



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:27 PM UTC

PDB ID : 8C6K / pdb_00008c6k
Title : Double mutant A(L53)C/I(L64)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 : 2023-01-12
Resolution : 2.86 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

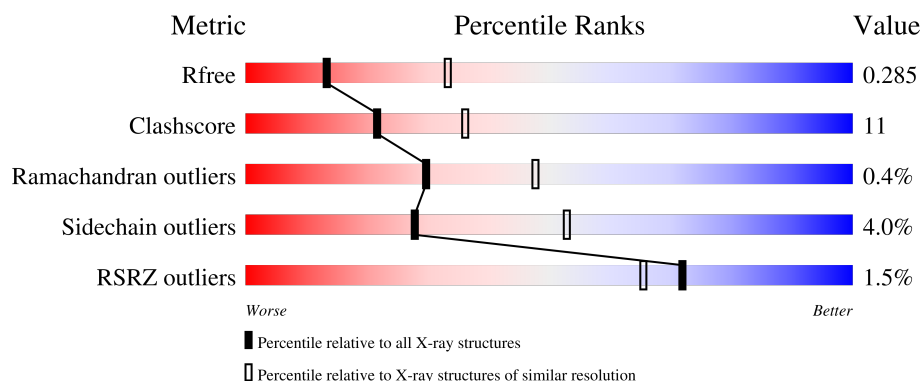
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	242	 76% 22% ..
2	L	281	 2% 74% 23% .
3	M	303	 % 73% 26% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7463 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	240	Total	C	N	O	S	0	3	0
			1848	1183	317	339	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	1	0
			2240	1511	356	363	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	53	CYS	ALA	engineered mutation	UNP P0C0Y8
L	64	CYS	ILE	engineered mutation	UNP P0C0Y8
L	178	THR	SER	conflict	UNP P0C0Y8

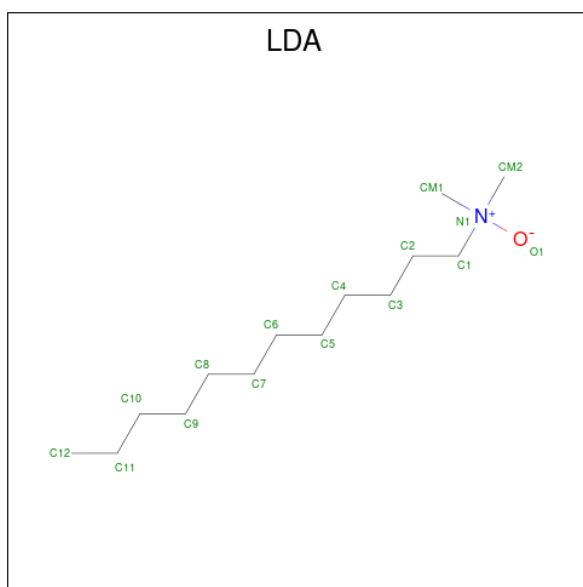
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	4	0
			2436	1630	397	399	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	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	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	4	Total	C	0	0
			51	51		
5	L	4	Total	C	0	0
			49	49		
5	M	2	Total	C	0	0
			27	27		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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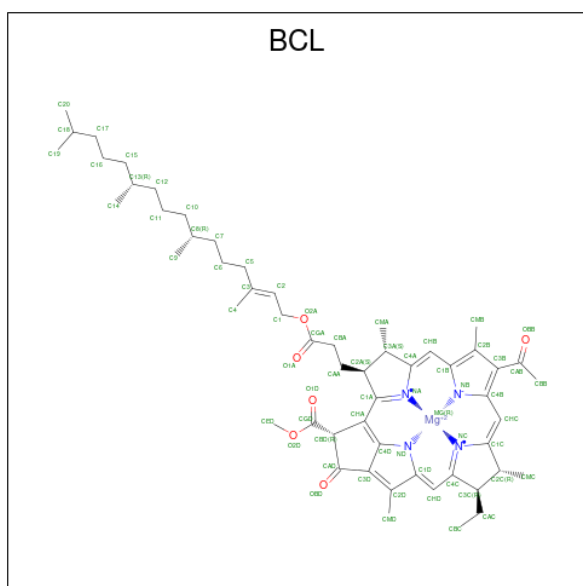
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	L	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	K	0	0
			1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



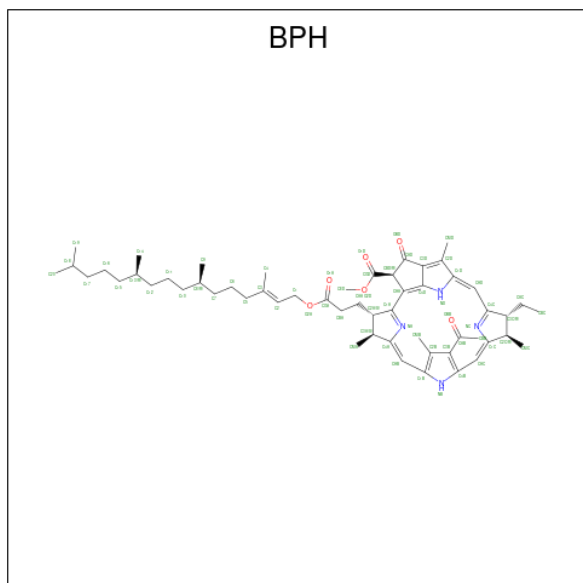
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	0
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	0

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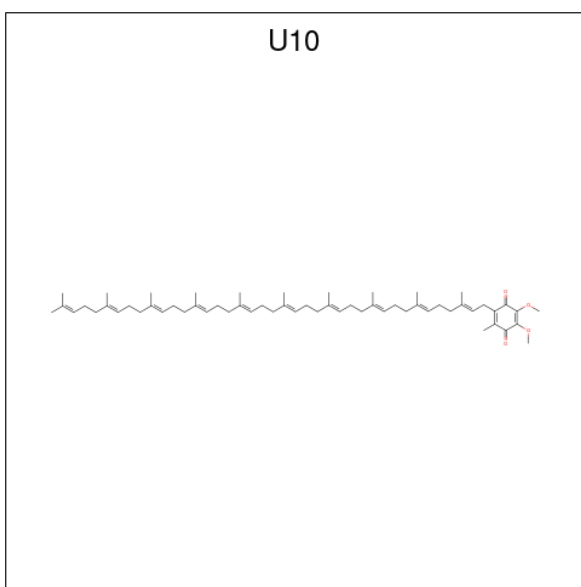
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



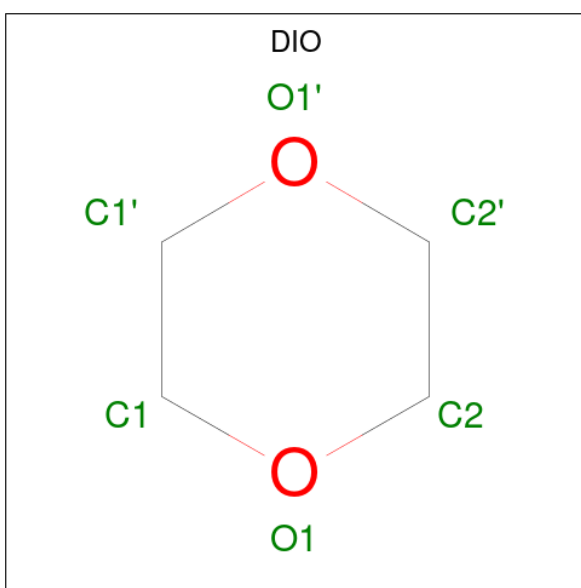
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



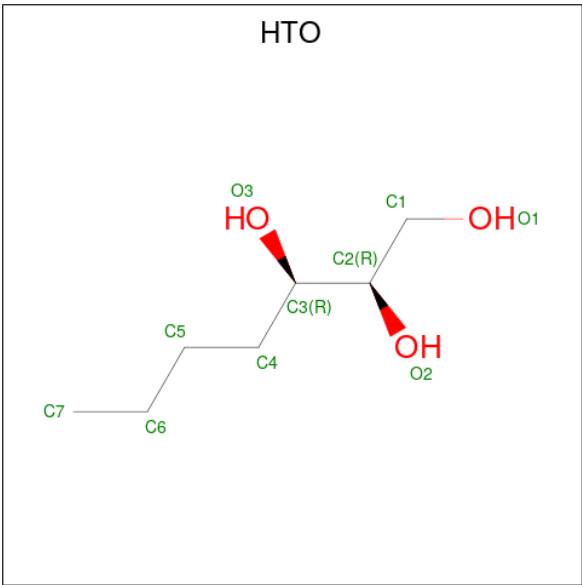
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			48	44	4		
11	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 12 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



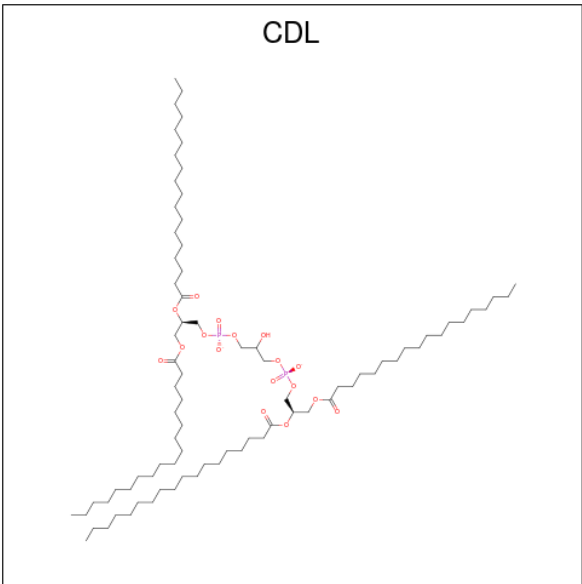
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			6	4	2		

- Molecule 13 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

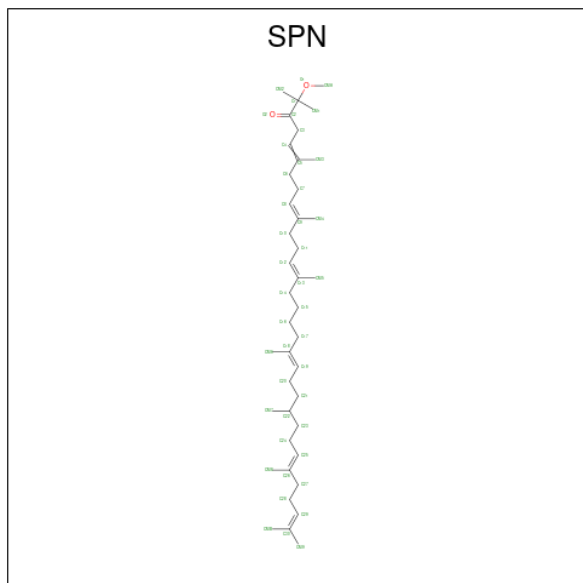


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 16 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂) (labeled as "Ligand of Interest" by depositor).



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

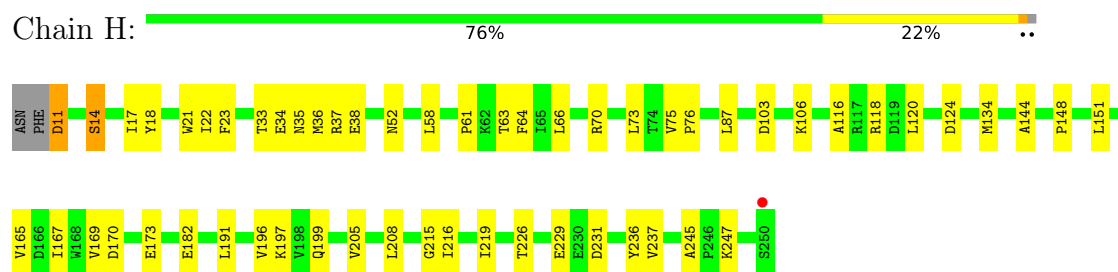
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	11	Total	O	0	0
			11	11		
17	L	12	Total	O	0	0
			12	12		
17	M	8	Total	O	0	0
			8	8		

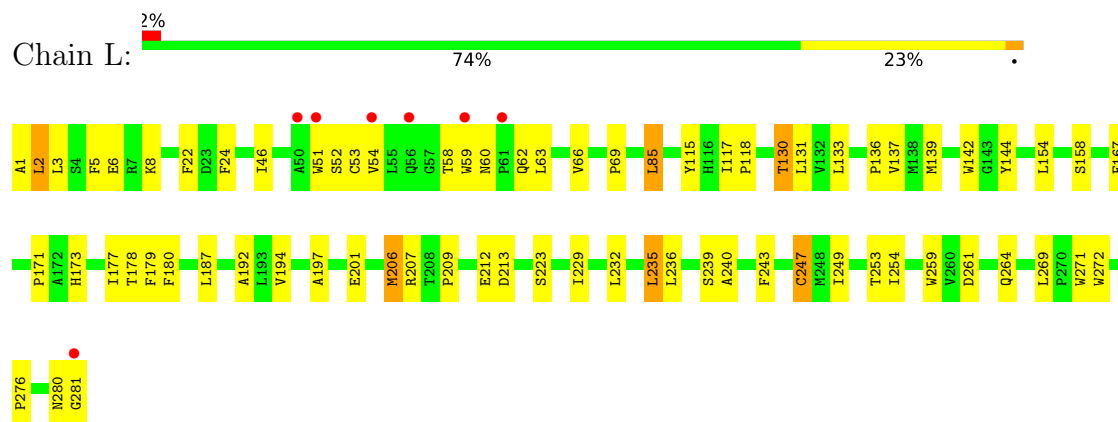
3 Residue-property plots [i](#)

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

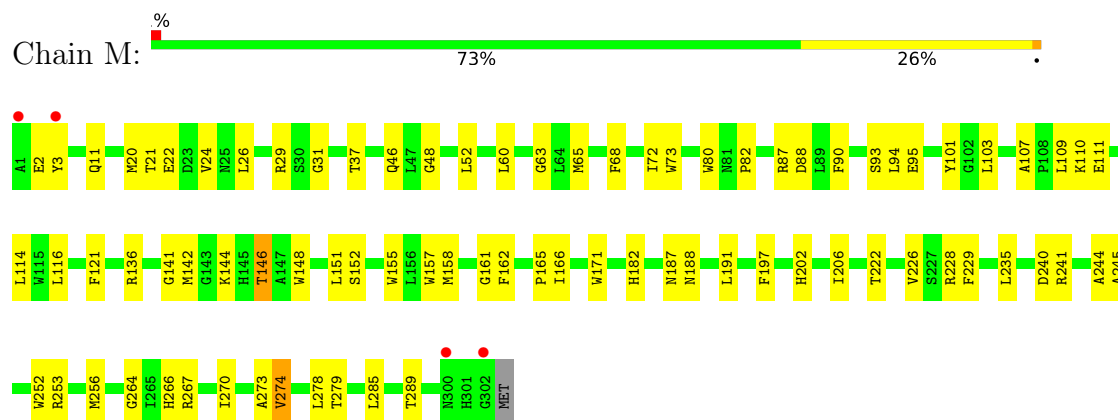
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.64Å 139.64Å 185.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 2.86 29.89 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.89-2.86) 99.4 (29.89-2.86)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.229 , 0.279 0.239 , 0.285	Depositor DCC
R_{free} test set	2466 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	7.5	Xtriage
Anisotropy	1.816	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/1905	0.65	0/2590
2	L	0.43	0/2328	0.62	0/3186
3	M	0.40	0/2541	0.59	0/3468
All	All	0.41	0/6774	0.62	0/9244

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1848	0	1866	38	0
2	L	2240	0	2191	57	0
3	M	2436	0	2362	67	0
4	H	16	0	31	3	0
4	M	80	0	155	4	0
5	H	51	0	0	0	0
5	L	49	0	0	0	0
5	M	27	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	16	0	24	2	0
7	L	4	0	6	0	0
7	M	8	0	12	2	0
8	H	1	0	0	0	0
9	L	132	0	148	7	0
9	M	132	0	148	9	0
10	L	65	0	76	1	0
10	M	65	0	76	4	0
11	L	48	0	63	3	0
11	M	48	0	63	3	0
12	L	6	0	8	1	0
13	L	20	0	32	0	0
14	M	81	0	106	10	0
15	M	1	0	0	0	0
16	M	43	0	70	6	0
17	H	11	0	0	0	0
17	L	12	0	0	0	0
17	M	8	0	0	0	0
All	All	7463	0	7437	160	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 11.

All (160) 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)
3:M:161:GLY:HA3	16:M:407:SPN:H201	1.60	0.82
9:L:301:BCL:H2C	9:M:403:BCL:HBC2	1.66	0.75
9:M:402:BCL:H202	16:M:407:SPN:H72	1.70	0.73
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.71	0.72
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.74	0.70
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.28	0.68
3:M:63:GLY:HA3	10:M:404:BPH:H5C1	1.73	0.68
9:M:402:BCL:CAB	16:M:407:SPN:H162	2.25	0.67
3:M:151:LEU:HD23	14:M:401:CDL:H781	1.77	0.66
3:M:148:TRP:HE1	14:M:401:CDL:HB32	1.60	0.65
1:H:134:MET:HE3	1:H:169:VAL:HG11	1.79	0.64
11:M:406:U10:H212	4:M:418:LDA:H71	1.79	0.64
2:L:6:GLU:OE1	3:M:253[B]:ARG:NH1	2.32	0.62
2:L:46:ILE:HG12	9:L:302:BCL:H191	1.82	0.62
3:M:20:MET:HE3	3:M:20:MET:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:GLN:HB3	7:H:308:EDO:H22	1.82	0.62
2:L:60:ASN:HB3	2:L:63:LEU:HB2	1.82	0.61
10:M:404:BPH:H102	10:M:404:BPH:H161	1.82	0.61
1:H:64:PHE:HB3	2:L:206:MET:HE2	1.84	0.60
4:H:301:LDA:H122	11:M:406:U10:H202	1.85	0.59
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.83	0.59
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.02	0.58
3:M:278:LEU:HD11	14:M:401:CDL:H791	1.86	0.58
3:M:157:TRP:CE2	16:M:407:SPN:HM73	2.39	0.57
3:M:228:ARG:HH12	7:M:416:EDO:H22	1.69	0.57
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.39	0.57
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.87	0.57
3:M:46:GLN:NE2	3:M:48:GLY:O	2.35	0.57
3:M:157:TRP:CH2	3:M:158:MET:HE3	2.40	0.57
11:L:304:U10:H28	11:L:304:U10:H251	1.87	0.56
3:M:73:TRP:HZ3	3:M:110:LYS:HG2	1.70	0.56
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.40	0.55
3:M:285:LEU:O	3:M:289:THR:OG1	2.21	0.55
1:H:70:ARG:O	1:H:118[A]:ARG:NH2	2.39	0.55
9:M:403:BCL:HHC	9:M:403:BCL:OBB	2.06	0.55
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.42	0.54
3:M:80:TRP:O	3:M:82:PRO:HD3	2.07	0.54
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.90	0.54
3:M:187:ASN:HA	9:M:403:BCL:HAC1	1.90	0.54
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.89	0.53
9:L:302:BCL:HBB3	10:L:303:BPH:H162	1.90	0.53
3:M:222:THR:O	3:M:226:VAL:HG22	2.09	0.53
2:L:54:VAL:CG1	2:L:59:TRP:HE1	2.21	0.53
3:M:103:LEU:HD11	3:M:166:ILE:HA	1.91	0.52
3:M:267:ARG:HA	3:M:270:ILE:HG22	1.91	0.52
3:M:197:PHE:CE1	9:M:403:BCL:HMC2	2.44	0.52
2:L:192:ALA:HB1	3:M:146:THR:N	2.25	0.52
1:H:14:SER:HA	1:H:17:ILE:HG22	1.91	0.51
1:H:66:LEU:HD22	2:L:206:MET:HE3	1.92	0.51
2:L:139:MET:HE2	2:L:144:TYR:HB3	1.92	0.51
1:H:64:PHE:CB	2:L:206:MET:HE2	2.41	0.51
2:L:167:PHE:HB3	9:L:301:BCL:HMC3	1.92	0.51
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.45	0.51
3:M:94:LEU:HD11	3:M:114:LEU:HB3	1.93	0.51
2:L:201:GLU:HG3	3:M:141:GLY:O	2.11	0.50
2:L:130:THR:HG22	2:L:131:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:LEU:HB3	2:L:6:GLU:HB3	1.92	0.50
2:L:197:ALA:HB3	3:M:235:LEU:HD21	1.94	0.50
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.94	0.50
3:M:109:LEU:HG	3:M:114:LEU:HD13	1.93	0.49
9:L:301:BCL:NA	9:M:403:BCL:HBB2	2.27	0.49
9:L:301:BCL:CGA	9:L:302:BCL:HBC1	2.42	0.49
2:L:139:MET:HE2	2:L:144:TYR:CG	2.47	0.49
1:H:118[A]:ARG:HD2	1:H:120:LEU:HB2	1.95	0.48
14:M:401:CDL:H312	14:M:401:CDL:H521	1.94	0.48
2:L:115:TYR:O	2:L:118:PRO:HD2	2.13	0.48
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.96	0.48
9:L:301:BCL:OBB	9:L:301:BCL:HHC	2.14	0.48
3:M:228:ARG:HH22	7:M:416:EDO:H22	1.78	0.48
3:M:158:MET:HE2	16:M:407:SPN:HM71	1.96	0.47
3:M:162:PHE:C	3:M:165:PRO:HD2	2.39	0.47
3:M:31:GLY:H	4:M:410:LDA:HM11	1.80	0.47
2:L:269:LEU:HD13	2:L:271:TRP:CZ2	2.50	0.47
3:M:24:VAL:HG11	3:M:29:ARG:NH2	2.30	0.47
1:H:73:LEU:HD11	1:H:75:VAL:HG13	1.97	0.47
2:L:139:MET:CE	2:L:144:TYR:CG	2.98	0.47
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.49	0.46
14:M:401:CDL:HB61	14:M:401:CDL:OA5	2.14	0.46
1:H:75:VAL:HA	1:H:76:PRO:C	2.40	0.46
2:L:201:GLU:HG3	3:M:141:GLY:C	2.40	0.46
1:H:33:THR:HA	1:H:36:MET:HE2	1.97	0.46
2:L:139:MET:HE2	2:L:144:TYR:CB	2.46	0.46
2:L:194:VAL:HG21	3:M:266:HIS:CD2	2.51	0.46
2:L:223:SER:HA	11:L:304:U10:H103	1.98	0.46
3:M:68[B]:PHE:CZ	3:M:72:ILE:HD11	2.51	0.46
3:M:157:TRP:CZ3	3:M:158:MET:HE3	2.51	0.46
1:H:11:ASP:OD2	1:H:14:SER:HB2	2.15	0.46
2:L:276:PRO:HA	2:L:281:GLY:O	2.14	0.46
3:M:148:TRP:NE1	14:M:401:CDL:HB32	2.28	0.46
1:H:64:PHE:CG	2:L:206:MET:HE2	2.51	0.46
2:L:3:LEU:C	2:L:5:PHE:H	2.24	0.46
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.51	0.46
3:M:256:MET:HE1	11:M:406:U10:H102	1.98	0.45
3:M:116:LEU:HD21	3:M:171:TRP:CD1	2.50	0.45
1:H:35:ASN:OD1	3:M:264:GLY:HA3	2.16	0.45
3:M:157:TRP:HE1	16:M:407:SPN:H211	1.82	0.45
3:M:188:ASN:O	3:M:191:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:171:PRO:HD2	2:L:259:TRP:CZ3	2.52	0.45
1:H:170:ASP:OD2	1:H:173:GLU:HG3	2.17	0.45
12:L:309:DIO:H21	3:M:90:PHE:CZ	2.52	0.45
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.52	0.45
1:H:118[B]:ARG:HH11	1:H:118[B]:ARG:HB2	1.82	0.45
2:L:281:GLY:H	3:M:87:ARG:NH2	2.15	0.44
2:L:52:SER:OG	2:L:66:VAL:HG22	2.17	0.44
2:L:209:PRO:HA	2:L:212:GLU:OE1	2.18	0.44
3:M:148:TRP:HB3	14:M:401:CDL:H741	1.99	0.44
2:L:178:THR:HG21	11:L:304:U10:H321	2.00	0.44
2:L:207:ARG:HG2	3:M:142:MET:HG2	2.00	0.43
2:L:51:TRP:CE3	2:L:85:LEU:HD11	2.53	0.43
3:M:152:SER:O	3:M:155:TRP:HB3	2.19	0.43
2:L:53:CYS:HB3	2:L:58:THR:O	2.19	0.43
2:L:235:LEU:O	2:L:239:SER:OG	2.29	0.43
2:L:280:ASN:ND2	3:M:88:ASP:OD1	2.51	0.43
1:H:21:TRP:HZ2	4:M:408:LDA:HM11	1.84	0.43
2:L:213:ASP:OD1	2:L:223:SER:OG	2.29	0.43
3:M:21:THR:O	3:M:22:GLU:C	2.61	0.43
4:H:301:LDA:H12	4:M:418:LDA:HM13	2.01	0.42
2:L:2:LEU:HD23	2:L:2:LEU:N	2.35	0.42
3:M:101:TYR:CG	3:M:107:ALA:HB2	2.54	0.42
1:H:197:LYS:HD3	3:M:3:TYR:HB2	2.00	0.42
2:L:179:PHE:HB3	2:L:240:ALA:HB2	2.01	0.42
1:H:103:ASP:OD2	1:H:106:LYS:HG3	2.20	0.42
1:H:120:LEU:HD23	1:H:120:LEU:HA	1.57	0.42
2:L:154:LEU:HD23	3:M:197:PHE:HB3	2.01	0.42
2:L:117:ILE:HB	2:L:118:PRO:HD3	2.02	0.42
1:H:215:GLY:O	1:H:216:ILE:C	2.62	0.41
1:H:215:GLY:HA3	1:H:236:TYR:OH	2.20	0.41
2:L:133:LEU:C	2:L:136:PRO:HD2	2.46	0.41
2:L:173:HIS:N	2:L:247:CYS:HB2	2.35	0.41
4:H:301:LDA:H22	4:H:301:LDA:HM11	1.52	0.41
2:L:249:ILE:HD12	2:L:249:ILE:HA	1.83	0.41
3:M:144:LYS:N	14:M:401:CDL:OB3	2.28	0.41
1:H:34:GLU:OE2	1:H:37:ARG:NH2	2.41	0.41
2:L:261:ASP:O	2:L:264:GLN:HG2	2.20	0.41
1:H:23:PHE:CE1	14:M:401:CDL:H362	2.56	0.41
14:M:401:CDL:HB61	14:M:401:CDL:HA4	2.03	0.41
1:H:87:LEU:HD11	2:L:8:LYS:HA	2.02	0.41
1:H:116:ALA:O	7:H:310:EDO:H12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ALA:HB3	3:M:11:GLN:HB2	2.02	0.41
1:H:208:LEU:HD11	1:H:237:VAL:HG22	2.02	0.41
2:L:187:LEU:HD23	3:M:273:ALA:HB2	2.02	0.41
2:L:232:LEU:HG	2:L:236:LEU:HD12	2.03	0.41
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.36	0.41
1:H:18:TYR:CZ	1:H:22:ILE:HD11	2.56	0.41
2:L:1:ALA:C	2:L:2:LEU:HD23	2.47	0.41
3:M:93:SER:OG	3:M:95:GLU:OE2	2.23	0.40
1:H:219:ILE:HG22	1:H:229:GLU:HB3	2.02	0.40
3:M:136:ARG:NH1	3:M:136:ARG:HA	2.36	0.40
9:M:403:BCL:H18	10:M:404:BPH:H8	2.03	0.40
9:M:402:BCL:H91	9:M:402:BCL:H111	1.77	0.40
2:L:62:GLN:O	2:L:63:LEU:HD12	2.22	0.40
2:L:243:PHE:O	2:L:247:CYS:HB3	2.22	0.40
2:L:253:THR:OG1	2:L:254:ILE:N	2.51	0.40
3:M:65:MET:HB3	3:M:121:PHE:CE2	2.56	0.40
1:H:165:VAL:HG11	1:H:182:GLU:HB2	2.02	0.40
3:M:63:GLY:HA3	10:M:404:BPH:C5	2.45	0.40
3:M:114:LEU:HA	3:M:114:LEU:HD12	1.88	0.40
3:M:187:ASN:O	3:M:191:LEU:HG	2.22	0.40
3:M:241:ARG:HG3	3:M:245:ALA:HB3	2.04	0.40
3:M:270:ILE:O	3:M:274:VAL:HB	2.21	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	241/242 (100%)	230 (95%)	9 (4%)	2 (1%)	16	31
2	L	280/281 (100%)	257 (92%)	23 (8%)	0	100	100
3	M	304/303 (100%)	285 (94%)	18 (6%)	1 (0%)	36	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	825/826 (100%)	772 (94%)	50 (6%)	3 (0%)	30	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
1	H	124	ASP
3	M	240	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/197 (100%)	190 (96%)	8 (4%)	28	53
2	L	222/221 (100%)	213 (96%)	9 (4%)	27	52
3	M	240/237 (101%)	229 (95%)	11 (5%)	24	48
All	All	660/655 (101%)	632 (96%)	28 (4%)	28	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	14	SER
1	H	52	ASN
1	H	58	LEU
1	H	63	THR
1	H	191	LEU
1	H	231	ASP
1	H	247	LYS
2	L	2	LEU
2	L	85	LEU
2	L	130	THR
2	L	137	VAL
2	L	158	SER

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Mol	Chain	Res	Type
2	L	206	MET
2	L	229	ILE
2	L	235	LEU
2	L	247	CYS
3	M	2[A]	GLU
3	M	2[B]	GLU
3	M	37	THR
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	60	LEU
3	M	111	GLU
3	M	146	THR
3	M	182	HIS
3	M	274	VAL
3	M	279	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	199	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 41 ligands modelled in this entry, 10 are unknown and 2 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	H	308	-	3,3,3	0.52	0	2,2,2	0.19	0
9	BCL	L	301	-	69,74,74	1.30	7 (10%)	79,115,115	1.36	10 (12%)
16	SPN	M	407	-	42,42,42	0.51	0	50,52,52	0.98	3 (6%)
7	EDO	M	416	-	3,3,3	0.46	0	2,2,2	0.43	0
12	DIO	L	309	-	6,6,6	1.22	1 (16%)	6,6,6	0.42	0
7	EDO	L	310	-	3,3,3	0.45	0	2,2,2	0.41	0
11	U10	M	406	-	48,48,63	2.67	14 (29%)	60,61,79	1.91	17 (28%)
9	BCL	M	403	-	69,74,74	1.25	7 (10%)	79,115,115	1.52	10 (12%)
9	BCL	M	402	-	69,74,74	1.31	7 (10%)	79,115,115	1.58	12 (15%)
6	PO4	M	415	-	4,4,4	0.85	0	6,6,6	1.03	0
4	LDA	M	408	-	13,15,15	2.04	2 (15%)	14,17,17	0.96	1 (7%)
4	LDA	M	410	-	13,15,15	2.18	2 (15%)	14,17,17	0.75	1 (7%)
13	HTO	L	311	-	9,9,9	0.58	0	10,10,10	1.45	2 (20%)
14	CDL	M	401	-	80,80,99	0.60	1 (1%)	86,92,111	0.42	0
10	BPH	M	404	-	59,70,70	1.23	8 (13%)	59,101,101	2.11	13 (22%)
6	PO4	H	306	-	4,4,4	0.81	0	6,6,6	0.65	0
4	LDA	H	301	-	13,15,15	2.49	2 (15%)	14,17,17	0.80	0
4	LDA	M	418	-	13,15,15	2.30	2 (15%)	14,17,17	0.52	0
13	HTO	L	312	-	9,9,9	0.50	0	10,10,10	0.89	1 (10%)
7	EDO	H	310	-	3,3,3	0.53	0	2,2,2	0.30	0
7	EDO	H	309	-	3,3,3	0.60	0	2,2,2	0.22	0
10	BPH	L	303	-	59,70,70	1.19	5 (8%)	59,101,101	2.11	13 (22%)
7	EDO	H	307	-	3,3,3	0.52	0	2,2,2	0.51	0
4	LDA	M	409	-	13,15,15	2.38	2 (15%)	14,17,17	0.55	0
7	EDO	M	417	-	3,3,3	0.50	0	2,2,2	0.51	0
11	U10	L	304	-	48,48,63	2.66	13 (27%)	60,61,79	1.99	13 (21%)
4	LDA	M	411	-	13,15,15	2.37	2 (15%)	14,17,17	0.51	0
9	BCL	L	302	-	69,74,74	1.23	5 (7%)	79,115,115	1.60	13 (16%)
6	PO4	M	414	-	4,4,4	0.73	0	6,6,6	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	308	-	-	0/1/1/1	-
9	BCL	L	301	-	-	3/41/137/137	-
16	SPN	M	407	-	-	12/50/51/51	-
7	EDO	M	416	-	-	1/1/1/1	-
12	DIO	L	309	-	-	-	0/1/1/1
7	EDO	L	310	-	-	1/1/1/1	-
11	U10	M	406	-	-	17/45/69/87	0/1/1/1
9	BCL	M	403	-	-	3/41/137/137	-
9	BCL	M	402	-	-	4/41/137/137	-
4	LDA	M	408	-	-	8/13/13/13	-
4	LDA	M	410	-	-	3/13/13/13	-
13	HTO	L	311	-	-	8/10/10/10	-
14	CDL	M	401	-	-	51/91/91/110	-
10	BPH	M	404	-	-	13/37/105/105	0/5/6/6
4	LDA	H	301	-	-	3/13/13/13	-
4	LDA	M	418	-	-	7/13/13/13	-
13	HTO	L	312	-	-	6/10/10/10	-
7	EDO	H	310	-	-	0/1/1/1	-
10	BPH	L	303	-	-	5/37/105/105	0/5/6/6
7	EDO	H	309	-	-	0/1/1/1	-
7	EDO	H	307	-	-	1/1/1/1	-
4	LDA	M	409	-	-	5/13/13/13	-
7	EDO	M	417	-	-	0/1/1/1	-
11	U10	L	304	-	-	19/45/69/87	0/1/1/1
4	LDA	M	411	-	-	7/13/13/13	-
9	BCL	L	302	-	-	2/41/137/137	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	411	LDA	O1-N1	-6.91	1.25	1.42
4	M	410	LDA	O1-N1	-6.79	1.25	1.42
4	M	418	LDA	O1-N1	-6.73	1.25	1.42
11	L	304	U10	C13-C14	6.72	1.48	1.33
4	M	408	LDA	O1-N1	-6.62	1.25	1.42
4	M	409	LDA	O1-N1	-6.55	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	LDA	C1-N1	-6.48	1.44	1.51
11	L	304	U10	C8-C9	6.32	1.47	1.33
11	M	406	U10	C13-C14	6.31	1.47	1.33
11	M	406	U10	C33-C34	6.28	1.47	1.33
11	M	406	U10	C28-C29	6.28	1.47	1.33
4	H	301	LDA	O1-N1	-6.19	1.27	1.42
11	M	406	U10	C18-C19	6.17	1.47	1.33
11	L	304	U10	C18-C19	6.15	1.47	1.33
11	M	406	U10	C8-C9	6.10	1.47	1.33
11	L	304	U10	C28-C29	6.05	1.47	1.33
11	L	304	U10	C23-C24	5.98	1.46	1.33
11	M	406	U10	C23-C24	5.93	1.46	1.33
11	L	304	U10	C33-C34	5.89	1.46	1.33
11	L	304	U10	C38-C39	5.47	1.48	1.32
4	M	409	LDA	C1-N1	-5.39	1.45	1.51
9	M	402	BCL	MG-NA	5.29	2.18	2.06
9	L	302	BCL	MG-NA	5.13	2.18	2.06
4	M	411	LDA	C1-N1	-4.90	1.46	1.51
11	L	304	U10	O4-C4	-4.90	1.25	1.36
11	M	406	U10	C38-C39	4.88	1.47	1.32
11	M	406	U10	O3-C3	-4.82	1.25	1.36
4	M	418	LDA	C1-N1	-4.72	1.46	1.51
9	M	403	BCL	MG-NA	4.64	2.17	2.06
9	L	301	BCL	MG-NA	4.62	2.17	2.06
11	M	406	U10	O4-C4	-4.60	1.25	1.36
11	L	304	U10	O3-C3	-4.57	1.25	1.36
10	L	303	BPH	CBD-CGD	-4.07	1.47	1.52
9	L	301	BCL	O1A-CGA	-3.85	1.11	1.22
9	L	302	BCL	C1D-ND	3.82	1.42	1.37
9	M	403	BCL	O1A-CGA	-3.78	1.11	1.22
4	M	410	LDA	C1-N1	-3.72	1.47	1.51
9	L	301	BCL	MG-NC	3.66	2.15	2.06
9	L	302	BCL	MG-NC	3.44	2.14	2.06
9	M	402	BCL	C3B-C4B	3.23	1.47	1.41
9	M	402	BCL	CHD-C1D	3.18	1.44	1.38
10	M	404	BPH	C1D-C2D	3.11	1.43	1.39
10	M	404	BPH	C3D-CAD	-3.07	1.41	1.47
9	M	402	BCL	OBD-CAD	3.05	1.27	1.22
9	M	403	BCL	MG-NC	2.97	2.13	2.06
4	M	408	LDA	C1-N1	-2.82	1.48	1.51
14	M	401	CDL	OA8-CA6	2.79	1.51	1.45
10	L	303	BPH	C3D-CAD	-2.75	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	BPH	C3B-C4B	2.70	1.45	1.41
11	M	406	U10	C1-C2	-2.68	1.38	1.47
9	M	403	BCL	C1D-ND	2.67	1.41	1.37
10	M	404	BPH	C3B-CAB	-2.64	1.42	1.49
9	M	402	BCL	MG-NC	2.63	2.12	2.06
9	L	301	BCL	C5-C3	2.63	1.56	1.51
9	L	301	BCL	OBD-CAD	2.56	1.26	1.22
10	M	404	BPH	CBD-CGD	-2.56	1.49	1.52
9	L	302	BCL	CHD-C1D	2.56	1.43	1.38
10	M	404	BPH	C1B-C2B	2.56	1.42	1.39
10	M	404	BPH	C4D-CHA	2.53	1.43	1.39
11	L	304	U10	C4-C5	-2.46	1.41	1.48
11	M	406	U10	C6-C1	2.46	1.39	1.35
11	M	406	U10	C3-C2	-2.43	1.41	1.48
11	M	406	U10	C4-C5	-2.43	1.41	1.48
10	L	303	BPH	OBD-CAD	2.42	1.25	1.22
9	L	301	BCL	C3B-C4B	2.40	1.45	1.41
11	L	304	U10	C3-C2	-2.39	1.41	1.48
11	M	406	U10	C6-C5	-2.37	1.39	1.46
9	L	302	BCL	C3B-C4B	2.36	1.45	1.41
9	M	402	BCL	CAA-C2A	2.34	1.58	1.54
11	L	304	U10	C6-C1	2.32	1.39	1.35
9	M	403	BCL	CHD-C1D	2.29	1.42	1.38
9	M	402	BCL	C1B-NB	2.22	1.40	1.37
10	L	303	BPH	C3B-C4B	2.21	1.45	1.41
11	L	304	U10	C6-C5	-2.19	1.40	1.46
10	L	303	BPH	C2C-C3C	-2.17	1.52	1.54
9	M	403	BCL	CMD-C2D	2.17	1.55	1.50
12	L	309	DIO	O1-C2	2.13	1.50	1.42
10	M	404	BPH	C2-C3	-2.09	1.28	1.33
9	M	403	BCL	C3D-C4D	-2.08	1.39	1.44
9	L	301	BCL	C1D-ND	2.05	1.40	1.37

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404	BPH	C4D-CHA-CBD	-10.49	103.42	108.45
10	L	303	BPH	C4D-CHA-CBD	-10.48	103.43	108.45
9	M	402	BCL	C1D-ND-C4D	-5.15	102.70	106.31
11	L	304	U10	C22-C23-C24	-5.10	115.94	127.62
9	L	302	BCL	C4D-CHA-C1A	4.98	127.19	121.24
9	M	403	BCL	C4D-CHA-C1A	4.88	127.06	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	304	U10	C7-C8-C9	-4.75	118.65	126.83
9	M	402	BCL	C4D-CHA-C1A	4.63	126.77	121.24
10	L	303	BPH	C11-C10-C8	-4.44	101.20	115.97
9	M	402	BCL	CHD-C1D-ND	-4.42	118.58	124.80
11	M	406	U10	C22-C23-C24	-4.29	117.80	127.62
11	L	304	U10	C32-C33-C34	-4.28	117.82	127.62
11	M	406	U10	C32-C33-C34	-4.15	118.13	127.62
9	L	302	BCL	CHD-C1D-ND	-4.12	119.00	124.80
9	L	302	BCL	C1D-ND-C4D	-4.09	103.44	106.31
11	L	304	U10	C7-C6-C1	-4.06	117.94	124.89
9	L	301	BCL	C4D-CHA-C1A	3.97	125.98	121.24
11	M	406	U10	C15-C14-C16	3.96	122.11	115.23
10	L	303	BPH	C4D-ND-C1D	-3.96	104.13	108.87
10	M	404	BPH	O2D-CGD-CBD	3.95	115.29	110.95
11	L	304	U10	C25-C24-C26	3.94	122.07	115.23
10	M	404	BPH	C17-C16-C15	3.92	130.86	113.28
9	M	403	BCL	C1D-ND-C4D	-3.89	103.58	106.31
11	L	304	U10	C12-C13-C14	-3.80	118.94	127.62
11	M	406	U10	C35-C34-C36	3.75	121.73	115.23
10	M	404	BPH	C4D-ND-C1D	-3.72	104.41	108.87
9	L	301	BCL	C1-C2-C3	-3.66	120.20	126.20
10	M	404	BPH	C1-C2-C3	-3.64	120.24	126.20
11	L	304	U10	C35-C34-C36	3.62	121.51	115.23
10	M	404	BPH	C3D-C4D-ND	3.56	112.27	107.71
11	M	406	U10	C17-C18-C19	-3.54	119.51	127.62
10	L	303	BPH	C3D-C4D-ND	3.54	112.25	107.71
9	M	403	BCL	CHD-C1D-ND	-3.51	119.86	124.80
9	L	302	BCL	C11-C10-C8	3.49	127.58	115.97
9	M	403	BCL	C11-C10-C8	-3.49	104.38	115.97
11	L	304	U10	C1M-C1-C6	-3.49	118.72	124.45
9	L	301	BCL	O2A-CGA-O1A	-3.47	114.94	123.63
10	M	404	BPH	OBD-CAD-CBD	-3.40	120.83	125.82
9	L	302	BCL	CHA-C1A-NA	-3.37	118.76	126.39
9	L	302	BCL	C2A-C1A-CHA	3.30	129.60	123.87
9	L	301	BCL	CHD-C1D-ND	-3.29	120.18	124.80
10	L	303	BPH	C6-C7-C8	-3.28	105.05	115.97
11	M	406	U10	C12-C13-C14	-3.25	120.18	127.62
11	M	406	U10	O2-C2-C1	-3.24	111.68	120.73
9	M	402	BCL	OBB-CAB-CBB	-3.21	112.59	119.77
9	L	302	BCL	O2D-CGD-CBD	3.20	116.82	111.23
10	L	303	BPH	OBD-CAD-CBD	-3.19	121.14	125.82
9	M	402	BCL	C6-C7-C8	3.17	126.52	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	403	BCL	CHA-C1A-NA	-3.17	119.20	126.39
11	L	304	U10	C17-C18-C19	-3.16	120.39	127.62
11	L	304	U10	C30-C29-C31	3.13	120.66	115.23
9	M	402	BCL	C2A-C1A-CHA	3.12	129.27	123.87
9	L	301	BCL	C1D-ND-C4D	-3.10	104.14	106.31
9	M	403	BCL	CAB-C3B-C2B	3.09	134.16	127.74
9	M	403	BCL	O2D-CGD-O1D	-3.05	117.92	123.85
10	L	303	BPH	C2D-C1D-ND	3.04	111.63	109.43
11	M	406	U10	C30-C29-C31	3.01	120.46	115.23
9	L	301	BCL	C2A-C1A-CHA	3.00	129.07	123.87
11	M	406	U10	C41-C39-C40	2.98	121.45	114.59
9	L	301	BCL	C1-O2A-CGA	2.96	123.82	116.65
11	M	406	U10	C25-C24-C26	2.96	120.36	115.23
11	L	304	U10	C20-C19-C21	2.91	120.28	115.23
11	M	406	U10	C10-C9-C11	2.90	120.26	115.23
9	M	402	BCL	CAA-CBA-CGA	2.89	121.42	113.21
11	M	406	U10	O5-C5-C6	-2.88	116.21	121.79
9	M	403	BCL	C2A-C1A-CHA	2.88	128.87	123.87
9	L	301	BCL	CHA-C1A-NA	-2.88	119.88	126.39
9	M	403	BCL	C4A-NA-C1A	2.83	107.97	106.68
9	M	402	BCL	CHA-C1A-NA	-2.81	120.02	126.39
9	M	402	BCL	O2A-CGA-O1A	-2.81	116.60	123.63
10	L	303	BPH	CMD-C2D-C3D	2.79	130.26	124.68
13	L	311	HTO	O3-C3-C4	2.75	115.39	109.14
9	L	302	BCL	OBb-CAB-CBB	-2.74	113.64	119.77
11	L	304	U10	C25-C24-C23	-2.69	116.72	123.63
10	L	303	BPH	O2D-CGD-CBD	2.67	113.89	110.95
11	M	406	U10	C37-C38-C39	-2.65	118.80	127.64
4	M	408	LDA	CM1-N1-C1	2.62	115.75	110.23
11	M	406	U10	C4M-O4-C4	2.60	125.61	116.47
16	M	407	SPN	CM6-C18-C17	2.57	119.69	115.23
9	L	302	BCL	O2D-CGD-O1D	-2.55	118.88	123.85
9	M	402	BCL	C16-C15-C13	2.55	124.43	115.97
10	L	303	BPH	CMB-C2B-C3B	2.52	129.73	124.68
9	L	302	BCL	C16-C17-C18	-2.51	104.72	115.94
16	M	407	SPN	C17-C18-C19	-2.50	115.56	121.17
11	M	406	U10	C7-C8-C9	-2.50	122.53	126.83
13	L	312	HTO	O1-C1-C2	-2.48	105.94	111.16
9	L	302	BCL	C11-C12-C13	-2.48	107.72	115.97
9	M	402	BCL	C1C-NC-C4C	2.47	107.81	106.68
10	M	404	BPH	CAA-CBA-CGA	2.44	120.13	113.21
13	L	311	HTO	C5-C4-C3	2.42	118.07	114.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404	BPH	O2D-CGD-O1D	-2.41	119.15	123.85
10	M	404	BPH	C1B-NB-C4B	-2.32	105.43	108.82
9	M	402	BCL	OBB-CAB-C3B	2.31	124.51	120.43
11	M	406	U10	C7-C6-C1	-2.30	120.95	124.89
9	L	301	BCL	O2A-CGA-CBA	2.29	118.80	111.83
10	M	404	BPH	C2D-C1D-ND	2.26	111.06	109.43
9	L	302	BCL	OBB-CAB-C3B	2.21	124.34	120.43
10	M	404	BPH	CMD-C2D-C3D	2.21	129.09	124.68
9	L	302	BCL	C16-C15-C13	2.19	123.24	115.97
10	L	303	BPH	C4C-C3C-C2C	-2.19	100.76	102.84
10	M	404	BPH	C2B-C1B-NB	2.18	111.00	109.43
9	M	403	BCL	C4D-C3D-CAD	-2.17	105.75	108.11
9	L	301	BCL	CAB-C3B-C2B	2.14	132.19	127.74
4	M	410	LDA	CM1-N1-C1	2.13	114.71	110.23
10	L	303	BPH	O2D-CGD-O1D	-2.08	119.79	123.85
16	M	407	SPN	C3-C4-C5	-2.08	123.25	126.83
11	L	304	U10	C37-C38-C39	-2.07	120.72	127.64
10	L	303	BPH	OBB-CAB-CBB	-2.05	115.81	120.19
11	M	406	U10	C22-C21-C19	-2.02	106.49	113.19

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	408	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-CM1
4	M	410	LDA	C2-C1-N1-CM2
4	M	418	LDA	C2-C1-N1-O1
4	M	418	LDA	C2-C1-N1-CM1
9	L	301	BCL	C2C-C3C-CAC-CBC
9	L	301	BCL	C4C-C3C-CAC-CBC
9	L	302	BCL	C4C-C3C-CAC-CBC
9	M	403	BCL	C2C-C3C-CAC-CBC
9	M	403	BCL	C4C-C3C-CAC-CBC
10	M	404	BPH	C2C-C3C-CAC-CBC
11	L	304	U10	C12-C13-C14-C15
11	L	304	U10	C12-C13-C14-C16
11	M	406	U10	C27-C28-C29-C30
11	M	406	U10	C27-C28-C29-C31
13	L	311	HTO	O1-C1-C2-O2
13	L	311	HTO	O1-C1-C2-C3
13	L	311	HTO	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	L	311	HTO	C1-C2-C3-C4
13	L	311	HTO	O2-C2-C3-O3
13	L	311	HTO	O2-C2-C3-C4
13	L	311	HTO	O3-C3-C4-C5
13	L	312	HTO	O1-C1-C2-O2
13	L	312	HTO	C1-C2-C3-O3
13	L	312	HTO	C1-C2-C3-C4
13	L	312	HTO	O2-C2-C3-O3
13	L	312	HTO	O2-C2-C3-C4
14	M	401	CDL	CB2-C1-CA2-OA2
14	M	401	CDL	CA2-OA2-PA1-OA3
14	M	401	CDL	CA2-OA2-PA1-OA4
14	M	401	CDL	CA3-OA5-PA1-OA2
14	M	401	CDL	CA3-OA5-PA1-OA4
14	M	401	CDL	CB3-OB5-PB2-OB2
14	M	401	CDL	CB3-OB5-PB2-OB3
14	M	401	CDL	CB3-OB5-PB2-OB4
14	M	401	CDL	OB6-CB4-CB6-OB8
16	M	407	SPN	CM1-C1-O1-CMA
16	M	407	SPN	CM2-C1-O1-CMA
11	M	406	U10	C37-C38-C39-C40
16	M	407	SPN	C16-C17-C18-CM6
13	L	312	HTO	O1-C1-C2-C3
11	M	406	U10	C37-C38-C39-C41
14	M	401	CDL	O1-C1-CA2-OA2
16	M	407	SPN	C16-C17-C18-C19
11	L	304	U10	C29-C31-C32-C33
11	M	406	U10	C14-C16-C17-C18
11	M	406	U10	C19-C21-C22-C23
11	M	406	U10	C24-C26-C27-C28
11	M	406	U10	C29-C31-C32-C33
14	M	401	CDL	C39-C40-C41-C42
11	L	304	U10	C37-C38-C39-C40
11	L	304	U10	C32-C33-C34-C35
16	M	407	SPN	C26-C27-C28-C29
10	M	404	BPH	C5-C6-C7-C8
14	M	401	CDL	C31-CA7-OA8-CA6
14	M	401	CDL	C71-CB7-OB8-CB6
9	M	402	BCL	C8-C10-C11-C12
16	M	407	SPN	C11-C10-C9-CM4
11	M	406	U10	C32-C33-C34-C35
14	M	401	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
14	M	401	CDL	OB9-CB7-OB8-CB6
4	M	411	LDA	C6-C7-C8-C9
14	M	401	CDL	C78-C79-C80-C81
4	H	301	LDA	C3-C4-C5-C6
4	M	418	LDA	C2-C3-C4-C5
14	M	401	CDL	C11-C12-C13-C14
4	M	418	LDA	C4-C5-C6-C7
14	M	401	CDL	CA5-C11-C12-C13
14	M	401	CDL	C71-C72-C73-C74
14	M	401	CDL	C17-C18-C19-C20
7	L	310	EDO	O1-C1-C2-O2
7	M	416	EDO	O1-C1-C2-O2
11	L	304	U10	C37-C38-C39-C41
14	M	401	CDL	C80-C81-C82-C83
16	M	407	SPN	C11-C10-C9-C8
14	M	401	CDL	C51-C52-C53-C54
14	M	401	CDL	CB7-C71-C72-C73
14	M	401	CDL	C72-C73-C74-C75
14	M	401	CDL	C11-CA5-OA6-CA4
4	M	411	LDA	C7-C8-C9-C10
9	M	403	BCL	C15-C16-C17-C18
14	M	401	CDL	C16-C17-C18-C19
14	M	401	CDL	C36-C37-C38-C39
4	M	409	LDA	C1-C2-C3-C4
4	M	418	LDA	C9-C10-C11-C12
14	M	401	CDL	C20-C21-C22-C23
4	H	301	LDA	C7-C8-C9-C10
11	L	304	U10	C9-C11-C12-C13
4	M	418	LDA	C5-C6-C7-C8
11	M	406	U10	C23-C24-C26-C27
4	M	408	LDA	C1-C2-C3-C4
14	M	401	CDL	OA7-CA5-OA6-CA4
4	M	409	LDA	C3-C4-C5-C6
4	M	418	LDA	C7-C8-C9-C10
14	M	401	CDL	CB3-CB4-CB6-OB8
4	M	411	LDA	C1-C2-C3-C4
11	M	406	U10	C25-C24-C26-C27
10	M	404	BPH	C2-C3-C5-C6
14	M	401	CDL	C77-C78-C79-C80
4	H	301	LDA	C1-C2-C3-C4
10	L	303	BPH	O2A-C1-C2-C3
14	M	401	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
10	M	404	BPH	C10-C11-C12-C13
10	M	404	BPH	C4-C3-C5-C6
16	M	407	SPN	CM3-C5-C6-C7
14	M	401	CDL	C55-C56-C57-C58
11	L	304	U10	C34-C36-C37-C38
11	L	304	U10	C30-C29-C31-C32
4	M	409	LDA	C4-C5-C6-C7
10	M	404	BPH	C6-C7-C8-C9
14	M	401	CDL	OB5-CB3-CB4-CB6
10	M	404	BPH	C6-C7-C8-C10
4	M	410	LDA	C4-C5-C6-C7
11	M	406	U10	C20-C19-C21-C22
11	L	304	U10	C28-C29-C31-C32
14	M	401	CDL	OB5-CB3-CB4-OB6
4	M	408	LDA	C6-C7-C8-C9
14	M	401	CDL	C40-C41-C42-C43
14	M	401	CDL	C19-C20-C21-C22
11	M	406	U10	C32-C33-C34-C36
11	M	406	U10	C18-C19-C21-C22
11	L	304	U10	C5-C4-O4-C4M
9	L	302	BCL	C15-C16-C17-C18
10	M	404	BPH	C8-C10-C11-C12
4	M	410	LDA	C2-C1-N1-CM1
13	L	311	HTO	C3-C4-C5-C6
11	L	304	U10	C32-C33-C34-C36
10	M	404	BPH	C16-C17-C18-C19
10	M	404	BPH	C4C-C3C-CAC-CBC
14	M	401	CDL	CA2-OA2-PA1-OA5
14	M	401	CDL	CA3-OA5-PA1-OA3
16	M	407	SPN	C4-C5-C6-C7
10	M	404	BPH	C16-C17-C18-C20
11	L	304	U10	C20-C19-C21-C22
4	M	411	LDA	C5-C6-C7-C8
16	M	407	SPN	CM5-C13-C14-C15
11	L	304	U10	C18-C19-C21-C22
4	M	409	LDA	C7-C8-C9-C10
9	M	402	BCL	C4-C3-C5-C6
14	M	401	CDL	C14-C15-C16-C17
11	L	304	U10	C3-C4-O4-C4M
11	M	406	U10	C3-C4-O4-C4M
14	M	401	CDL	C51-CB5-OB6-CB4
10	L	303	BPH	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	L	304	U10	C35-C34-C36-C37
14	M	401	CDL	OB7-CB5-OB6-CB4
14	M	401	CDL	C52-C53-C54-C55
11	M	406	U10	C5-C4-O4-C4M
10	L	303	BPH	C2-C3-C5-C6
4	M	411	LDA	C11-C10-C9-C8
10	L	303	BPH	C4-C3-C5-C6
10	L	303	BPH	C16-C17-C18-C19
11	L	304	U10	C15-C14-C16-C17
14	M	401	CDL	CB5-C51-C52-C53
4	M	408	LDA	C9-C10-C11-C12
14	M	401	CDL	C18-C19-C20-C21
7	H	307	EDO	O1-C1-C2-O2
14	M	401	CDL	C32-C31-CA7-OA8
14	M	401	CDL	OA5-CA3-CA4-CA6
4	M	408	LDA	C5-C6-C7-C8
10	M	404	BPH	C2-C1-O2A-CGA
4	M	408	LDA	C2-C1-N1-CM2
11	L	304	U10	C33-C34-C36-C37
16	M	407	SPN	C12-C13-C14-C15
9	L	301	BCL	C2A-CAA-CBA-CGA
16	M	407	SPN	C2-C3-C4-C5
4	M	411	LDA	C9-C10-C11-C12
14	M	401	CDL	C72-C71-CB7-OB8
11	M	406	U10	C22-C23-C24-C25
9	M	402	BCL	C2-C1-O2A-CGA
9	M	402	BCL	C2-C3-C5-C6
4	M	408	LDA	C7-C8-C9-C10
14	M	401	CDL	C32-C31-CA7-OA9
14	M	401	CDL	OA5-CA3-CA4-OA6
14	M	401	CDL	C72-C71-CB7-OB9
4	M	411	LDA	C4-C5-C6-C7
4	M	408	LDA	C2-C1-N1-O1
10	M	404	BPH	CAD-CBD-CGD-O2D
11	L	304	U10	C16-C17-C18-C19

There are no ring outliers.

18 monomers are involved in 46 short contacts:

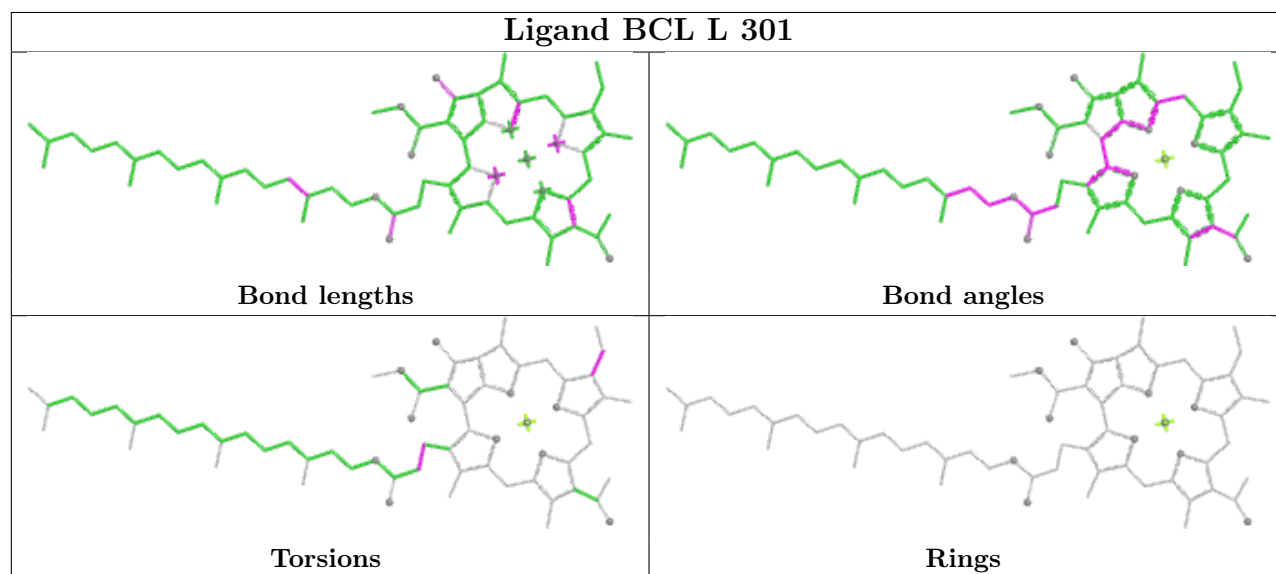
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	308	EDO	1	0
9	L	301	BCL	5	0

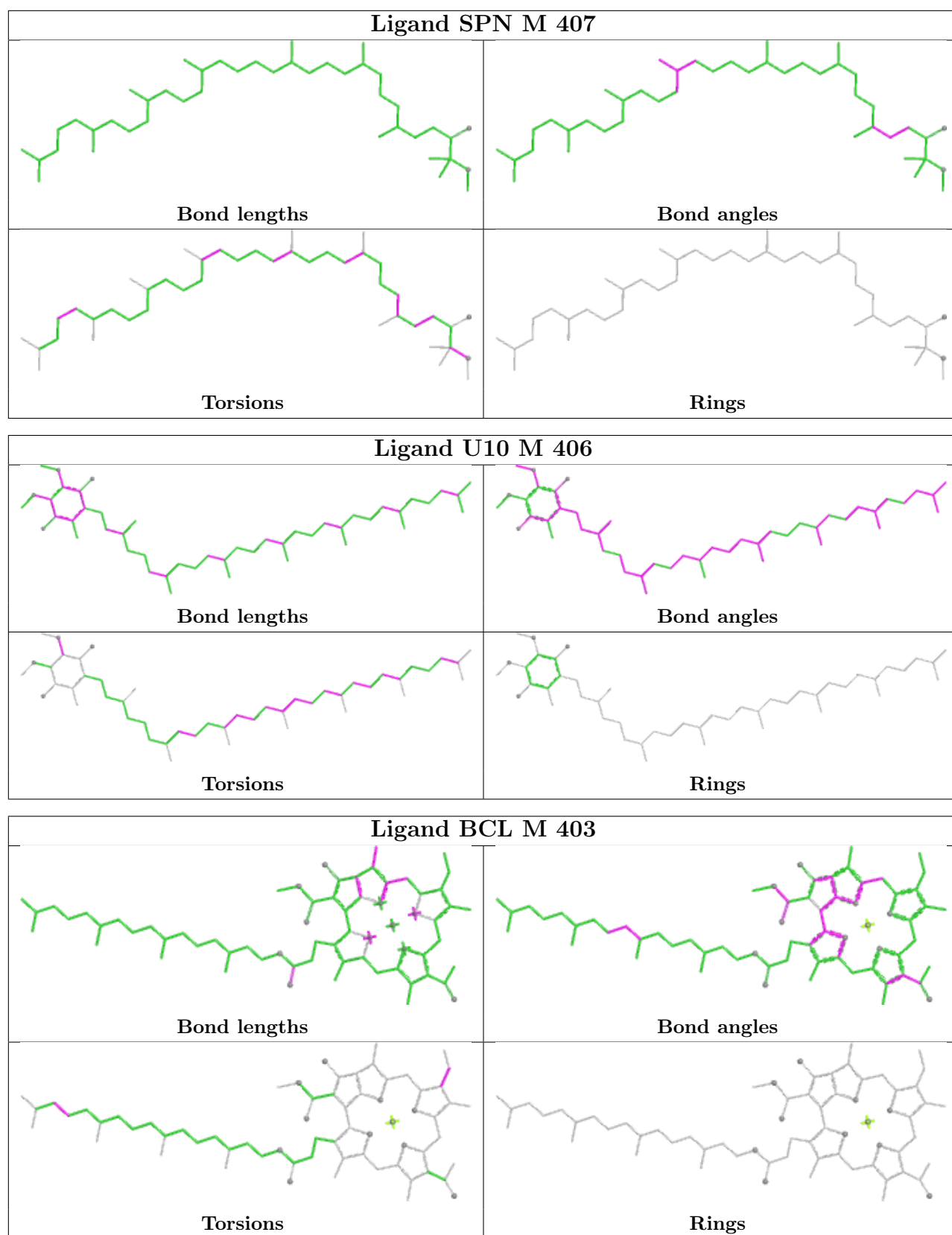
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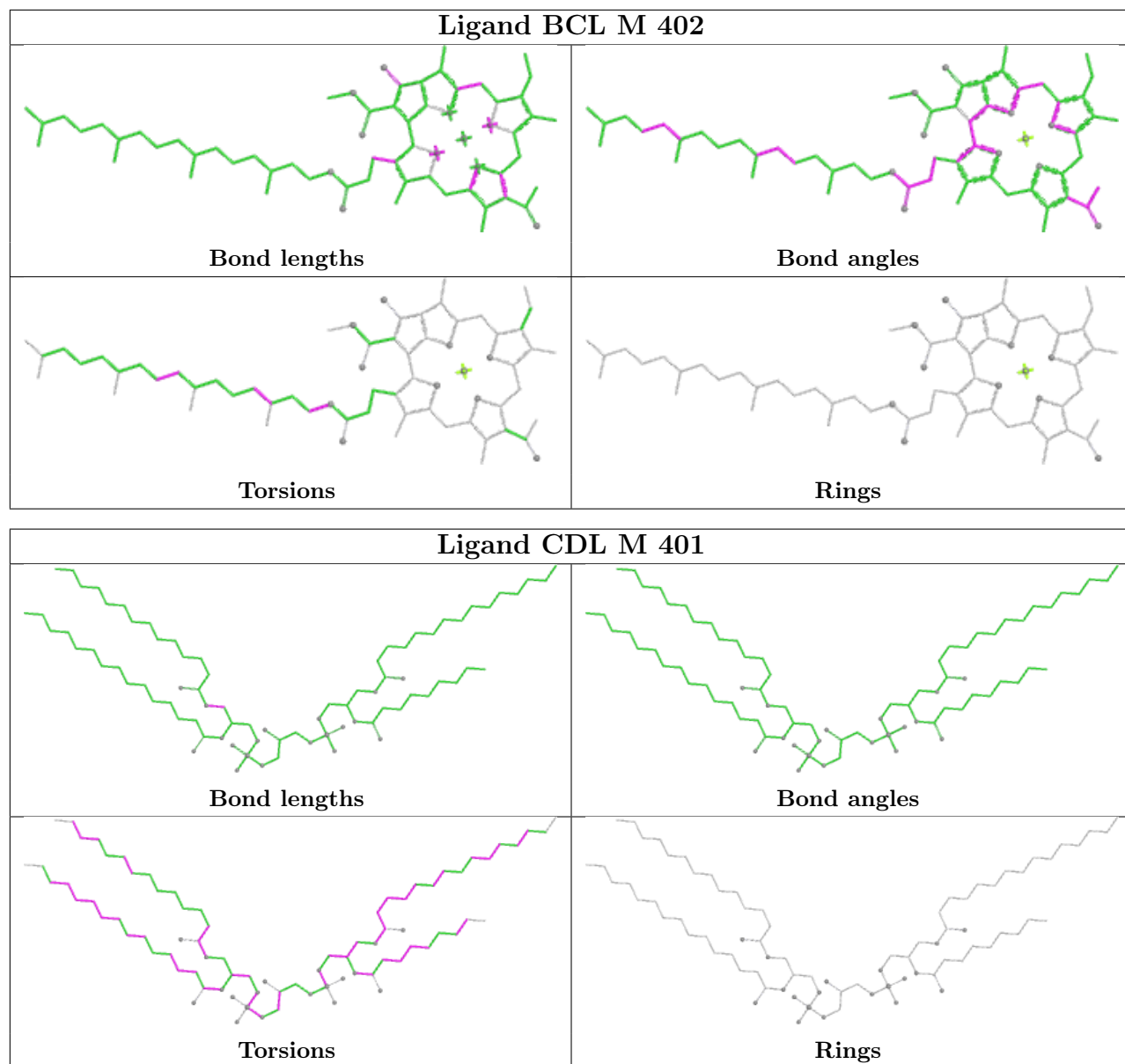
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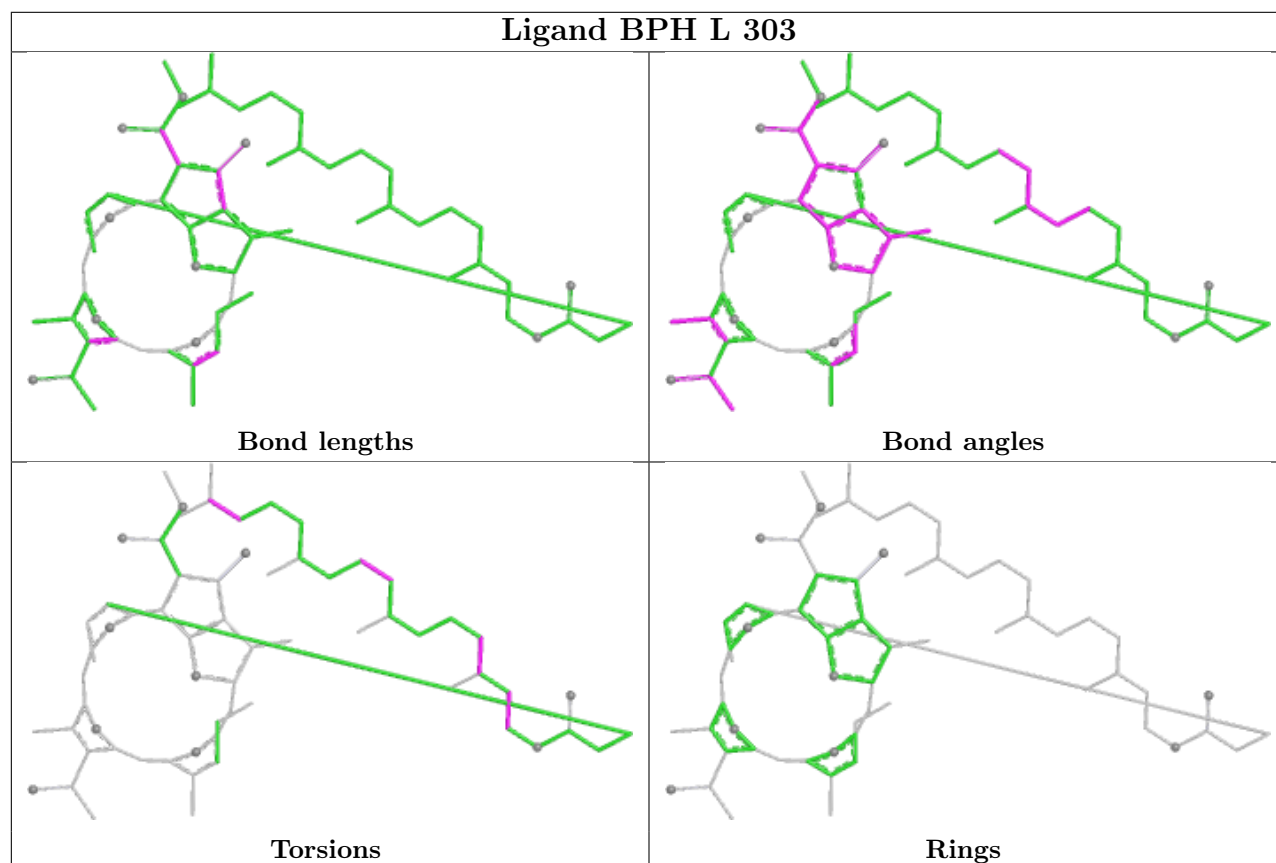
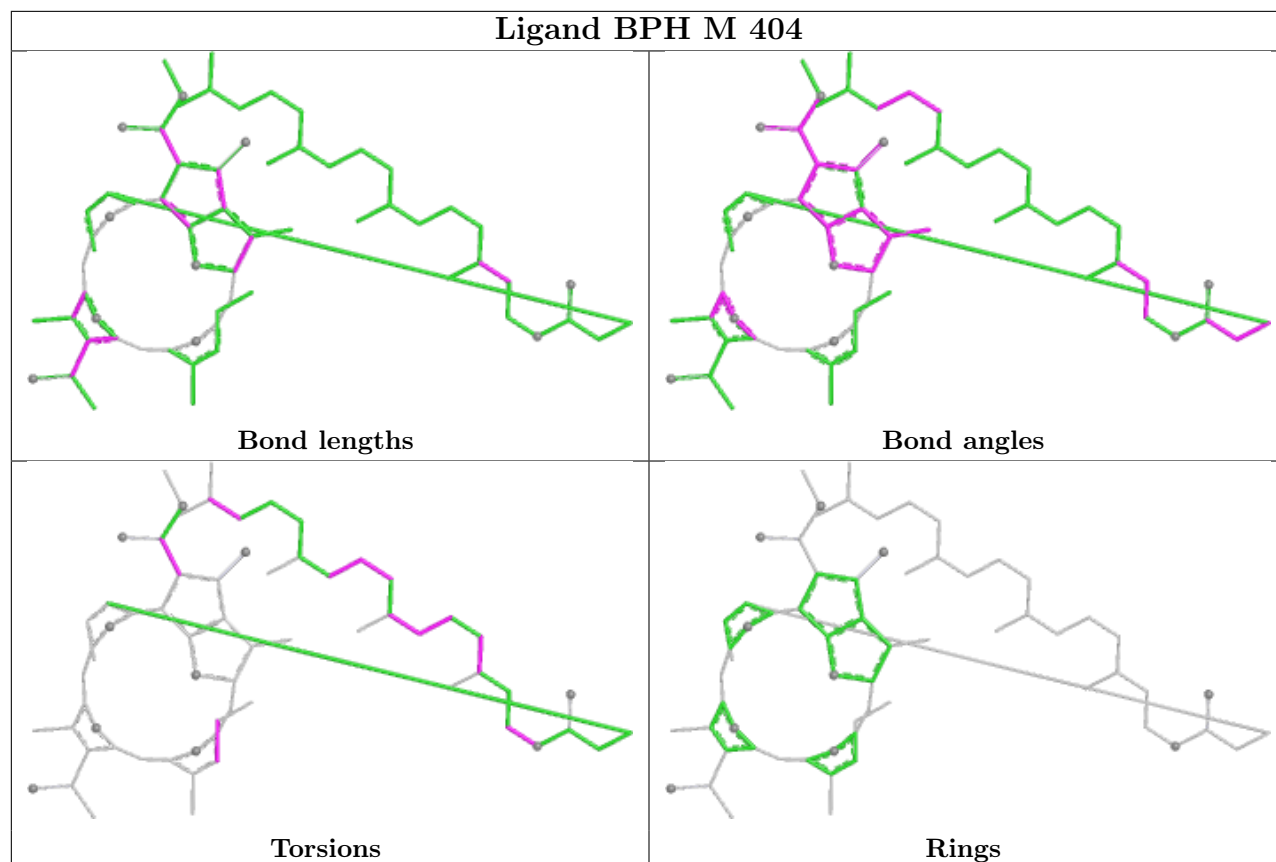
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	407	SPN	6	0
7	M	416	EDO	2	0
12	L	309	DIO	1	0
11	M	406	U10	3	0
9	M	403	BCL	6	0
9	M	402	BCL	3	0
4	M	408	LDA	1	0
4	M	410	LDA	1	0
14	M	401	CDL	10	0
10	M	404	BPH	4	0
4	H	301	LDA	3	0
4	M	418	LDA	2	0
7	H	310	EDO	1	0
10	L	303	BPH	1	0
11	L	304	U10	3	0
9	L	302	BCL	3	0

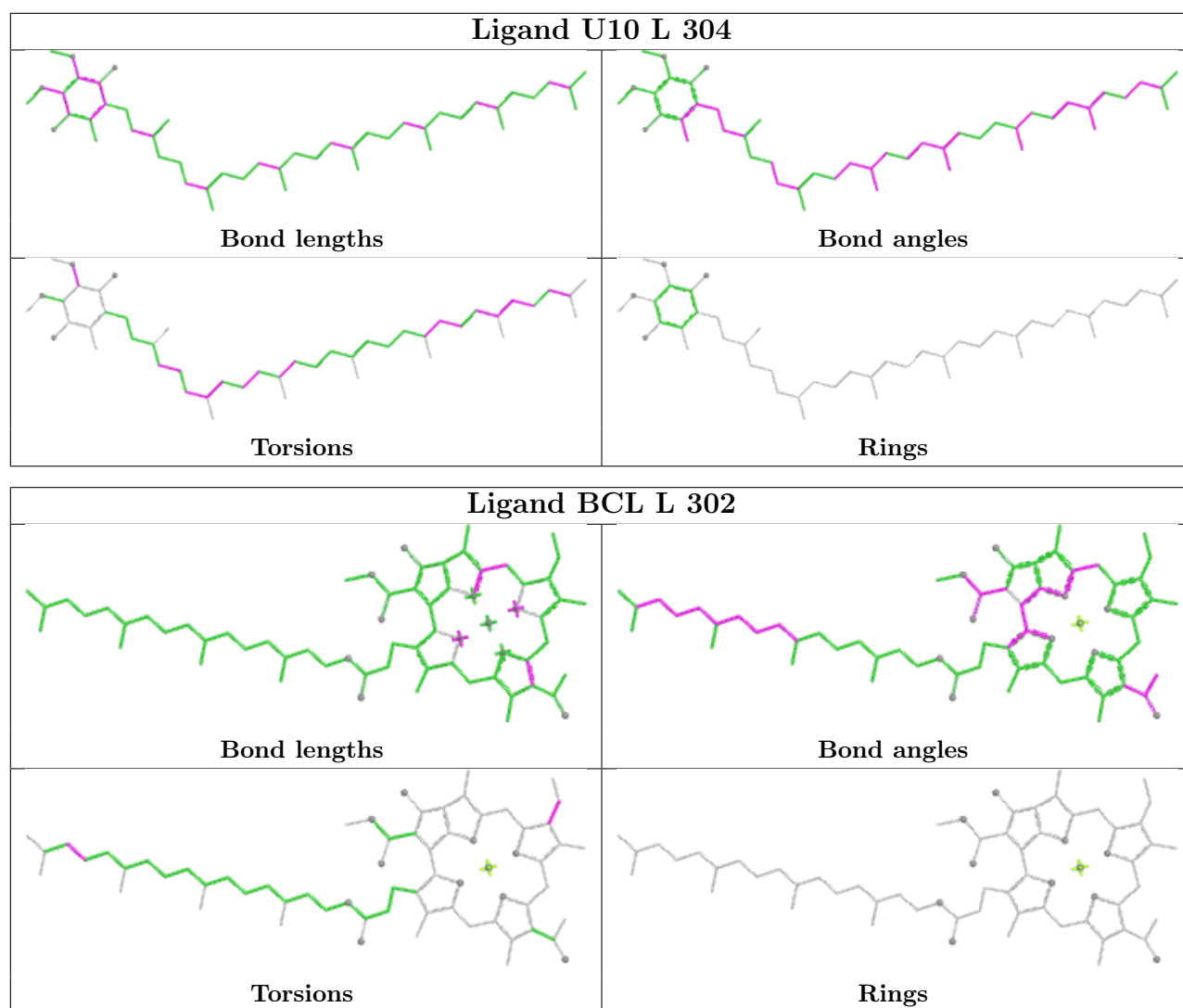
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	240/242 (99%)	-0.14	1 (0%) 88 87	3, 12, 31, 88	3 (1%)
2	L	281/281 (100%)	0.03	7 (2%) 58 49	2, 11, 45, 99	1 (0%)
3	M	302/303 (99%)	-0.02	4 (1%) 75 68	2, 12, 33, 64	4 (1%)
All	All	823/826 (99%)	-0.04	12 (1%) 72 65	2, 12, 36, 99	8 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	8.4
3	M	302	GLY	5.5
1	H	250	SER	4.9
2	L	51	TRP	3.5
2	L	56	GLN	3.1
2	L	54	VAL	2.5
2	L	50	ALA	2.5
3	M	300	ASN	2.5
2	L	61	PRO	2.4
2	L	281	GLY	2.3
3	M	3	TYR	2.2
3	M	1	ALA	2.1

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
4	LDA	M	409	16/16	0.77	0.22	6,25,61,69	0
4	LDA	M	411	16/16	0.77	0.26	22,46,70,71	0
6	PO4	M	415	5/5	0.78	0.27	16,32,55,61	5
4	LDA	M	410	16/16	0.79	0.22	12,22,71,79	0
4	LDA	M	418	16/16	0.80	0.22	31,42,60,62	0
11	U10	L	304	48/63	0.80	0.21	7,25,39,51	0
14	CDL	M	401	81/100	0.80	0.23	5,45,99,121	0
5	UNL	M	413	12/-	0.81	0.22	12,25,37,40	0
13	HTO	L	311	10/10	0.81	0.24	13,40,50,61	10
5	UNL	L	308	12/-	0.81	0.23	6,30,58,62	0
13	HTO	L	312	10/10	0.82	0.38	22,64,78,78	0
5	UNL	L	307	10/-	0.82	0.32	19,42,59,70	0
7	EDO	H	310	4/4	0.85	0.18	17,21,30,33	0
5	UNL	H	303	12/-	0.85	0.22	18,25,44,56	0
12	DIO	L	309	6/6	0.85	0.19	25,31,37,37	0
5	UNL	H	304	12/-	0.86	0.16	14,34,46,52	0
5	UNL	H	305	15/-	0.86	0.20	1,31,51,60	0
4	LDA	H	301	16/16	0.87	0.16	14,27,43,44	0
5	UNL	M	412	15/-	0.87	0.15	15,20,35,39	0
5	UNL	L	305	12/-	0.88	0.20	15,30,40,48	0
7	EDO	H	309	4/4	0.89	0.17	12,16,34,35	0
6	PO4	H	306	5/5	0.90	0.15	29,55,63,72	0
5	UNL	H	302	12/-	0.90	0.12	6,17,24,39	0
5	UNL	L	306	15/-	0.90	0.17	5,18,41,48	0
4	LDA	M	408	16/16	0.92	0.12	1,9,25,26	0
7	EDO	L	310	4/4	0.92	0.16	19,31,40,44	0
7	EDO	M	417	4/4	0.92	0.14	6,8,9,10	0
6	PO4	M	414	5/5	0.92	0.09	22,24,52,58	0
7	EDO	H	308	4/4	0.93	0.13	20,43,44,55	0
7	EDO	H	307	4/4	0.93	0.14	9,14,15,19	0
16	SPN	M	407	43/43	0.93	0.13	2,14,30,56	0
11	U10	M	406	48/63	0.94	0.11	1,8,26,43	0
10	BPH	M	404	65/65	0.94	0.11	2,12,48,64	0
8	K	H	311	1/1	0.94	0.06	19,19,19,19	0
9	BCL	M	403	66/66	0.95	0.10	1,4,19,28	0
7	EDO	M	416	4/4	0.95	0.14	19,23,27,36	0
9	BCL	L	302	66/66	0.95	0.09	1,7,18,30	0

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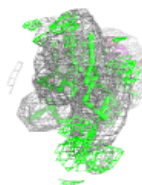
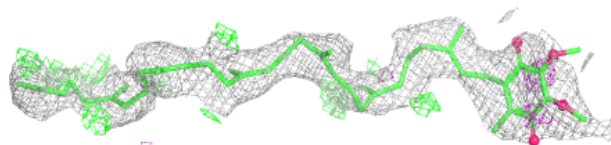
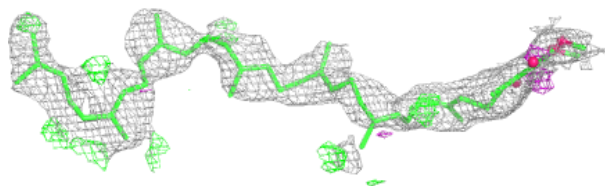
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	BPH	L	303	65/65	0.96	0.08	1,5,13,22	0
9	BCL	M	402	66/66	0.96	0.09	1,7,30,41	0
9	BCL	L	301	66/66	0.96	0.09	1,3,11,24	0
15	FE	M	405	1/1	1.00	0.02	6,6,6,6	0

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

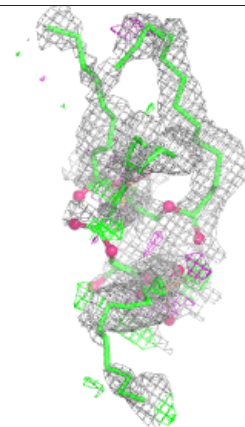
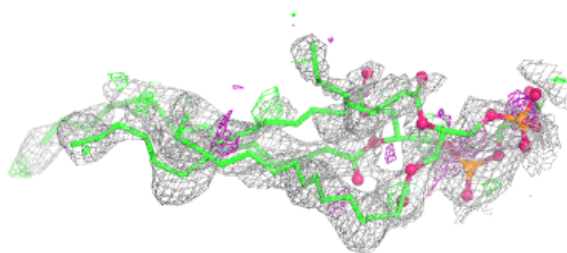
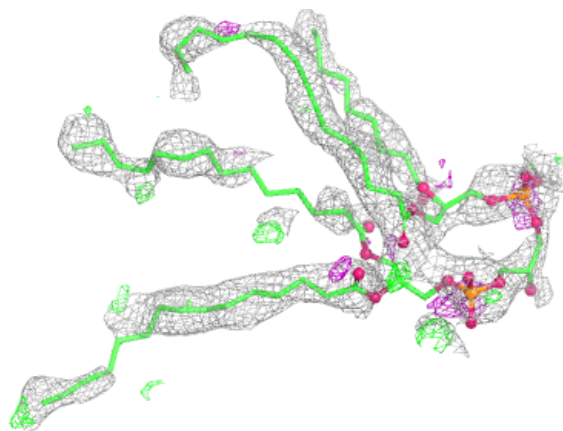
Electron density around U10 L 304:

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

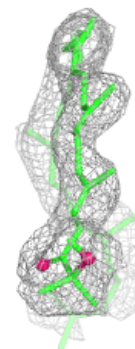
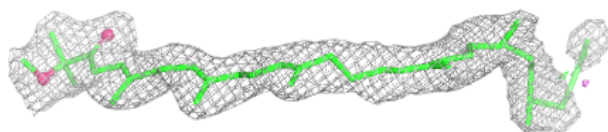
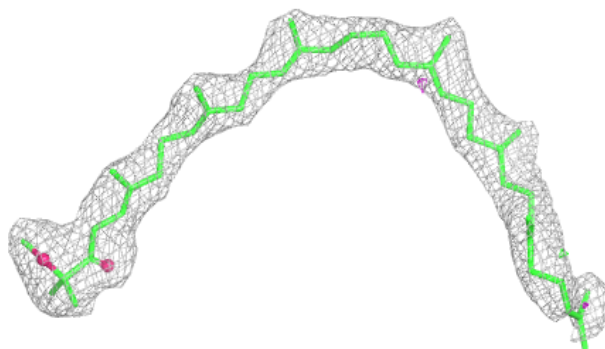


Electron density around CDL M 401:

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

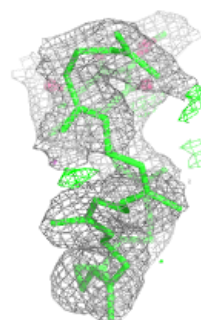
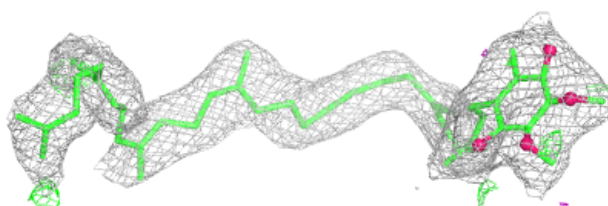
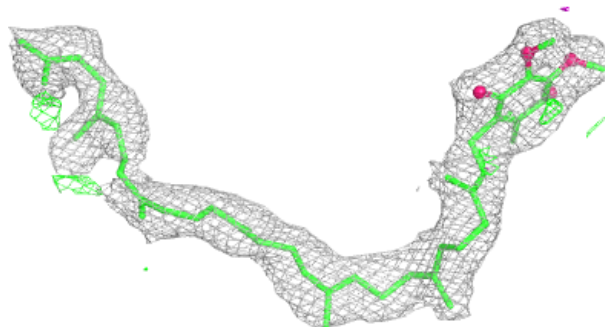
**Electron density around SPN M 407:**

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

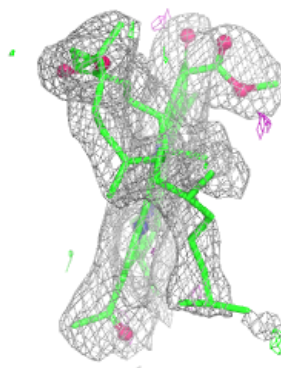
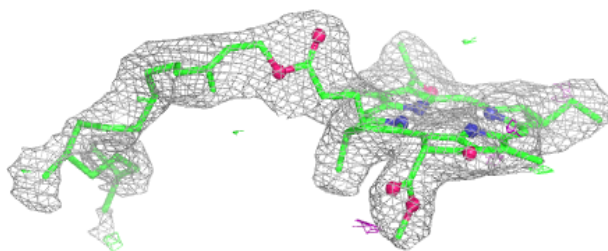
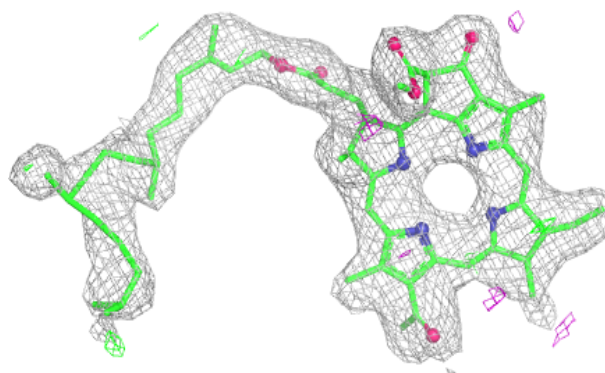


Electron density around U10 M 406:

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

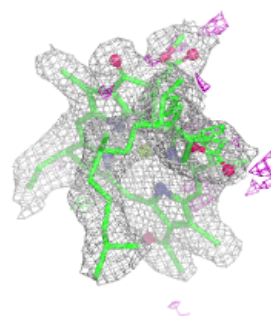
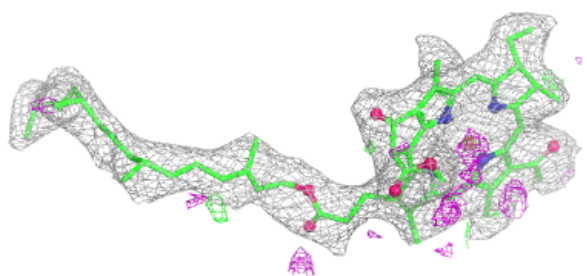
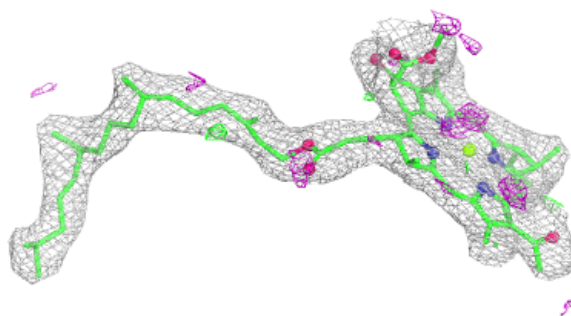
**Electron density around BPH M 404:**

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and green (positive)

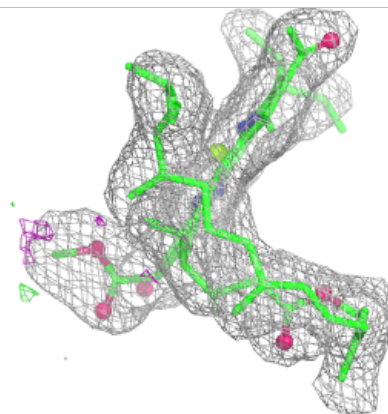
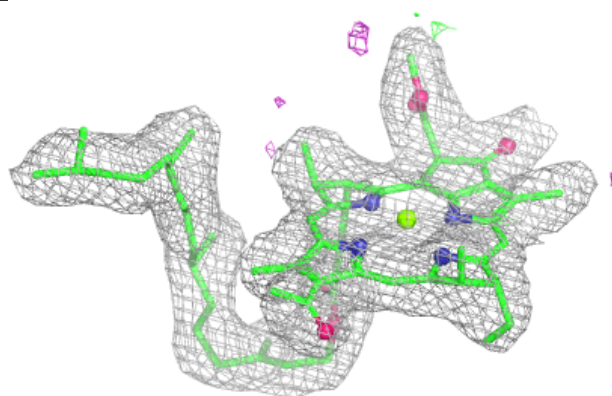
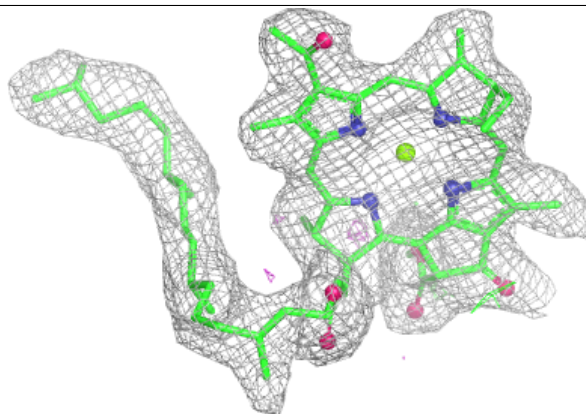


Electron density around BCL M 403:

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

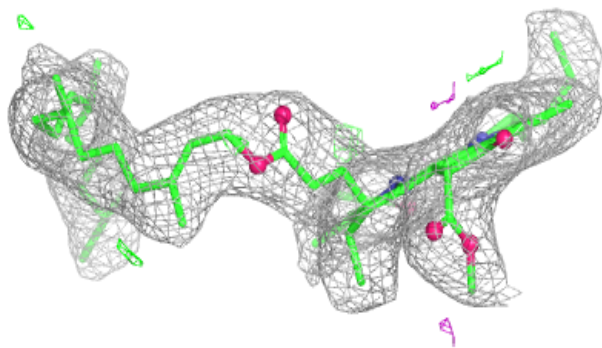
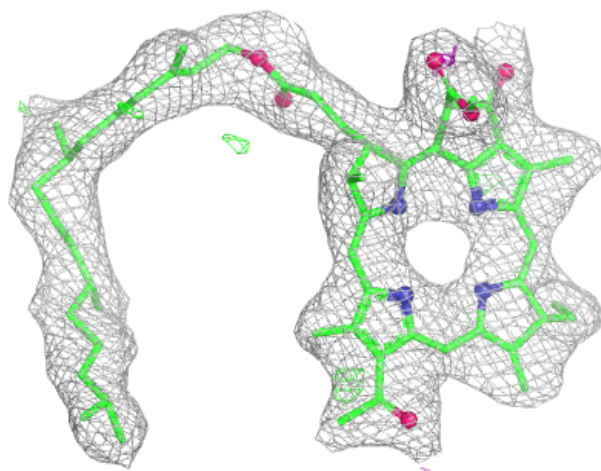
**Electron density around BCL L 302:**

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



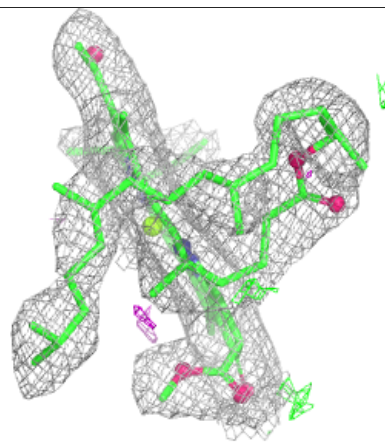
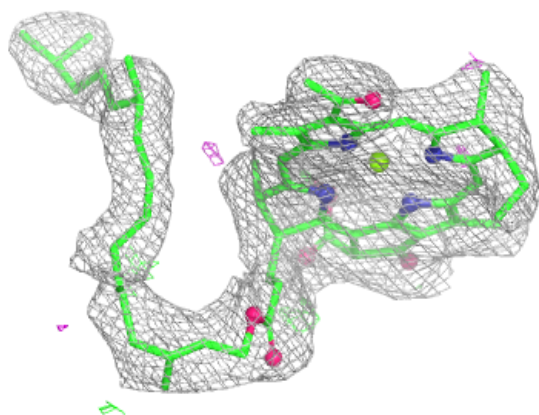
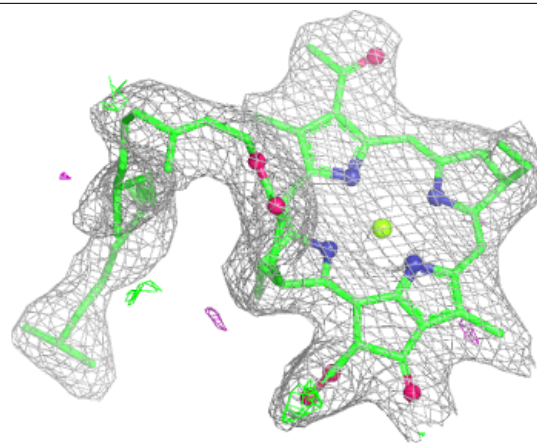
Electron density around BPH L 303:

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



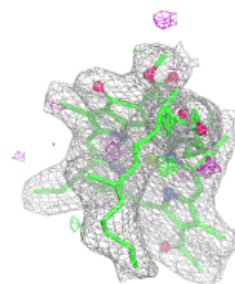
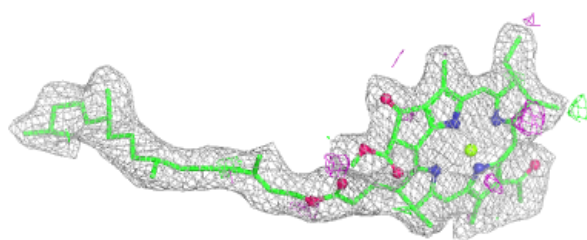
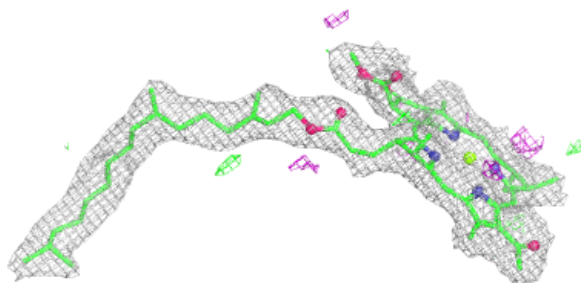
Electron density around BCL M 402:

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



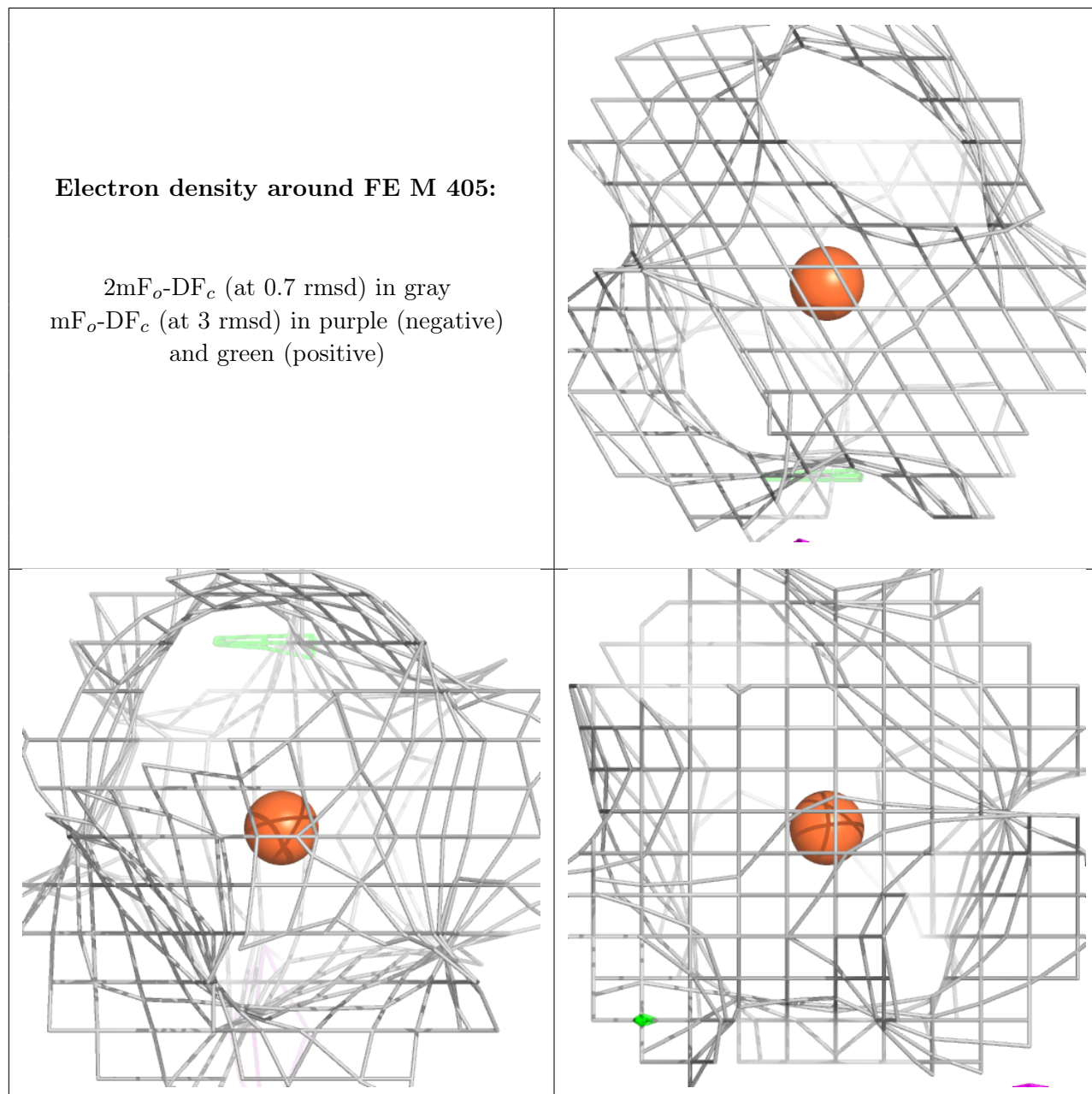
Electron density around BCL L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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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.