	2.01	120.48	115.92
7	L	301	BCL	O2A-CGA-O1A	-2.00	118.62	123.63

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	408	LDA	C2-C1-N1-O1
4	M	408	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-O1
4	M	409	LDA	C2-C1-N1-CM1
4	M	413	LDA	C2-C1-N1-O1
4	M	413	LDA	C2-C1-N1-CM1
7	M	402	BCL	C1A-C2A-CAA-CBA
7	M	402	BCL	C4C-C3C-CAC-CBC
9	L	310	HTO	C1-C2-C3-O3
9	L	310	HTO	O2-C2-C3-O3
10	M	401	CDL	CA2-OA2-PA1-OA5
10	M	401	CDL	CB3-OB5-PB2-OB2
10	M	401	CDL	CB3-OB5-PB2-OB3
10	M	401	CDL	CB3-OB5-PB2-OB4
13	M	407	SPN	CM1-C1-O1-CMA
13	M	407	SPN	C2-C1-O1-CMA
13	M	407	SPN	C11-C10-C9-CM4
13	M	407	SPN	C11-C10-C9-C8
10	M	401	CDL	C71-CB7-OB8-CB6
13	M	407	SPN	C16-C17-C18-CM6
13	M	407	SPN	C16-C17-C18-C19
10	M	401	CDL	OB9-CB7-OB8-CB6
12	M	406	U10	C24-C26-C27-C28
10	M	401	CDL	C78-C79-C80-C81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C5-C6-C7-C8
13	M	407	SPN	CM3-C5-C6-C7
13	M	407	SPN	C4-C5-C6-C7
7	M	402	BCL	C2A-CAA-CBA-CGA
10	M	401	CDL	CA5-C11-C12-C13
8	M	404	BPH	C8-C10-C11-C12
8	M	404	BPH	C5-C6-C7-C8
10	M	401	CDL	O1-C1-CB2-OB2
4	M	409	LDA	C7-C8-C9-C10
4	M	413	LDA	C2-C3-C4-C5
7	M	402	BCL	C3A-C2A-CAA-CBA
4	M	409	LDA	C4-C5-C6-C7
10	M	401	CDL	C16-C17-C18-C19
10	M	401	CDL	C39-C40-C41-C42
4	M	408	LDA	C1-C2-C3-C4
4	M	413	LDA	C4-C5-C6-C7
10	M	401	CDL	C11-CA5-OA6-CA4
4	H	301	LDA	C1-C2-C3-C4
10	M	401	CDL	C74-C75-C76-C77
10	M	401	CDL	C20-C21-C22-C23
10	M	401	CDL	CA2-C1-CB2-OB2
13	M	407	SPN	C19-C20-C21-C22
10	M	401	CDL	OB5-CB3-CB4-CB6
10	M	401	CDL	OA7-CA5-OA6-CA4
10	M	401	CDL	C36-C37-C38-C39
12	M	406	U10	C35-C34-C36-C37
12	M	406	U10	C33-C34-C36-C37
7	M	402	BCL	C6-C7-C8-C9
4	L	304	LDA	C2-C3-C4-C5
10	M	401	CDL	C11-C12-C13-C14
10	M	401	CDL	CB3-CB4-CB6-OB8
10	M	401	CDL	C34-C35-C36-C37
10	M	401	CDL	C71-C72-C73-C74
4	M	409	LDA	C5-C6-C7-C8
10	M	401	CDL	C54-C55-C56-C57
4	L	304	LDA	C7-C8-C9-C10
4	M	413	LDA	C7-C8-C9-C10
13	M	407	SPN	CM5-C13-C14-C15
12	M	406	U10	C36-C37-C38-C39
13	M	407	SPN	C23-C24-C25-C26
10	M	401	CDL	C40-C41-C42-C43
10	M	401	CDL	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C7-C8-C9-C10
13	M	407	SPN	C20-C21-C22-CM7
13	M	407	SPN	C22-C23-C24-C25
10	M	401	CDL	C55-C56-C57-C58
7	M	402	BCL	C6-C7-C8-C10
8	M	404	BPH	C12-C13-C15-C16
13	M	407	SPN	C20-C21-C22-C23
10	M	401	CDL	C79-C80-C81-C82
4	M	408	LDA	C7-C8-C9-C10
6	L	309	EDO	O1-C1-C2-O2
4	M	413	LDA	C5-C6-C7-C8
10	M	401	CDL	OB5-CB3-CB4-OB6
10	M	401	CDL	OB6-CB4-CB6-OB8
7	M	403	BCL	C14-C13-C15-C16
13	M	407	SPN	CM7-C22-C23-C24
13	M	407	SPN	O1-C1-C2-O2
10	M	401	CDL	C33-C34-C35-C36
4	H	301	LDA	C9-C10-C11-C12
8	L	303	BPH	O2A-C1-C2-C3
13	M	407	SPN	C12-C13-C14-C15
10	M	401	CDL	C18-C19-C20-C21
4	M	408	LDA	C2-C1-N1-CM2
4	M	409	LDA	C2-C1-N1-CM2
4	M	413	LDA	C2-C1-N1-CM2
10	M	401	CDL	OA5-CA3-CA4-CA6
4	M	413	LDA	C3-C4-C5-C6
10	M	401	CDL	OA5-CA3-CA4-OA6
8	M	404	BPH	C14-C13-C15-C16
8	L	303	BPH	C4C-C3C-CAC-CBC
7	L	302	BCL	CHA-CBD-CGD-O1D
7	L	302	BCL	CHA-CBD-CGD-O2D
10	M	401	CDL	CA2-OA2-PA1-OA3
10	M	401	CDL	CA2-OA2-PA1-OA4
13	M	407	SPN	CM2-C1-O1-CMA
10	M	401	CDL	C14-C15-C16-C17
7	M	403	BCL	C16-C17-C18-C19
10	M	401	CDL	C12-C13-C14-C15
13	M	407	SPN	CM2-C1-C2-C3
10	M	401	CDL	C1-CA2-OA2-PA1
12	M	406	U10	C5-C4-O4-C4M
4	M	409	LDA	C2-C3-C4-C5
7	M	402	BCL	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	401	CDL	CA3-CA4-CA6-OA8
7	M	402	BCL	C3-C5-C6-C7
10	M	401	CDL	C75-C76-C77-C78
10	M	401	CDL	C72-C73-C74-C75
8	L	303	BPH	C2-C3-C5-C6
12	M	406	U10	C37-C38-C39-C40
8	L	303	BPH	C4-C3-C5-C6
10	M	401	CDL	C17-C18-C19-C20
8	M	404	BPH	C10-C11-C12-C13
13	M	407	SPN	CM2-C1-C2-O2
9	L	310	HTO	O2-C2-C3-C4
8	M	404	BPH	CAD-CBD-CGD-O2D

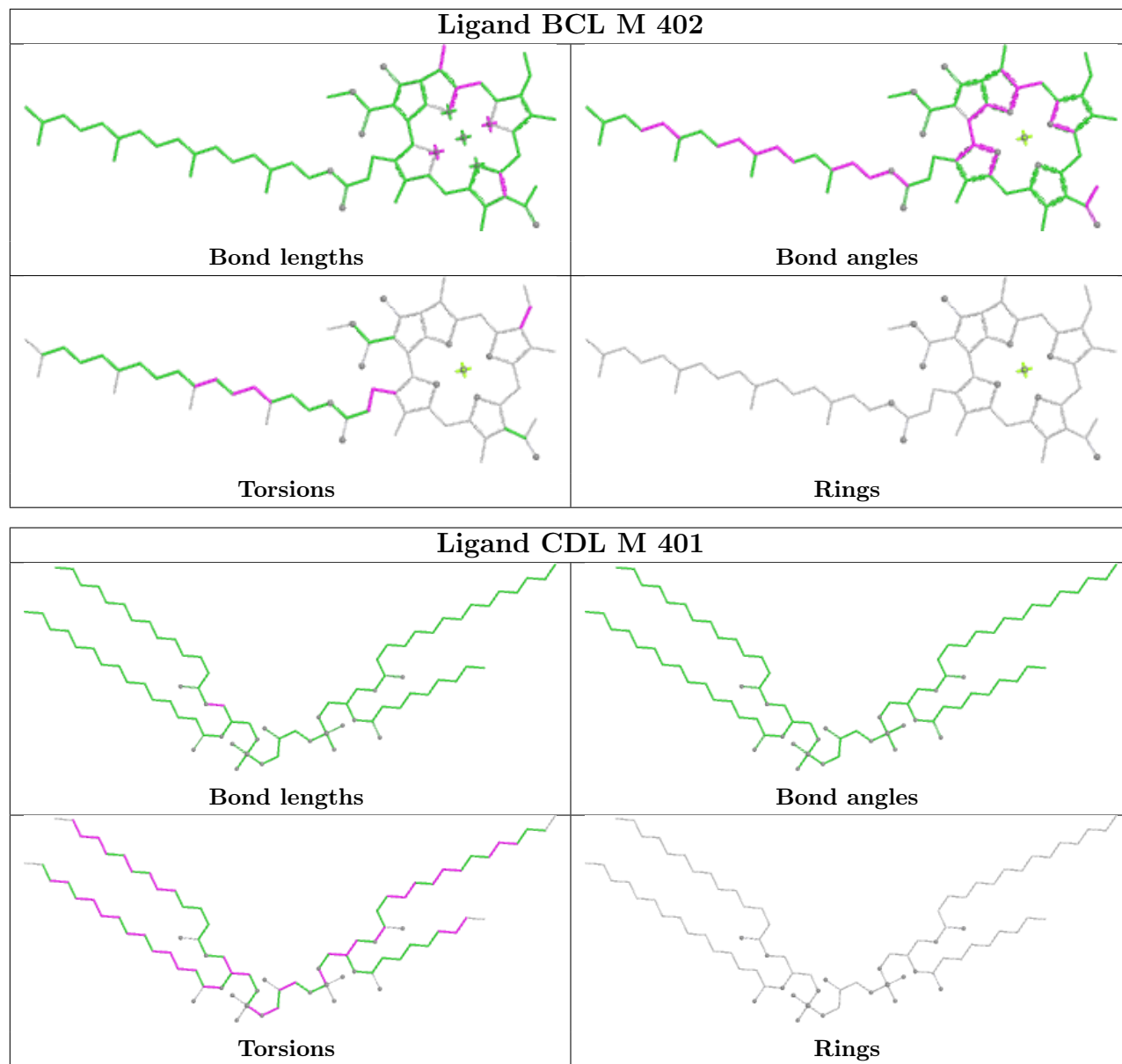
There are no ring outliers.

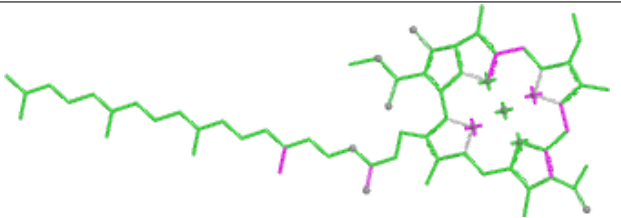
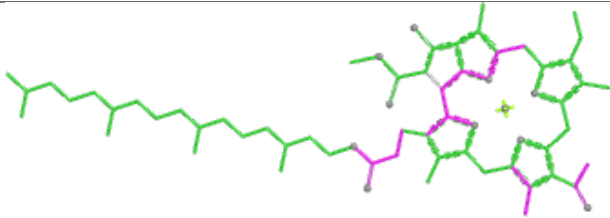
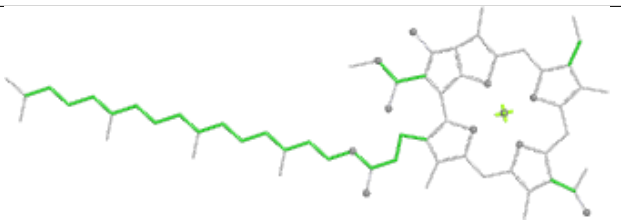
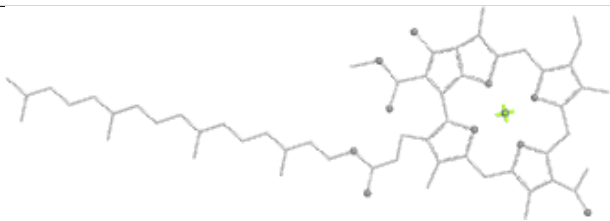
13 monomers are involved in 33 short contacts:

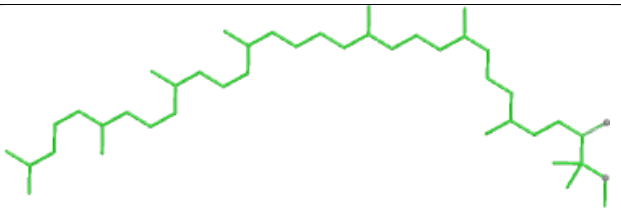
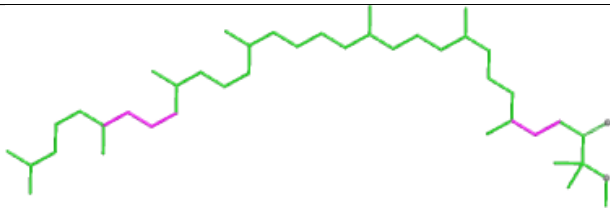
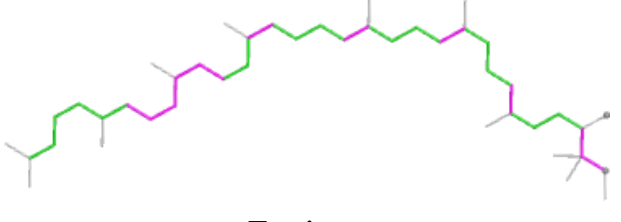
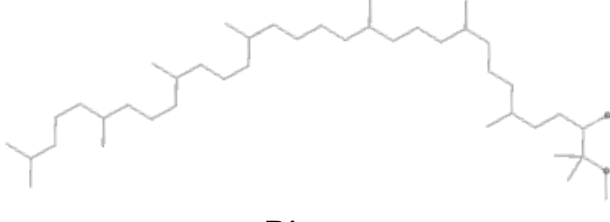
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	402	BCL	2	0
10	M	401	CDL	6	0
4	H	301	LDA	2	0
7	L	301	BCL	3	0
13	M	407	SPN	10	0
6	H	304	EDO	1	0
6	L	309	EDO	5	0
7	L	302	BCL	2	0
7	M	403	BCL	1	0
4	M	408	LDA	1	0
8	L	303	BPH	2	0
8	M	404	BPH	1	0
12	M	406	U10	2	0

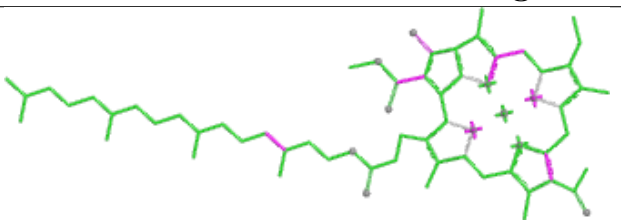
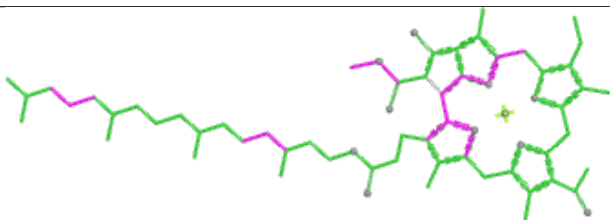
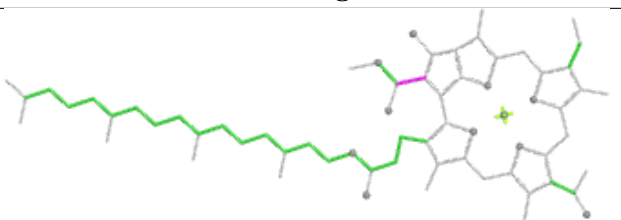
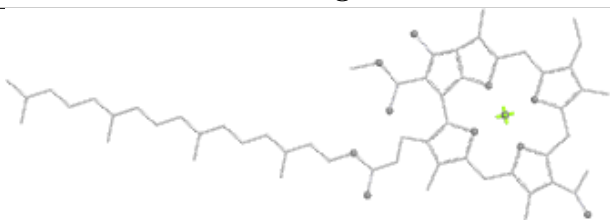
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

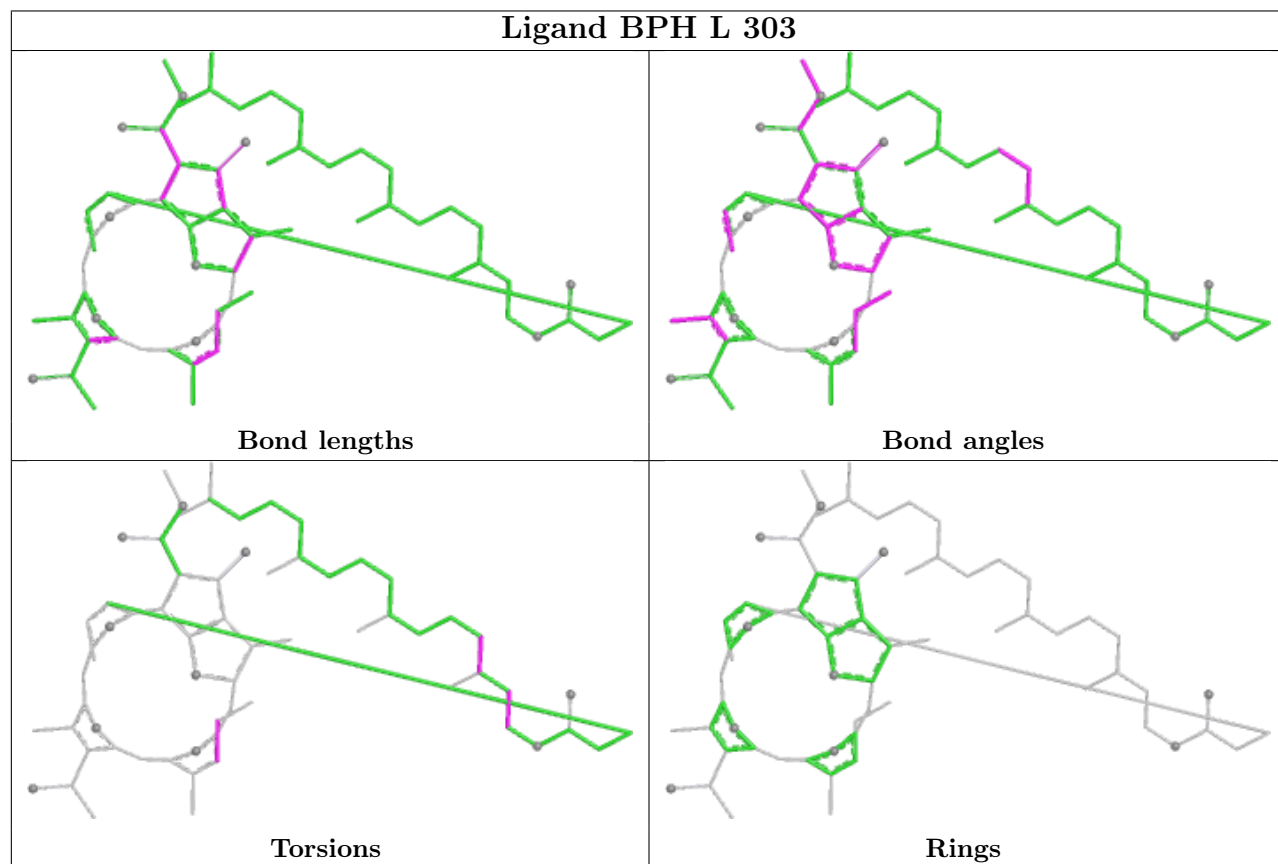
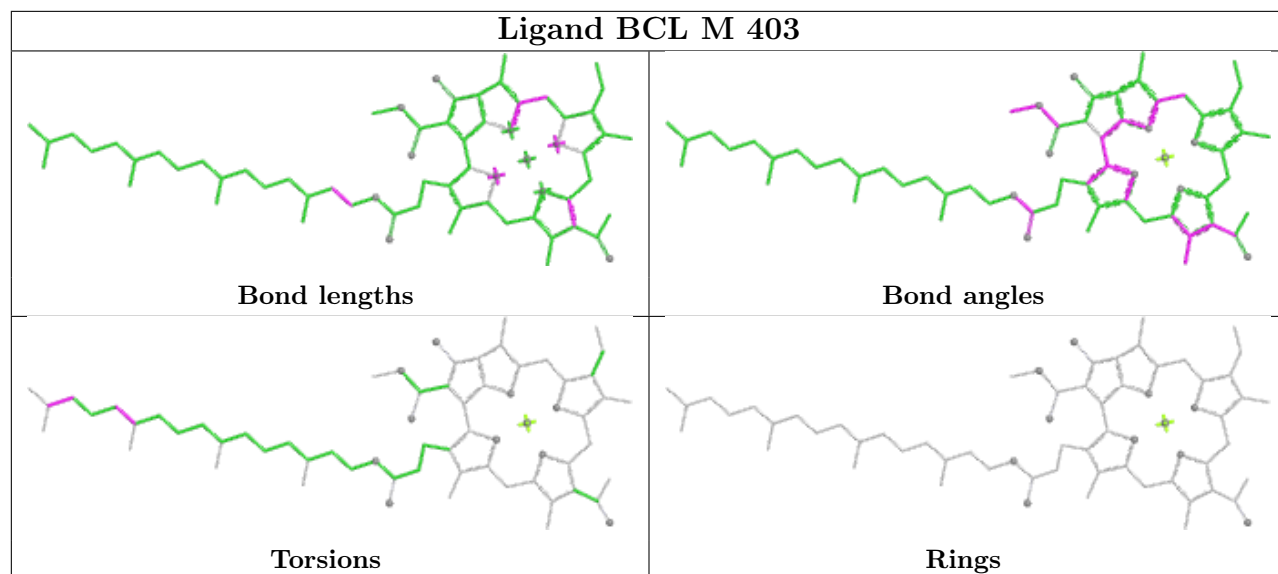
equivalents in the CSD to analyse the geometry.

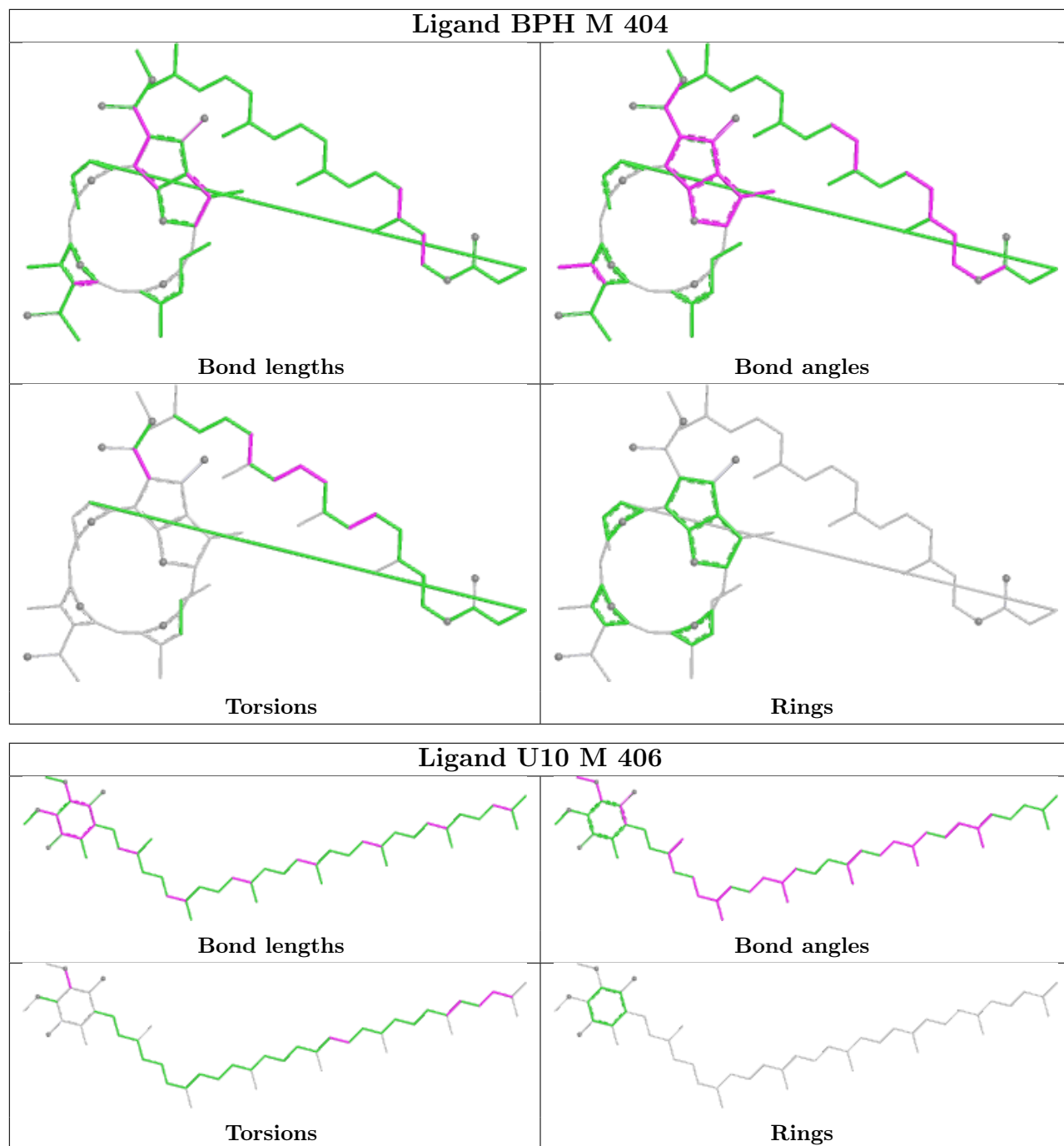


Ligand BCL L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SPN M 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL L 302	
	
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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	H	250/251 (99%)	-0.26	0	100	100	39, 66, 86, 105	2 (0%)
2	L	281/281 (100%)	-0.01	9 (3%)	50	44	41, 72, 162, 199	2 (0%)
3	M	302/303 (99%)	-0.09	3 (0%)	79	76	37, 68, 106, 149	2 (0%)
All	All	833/835 (99%)	-0.11	12 (1%)	73	69	37, 69, 110, 199	6 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	4.0
2	L	266	TRP	3.9
3	M	148	TRP	3.8
2	L	271	TRP	3.2
2	L	270	PRO	3.1
2	L	259	TRP	2.9
2	L	265	TRP	2.8
2	L	272	TRP	2.7
2	L	269	LEU	2.6
2	L	279	ILE	2.3
3	M	85	PHE	2.3
2	L	276	PRO	2.2

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 ⓘ

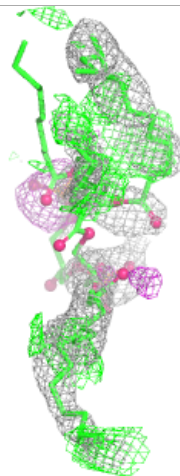
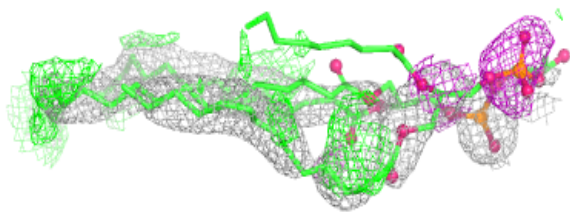
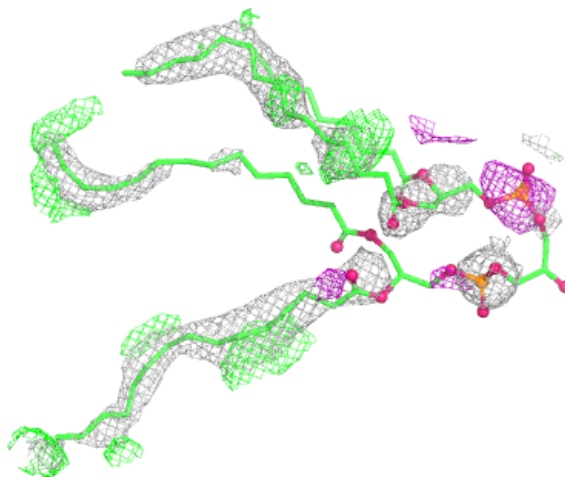
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UNL	H	302	12/-	0.64	0.21	88,95,108,111	0
10	CDL	M	401	81/100	0.67	0.29	58,87,106,116	81
5	UNL	M	412	12/-	0.74	0.30	66,80,97,99	0
5	UNL	H	303	15/-	0.75	0.26	85,99,116,118	0
4	LDA	M	413	16/16	-	-	68,72,88,92	16
5	UNL	M	411	12/-	0.75	0.29	84,95,99,101	0
9	HTO	L	310	10/10	0.76	0.23	90,100,105,109	0
5	UNL	L	306	15/-	0.79	0.23	55,89,108,108	0
4	LDA	L	304	16/16	0.80	0.18	76,88,102,110	0
5	UNL	L	307	10/-	0.80	0.20	77,93,98,100	0
4	LDA	M	409	16/16	0.81	0.21	70,84,94,98	0
5	UNL	M	410	15/-	0.81	0.24	76,92,103,104	0
4	LDA	M	408	16/16	0.81	0.24	60,85,93,94	0
6	EDO	L	309	4/4	0.83	0.21	73,75,79,83	0
6	EDO	H	304	4/4	0.85	0.20	71,73,75,83	0
6	EDO	L	308	4/4	-	-	65,66,66,67	4
6	EDO	H	305	4/4	0.86	0.14	66,68,84,90	0
4	LDA	H	301	16/16	0.87	0.17	71,78,96,97	0
13	SPN	M	407	43/43	0.88	0.16	71,86,110,114	0
5	UNL	L	305	12/-	0.89	0.15	77,83,86,86	0
8	BPH	M	404	65/65	0.91	0.12	49,68,125,132	0
12	U10	M	406	48/63	0.92	0.14	55,68,90,95	0
7	BCL	M	403	66/66	0.94	0.10	58,71,85,97	0
8	BPH	L	303	65/65	0.95	0.09	47,62,78,88	0
7	BCL	M	402	66/66	0.95	0.11	63,75,98,104	0
7	BCL	L	301	66/66	0.95	0.09	57,70,78,82	0
7	BCL	L	302	66/66	0.97	0.09	57,69,92,96	0
11	FE	M	405	1/1	1.00	0.05	62,62,62,62	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.

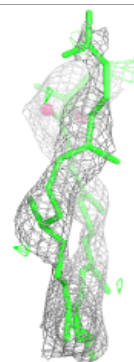
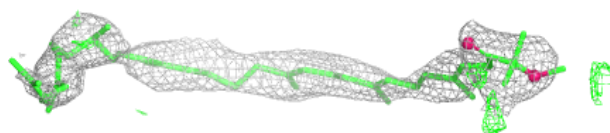
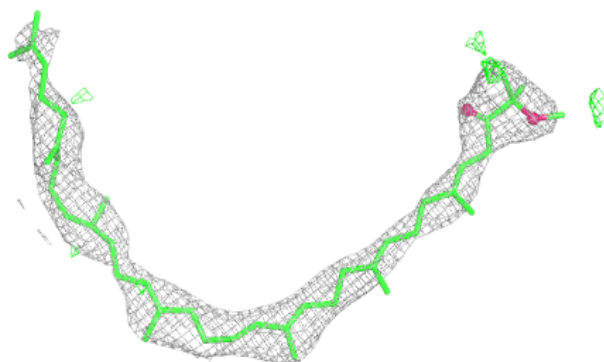
Electron density around CDL M 401:

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

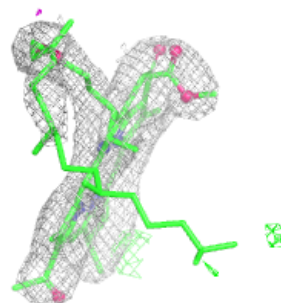
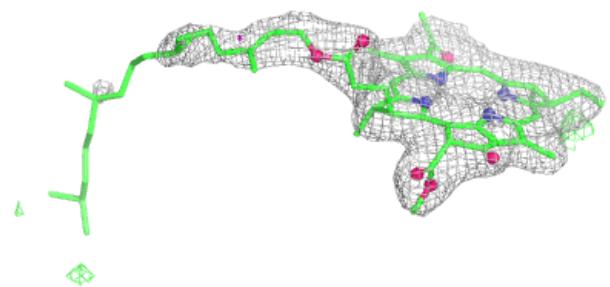
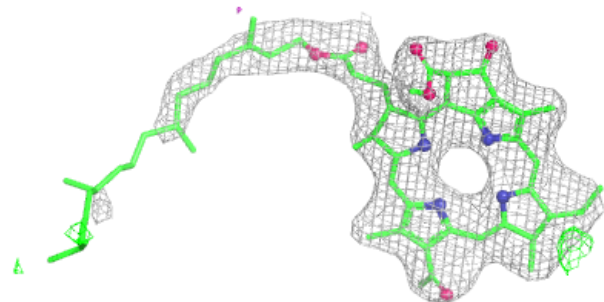


Electron density around SPN M 407:

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

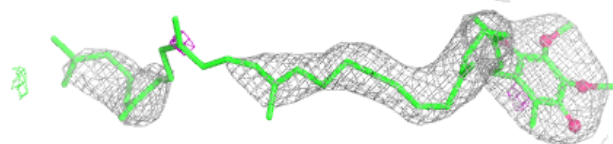
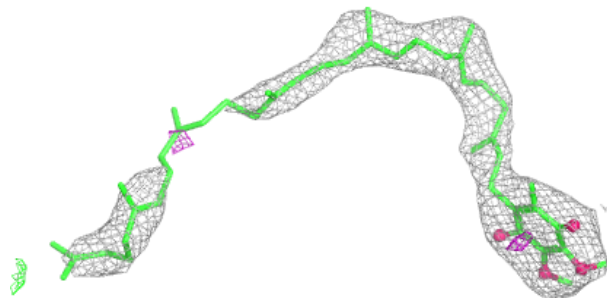
**Electron density around BPH M 404:**

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

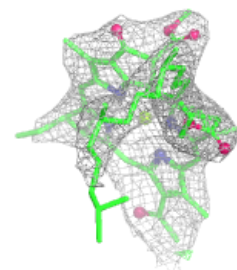
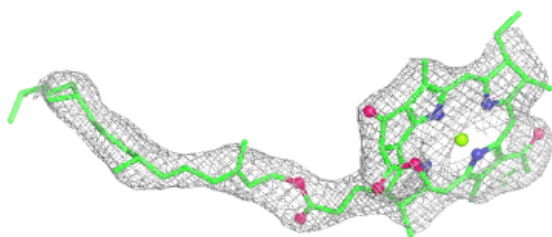
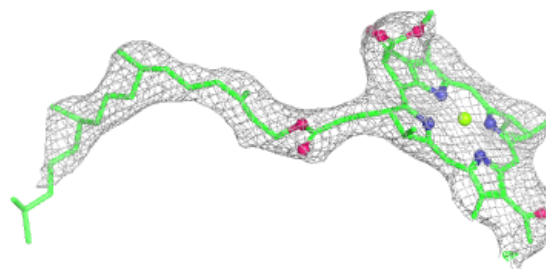


Electron density around U10 M 406:

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

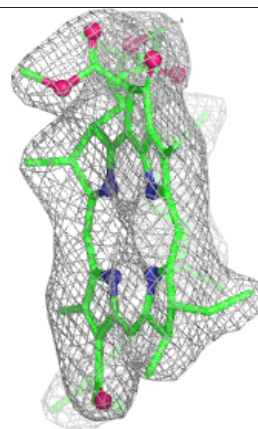
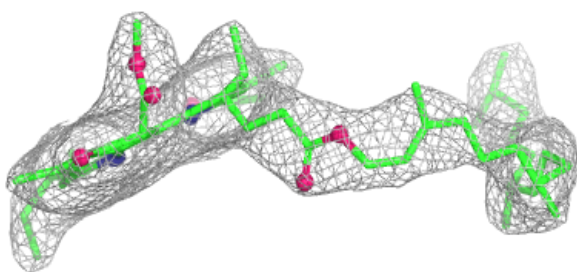
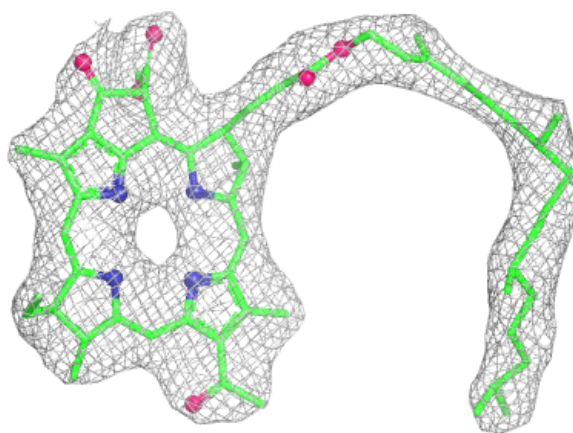
**Electron density around BCL M 403:**

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



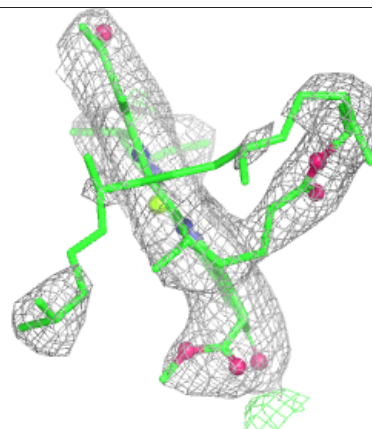
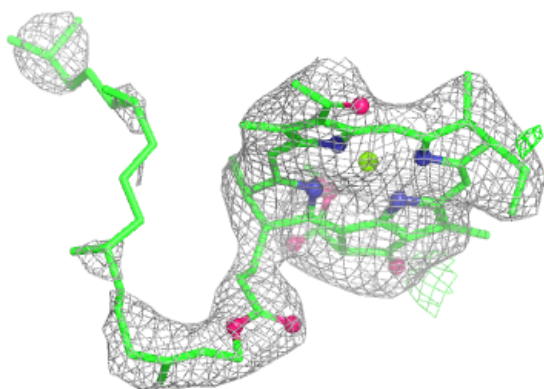
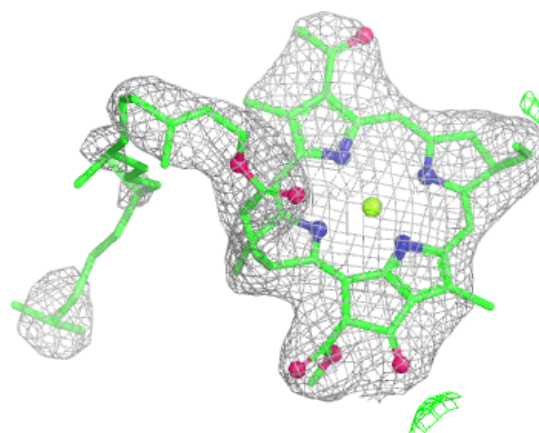
Electron density around BPH L 303:

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

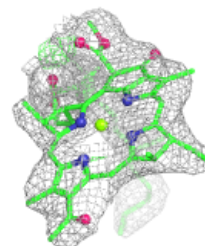
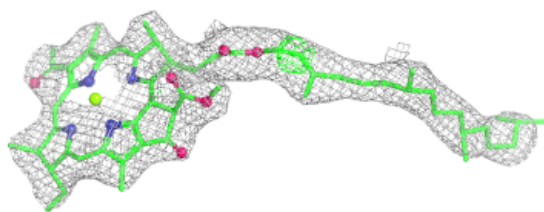
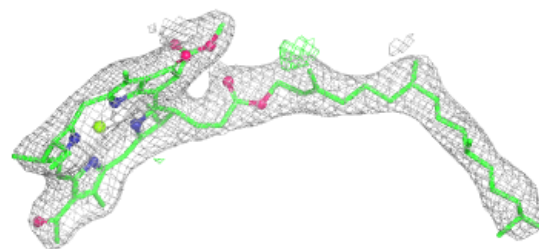


Electron density around BCL M 402:

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

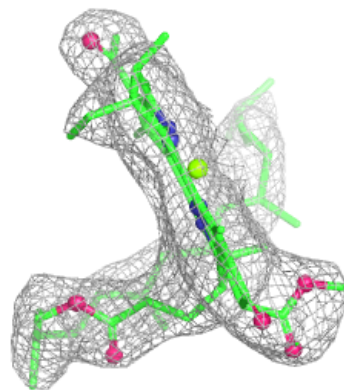
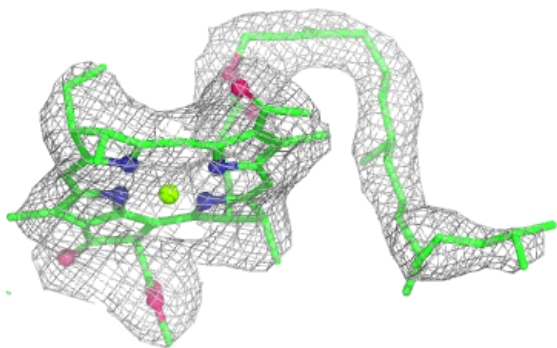
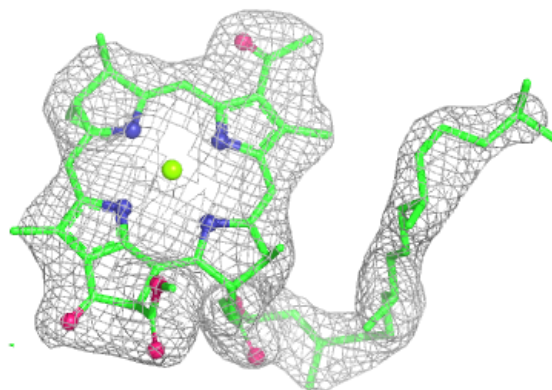
**Electron density around BCL L 301:**

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



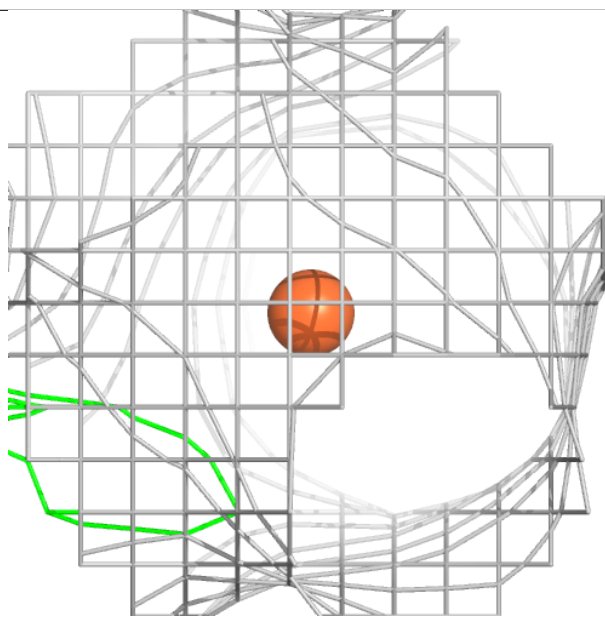
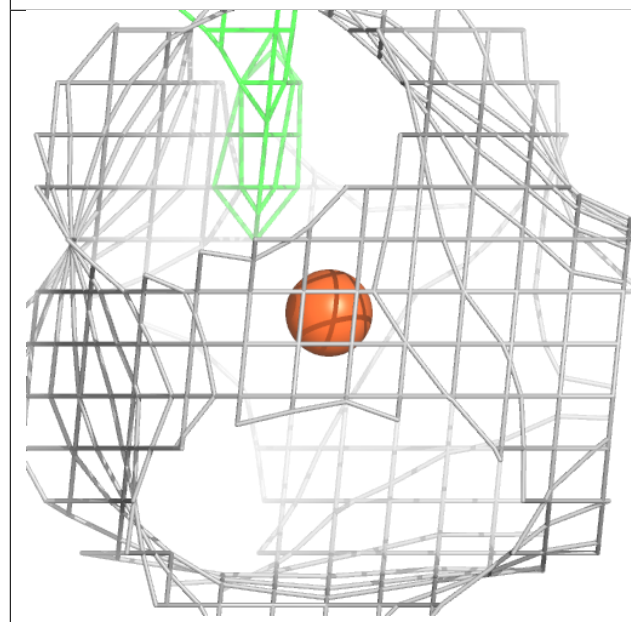
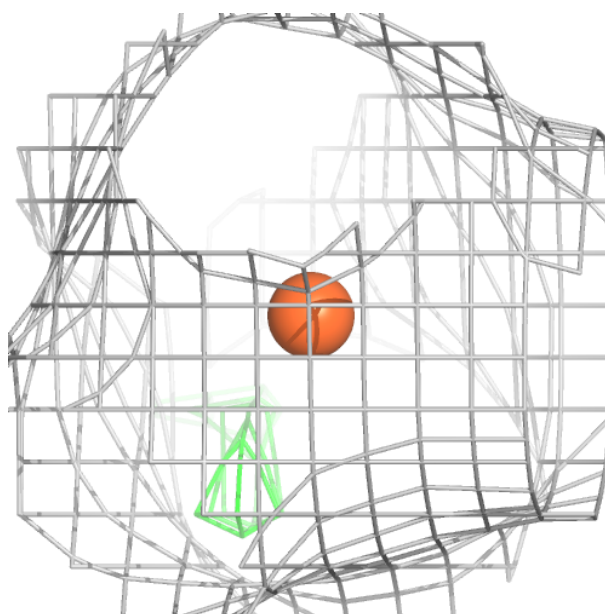
Electron density around BCL L 302:

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



Electron density around FE M 405:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.