



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 08:58 pm BST

PDB ID : 8C3F / pdb_00008c3f
Title : Double mutant I(L177)H/F(M197)H structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors : Gabdulkhakov, A.G.; Selikhanov, G.K.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on : 2022-12-23
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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

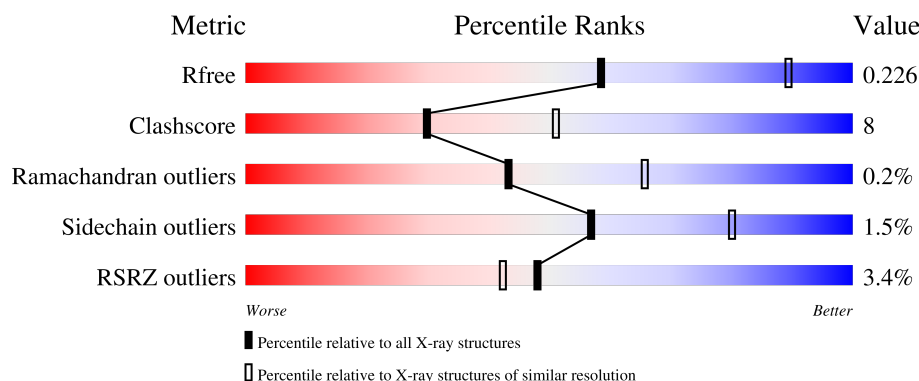
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

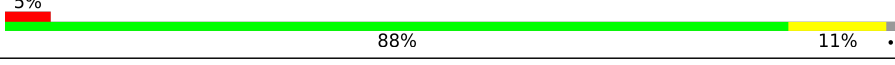
The reported resolution of this entry is 2.60 Å.

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	L	281	
2	M	303	
3	H	241	

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	HTO	M	402	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 7413 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
			2234	1508	357	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	177	HIS	ILE	engineered mutation	UNP P0C0Y8
L	178	THR	SER	engineered mutation	UNP P0C0Y8

- 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
			2416	1610	397	398	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

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

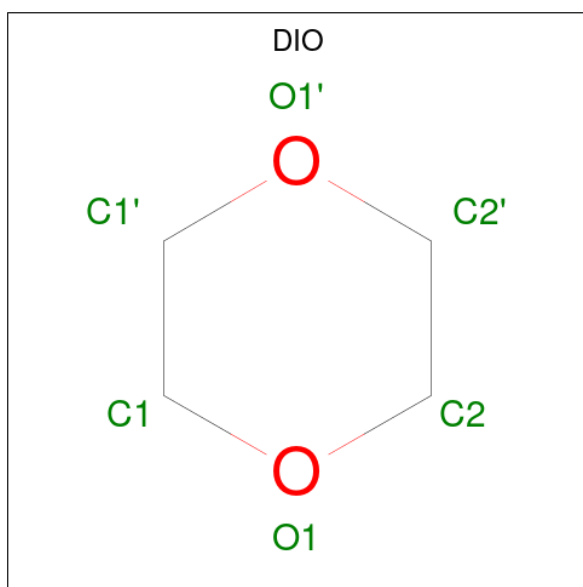
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	0	0
			1823	1166	313	335	9			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



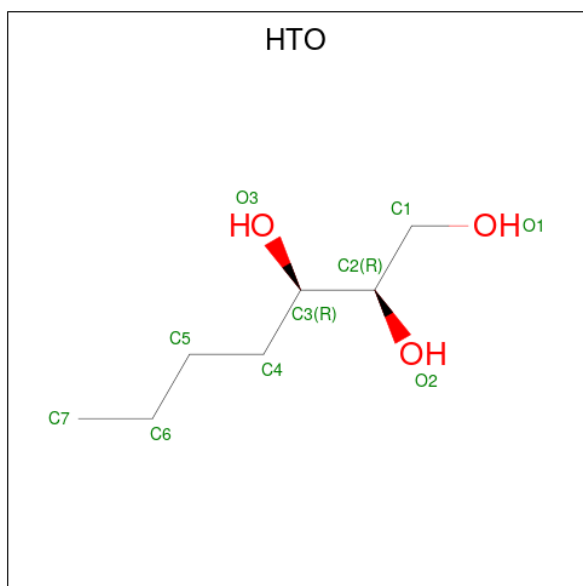
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



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

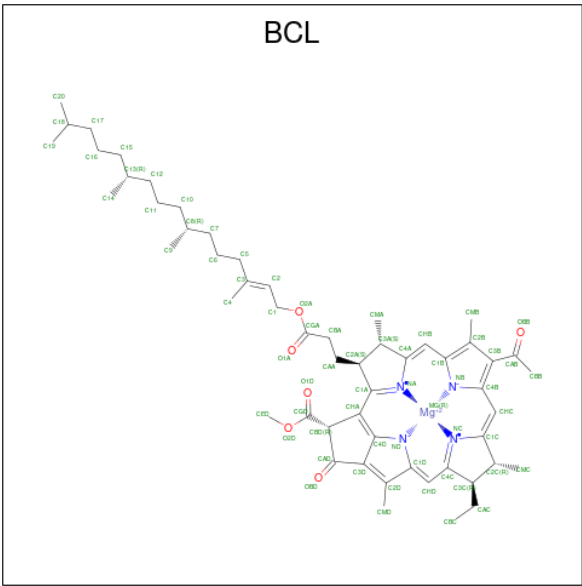
- Molecule 6 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

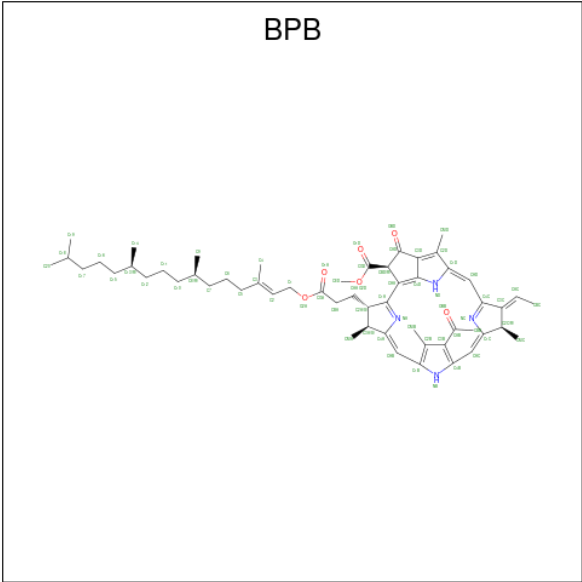
- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$)

(labeled as "Ligand of Interest" by depositor).



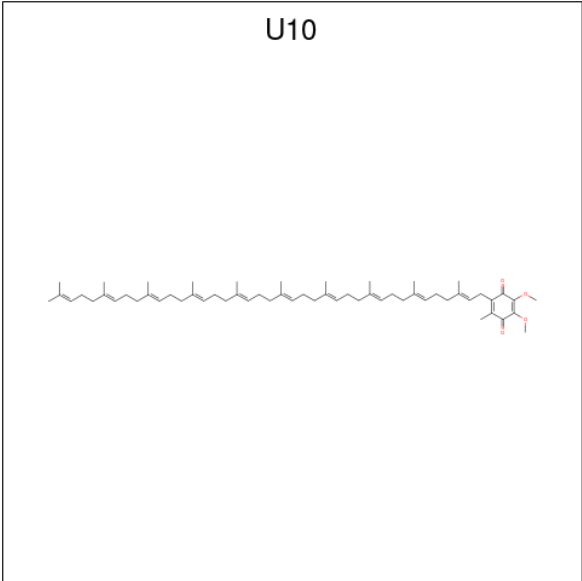
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆) (la-
beled 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 UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



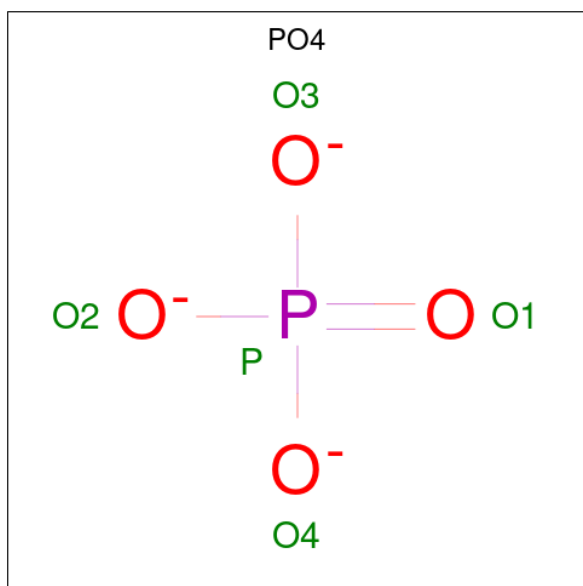
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			48	44	4		

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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



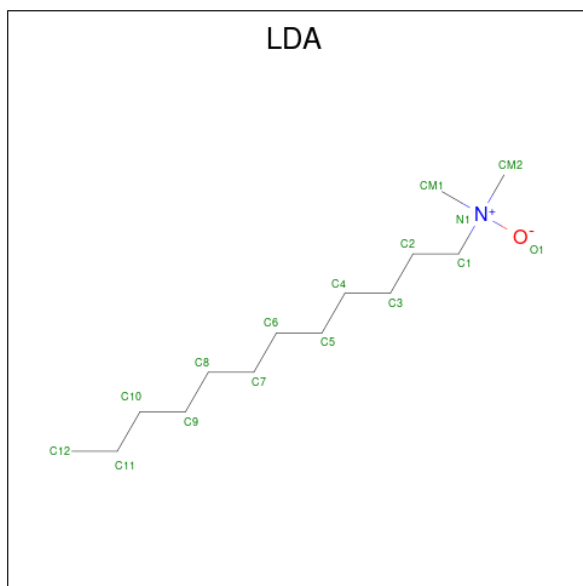
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	O	P	0	0
			5	4	1		
10	L	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

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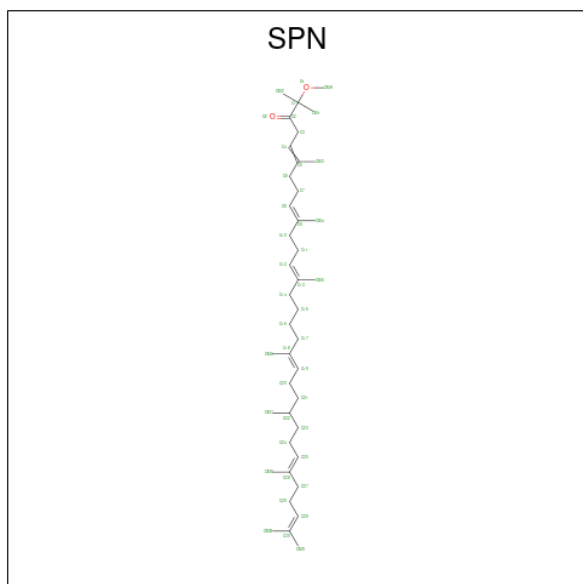
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	H	1	Total	C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

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 14 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂) (labeled as "Ligand of Interest" by depositor).



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

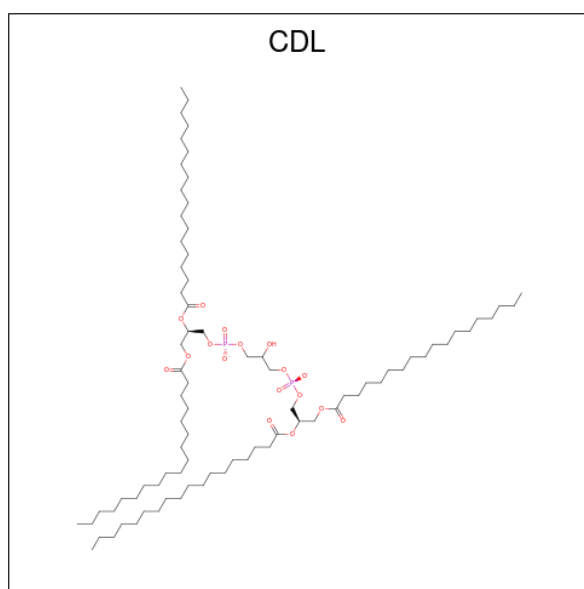
- Molecule 15 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total K 1 1	0	0
15	H	1	Total K 1 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

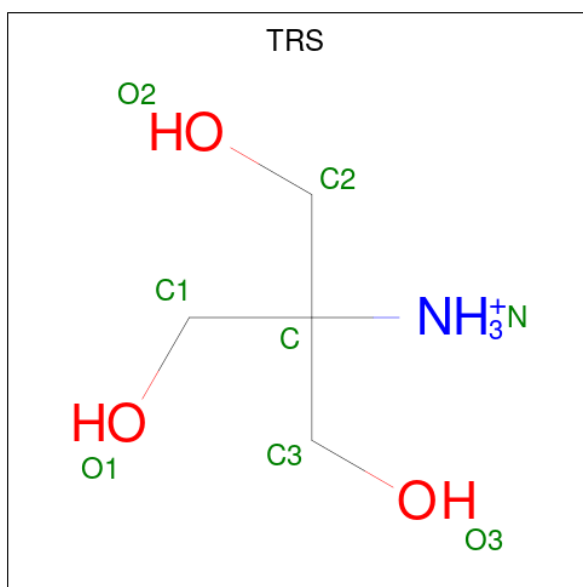
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total Cl 1 1	0	0

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	H	1	Total	C	N	O	0	0
			8	4	1	3		

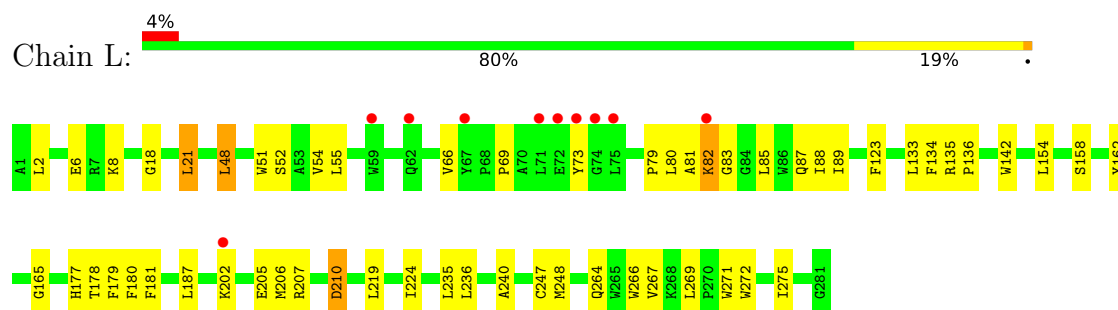
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	32	Total	O	0	0
			32	32		
19	M	39	Total	O	0	0
			39	39		
19	H	40	Total	O	0	0
			40	40		

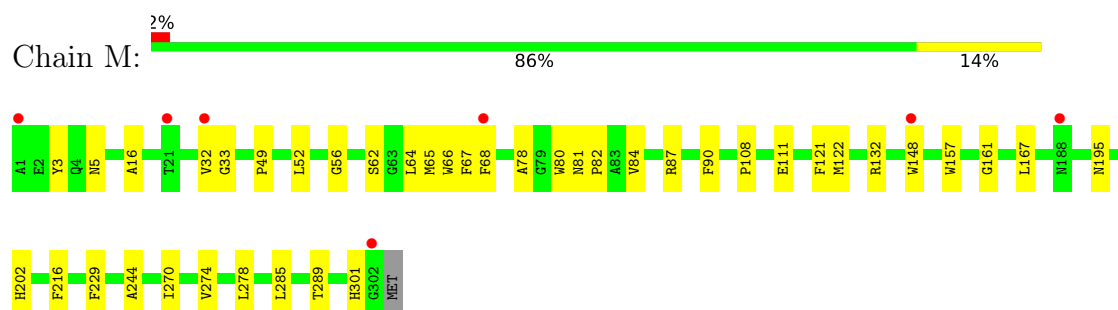
3 Residue-property plots [i](#)

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.

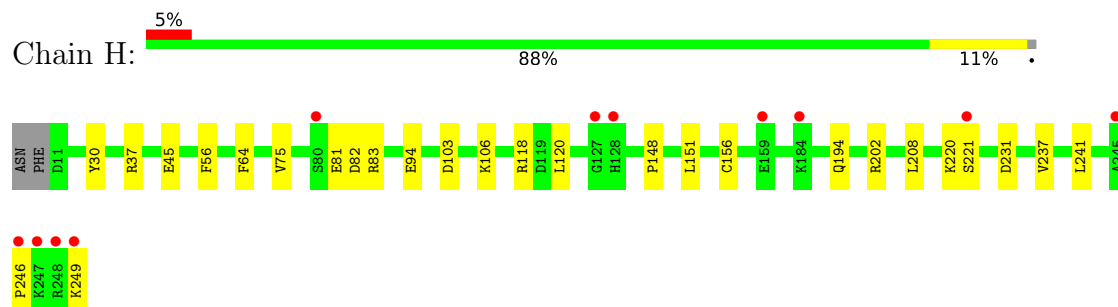
- Molecule 1: Reaction center protein L chain



- 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	139.35Å 139.35Å 184.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.12 – 2.60 46.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.12-2.60) 100.0 (46.12-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.220 0.197 , 0.226	Depositor DCC
R_{free} test set	3442 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7413	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, SPN, BCL, CDL, U10, HTO, BPB, CL, LDA, GOL, K, PO4, TRS, EDO, DIO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.34	0/2323	0.53	1/3181 (0.0%)
2	M	0.31	0/2508	0.50	0/3424
3	H	0.35	0/1871	0.54	0/2545
All	All	0.33	0/6702	0.52	1/9150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	48	LEU	CA-CB-CG	-5.37	97.49	116.30

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	L	2234	0	2185	57	0
2	M	2416	0	2329	33	0
3	H	1823	0	1831	22	0
4	H	8	0	12	1	0
4	L	8	0	12	1	0
4	M	12	0	18	0	0
5	L	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	10	0	16	0	0
6	M	10	0	16	6	0
7	L	132	0	148	10	0
7	M	132	0	148	3	0
8	L	65	0	74	0	0
8	M	65	0	74	2	0
9	L	48	0	63	8	0
9	M	48	0	63	2	0
10	L	10	0	0	0	0
10	M	5	0	0	0	0
11	L	6	0	8	0	0
12	H	16	0	31	3	0
12	L	32	0	62	1	0
12	M	80	0	155	7	0
13	M	1	0	0	0	0
14	M	43	0	70	7	0
15	H	1	0	0	0	0
15	M	1	0	0	0	0
16	M	1	0	0	0	0
17	M	81	0	106	8	0
18	H	8	0	12	4	0
19	H	40	0	0	2	0
19	L	32	0	0	1	0
19	M	39	0	0	2	0
All	All	7413	0	7441	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:177:HIS:ND1	7:L:305:BCL:HMB2	1.23	1.43
1:L:177:HIS:ND1	7:L:305:BCL:CMB	2.06	1.18
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.53	0.90
1:L:266:TRP:CD1	6:M:402:HTO:H2	2.19	0.78
3:H:202:ARG:HH12	18:H:303:TRS:H12	1.49	0.77
1:L:48:LEU:HD13	1:L:88:ILE:CD1	2.16	0.75
3:H:202:ARG:HH22	18:H:303:TRS:H21	1.52	0.72
7:L:313:BCL:CAB	14:M:410:SPN:H162	2.18	0.72
2:M:81:ASN:HB3	2:M:84:VAL:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:LEU:HD13	1:L:88:ILE:HD13	1.73	0.70
2:M:78:ALA:HB1	2:M:84:VAL:HG23	1.73	0.70
7:L:313:BCL:H141	14:M:410:SPN:H101	1.74	0.69
17:M:414:CDL:H312	17:M:414:CDL:H521	1.73	0.69
1:L:177:HIS:CE1	7:L:305:BCL:CMB	2.77	0.68
17:M:414:CDL:H542	17:M:414:CDL:H332	1.78	0.65
12:L:312:LDA:HM13	2:M:33:GLY:HA2	1.78	0.65
2:M:32:VAL:HG12	2:M:49:PRO:HD3	1.79	0.64
1:L:178:THR:HG22	9:L:307:U10:H262	1.81	0.62
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.80	0.62
7:L:313:BCL:OBB	14:M:410:SPN:H162	1.99	0.61
2:M:278:LEU:HD21	17:M:414:CDL:H391	1.81	0.61
2:M:202:HIS:HD2	19:M:535:HOH:O	1.84	0.61
2:M:90:PHE:CG	6:M:402:HTO:H12	2.36	0.60
3:H:220:LYS:HD3	19:H:409:HOH:O	2.02	0.60
3:H:208:LEU:HD11	3:H:237:VAL:HG22	1.84	0.59
1:L:55:LEU:HD23	1:L:81:ALA:HA	1.85	0.58
2:M:161:GLY:HA3	14:M:410:SPN:H201	1.87	0.56
3:H:220:LYS:HE2	19:H:415:HOH:O	2.04	0.56
1:L:266:TRP:CE2	6:M:402:HTO:H3	2.41	0.55
3:H:156:CYS:SG	3:H:249:LYS:O	2.63	0.55
1:L:73:TYR:OH	1:L:82:LYS:HD2	2.07	0.55
9:M:409:U10:H202	12:H:304:LDA:H112	1.88	0.54
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.43	0.54
2:M:148:TRP:HD1	17:M:414:CDL:H752	1.72	0.54
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.89	0.54
1:L:202:LYS:H	1:L:202:LYS:CD	2.21	0.54
17:M:414:CDL:H112	3:H:30:TYR:CZ	2.43	0.53
1:L:236:LEU:HD21	9:L:307:U10:H203	1.91	0.52
1:L:133:LEU:HD23	1:L:134:PHE:CE1	2.44	0.52
1:L:177:HIS:CE1	7:L:305:BCL:HMB3	2.44	0.52
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.91	0.51
2:M:289:THR:HA	12:M:417:LDA:H11	1.93	0.51
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.36	0.51
8:M:407:BPB:H12A	8:M:407:BPB:H17A	1.92	0.51
1:L:79:PRO:HB2	1:L:82:LYS:HG2	1.93	0.51
2:M:285:LEU:HD23	12:M:417:LDA:H123	1.93	0.51
3:H:56:PHE:HE2	12:H:304:LDA:H42	1.76	0.51
2:M:157:TRP:CE2	14:M:410:SPN:HM73	2.48	0.49
3:H:37:ARG:HB3	3:H:75:VAL:HB	1.95	0.48
2:M:80:TRP:O	2:M:82:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:PHE:CZ	9:L:307:U10:H272	2.48	0.48
1:L:51:TRP:O	1:L:54:VAL:HG22	2.14	0.48
2:M:148:TRP:NE1	17:M:414:CDL:H522	2.28	0.48
2:M:90:PHE:CD1	6:M:402:HTO:H12	2.49	0.47
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.14	0.47
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.95	0.47
1:L:88:ILE:HD12	1:L:89:ILE:N	2.28	0.47
1:L:206:MET:HE3	3:H:64:PHE:CD2	2.48	0.47
2:M:270:ILE:O	2:M:274:VAL:HG13	2.15	0.47
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.42	0.47
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.97	0.47
3:H:81:GLU:O	3:H:83:ARG:HG2	2.15	0.46
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.97	0.46
2:M:67:PHE:CE1	14:M:410:SPN:H61	2.50	0.46
3:H:82:ASP:OD2	4:H:302:EDO:H21	2.15	0.46
3:H:194:GLN:H	3:H:194:GLN:CD	2.23	0.46
7:M:406:BCL:HAA2	7:M:406:BCL:HBD	1.98	0.46
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.49	0.46
2:M:52:LEU:HD23	2:M:52:LEU:HA	1.79	0.46
1:L:202:LYS:H	1:L:202:LYS:CE	2.28	0.46
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.52	0.45
1:L:269:LEU:HD13	1:L:271:TRP:CZ2	2.52	0.45
7:L:313:BCL:C4A	7:L:313:BCL:HBA2	2.46	0.45
17:M:414:CDL:OA3	17:M:414:CDL:HA4	2.17	0.45
1:L:2:LEU:HB3	1:L:6:GLU:HB3	1.99	0.45
7:L:313:BCL:H2	8:M:407:BPB:CMB	2.47	0.45
3:H:202:ARG:HH22	18:H:303:TRS:H32	1.81	0.45
3:H:202:ARG:NH1	18:H:303:TRS:H12	2.24	0.45
1:L:123:PHE:CE2	5:L:303:DIO:H2'2	2.52	0.44
12:M:404:LDA:H101	9:M:409:U10:H201	1.98	0.44
1:L:224:ILE:H	9:L:307:U10:H103	1.82	0.44
3:H:148:PRO:HA	3:H:151:LEU:HD12	2.00	0.44
1:L:88:ILE:HD12	1:L:88:ILE:C	2.43	0.44
1:L:83:GLY:O	1:L:87:GLN:HG3	2.17	0.44
3:H:56:PHE:CE2	12:H:304:LDA:H42	2.53	0.44
1:L:69:PRO:HD3	1:L:83:GLY:O	2.17	0.44
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.71	0.44
2:M:64:LEU:HB3	2:M:68:PHE:CE2	2.54	0.43
1:L:82:LYS:O	1:L:82:LYS:HG3	2.18	0.43
1:L:219:LEU:O	2:M:132:ARG:NH2	2.40	0.43
12:M:417:LDA:H21	12:M:417:LDA:HM23	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:289:THR:O	12:M:417:LDA:H22	2.18	0.43
9:L:307:U10:H4M3	9:L:307:U10:H3M2	2.00	0.43
2:M:16:ALA:HB1	2:M:32:VAL:HG11	2.01	0.43
7:M:406:BCL:H201	12:M:418:LDA:H112	2.00	0.43
1:L:154:LEU:HD11	7:M:403:BCL:C3D	2.48	0.43
4:L:301:EDO:H11	3:H:241:LEU:HD13	2.01	0.43
1:L:202:LYS:H	1:L:202:LYS:HE2	1.84	0.43
1:L:18:GLY:O	1:L:21:LEU:HB2	2.19	0.42
1:L:266:TRP:NE1	6:M:402:HTO:H2	2.35	0.42
1:L:202:LYS:H	1:L:202:LYS:HD3	1.84	0.42
2:M:167:LEU:HD13	12:M:417:LDA:H92	2.01	0.42
2:M:301:HIS:NE2	19:M:501:HOH:O	2.25	0.42
14:M:410:SPN:C25	14:M:410:SPN:H29	2.49	0.42
1:L:123:PHE:HE2	5:L:303:DIO:H2'2	1.85	0.41
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.55	0.41
1:L:272:TRP:CD1	2:M:87:ARG:HG3	2.55	0.41
2:M:56:GLY:HA2	2:M:132:ARG:HD2	2.02	0.41
1:L:177:HIS:CE1	1:L:181:PHE:CZ	3.08	0.41
1:L:210:ASP:OD1	1:L:210:ASP:N	2.52	0.41
7:L:305:BCL:OBB	7:L:305:BCL:HHC	2.19	0.41
9:L:307:U10:H321	9:L:307:U10:H28	1.73	0.41
1:L:162:TYR:HA	1:L:165:GLY:O	2.21	0.41
1:L:205:GLU:HG3	19:L:421:HOH:O	2.20	0.41
1:L:52:SER:OG	1:L:66:VAL:HG22	2.21	0.41
1:L:178:THR:HG21	9:L:307:U10:H28	2.03	0.41
1:L:248:MET:HE3	1:L:248:MET:HB3	1.97	0.41
1:L:80:LEU:HB3	1:L:85:LEU:HG	2.03	0.41
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.56	0.40
2:M:148:TRP:HE1	17:M:414:CDL:C55	2.34	0.40
3:H:118:ARG:HD2	3:H:120:LEU:HD12	2.02	0.40
1:L:224:ILE:N	9:L:307:U10:H103	2.37	0.40
2:M:66:TRP:CZ2	2:M:122:MET:HE3	2.57	0.40
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.03	0.40
1:L:266:TRP:CG	6:M:402:HTO:H2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	301/303 (99%)	290 (96%)	10 (3%)	1 (0%)	36	58
3	H	237/241 (98%)	232 (98%)	4 (2%)	1 (0%)	30	51
All	All	817/825 (99%)	789 (97%)	26 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	246	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%)	213 (97%)	7 (3%)	34	62
2	M	237/237 (100%)	236 (100%)	1 (0%)	84	93
3	H	194/196 (99%)	192 (99%)	2 (1%)	68	86
All	All	651/653 (100%)	641 (98%)	10 (2%)	57	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU

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Mol	Chain	Res	Type
1	L	82	LYS
1	L	158	SER
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	247	CYS
2	M	62	SER
3	H	221	SER
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN
2	M	300	ASN
3	H	129	ASN
3	H	206	ASN

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 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 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	U10	M	409	-	48,48,63	2.67	13 (27%)	58,61,79	1.74	15 (25%)
12	LDA	M	404	-	12,15,15	2.00	1 (8%)	14,17,17	0.55	0
7	BCL	M	403	1	69,74,74	1.23	8 (11%)	83,115,115	1.51	12 (14%)
4	EDO	L	302	-	3,3,3	0.63	0	2,2,2	0.09	0
6	HTO	M	402	-	9,9,9	0.49	0	10,10,10	0.95	0
12	LDA	M	418	-	12,15,15	2.04	1 (8%)	14,17,17	0.51	0
12	LDA	M	417	-	12,15,15	1.96	1 (8%)	14,17,17	0.54	0
18	TRS	H	303	-	7,7,7	0.30	0	9,9,9	0.33	0
4	EDO	M	401	-	3,3,3	0.65	0	2,2,2	0.27	0
8	BPB	L	306	-	57,70,70	1.62	6 (10%)	56,101,101	2.20	11 (19%)
7	BCL	M	406	-	69,74,74	1.26	6 (8%)	83,115,115	1.56	9 (10%)
12	LDA	H	304	-	12,15,15	1.96	1 (8%)	14,17,17	0.70	0
4	EDO	H	302	-	3,3,3	0.51	0	2,2,2	0.36	0
17	CDL	M	414	-	80,80,99	1.14	4 (5%)	86,92,111	1.13	5 (5%)
7	BCL	L	313	19,2	69,74,74	1.21	6 (8%)	83,115,115	1.88	15 (18%)
10	PO4	L	308	-	4,4,4	0.77	0	6,6,6	0.42	0
12	LDA	L	312	-	12,15,15	1.99	1 (8%)	14,17,17	0.81	0
14	SPN	M	410	-	40,42,42	0.74	1 (2%)	50,52,52	1.90	16 (32%)
11	GOL	L	310	-	5,5,5	0.76	0	5,5,5	1.03	0
10	PO4	L	309	-	4,4,4	0.81	0	6,6,6	0.48	0
7	BCL	L	305	1	69,74,74	1.34	8 (11%)	83,115,115	1.41	9 (10%)
12	LDA	L	311	-	12,15,15	2.05	1 (8%)	14,17,17	0.59	0
6	HTO	L	304	-	9,9,9	0.26	0	10,10,10	1.10	1 (10%)
12	LDA	M	415	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
4	EDO	L	301	-	3,3,3	0.59	0	2,2,2	0.29	0
10	PO4	M	413	-	4,4,4	0.76	0	6,6,6	0.43	0
4	EDO	M	419	-	3,3,3	0.40	0	2,2,2	0.74	0
5	DIO	L	303	-	6,6,6	0.57	0	6,6,6	1.21	1 (16%)
9	U10	L	307	-	48,48,63	2.60	13 (27%)	58,61,79	1.90	17 (29%)
8	BPB	M	407	-	57,70,70	1.50	8 (14%)	56,101,101	2.46	14 (25%)
12	LDA	M	416	-	12,15,15	1.98	1 (8%)	14,17,17	0.41	0
4	EDO	M	405	-	3,3,3	0.50	0	2,2,2	0.43	0
4	EDO	H	301	-	3,3,3	0.40	0	2,2,2	0.47	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
9	U10	M	409	-	-	15/45/69/87	0/1/1/1
12	LDA	M	404	-	-	4/13/13/13	-
7	BCL	M	403	1	-	1/41/137/137	-
4	EDO	L	302	-	-	1/1/1/1	-
6	HTO	M	402	-	-	5/10/10/10	-
12	LDA	M	418	-	-	5/13/13/13	-
12	LDA	M	417	-	-	9/13/13/13	-
18	TRS	H	303	-	-	5/9/9/9	-
4	EDO	M	401	-	-	0/1/1/1	-
8	BPB	L	306	-	-	8/37/105/105	0/5/6/6
7	BCL	M	406	-	-	1/41/137/137	-
12	LDA	H	304	-	-	8/13/13/13	-
4	EDO	H	302	-	-	0/1/1/1	-
17	CDL	M	414	-	-	39/91/91/110	-
7	BCL	L	313	19,2	-	10/41/137/137	-
12	LDA	L	312	-	-	6/13/13/13	-
14	SPN	M	410	-	-	16/50/51/51	-
11	GOL	L	310	-	-	0/4/4/4	-
7	BCL	L	305	1	-	2/41/137/137	-
12	LDA	L	311	-	-	8/13/13/13	-
6	HTO	L	304	-	-	2/10/10/10	-
12	LDA	M	415	-	-	10/13/13/13	-
4	EDO	L	301	-	-	1/1/1/1	-
4	EDO	M	419	-	-	0/1/1/1	-
9	U10	L	307	-	-	16/45/69/87	0/1/1/1
5	DIO	L	303	-	-	-	0/1/1/1
8	BPB	M	407	-	-	7/37/105/105	0/5/6/6
12	LDA	M	416	-	-	3/13/13/13	-
4	EDO	M	405	-	-	1/1/1/1	-
4	EDO	H	301	-	-	1/1/1/1	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	306	BPB	CAC-C3C	9.16	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	407	BPB	CAC-C3C	8.13	1.54	1.33
12	L	311	LDA	O1-N1	-6.99	1.25	1.42
12	M	418	LDA	O1-N1	-6.97	1.25	1.42
12	M	404	LDA	O1-N1	-6.83	1.26	1.42
12	M	415	LDA	O1-N1	-6.82	1.26	1.42
12	L	312	LDA	O1-N1	-6.81	1.26	1.42
12	M	417	LDA	O1-N1	-6.75	1.26	1.42
12	M	416	LDA	O1-N1	-6.73	1.26	1.42
12	H	304	LDA	O1-N1	-6.72	1.26	1.42
9	M	409	U10	C13-C14	6.68	1.49	1.33
9	M	409	U10	C33-C34	6.36	1.48	1.33
9	L	307	U10	C33-C34	6.29	1.48	1.33
9	M	409	U10	C8-C9	6.19	1.47	1.33
9	M	409	U10	C28-C29	6.17	1.47	1.33
9	M	409	U10	C18-C19	6.09	1.47	1.33
9	L	307	U10	C28-C29	5.97	1.47	1.33
9	L	307	U10	C18-C19	5.86	1.47	1.33
9	L	307	U10	C13-C14	5.75	1.46	1.33
9	L	307	U10	C8-C9	5.75	1.46	1.33
9	M	409	U10	C23-C24	5.71	1.46	1.33
9	L	307	U10	C23-C24	5.70	1.46	1.33
9	M	409	U10	C38-C39	5.42	1.47	1.32
7	M	406	BCL	MG-NA	5.40	2.19	2.06
9	L	307	U10	C38-C39	5.18	1.47	1.32
9	L	307	U10	O4-C4	-5.12	1.24	1.36
7	L	305	BCL	MG-NA	4.90	2.17	2.06
17	M	414	CDL	OB8-CB7	4.80	1.47	1.33
17	M	414	CDL	OA6-CA5	4.72	1.47	1.34
9	M	409	U10	O4-C4	-4.68	1.25	1.36
9	M	409	U10	O3-C3	-4.56	1.25	1.36
17	M	414	CDL	OB6-CB5	4.46	1.46	1.34
17	M	414	CDL	OA8-CA7	4.40	1.46	1.33
7	L	313	BCL	MG-NA	4.34	2.16	2.06
9	L	307	U10	O3-C3	-4.34	1.26	1.36
7	M	403	BCL	MG-NA	4.16	2.16	2.06
7	L	305	BCL	C3B-C4B	3.51	1.47	1.41
7	L	305	BCL	C5-C3	3.41	1.58	1.51
7	M	403	BCL	C3B-C4B	3.31	1.47	1.41
8	L	306	BPB	CBD-CGD	-3.29	1.48	1.52
9	L	307	U10	C6-C1	3.23	1.41	1.35
9	M	409	U10	C6-C1	3.14	1.40	1.35
7	L	305	BCL	MG-NC	3.12	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	307	U10	C3-C2	-3.07	1.40	1.48
7	M	406	BCL	MG-NC	3.07	2.13	2.06
9	L	307	U10	C4-C5	-3.05	1.40	1.48
7	L	313	BCL	C3B-C4B	2.95	1.46	1.41
7	M	406	BCL	C1D-ND	2.95	1.41	1.37
8	L	306	BPB	C3D-CAD	-2.84	1.41	1.47
8	M	407	BPB	CBD-CGD	-2.81	1.48	1.52
7	M	403	BCL	CHD-C1D	2.77	1.43	1.38
8	L	306	BPB	C1D-C2D	2.71	1.42	1.39
7	L	313	BCL	CHD-C1D	2.70	1.43	1.38
9	M	409	U10	C4-C5	-2.63	1.41	1.48
7	M	403	BCL	C1D-ND	2.59	1.41	1.37
7	M	403	BCL	O1A-CGA	-2.58	1.14	1.22
7	M	406	BCL	OBD-CAD	2.53	1.26	1.22
7	L	305	BCL	C1B-NB	2.46	1.40	1.37
8	M	407	BPB	C3D-CAD	-2.43	1.42	1.47
8	M	407	BPB	C3B-C4B	2.43	1.45	1.41
7	L	305	BCL	CHD-C1D	2.41	1.43	1.38
7	M	403	BCL	MG-NC	2.41	2.12	2.06
7	M	406	BCL	CHD-C1D	2.41	1.43	1.38
7	L	313	BCL	MG-NC	2.37	2.11	2.06
7	L	313	BCL	C1D-ND	2.32	1.40	1.37
7	M	403	BCL	OBD-CAD	2.31	1.26	1.22
8	M	407	BPB	OBD-CAD	2.30	1.25	1.22
7	M	406	BCL	O1A-CGA	-2.29	1.15	1.22
9	L	307	U10	C6-C5	-2.27	1.40	1.46
9	M	409	U10	C3-C2	-2.24	1.42	1.48
8	M	407	BPB	CHA-CBD	2.24	1.54	1.51
14	M	410	SPN	CM9-C30	2.24	1.56	1.50
8	M	407	BPB	C1D-C2D	2.23	1.42	1.39
7	L	305	BCL	C1D-C2D	-2.21	1.41	1.45
8	L	306	BPB	OBD-CAD	2.20	1.25	1.22
7	L	305	BCL	CMB-C2B	2.18	1.55	1.50
7	L	313	BCL	C1B-NB	2.18	1.40	1.37
8	M	407	BPB	C1B-C2B	2.11	1.41	1.39
7	M	403	BCL	OBB-CAB	2.07	1.27	1.23
8	L	306	BPB	C3B-C4B	2.05	1.45	1.41
9	M	409	U10	C6-C5	-2.03	1.41	1.46

All (125) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	407	BPB	C4D-CHA-CBD	-11.40	103.36	108.52
8	L	306	BPB	C4D-CHA-CBD	-11.30	103.41	108.52
7	L	313	BCL	C1-O2A-CGA	8.26	138.12	116.44
8	M	407	BPB	CBC-CAC-C3C	-6.25	110.11	126.70
7	L	313	BCL	CHD-C1D-ND	-5.79	119.14	124.45
7	M	406	BCL	C4D-CHA-C1A	5.49	127.93	121.25
7	L	305	BCL	CHD-C1D-ND	-5.34	119.55	124.45
7	L	313	BCL	C4D-CHA-C1A	5.25	127.64	121.25
7	M	403	BCL	CHD-C1D-ND	-5.15	119.72	124.45
7	M	406	BCL	CHD-C1D-ND	-4.94	119.92	124.45
7	M	403	BCL	C4D-CHA-C1A	4.86	127.17	121.25
9	L	307	U10	C17-C18-C19	-4.84	116.02	127.66
7	M	406	BCL	C1-C2-C3	-4.83	117.69	126.04
8	L	306	BPB	C4D-ND-C1D	-4.75	103.99	108.83
7	L	305	BCL	C4D-CHA-C1A	4.74	127.02	121.25
8	M	407	BPB	C4D-ND-C1D	-4.66	104.09	108.83
17	M	414	CDL	OB6-CB5-C51	4.66	121.53	111.50
8	M	407	BPB	C11-C10-C8	4.52	130.53	115.92
14	M	410	SPN	CM3-C5-C6	4.25	122.42	115.27
8	L	306	BPB	CBC-CAC-C3C	-4.20	115.56	126.70
9	M	409	U10	C32-C33-C34	-4.14	117.69	127.66
14	M	410	SPN	C7-C8-C9	-4.14	117.70	127.66
7	M	403	BCL	C1D-ND-C4D	-4.07	103.44	106.33
9	L	307	U10	C22-C23-C24	-4.07	117.86	127.66
7	L	313	BCL	CAA-CBA-CGA	4.05	125.10	113.25
9	L	307	U10	C10-C9-C11	3.98	121.97	115.27
14	M	410	SPN	CM4-C9-C10	3.88	121.79	115.27
8	M	407	BPB	O2D-CGD-CBD	3.84	115.86	111.00
7	L	313	BCL	O2A-C1-C2	-3.84	98.55	108.64
9	L	307	U10	C12-C13-C14	-3.81	118.48	127.66
17	M	414	CDL	OA6-CA5-C11	3.77	119.62	111.50
7	M	406	BCL	C4A-NA-C1A	3.76	108.40	106.71
7	L	313	BCL	C1D-ND-C4D	-3.62	103.76	106.33
14	M	410	SPN	CM5-C13-C14	3.61	121.34	115.27
8	M	407	BPB	C1-O2A-CGA	3.59	125.87	116.44
9	M	409	U10	C10-C9-C11	3.58	121.30	115.27
9	L	307	U10	C30-C29-C31	3.56	121.25	115.27
9	M	409	U10	C17-C18-C19	-3.49	119.26	127.66
8	L	306	BPB	O2D-CGD-CBD	3.44	115.35	111.00
8	L	306	BPB	C11-C10-C8	-3.41	104.89	115.92
8	M	407	BPB	C3D-C4D-ND	3.39	112.35	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	409	U10	C22-C23-C24	-3.31	119.69	127.66
9	L	307	U10	C25-C24-C26	3.30	120.81	115.27
7	M	406	BCL	CHA-C1A-NA	-3.27	118.91	126.40
9	M	409	U10	C30-C29-C31	3.25	120.73	115.27
8	L	306	BPB	C3D-C4D-ND	3.23	112.12	107.72
7	L	305	BCL	C1D-ND-C4D	-3.21	104.05	106.33
7	M	406	BCL	C1D-ND-C4D	-3.18	104.08	106.33
8	M	407	BPB	OBD-CAD-CBD	-3.17	121.18	125.82
9	M	409	U10	C35-C34-C36	3.16	120.59	115.27
8	M	407	BPB	C17-C16-C15	3.15	127.73	113.24
8	M	407	BPB	C2D-C1D-ND	3.15	111.70	109.53
7	L	313	BCL	C16-C15-C13	3.15	126.09	115.92
9	L	307	U10	C27-C28-C29	-3.12	120.14	127.66
8	L	306	BPB	OBD-CAD-CBD	-3.05	121.34	125.82
14	M	410	SPN	C11-C12-C13	-3.04	120.33	127.66
14	M	410	SPN	C20-C19-C18	-3.04	120.34	127.66
7	L	305	BCL	C2A-C1A-CHA	3.01	129.12	123.86
7	M	403	BCL	CHA-C1A-NA	-2.99	119.56	126.40
8	M	407	BPB	CMD-C2D-C3D	2.96	130.21	124.68
9	L	307	U10	C32-C33-C34	-2.94	120.58	127.66
7	M	406	BCL	CAB-C3B-C2B	2.94	132.75	128.34
6	L	304	HTO	C5-C4-C3	-2.92	109.38	114.18
7	L	305	BCL	CHA-C1A-NA	-2.89	119.77	126.40
7	L	313	BCL	CHA-C1A-NA	-2.87	119.81	126.40
9	M	409	U10	C37-C38-C39	-2.85	118.02	127.75
14	M	410	SPN	CM6-C18-C17	2.83	120.03	115.27
9	M	409	U10	C25-C24-C26	2.79	119.97	115.27
14	M	410	SPN	CMB-C30-CM9	2.77	120.73	114.60
7	M	403	BCL	C2A-C1A-CHA	2.76	128.69	123.86
5	L	303	DIO	C2'-O1'-C1'	2.75	119.08	109.89
7	M	406	BCL	C2A-C1A-CHA	2.73	128.63	123.86
9	M	409	U10	C41-C39-C40	2.71	120.60	114.60
7	M	406	BCL	CAA-CBA-CGA	-2.69	105.40	113.25
9	L	307	U10	C20-C19-C21	2.65	119.73	115.27
17	M	414	CDL	CB4-OB6-CB5	-2.64	111.29	117.79
14	M	410	SPN	C10-C11-C12	-2.62	103.28	111.88
14	M	410	SPN	C3-C4-C5	-2.62	122.44	126.79
14	M	410	SPN	C21-C20-C19	-2.61	105.33	112.23
8	L	306	BPB	C1-C2-C3	-2.58	121.59	126.04
7	L	305	BCL	CAB-C3B-C2B	2.57	132.20	128.34
9	L	307	U10	C15-C14-C16	2.57	119.60	115.27
7	L	313	BCL	OBB-CAB-CBB	-2.57	114.04	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	307	U10	C3M-O3-C3	2.57	125.56	116.47
7	L	313	BCL	C6-C7-C8	2.55	124.16	115.92
8	L	306	BPB	C2D-C1D-ND	2.55	111.28	109.53
7	L	305	BCL	C1C-NC-C4C	2.54	107.85	106.71
7	M	403	BCL	CHC-C4B-NB	-2.53	121.57	124.26
14	M	410	SPN	C20-C21-C22	-2.52	107.02	115.76
7	M	403	BCL	O2A-C1-C2	-2.50	102.07	108.64
7	L	313	BCL	CHC-C4B-NB	-2.45	121.66	124.26
9	L	307	U10	C41-C39-C40	2.43	119.97	114.60
14	M	410	SPN	CM8-C26-C27	2.40	119.30	115.27
7	L	305	BCL	CHC-C4B-NB	-2.39	121.72	124.26
17	M	414	CDL	OB8-CB7-C71	2.38	119.38	111.91
9	M	409	U10	C15-C14-C16	2.36	119.24	115.27
9	M	409	U10	C26-C27-C28	-2.35	104.14	111.88
7	M	403	BCL	CAA-CBA-CGA	2.33	120.06	113.25
8	M	407	BPB	CMB-C2B-C3B	2.32	129.01	124.68
9	L	307	U10	C37-C38-C39	-2.30	119.88	127.75
9	M	409	U10	C4M-O4-C4	2.30	124.62	116.47
7	L	313	BCL	C2A-C1A-CHA	2.30	127.88	123.86
9	L	307	U10	C1M-C1-C6	-2.29	120.66	124.40
7	M	403	BCL	O2D-CGD-CBD	2.28	115.32	111.27
7	L	313	BCL	CAB-C3B-C2B	2.26	131.73	128.34
17	M	414	CDL	OA8-CA7-C31	2.26	119.00	111.91
14	M	410	SPN	C23-C24-C25	-2.25	106.29	112.23
7	L	313	BCL	C4B-C3B-C2B	-2.24	104.76	108.36
14	M	410	SPN	C28-C27-C26	-2.24	105.62	112.98
8	L	306	BPB	CMB-C2B-C3B	2.23	128.85	124.68
7	M	403	BCL	C4B-C3B-C2B	-2.21	104.80	108.36
8	M	407	BPB	O2A-C1-C2	-2.20	102.86	108.64
7	M	403	BCL	C4A-NA-C1A	2.19	107.69	106.71
9	M	409	U10	C20-C19-C21	2.18	118.93	115.27
9	L	307	U10	C20-C19-C18	-2.17	118.11	123.68
8	L	306	BPB	CMD-C2D-C3D	2.17	128.73	124.68
9	M	409	U10	C27-C28-C29	-2.16	122.45	127.66
9	L	307	U10	C12-C11-C9	-2.16	105.87	112.98
9	M	409	U10	C7-C8-C9	-2.14	123.23	126.79
9	L	307	U10	C35-C34-C36	2.07	118.75	115.27
14	M	410	SPN	C28-C29-C30	-2.07	120.69	127.75
7	L	305	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
7	M	403	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
7	L	313	BCL	CHD-C1D-C2D	2.01	129.69	125.48
8	M	407	BPB	C1A-C2A-C3A	-2.00	100.93	102.84

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	304	HTO	C2-C3-C4-C5
6	M	402	HTO	C1-C2-C3-O3
6	M	402	HTO	C1-C2-C3-C4
6	M	402	HTO	O2-C2-C3-O3
6	M	402	HTO	O2-C2-C3-C4
8	L	306	BPB	C2C-C3C-CAC-CBC
8	L	306	BPB	C4C-C3C-CAC-CBC
8	M	407	BPB	C2C-C3C-CAC-CBC
9	L	307	U10	C27-C28-C29-C30
9	M	409	U10	C27-C28-C29-C30
9	M	409	U10	C27-C28-C29-C31
9	M	409	U10	C32-C33-C34-C36
12	L	312	LDA	C2-C1-N1-O1
12	L	312	LDA	C2-C1-N1-CM1
12	M	404	LDA	N1-C1-C2-C3
12	M	415	LDA	C2-C1-N1-O1
12	M	415	LDA	C2-C1-N1-CM1
12	M	417	LDA	C2-C1-N1-CM1
12	M	417	LDA	C2-C1-N1-CM2
12	M	418	LDA	C2-C1-N1-CM1
12	H	304	LDA	C2-C1-N1-O1
12	H	304	LDA	C2-C1-N1-CM1
14	M	410	SPN	CM1-C1-O1-CMA
14	M	410	SPN	CM2-C1-O1-CMA
14	M	410	SPN	C2-C1-O1-CMA
14	M	410	SPN	O1-C1-C2-O2
14	M	410	SPN	C4-C5-C6-C7
14	M	410	SPN	CM3-C5-C6-C7
14	M	410	SPN	C11-C10-C9-CM4
17	M	414	CDL	CA2-OA2-PA1-OA5
17	M	414	CDL	CA4-CA3-OA5-PA1
17	M	414	CDL	CB2-OB2-PB2-OB4
17	M	414	CDL	CB2-OB2-PB2-OB5
17	M	414	CDL	CB3-OB5-PB2-OB2
17	M	414	CDL	CB3-OB5-PB2-OB3
17	M	414	CDL	CB3-OB5-PB2-OB4
18	H	303	TRS	N-C-C2-O2
18	H	303	TRS	C1-C-C3-O3
18	H	303	TRS	C2-C-C3-O3
18	H	303	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
14	M	410	SPN	CM5-C13-C14-C15
7	L	313	BCL	C2A-CAA-CBA-CGA
9	M	409	U10	C32-C33-C34-C35
9	L	307	U10	C27-C28-C29-C31
14	M	410	SPN	C16-C17-C18-CM6
14	M	410	SPN	C11-C10-C9-C8
14	M	410	SPN	C16-C17-C18-C19
9	L	307	U10	C14-C16-C17-C18
9	L	307	U10	C29-C31-C32-C33
17	M	414	CDL	C31-CA7-OA8-CA6
17	M	414	CDL	OA9-CA7-OA8-CA6
14	M	410	SPN	C12-C13-C14-C15
8	M	407	BPB	C5-C6-C7-C8
9	M	409	U10	C37-C38-C39-C40
4	L	302	EDO	O1-C1-C2-O2
9	L	307	U10	C24-C26-C27-C28
9	M	409	U10	C24-C26-C27-C28
17	M	414	CDL	O1-C1-CB2-OB2
14	M	410	SPN	C14-C15-C16-C17
17	M	414	CDL	CA2-C1-CB2-OB2
12	L	311	LDA	C11-C10-C9-C8
12	M	415	LDA	C2-C3-C4-C5
12	M	417	LDA	C5-C6-C7-C8
17	M	414	CDL	C18-C19-C20-C21
12	H	304	LDA	C6-C7-C8-C9
17	M	414	CDL	C11-C12-C13-C14
17	M	414	CDL	C53-C54-C55-C56
17	M	414	CDL	C52-C53-C54-C55
17	M	414	CDL	C72-C73-C74-C75
9	L	307	U10	C34-C36-C37-C38
12	M	416	LDA	C4-C5-C6-C7
12	L	312	LDA	C4-C5-C6-C7
6	L	304	HTO	O3-C3-C4-C5
8	L	306	BPB	C2-C3-C5-C6
9	L	307	U10	C28-C29-C31-C32
12	M	418	LDA	C5-C6-C7-C8
12	M	418	LDA	C1-C2-C3-C4
17	M	414	CDL	C17-C18-C19-C20
8	M	407	BPB	C15-C16-C17-C18
12	M	418	LDA	C4-C5-C6-C7
12	H	304	LDA	C1-C2-C3-C4
4	H	301	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
12	M	417	LDA	C11-C10-C9-C8
9	M	409	U10	C37-C38-C39-C41
12	M	404	LDA	C1-C2-C3-C4
8	L	306	BPB	C4-C3-C5-C6
12	M	418	LDA	C9-C10-C11-C12
17	M	414	CDL	CB7-C71-C72-C73
12	M	404	LDA	C7-C8-C9-C10
12	M	415	LDA	C7-C8-C9-C10
12	M	416	LDA	C1-C2-C3-C4
17	M	414	CDL	C38-C39-C40-C41
7	L	313	BCL	C15-C16-C17-C18
17	M	414	CDL	C71-CB7-OB8-CB6
17	M	414	CDL	OA5-CA3-CA4-CA6
12	L	312	LDA	C3-C4-C5-C6
9	L	307	U10	C30-C29-C31-C32
17	M	414	CDL	C74-C75-C76-C77
12	L	312	LDA	C5-C6-C7-C8
17	M	414	CDL	OB9-CB7-OB8-CB6
17	M	414	CDL	C75-C76-C77-C78
12	M	417	LDA	C1-C2-C3-C4
9	M	409	U10	C14-C16-C17-C18
17	M	414	CDL	C78-C79-C80-C81
12	M	404	LDA	C9-C10-C11-C12
12	H	304	LDA	C7-C8-C9-C10
8	L	306	BPB	O2A-C1-C2-C3
12	M	415	LDA	C5-C6-C7-C8
12	M	415	LDA	C1-C2-C3-C4
9	L	307	U10	C12-C11-C9-C10
9	L	307	U10	C12-C11-C9-C8
12	M	417	LDA	C2-C3-C4-C5
17	M	414	CDL	OB5-CB3-CB4-CB6
8	M	407	BPB	C6-C7-C8-C10
12	H	304	LDA	C3-C4-C5-C6
9	M	409	U10	C29-C31-C32-C33
12	L	311	LDA	C2-C1-N1-CM1
12	L	311	LDA	C2-C1-N1-CM2
12	L	312	LDA	C2-C1-N1-CM2
12	M	415	LDA	C2-C1-N1-CM2
12	H	304	LDA	C2-C1-N1-CM2
12	M	415	LDA	C3-C4-C5-C6
9	M	409	U10	C25-C24-C26-C27
7	L	313	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	H	303	TRS	C1-C-C2-O2
17	M	414	CDL	CA2-OA2-PA1-OA3
12	L	311	LDA	C2-C1-N1-O1
12	M	417	LDA	C2-C1-N1-O1
17	M	414	CDL	C79-C80-C81-C82
7	L	313	BCL	C6-C7-C8-C10
7	L	313	BCL	C12-C13-C15-C16
17	M	414	CDL	OA5-CA3-CA4-OA6
17	M	414	CDL	OB5-CB3-CB4-OB6
17	M	414	CDL	C81-C82-C83-C84
12	M	417	LDA	C6-C7-C8-C9
7	L	313	BCL	C13-C15-C16-C17
12	H	304	LDA	C4-C5-C6-C7
9	M	409	U10	C23-C24-C26-C27
12	M	417	LDA	N1-C1-C2-C3
14	M	410	SPN	CM2-C1-C2-C3
9	M	409	U10	C5-C4-O4-C4M
12	M	416	LDA	C2-C3-C4-C5
12	L	311	LDA	C7-C8-C9-C10
12	M	415	LDA	C4-C5-C6-C7
9	L	307	U10	C20-C19-C21-C22
4	L	301	EDO	O1-C1-C2-O2
9	L	307	U10	C15-C14-C16-C17
12	M	415	LDA	C9-C10-C11-C12
9	M	409	U10	C28-C29-C31-C32
17	M	414	CDL	C32-C31-CA7-OA8
9	M	409	U10	C30-C29-C31-C32
17	M	414	CDL	C80-C81-C82-C83
9	L	307	U10	C18-C19-C21-C22
8	M	407	BPB	C6-C7-C8-C9
7	L	313	BCL	C3A-C2A-CAA-CBA
17	M	414	CDL	C76-C77-C78-C79
7	L	305	BCL	CAD-CBD-CGD-O2D
7	L	313	BCL	CAD-CBD-CGD-O2D
8	L	306	BPB	CAD-CBD-CGD-O2D
8	M	407	BPB	CAD-CBD-CGD-O2D
7	L	313	BCL	C4-C3-C5-C6
17	M	414	CDL	C1-CB2-OB2-PB2
17	M	414	CDL	C13-C14-C15-C16
4	M	405	EDO	O1-C1-C2-O2
7	M	403	BCL	CHA-CBD-CGD-O1D
17	M	414	CDL	OB6-CB4-CB6-OB8

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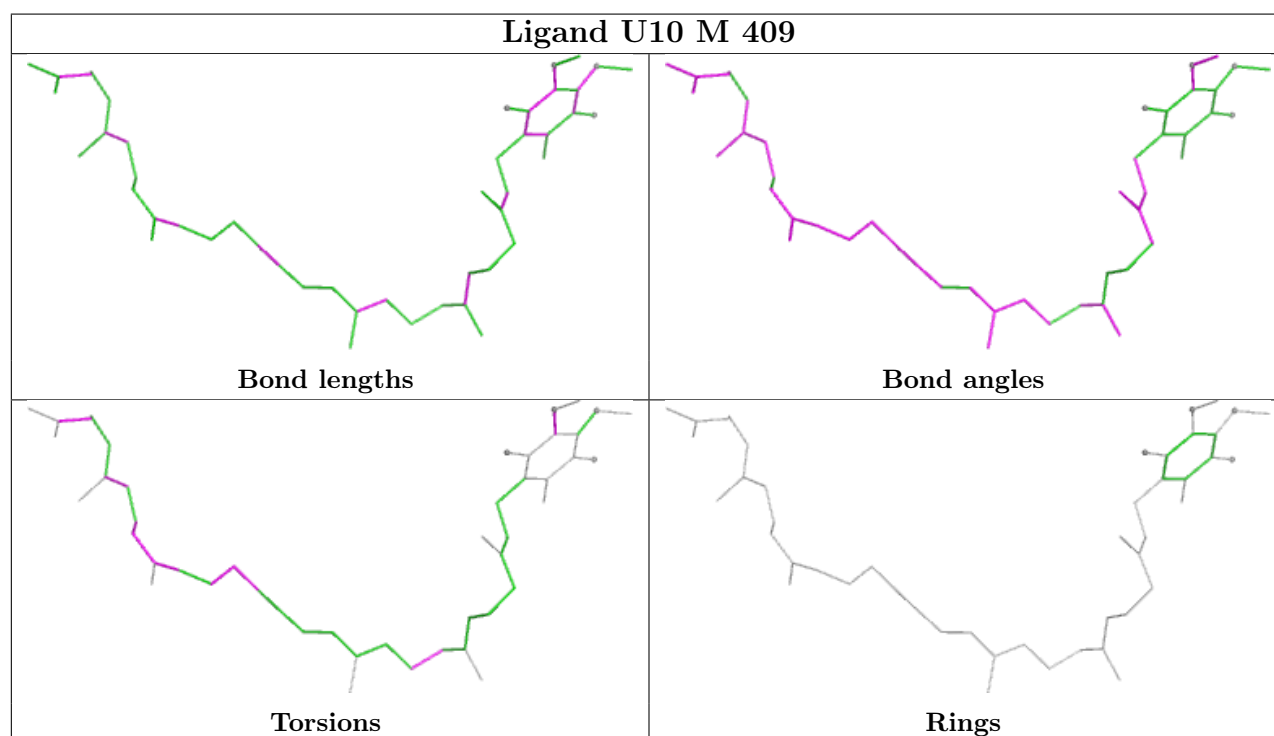
Mol	Chain	Res	Type	Atoms
12	L	311	LDA	C4-C5-C6-C7
9	L	307	U10	C13-C14-C16-C17
8	L	306	BPB	C11-C10-C8-C9
12	L	311	LDA	C5-C6-C7-C8
9	L	307	U10	C3-C4-O4-C4M
9	L	307	U10	C5-C4-O4-C4M
6	M	402	HTO	C4-C5-C6-C7
17	M	414	CDL	C32-C31-CA7-OA9
7	L	313	BCL	C1A-C2A-CAA-CBA
12	L	311	LDA	C1-C2-C3-C4
7	L	305	BCL	C2-C1-O2A-CGA
17	M	414	CDL	CB2-OB2-PB2-OB3
8	M	407	BPB	C16-C17-C18-C19
14	M	410	SPN	CM2-C1-C2-O2
14	M	410	SPN	C18-C19-C20-C21
9	M	409	U10	C3-C4-O4-C4M
8	L	306	BPB	C8-C10-C11-C12
7	M	406	BCL	C5-C6-C7-C8

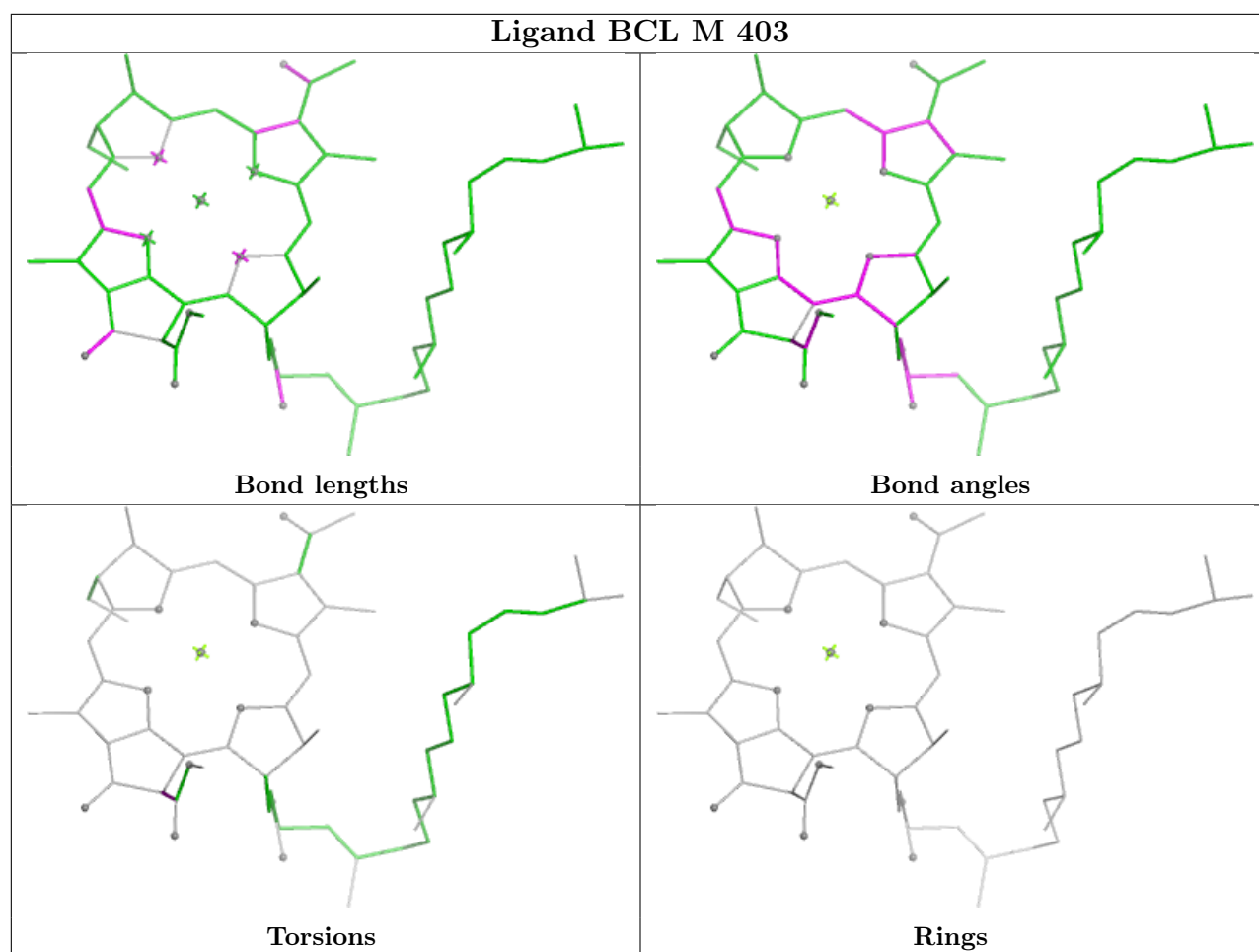
There are no ring outliers.

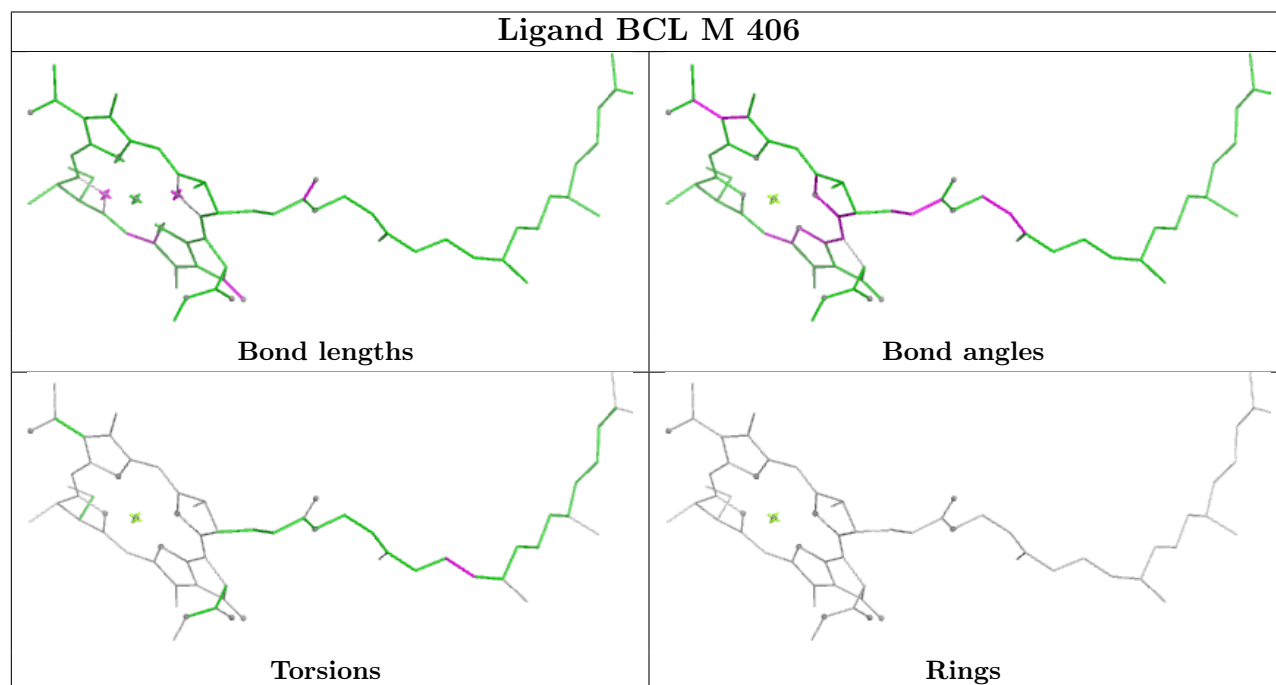
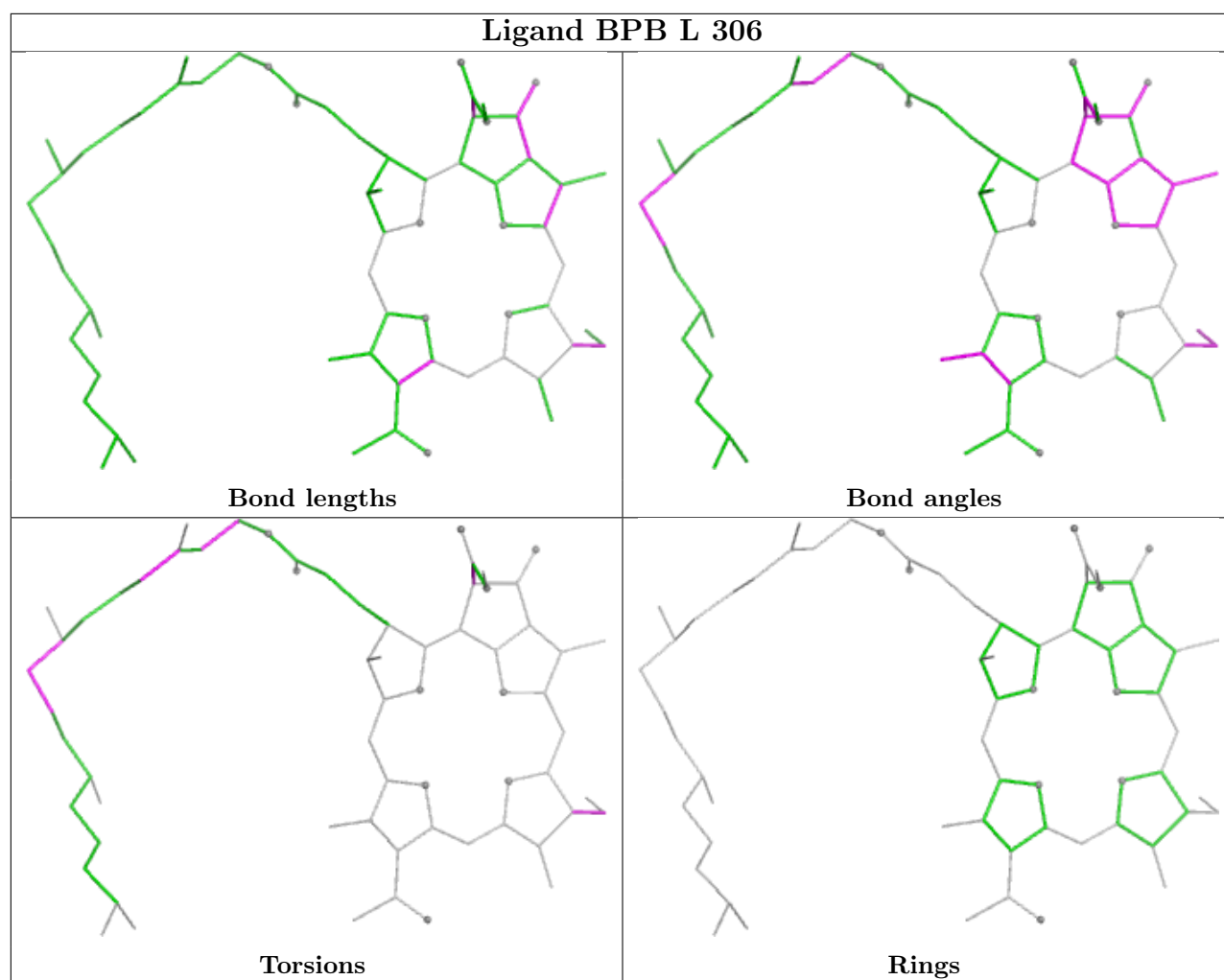
19 monomers are involved in 58 short contacts:

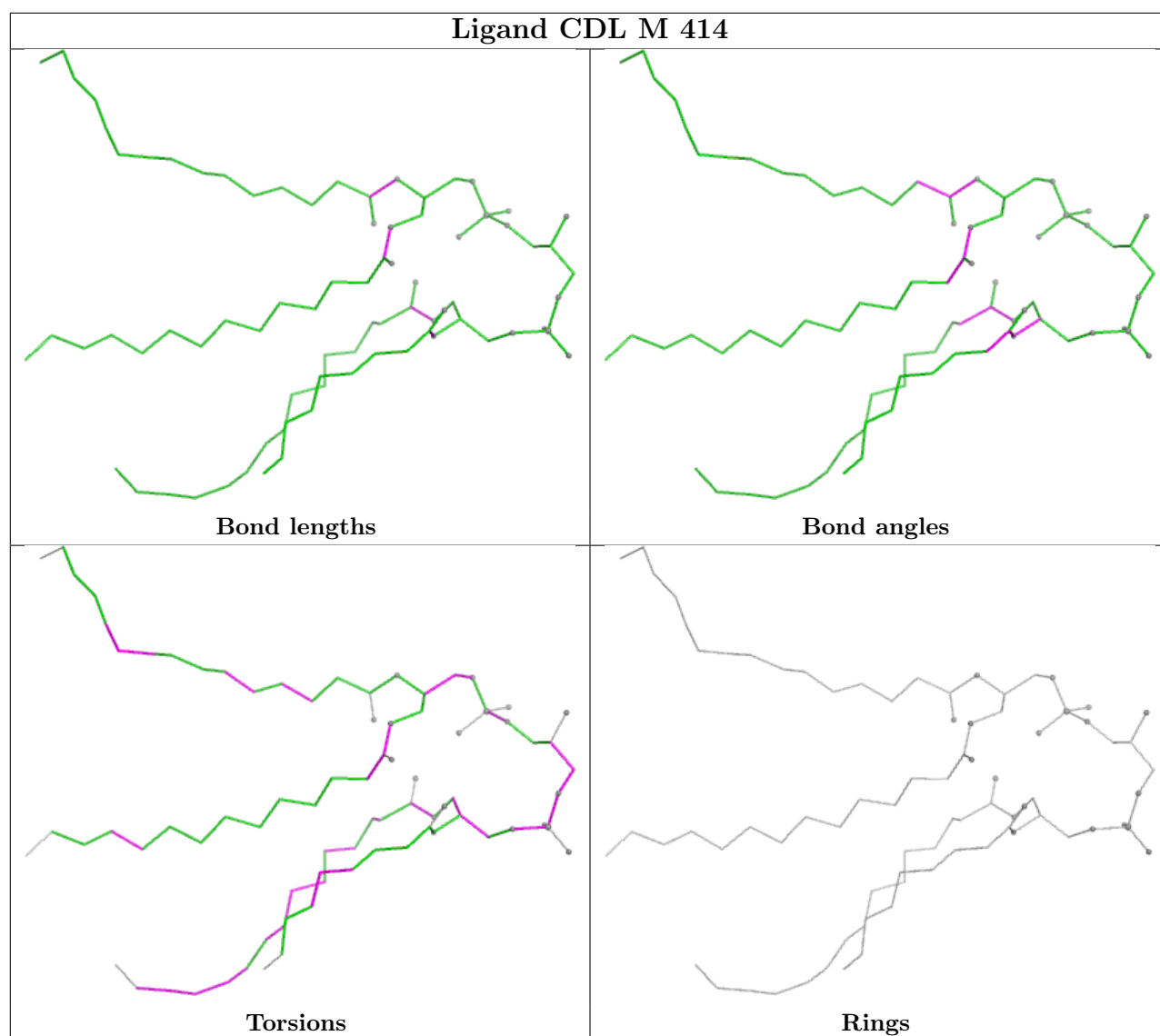
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	409	U10	2	0
12	M	404	LDA	1	0
7	M	403	BCL	1	0
6	M	402	HTO	6	0
12	M	418	LDA	1	0
12	M	417	LDA	5	0
18	H	303	TRS	4	0
7	M	406	BCL	2	0
12	H	304	LDA	3	0
4	H	302	EDO	1	0
17	M	414	CDL	8	0
7	L	313	BCL	5	0
12	L	312	LDA	1	0
14	M	410	SPN	7	0
7	L	305	BCL	5	0
4	L	301	EDO	1	0
5	L	303	DIO	2	0
9	L	307	U10	8	0
8	M	407	BPB	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.

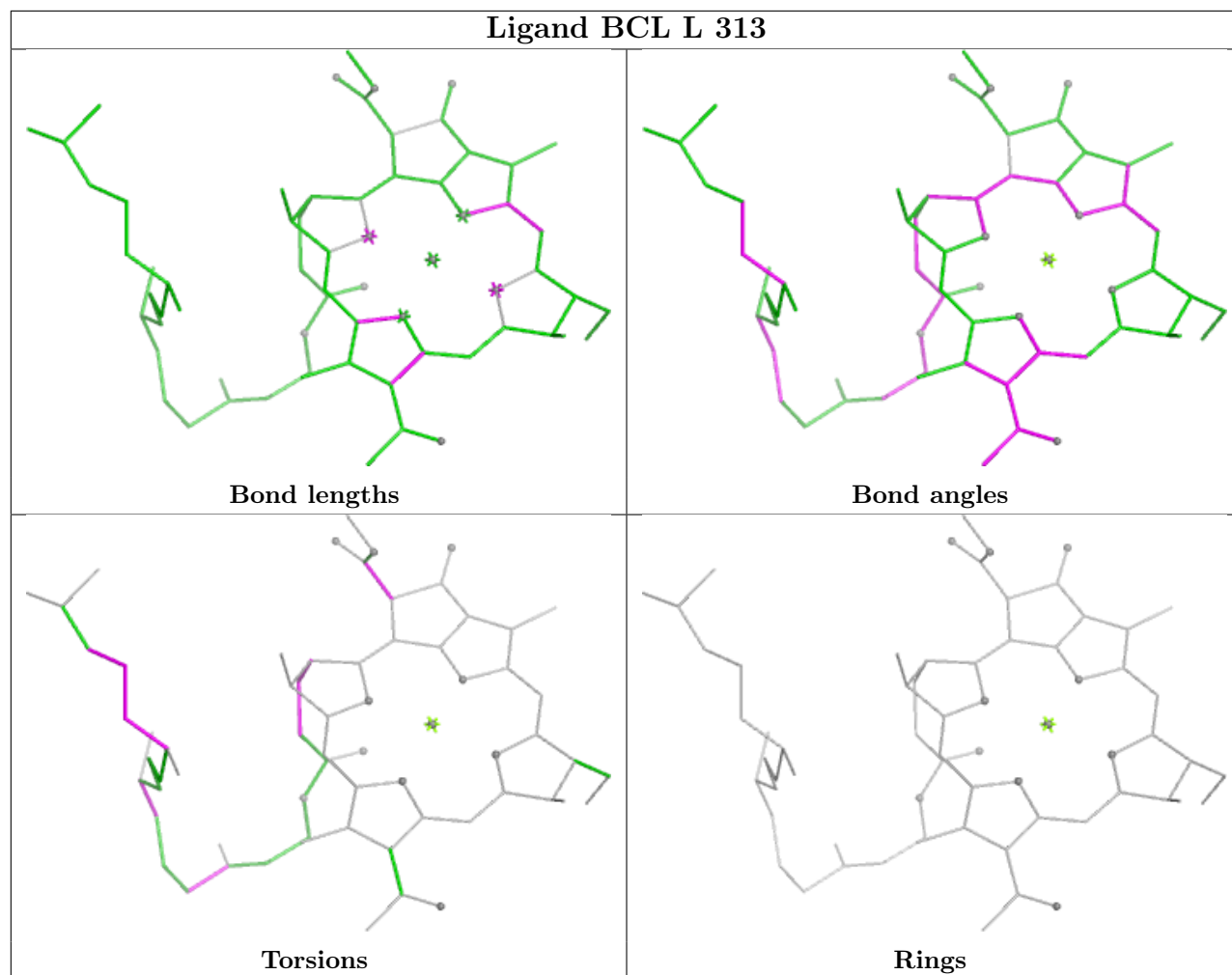


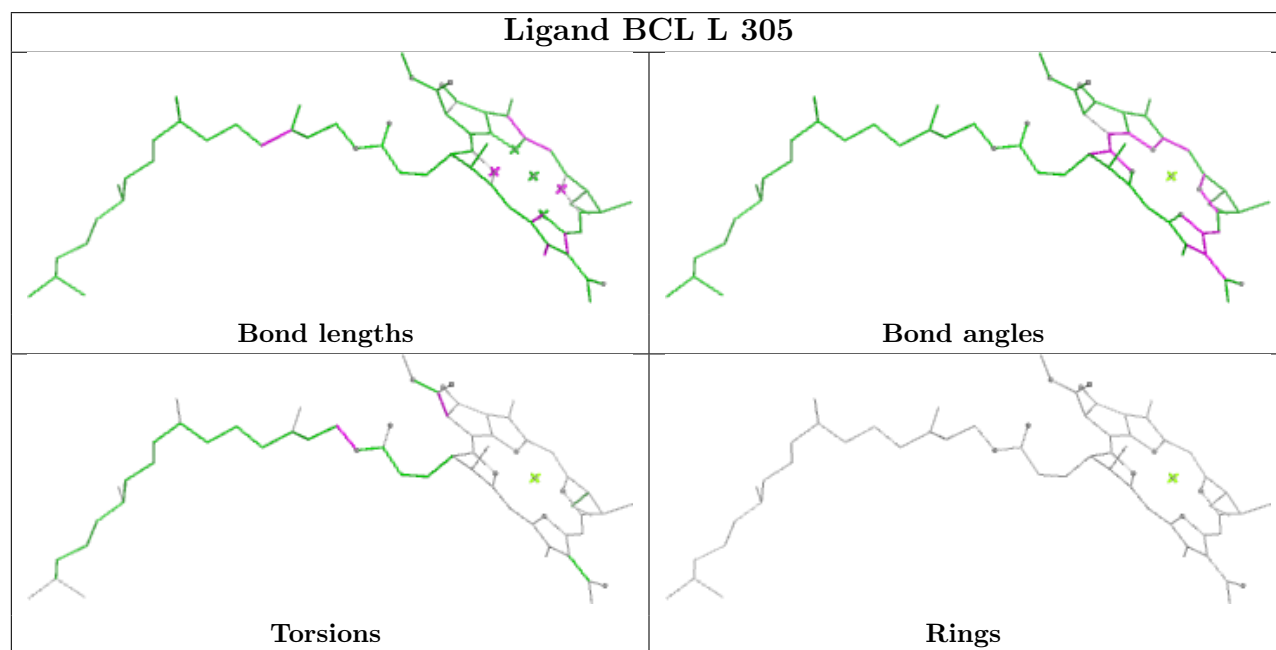
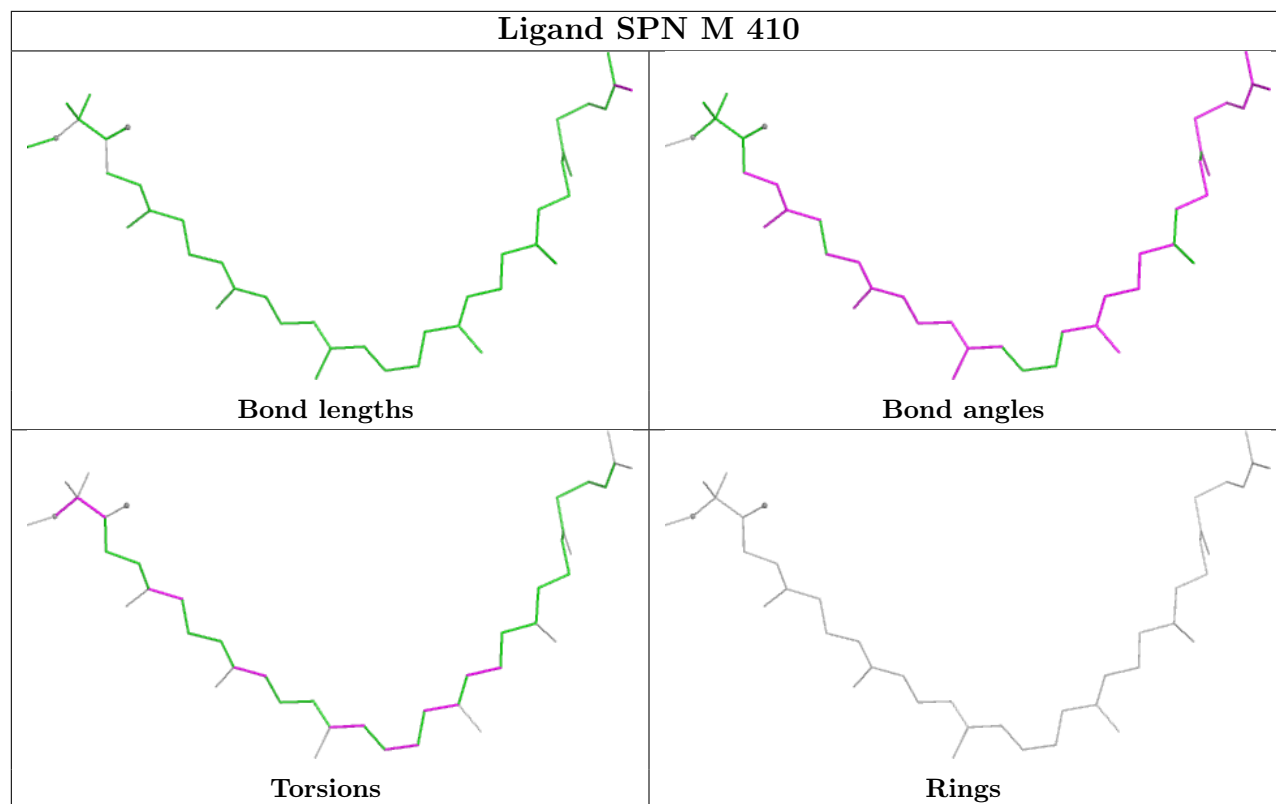


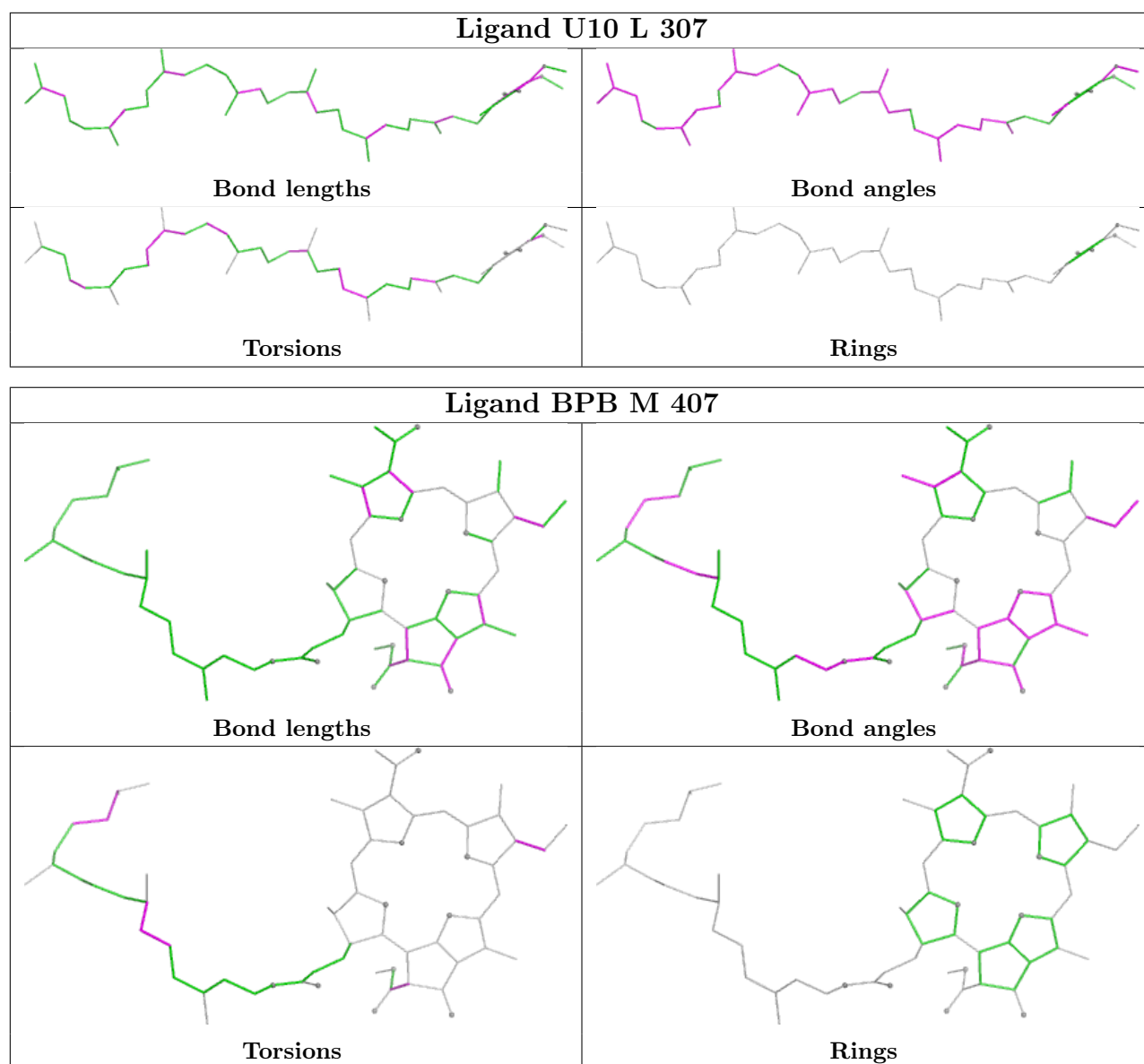




Ligand BCL L 313







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%)	0.10	10 (3%) 46 40	47, 60, 89, 104	0
2	M	302/303 (99%)	-0.12	7 (2%) 61 55	33, 63, 88, 104	1 (0%)
3	H	239/241 (99%)	-0.01	11 (4%) 37 32	50, 60, 75, 129	0
All	All	822/825 (99%)	-0.01	28 (3%) 48 42	33, 61, 88, 129	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	72	GLU	6.3
1	L	73	TYR	4.9
3	H	249	LYS	4.8
3	H	247	LYS	4.1
3	H	246	PRO	4.0
3	H	245	ALA	4.0
2	M	302	GLY	3.1
1	L	59	TRP	3.0
2	M	1	ALA	2.9
2	M	68	PHE	2.9
1	L	62	GLN	2.9
3	H	159	GLU	2.8
3	H	80	SER	2.8
3	H	248	ARG	2.8
3	H	184	LYS	2.7
1	L	71	LEU	2.7
3	H	221	SER	2.7
2	M	188	ASN	2.6
1	L	67	TYR	2.5
3	H	128	HIS	2.3
1	L	74	GLY	2.3
1	L	82	LYS	2.2
2	M	32	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	148	TRP	2.1
3	H	127	GLY	2.1
1	L	75	LEU	2.0
1	L	202	LYS	2.0
2	M	21	THR	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
4	EDO	H	302	4/4	0.56	0.38	68,82,86,96	0
10	PO4	L	308	5/5	0.64	0.14	111,111,117,127	0
18	TRS	H	303	8/8	0.65	0.14	83,88,93,93	0
12	LDA	M	417	16/16	0.75	0.35	82,92,136,138	0
12	LDA	L	311	16/16	0.77	0.31	58,85,101,107	0
12	LDA	M	418	16/16	0.78	0.39	74,96,122,123	0
6	HTO	M	402	10/10	0.80	0.28	78,86,96,97	0
6	HTO	L	304	10/10	0.80	0.22	79,91,99,104	0
4	EDO	L	302	4/4	0.82	0.38	73,79,83,87	0
12	LDA	L	312	16/16	0.83	0.27	67,79,107,107	0
4	EDO	L	301	4/4	0.84	0.23	60,70,71,74	0
5	DIO	L	303	6/6	0.85	0.28	73,76,85,89	0
12	LDA	M	404	16/16	0.85	0.30	69,79,110,111	0
17	CDL	M	414	81/100	0.85	0.23	60,91,123,138	0
12	LDA	M	416	16/16	0.85	0.24	59,74,97,101	0
4	EDO	M	419	4/4	0.87	0.17	53,57,60,62	0
4	EDO	H	301	4/4	0.87	0.19	71,80,84,92	0
9	U10	L	307	48/63	0.87	0.33	47,71,80,84	48

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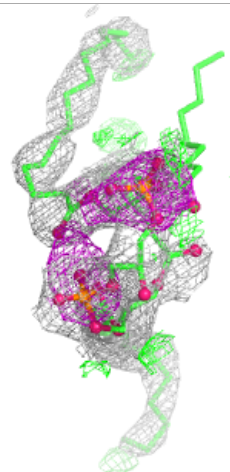
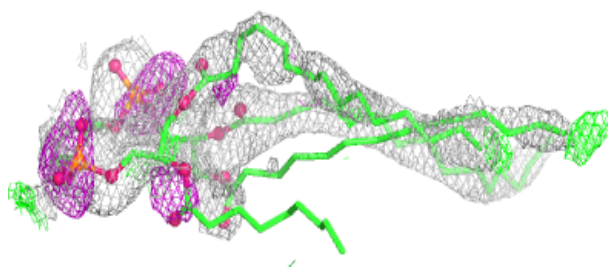
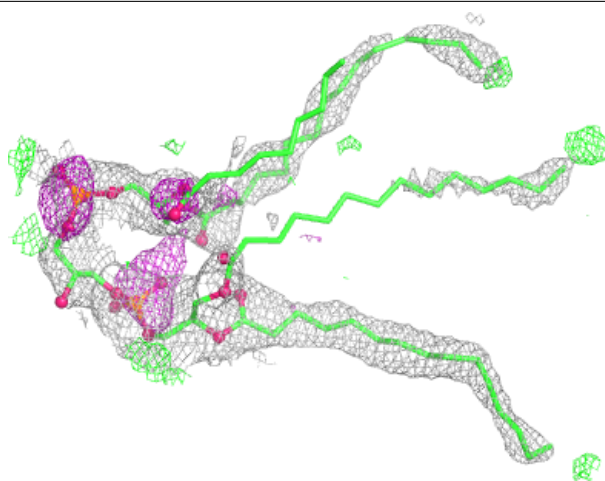
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	M	405	4/4	0.88	0.16	59,68,71,78	0
10	PO4	L	309	5/5	0.88	0.42	82,88,105,111	0
11	GOL	L	310	6/6	0.89	0.16	80,84,89,90	0
14	SPN	M	410	43/43	0.91	0.17	57,74,85,93	0
12	LDA	M	415	16/16	0.92	0.19	49,69,78,79	0
10	PO4	M	413	5/5	0.93	0.06	80,83,95,95	0
9	U10	M	409	48/63	0.93	0.15	45,58,77,84	0
7	BCL	L	313	66/66	0.94	0.17	54,66,112,119	0
4	EDO	M	401	4/4	0.94	0.15	56,58,63,64	0
12	LDA	H	304	16/16	0.94	0.18	65,73,83,88	0
15	K	M	411	1/1	0.95	0.12	87,87,87,87	0
16	CL	M	412	1/1	0.95	0.15	70,70,70,70	0
8	BPB	M	407	65/65	0.96	0.12	47,66,116,124	0
8	BPB	L	306	65/65	0.96	0.09	44,51,63,70	0
7	BCL	M	406	66/66	0.97	0.10	52,59,76,96	0
7	BCL	L	305	66/66	0.97	0.08	48,56,61,65	0
15	K	H	305	1/1	0.98	0.04	69,69,69,69	0
7	BCL	M	403	66/66	0.98	0.08	40,51,64,76	0
13	FE	M	408	1/1	1.00	0.01	50,50,50,50	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.

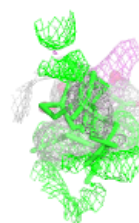
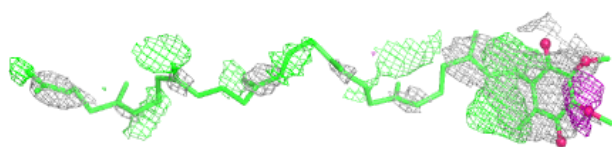
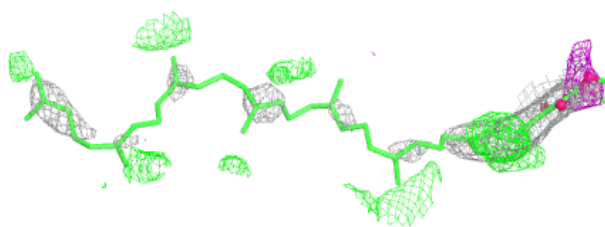
Electron density around CDL M 414:

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

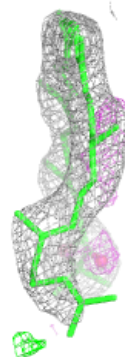
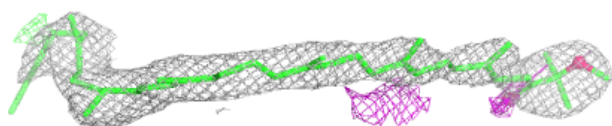
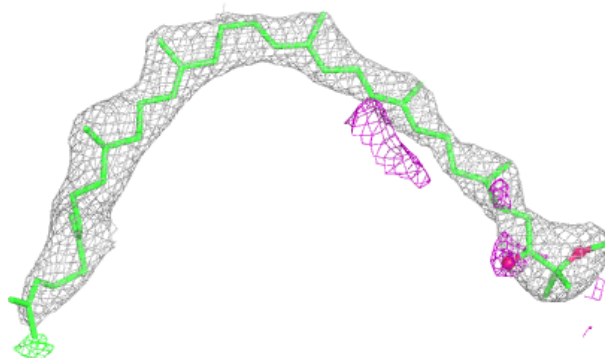


Electron density around U10 L 307:

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

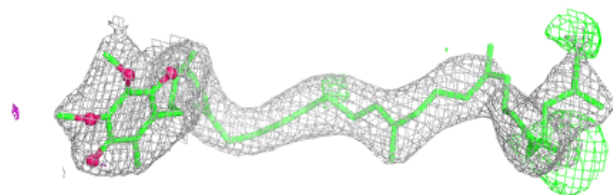
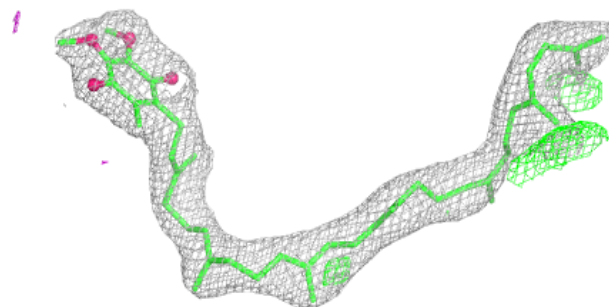
**Electron density around SPN M 410:**

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

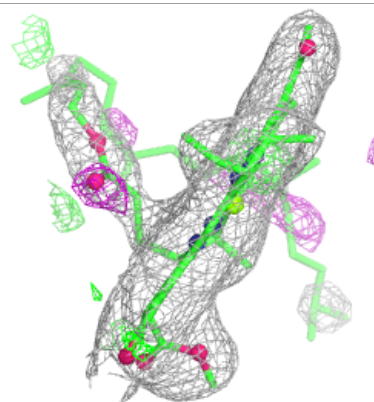
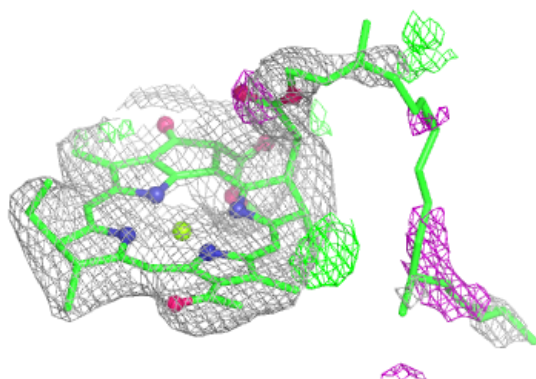
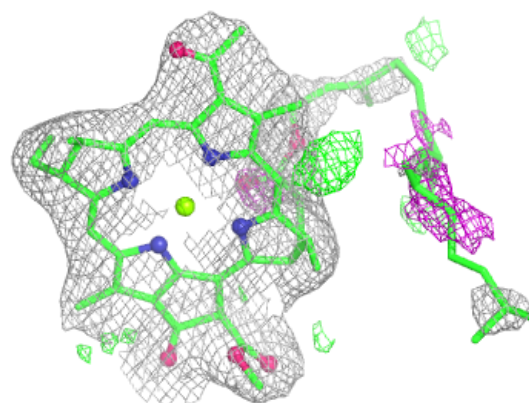


Electron density around U10 M 409:

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

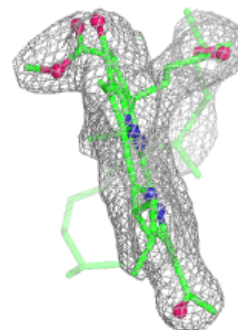
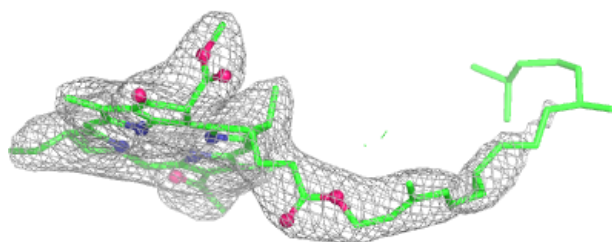
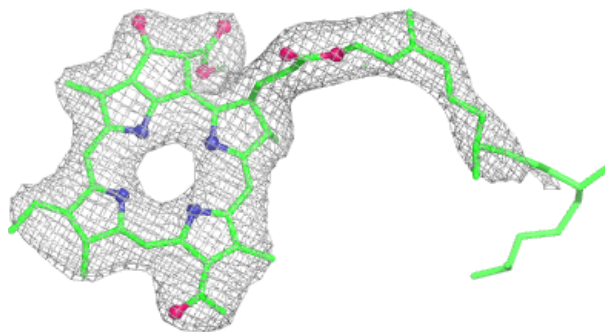
**Electron density around BCL L 313:**

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



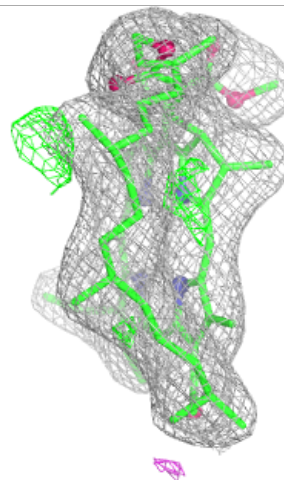
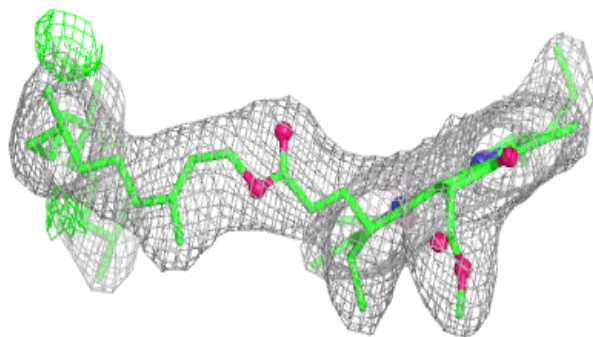
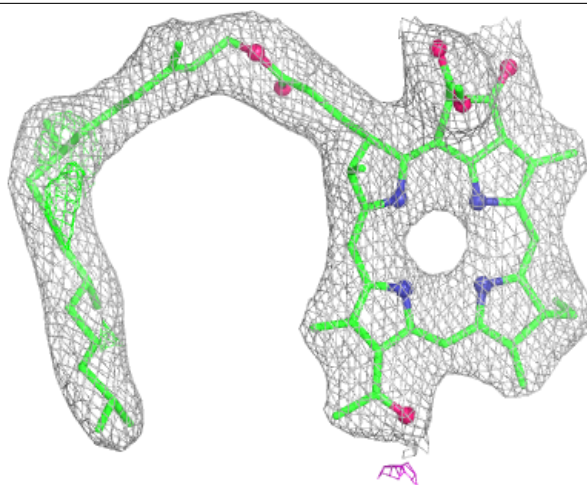
Electron density around BPB M 407:

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



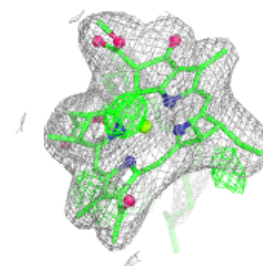
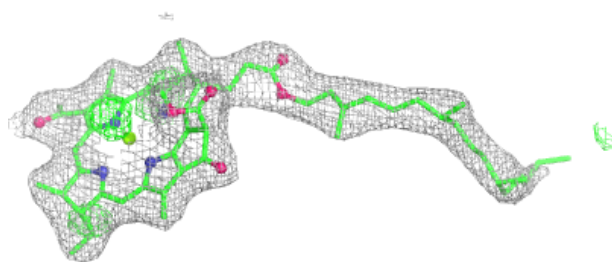
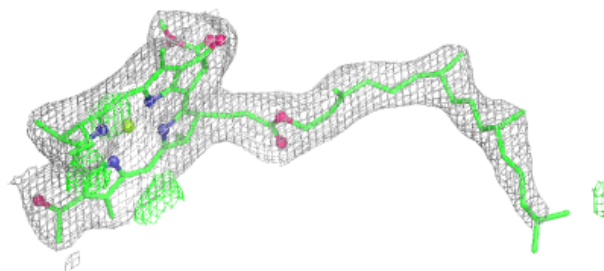
Electron density around BPB L 306:

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

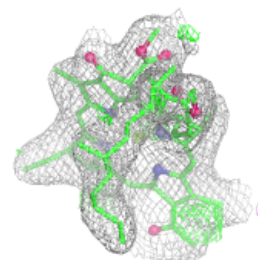
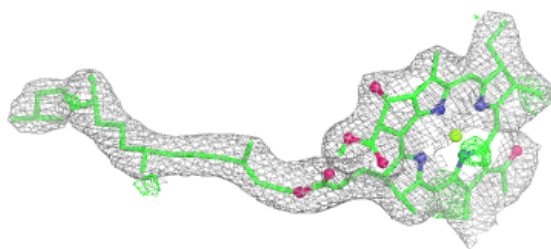
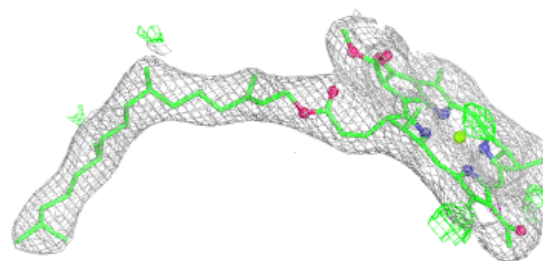


Electron density around BCL M 406:

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

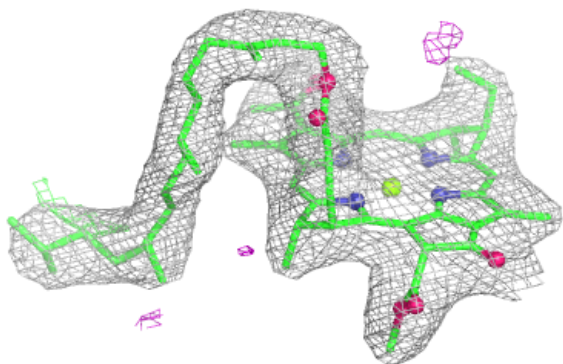
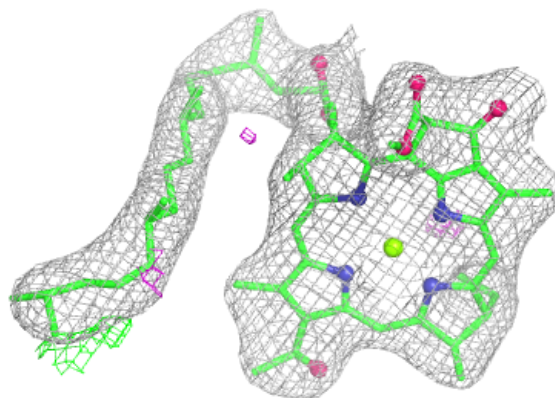
**Electron density around BCL L 305:**

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



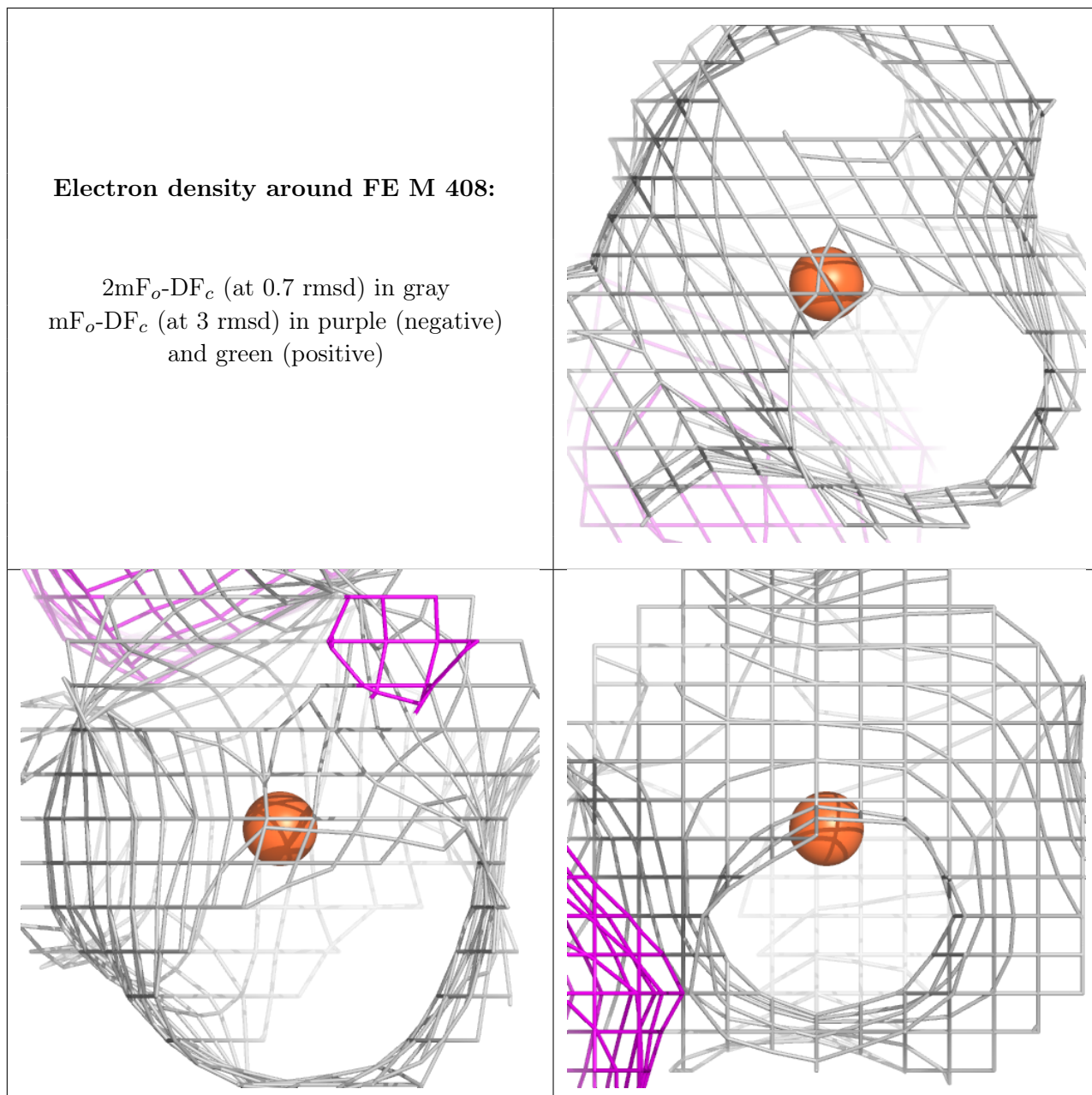
Electron density around BCL M 403:

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



Electron density around FE M 408:

$2mF_o-DF_c$ (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.