



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:39 PM EDT

PDB ID : 4LWY / pdb_00004lwy
Title : L(M196)H,H(M202)L Double Mutant Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors : Gabdulkhakov, A.G.
Deposited on : 2013-07-29
Resolution : 2.90 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	:	9.0.015 (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

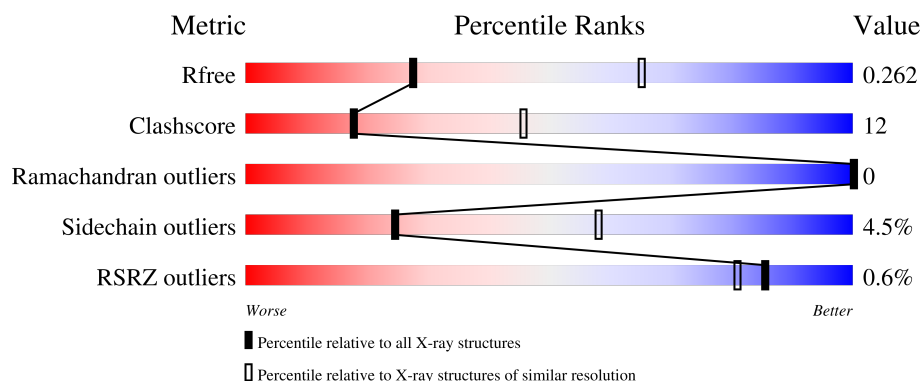
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	260	
2	L	282	
3	M	303	

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
12	BPH	L	303	X	-	-	-
12	BPH	M	402	X	-	-	-
12	BPH	M	404	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7434 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	0	0
			1829	1169	314	337	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	0	0
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

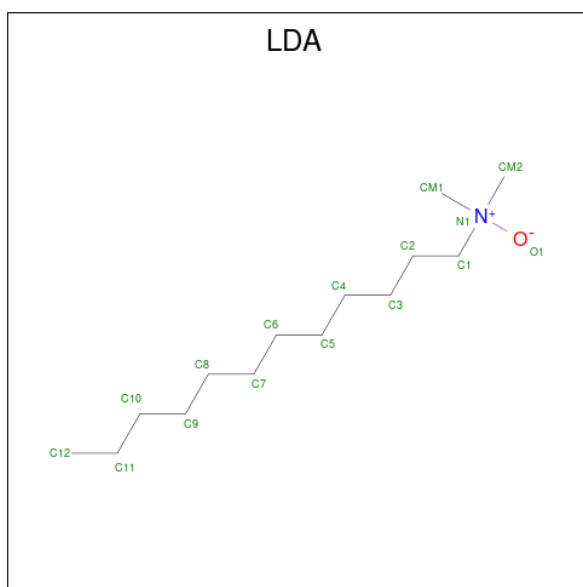
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9
M	196	HIS	LEU	engineered mutation	UNP P0C0Y9
M	202	LEU	HIS	engineered mutation	UNP P0C0Y9

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

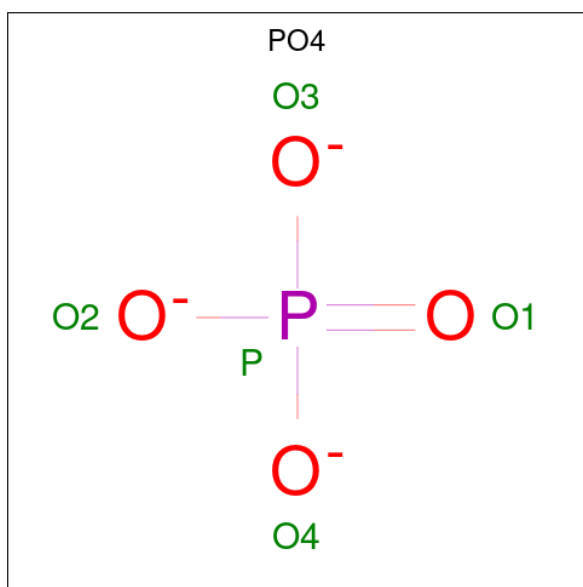


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

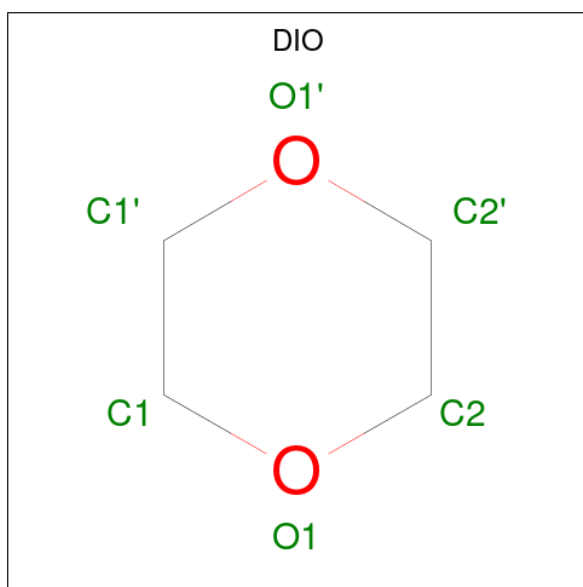
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	4	Total	C	0	0
			48	48		
5	L	4	Total	C	0	0
			46	46		
5	M	3	Total	C	0	0
			36	36		

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



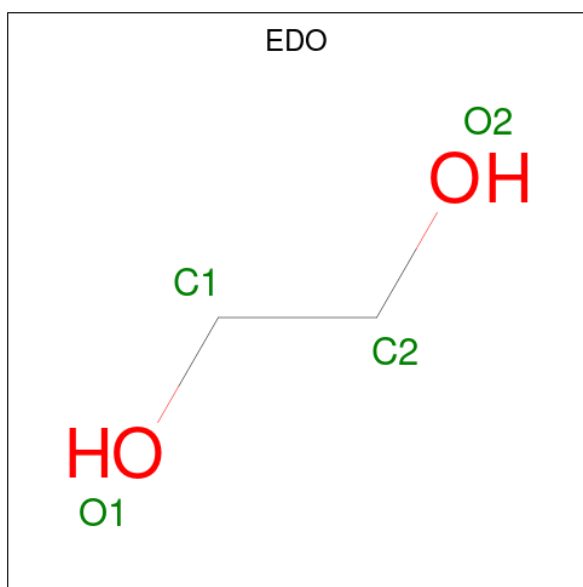
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	4	2		

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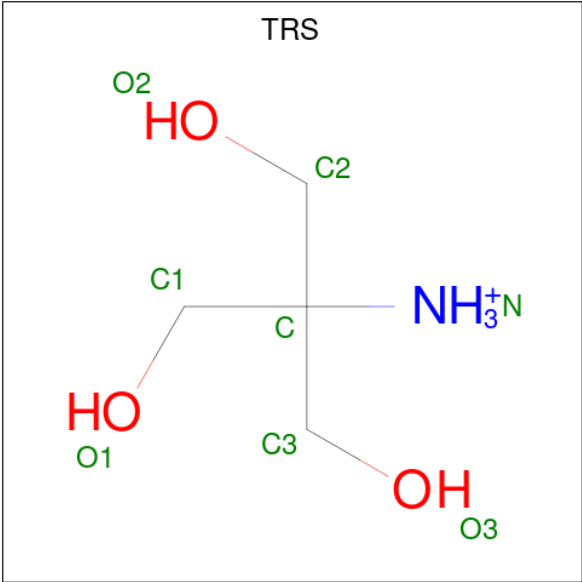
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	4	2		
7	L	1	Total	C	O	0	0
			6	4	2		
7	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

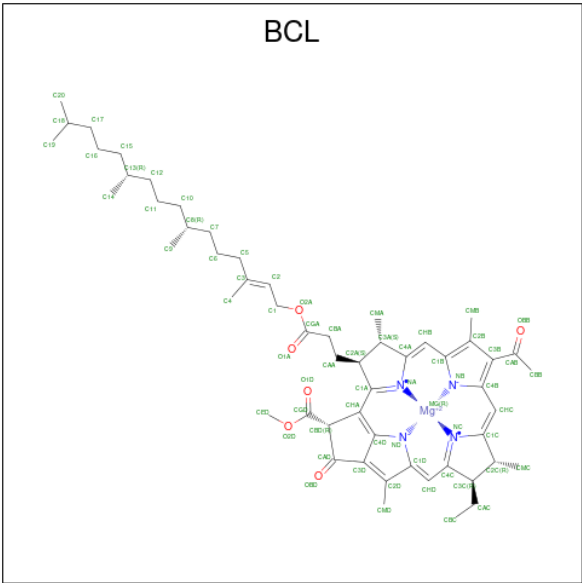


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			8	4	1	3		
9	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

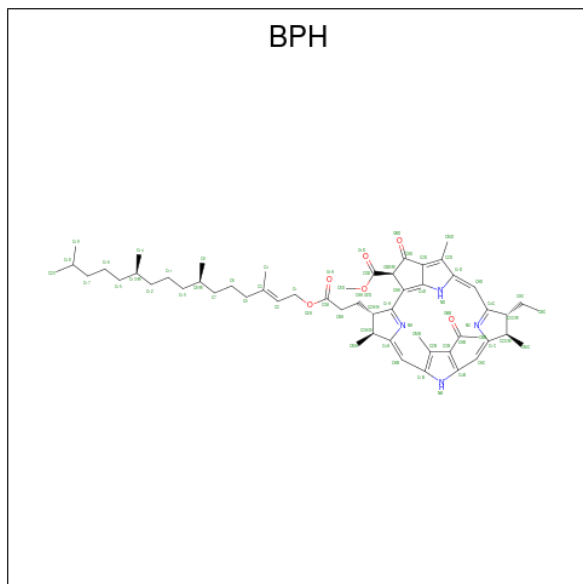
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total	K	0	0
			1	1		

- Molecule 11 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



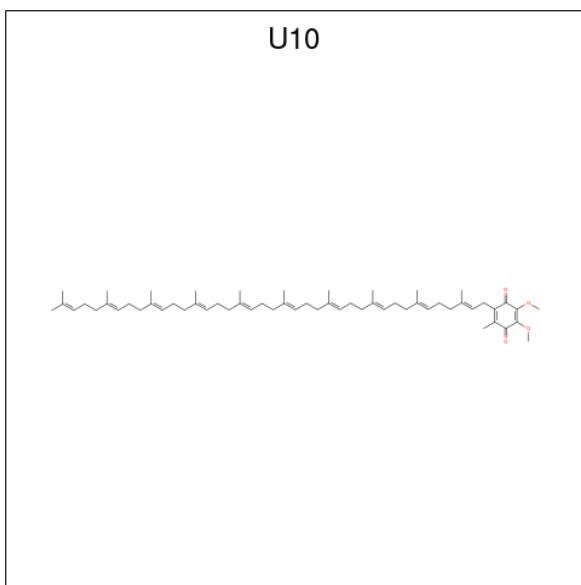
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 12 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



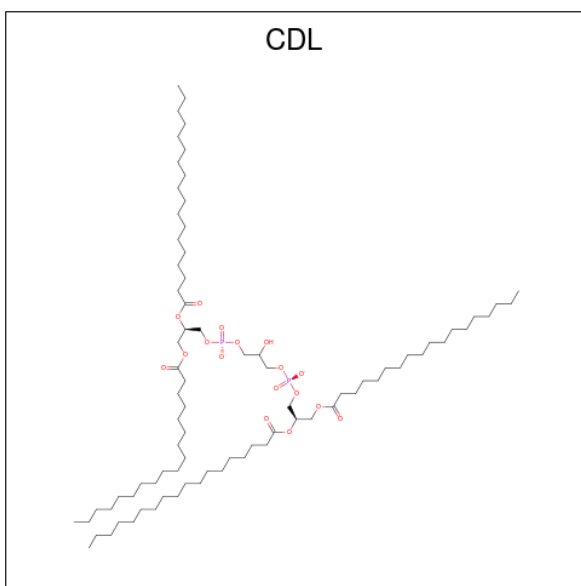
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

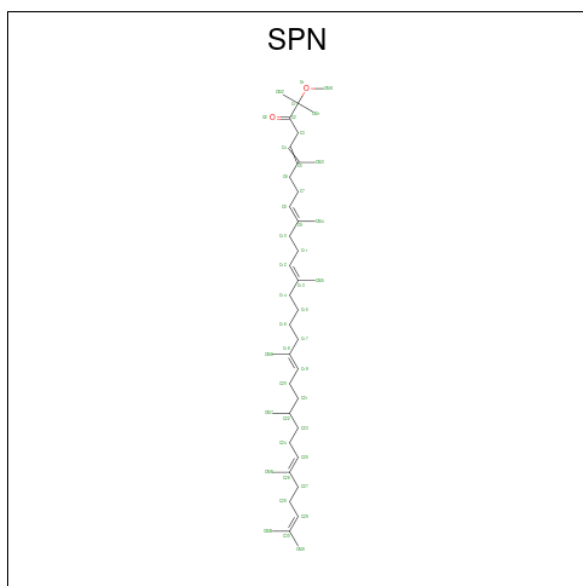


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 16 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



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

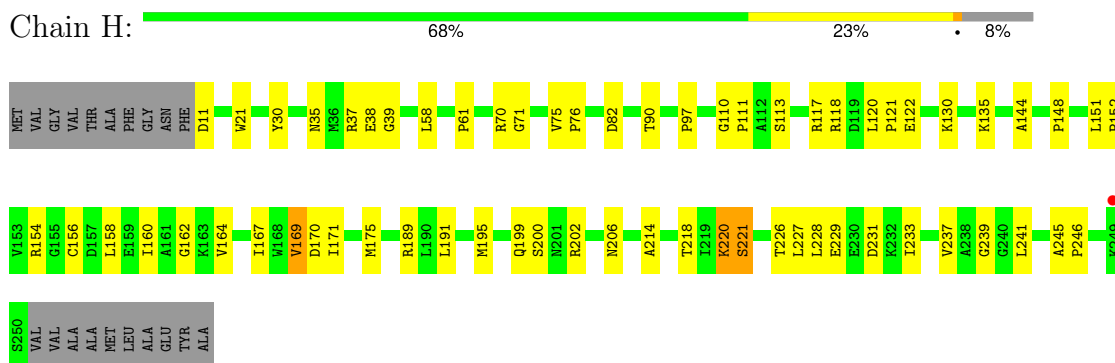
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	11	Total	O	0	0
			11	11		
17	L	10	Total	O	0	0
			10	10		
17	M	18	Total	O	0	0
			18	18		

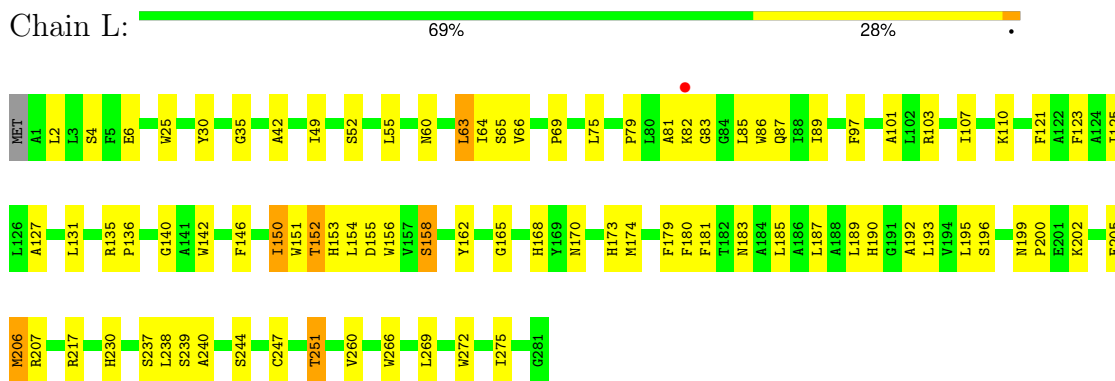
3 Residue-property plots

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

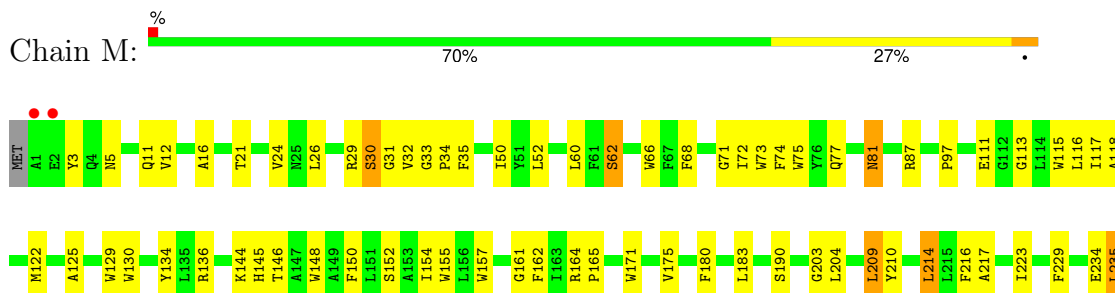
• Molecule 1: Reaction center protein H chain

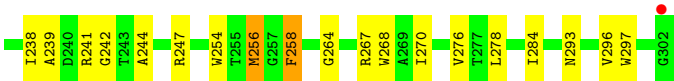


• Molecule 2: Reaction center protein L chain



• 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	140.04Å 140.04Å 184.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.19 – 2.90 43.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.90) 99.8 (43.19-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, R_{free}	0.214 , 0.262 0.215 , 0.262	Depositor DCC
R_{free} test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, EDO, SPN, LDA, BCL, U10, DIO, K, TRS, BPH, UNL, CDL, 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	0.54	0/1877	0.99	5/2553 (0.2%)
2	L	0.57	0/2321	0.89	5/3177 (0.2%)
3	M	0.55	0/2501	0.94	5/3415 (0.1%)
All	All	0.56	0/6699	0.94	15/9145 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	81	ASN	CA-C-N	7.01	127.61	119.47
3	M	81	ASN	C-N-CA	7.01	127.61	119.47
1	H	221	SER	CA-C-N	-6.99	111.10	119.84
1	H	221	SER	C-N-CA	-6.99	111.10	119.84
1	H	171	ILE	CA-C-N	-6.32	113.18	119.56
1	H	171	ILE	C-N-CA	-6.32	113.18	119.56
2	L	155	ASP	N-CA-C	-6.12	104.53	111.14
3	M	175	VAL	CA-C-N	5.97	126.44	119.99
3	M	175	VAL	C-N-CA	5.97	126.44	119.99
2	L	269	LEU	CA-C-N	5.63	125.30	119.05
2	L	269	LEU	C-N-CA	5.63	125.30	119.05
1	H	164	VAL	CB-CA-C	-5.53	104.23	111.25
2	L	35	GLY	N-CA-C	-5.17	106.15	112.77
3	M	256	MET	N-CA-C	5.10	119.19	112.92
2	L	131	LEU	N-CA-C	5.08	117.20	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	42	0
2	L	2233	0	2189	67	0
3	M	2409	0	2323	79	0
4	H	16	0	31	2	0
4	M	80	0	155	9	0
5	H	48	0	0	0	0
5	L	46	0	0	0	0
5	M	36	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0
7	H	6	0	8	0	0
7	L	12	0	16	3	0
7	M	6	0	8	1	0
8	H	16	0	24	3	0
8	L	4	0	6	1	0
8	M	8	0	12	1	0
9	H	8	0	12	1	0
9	L	8	0	12	0	0
10	H	1	0	0	0	0
11	L	132	0	148	10	0
11	M	66	0	74	3	0
12	L	65	0	76	10	0
12	M	130	0	152	12	0
13	L	48	0	63	1	0
13	M	48	0	63	5	0
14	M	81	0	106	7	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	10	0	0	0	0
17	M	18	0	0	1	0
All	All	7434	0	7384	181	0

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

All (181) 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:34:PRO:HA	4:M:412:LDA:H71	1.55	0.89
2:L:200:PRO:HD2	7:L:309:DIO:H22	1.64	0.80
1:H:202:ARG:HH12	9:H:312:TRS:H21	1.53	0.73
2:L:42:ALA:HA	12:L:303:BPH:H9C3	1.71	0.73
2:L:65:SER:HB2	2:L:152:THR:HG21	1.70	0.72
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.74	0.70
2:L:199:ASN:HA	7:L:309:DIO:H21	1.74	0.70
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.75	0.68
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.73	0.68
2:L:55:LEU:HD13	2:L:81:ALA:HB2	1.74	0.68
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.75	0.68
3:M:35:PHE:H	4:M:412:LDA:H51	1.61	0.66
12:M:404:BPH:HHC	12:M:404:BPH:HBB3	1.78	0.66
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.79	0.64
2:L:60:ASN:HB3	2:L:63:LEU:HB2	1.80	0.64
1:H:152:PRO:HB2	1:H:160:ILE:HD12	1.79	0.63
2:L:205:GLU:O	2:L:207:ARG:NH1	2.32	0.63
12:L:303:BPH:H7C2	11:M:403:BCL:H201	1.81	0.63
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.31	0.62
1:H:160:ILE:HG22	1:H:162:GLY:H	1.65	0.62
3:M:75:TRP:HE1	16:M:407:SPN:HMA2	1.65	0.60
2:L:266:TRP:CD2	7:M:418:DIO:H11	2.36	0.60
12:M:402:BPH:H172	12:M:404:BPH:H9C2	1.83	0.60
12:L:303:BPH:H112	11:M:403:BCL:H201	1.84	0.59
1:H:121:PRO:HA	1:H:226:THR:HA	1.84	0.58
1:H:71:GLY:H	8:H:310:EDO:H22	1.68	0.58
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.39	0.58
2:L:2:LEU:HB3	2:L:6:GLU:HB3	1.87	0.57
4:H:301:LDA:H121	4:M:408:LDA:H91	1.86	0.57
3:M:152:SER:O	3:M:155:TRP:HB3	2.05	0.57
1:H:117:ARG:O	1:H:228:LEU:HB2	2.05	0.56
2:L:146:PHE:HA	2:L:156:TRP:CD1	2.40	0.56
12:L:303:BPH:HBB2	3:M:210:TYR:HB3	1.87	0.56
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.87	0.56
2:L:150:ILE:HG22	2:L:151:TRP:CD1	2.40	0.56
12:L:303:BPH:HMA1	13:M:406:U10:H252	1.88	0.56
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.88	0.56
3:M:31:GLY:H	4:M:410:LDA:HM11	1.70	0.55
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.42	0.55
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.89	0.55
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.89	0.55
2:L:60:ASN:O	2:L:63:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:THR:OG1	1:H:97:PRO:O	2.22	0.54
1:H:156:CYS:HB3	1:H:206:ASN:O	2.08	0.54
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.90	0.54
1:H:11:ASP:OD2	3:M:297:TRP:NE1	2.41	0.54
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.42	0.53
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.88	0.53
3:M:122:MET:HE2	12:M:402:BPH:H142	1.91	0.53
3:M:190:SER:HB2	12:M:402:BPH:H3C	1.89	0.53
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.90	0.53
2:L:179:PHE:CD2	2:L:239:SER:HB3	2.45	0.52
3:M:148:TRP:HB3	14:M:401:CDL:H761	1.92	0.52
3:M:256:MET:HE3	3:M:258:PHE:CZ	2.45	0.51
2:L:180:PHE:HB3	3:M:209:LEU:HD21	1.91	0.51
3:M:157:TRP:CZ2	16:M:407:SPN:HM73	2.46	0.51
12:L:303:BPH:H152	11:M:403:BCL:H202	1.92	0.51
1:H:21:TRP:HZ2	4:M:408:LDA:HM13	1.75	0.51
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.46	0.51
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.93	0.50
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.45	0.50
4:H:301:LDA:H112	13:M:406:U10:H202	1.92	0.50
2:L:127:ALA:HB3	11:L:302:BCL:H43	1.94	0.50
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.94	0.50
1:H:113:SER:O	3:M:247:ARG:NH1	2.45	0.50
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.09	0.49
12:L:303:BPH:H3C	3:M:214:LEU:HA	1.93	0.49
1:H:30:TYR:OH	3:M:267:ARG:NH1	2.45	0.49
2:L:181:PHE:CD2	12:M:404:BPH:HBB1	2.48	0.49
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.12	0.49
2:L:190:HIS:HA	13:L:304:U10:O2	2.13	0.49
3:M:268:TRP:CD1	13:M:406:U10:H111	2.48	0.49
2:L:97:PHE:CE1	11:L:302:BCL:H121	2.48	0.49
2:L:153:HIS:CE1	12:L:303:BPH:H201	2.47	0.49
3:M:203:GLY:HA3	4:M:408:LDA:HM21	1.95	0.49
3:M:130:TRP:HD1	3:M:150:PHE:HD2	1.61	0.49
3:M:278:LEU:HD11	14:M:401:CDL:H811	1.94	0.49
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.95	0.48
2:L:185:LEU:HD13	12:M:404:BPH:ND	2.28	0.48
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.96	0.48
11:L:301:BCL:H61	12:M:402:BPH:H203	1.95	0.47
2:L:123:PHE:CD1	2:L:238:LEU:HD13	2.48	0.47
2:L:162:TYR:HA	2:L:165:GLY:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:204:LEU:HG	4:M:408:LDA:HM11	1.97	0.47
1:H:189:ARG:NH2	1:H:214:ALA:O	2.40	0.47
3:M:130:TRP:HD1	3:M:150:PHE:CD2	2.32	0.47
1:H:154:ARG:HG2	1:H:158:LEU:HA	1.97	0.47
2:L:60:ASN:O	2:L:64:ILE:HG13	2.15	0.47
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.96	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.50	0.47
2:L:75:LEU:HD11	2:L:140:GLY:HA2	1.96	0.47
2:L:79:PRO:HB2	2:L:82:LYS:HG3	1.97	0.47
3:M:164:ARG:HD2	3:M:284:ILE:HG22	1.96	0.47
11:L:301:BCL:HHC	12:M:402:BPH:H4C2	1.97	0.46
3:M:157:TRP:CE2	16:M:407:SPN:HM73	2.50	0.46
14:M:401:CDL:H391	14:M:401:CDL:H422	1.69	0.46
1:H:199:GLN:OE1	1:H:202:ARG:NH1	2.48	0.46
2:L:69:PRO:HD3	2:L:83:GLY:O	2.16	0.46
1:H:35:ASN:OD1	3:M:264:GLY:HA3	2.16	0.46
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.98	0.46
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.51	0.46
3:M:144:LYS:NZ	14:M:401:CDL:OB4	2.49	0.46
1:H:220:LYS:HG3	1:H:229:GLU:OE2	2.16	0.45
2:L:97:PHE:HB3	2:L:125:ILE:HD11	1.98	0.45
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.98	0.45
2:L:199:ASN:HA	7:L:309:DIO:C2	2.46	0.45
1:H:118:ARG:HG2	1:H:120:LEU:HG	1.99	0.45
12:L:303:BPH:CBB	3:M:210:TYR:HB3	2.47	0.45
3:M:234:GLU:O	3:M:238:ILE:HG13	2.17	0.45
13:M:406:U10:H28	13:M:406:U10:H322	1.44	0.45
1:H:110:GLY:HA3	1:H:111:PRO:HD2	1.83	0.45
4:M:412:LDA:H21	4:M:412:LDA:HM23	1.61	0.45
3:M:144:LYS:HB2	14:M:401:CDL:HB32	1.98	0.45
1:H:70:ARG:O	1:H:118:ARG:NH2	2.50	0.45
3:M:256:MET:CE	13:M:406:U10:H102	2.47	0.45
11:L:301:BCL:HBB2	12:M:402:BPH:H102	1.98	0.44
11:L:302:BCL:H161	11:L:302:BCL:H192	1.68	0.44
3:M:24:VAL:HG11	3:M:29:ARG:HH11	1.82	0.44
1:H:241:LEU:HD13	8:M:419:EDO:H11	1.98	0.44
2:L:244:SER:OG	11:L:302:BCL:HMA2	2.18	0.44
3:M:35:PHE:N	4:M:412:LDA:H51	2.30	0.44
1:H:245:ALA:N	1:H:246:PRO:HD2	2.32	0.44
2:L:189:LEU:HD23	2:L:189:LEU:HA	1.85	0.44
2:L:237:SER:HB3	3:M:217:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:66:VAL:HG12	2:L:86:TRP:HB2	2.00	0.44
2:L:52:SER:OG	8:L:311:EDO:O2	2.29	0.43
3:M:113:GLY:O	3:M:117:ILE:HG13	2.17	0.43
2:L:101:ALA:HB2	2:L:121:PHE:HD2	1.83	0.43
3:M:60:LEU:HA	12:M:404:BPH:C4	2.48	0.43
1:H:82:ASP:OD2	8:H:311:EDO:H12	2.18	0.43
2:L:25:TRP:CD1	2:L:30:TYR:HA	2.53	0.43
2:L:193:LEU:O	2:L:196:SER:OG	2.30	0.43
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.33	0.43
3:M:162:PHE:HD1	16:M:407:SPN:H242	1.84	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.44	0.43
1:H:144:ALA:HB3	3:M:11:GLN:HG3	2.00	0.43
2:L:158:SER:HA	11:L:302:BCL:HBC1	2.00	0.43
3:M:32:VAL:HG12	3:M:33:GLY:O	2.18	0.43
1:H:37:ARG:O	1:H:38:GLU:HG2	2.19	0.43
2:L:179:PHE:CE2	2:L:239:SER:HB3	2.54	0.42
2:L:192:ALA:HB1	3:M:146:THR:N	2.34	0.42
1:H:195:MET:HE3	1:H:195:MET:HB3	1.80	0.42
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.49	0.42
2:L:127:ALA:CB	11:L:302:BCL:H43	2.49	0.42
3:M:235:LEU:HD12	17:M:506:HOH:O	2.18	0.42
3:M:209:LEU:N	3:M:276:VAL:HG22	2.35	0.42
3:M:115:TRP:CE3	3:M:116:LEU:HD23	2.55	0.42
3:M:66:TRP:HD1	3:M:118:ALA:O	2.03	0.42
2:L:181:PHE:HB3	12:M:404:BPH:HBB2	2.02	0.41
2:L:217:ARG:O	3:M:50:ILE:HA	2.20	0.41
3:M:68:PHE:O	3:M:72:ILE:HG12	2.20	0.41
1:H:220:LYS:HG3	1:H:220:LYS:H	1.61	0.41
2:L:87:GLN:HE21	2:L:142:TRP:CD1	2.39	0.41
2:L:153:HIS:O	2:L:156:TRP:HB3	2.21	0.41
3:M:71:GLY:HA2	3:M:74:PHE:HB2	2.02	0.41
3:M:161:GLY:HA3	16:M:407:SPN:H201	2.02	0.41
1:H:39:GLY:HA2	2:L:4:SER:OG	2.20	0.41
3:M:30:SER:OG	3:M:31:GLY:N	2.52	0.41
3:M:293:ASN:HB3	3:M:296:VAL:HB	2.03	0.41
1:H:148:PRO:HD2	1:H:167:ILE:HD11	2.03	0.41
2:L:110:LYS:HD2	3:M:254:TRP:CZ3	2.56	0.41
2:L:174:MET:SD	11:L:301:BCL:HED3	2.61	0.41
2:L:195:LEU:HB3	3:M:145:HIS:CD2	2.56	0.41
3:M:162:PHE:C	3:M:165:PRO:HD2	2.46	0.41
2:L:103:ARG:O	2:L:107:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:303:BPH:HBB1	3:M:210:TYR:CD2	2.55	0.41
14:M:401:CDL:HB31	14:M:401:CDL:HB21	2.03	0.41
3:M:154:ILE:HG23	3:M:157:TRP:CE3	2.56	0.41
1:H:58:LEU:HA	1:H:58:LEU:HD23	1.85	0.40
1:H:71:GLY:N	8:H:310:EDO:H22	2.35	0.40
1:H:233:ILE:O	1:H:237:VAL:HG23	2.21	0.40
2:L:135:ARG:HH21	2:L:251:THR:HG22	1.86	0.40
3:M:129:TRP:CD1	12:M:404:BPH:HBA1	2.56	0.40
3:M:136:ARG:HA	3:M:136:ARG:NH1	2.36	0.40
3:M:148:TRP:NE1	14:M:401:CDL:OB6	2.53	0.40
2:L:107:ILE:HG23	3:M:254:TRP:HE3	1.86	0.40
2:L:174:MET:HE1	3:M:180:PHE:HE1	1.86	0.40
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.57	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.56	0.40
1:H:175:MET:HE3	1:H:175:MET:HB2	1.96	0.40
2:L:192:ALA:O	3:M:145:HIS:HB2	2.22	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	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/282 (99%)	261 (94%)	18 (6%)	0	100	100
3	M	300/303 (99%)	280 (93%)	20 (7%)	0	100	100
All	All	817/845 (97%)	774 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	195/208 (94%)	187 (96%)	8 (4%)	27	61
2	L	220/221 (100%)	209 (95%)	11 (5%)	22	53
3	M	236/237 (100%)	226 (96%)	10 (4%)	26	60
All	All	651/666 (98%)	622 (96%)	29 (4%)	24	58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	135	LYS
1	H	169	VAL
1	H	191	LEU
1	H	200	SER
1	H	218	THR
1	H	220	LYS
1	H	221	SER
1	H	231	ASP
2	L	63	LEU
2	L	150	ILE
2	L	152	THR
2	L	154	LEU
2	L	158	SER
2	L	183	ASN
2	L	202	LYS
2	L	206	MET
2	L	247	CYS
2	L	251	THR
2	L	260	VAL
3	M	12	VAL
3	M	30	SER
3	M	52	LEU
3	M	62	SER
3	M	111	GLU
3	M	209	LEU
3	M	214	LEU

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Mol	Chain	Res	Type
3	M	235	LEU
3	M	258	PHE
3	M	270	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	52	ASN
1	H	68	HIS
1	H	141	HIS
2	L	87	GLN
2	L	258	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 11 are unknown and 2 are monoatomic - leaving 32 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	DIO	L	309	-	6,6,6	0.84	0	6,6,6	0.83	0
11	BCL	L	301	3	69,74,74	1.32	6 (8%)	79,115,115	1.90	14 (17%)
13	U10	M	406	-	48,48,63	2.70	14 (29%)	60,61,79	1.82	14 (23%)
4	LDA	M	408	-	13,15,15	2.34	2 (15%)	14,17,17	0.57	0
7	DIO	M	418	-	6,6,6	0.88	0	6,6,6	0.88	0
6	PO4	M	417	-	4,4,4	0.92	0	6,6,6	0.38	0
9	TRS	H	312	-	7,7,7	0.32	0	9,9,9	0.43	0
11	BCL	M	403	2	69,74,74	1.31	7 (10%)	79,115,115	2.12	20 (25%)
8	EDO	H	310	-	3,3,3	0.43	0	2,2,2	0.52	0
7	DIO	L	310	-	6,6,6	0.72	0	6,6,6	1.11	0
4	LDA	M	409	-	13,15,15	2.28	2 (15%)	14,17,17	0.43	0
7	DIO	H	307	-	6,6,6	0.89	0	6,6,6	0.79	0
16	SPN	M	407	-	42,42,42	1.26	8 (19%)	50,52,52	1.66	14 (28%)
4	LDA	M	410	-	13,15,15	2.36	2 (15%)	14,17,17	0.60	0
8	EDO	L	311	-	3,3,3	0.51	0	2,2,2	0.15	0
8	EDO	H	309	-	3,3,3	0.41	0	2,2,2	0.58	0
4	LDA	M	411	-	13,15,15	2.34	2 (15%)	14,17,17	0.38	0
6	PO4	M	416	-	4,4,4	0.88	0	6,6,6	0.46	0
11	BCL	L	302	2	69,74,74	1.34	6 (8%)	79,115,115	1.83	18 (22%)
12	BPH	M	402	-	59,70,70	1.47	8 (13%)	59,101,101	1.65	12 (20%)
12	BPH	M	404	-	59,70,70	1.53	7 (11%)	59,101,101	1.75	13 (22%)
13	U10	L	304	-	48,48,63	2.66	13 (27%)	60,61,79	1.84	16 (26%)
8	EDO	M	420	-	3,3,3	0.49	0	2,2,2	0.25	0
8	EDO	H	308	-	3,3,3	0.44	0	2,2,2	0.33	0
12	BPH	L	303	-	59,70,70	1.55	7 (11%)	59,101,101	1.76	14 (23%)
8	EDO	M	419	-	3,3,3	0.47	0	2,2,2	0.32	0
6	PO4	H	306	-	4,4,4	0.98	0	6,6,6	0.34	0
4	LDA	M	412	-	13,15,15	2.32	2 (15%)	14,17,17	0.34	0
14	CDL	M	401	-	80,80,99	0.91	5 (6%)	86,92,111	1.32	7 (8%)
4	LDA	H	301	-	13,15,15	2.31	2 (15%)	14,17,17	0.54	0
9	TRS	L	312	-	7,7,7	0.34	0	9,9,9	0.35	0
8	EDO	H	311	-	3,3,3	0.51	0	2,2,2	0.22	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	DIO	L	309	-	-	-	0/1/1/1
11	BCL	L	301	3	-	8/41/137/137	-
13	U10	M	406	-	-	11/45/69/87	0/1/1/1
4	LDA	M	408	-	-	2/13/13/13	-
7	DIO	M	418	-	-	-	0/1/1/1
9	TRS	H	312	-	-	6/9/9/9	-
11	BCL	M	403	2	-	7/41/137/137	-
8	EDO	H	310	-	-	0/1/1/1	-
7	DIO	L	310	-	-	-	0/1/1/1
4	LDA	M	409	-	-	5/13/13/13	-
7	DIO	H	307	-	-	-	0/1/1/1
16	SPN	M	407	-	-	18/50/51/51	-
4	LDA	M	410	-	-	1/13/13/13	-
8	EDO	L	311	-	-	0/1/1/1	-
8	EDO	H	309	-	-	1/1/1/1	-
4	LDA	M	411	-	-	7/13/13/13	-
11	BCL	L	302	2	-	5/41/137/137	-
12	BPH	M	402	-	2/2/18/22	8/37/105/105	0/5/6/6
12	BPH	M	404	-	2/2/18/22	4/37/105/105	0/5/6/6
13	U10	L	304	-	-	9/45/69/87	0/1/1/1
8	EDO	M	420	-	-	1/1/1/1	-
8	EDO	H	308	-	-	0/1/1/1	-
12	BPH	L	303	-	2/2/18/22	7/37/105/105	0/5/6/6
8	EDO	M	419	-	-	1/1/1/1	-
4	LDA	M	412	-	-	6/13/13/13	-
14	CDL	M	401	-	-	42/91/91/110	-
4	LDA	H	301	-	-	8/13/13/13	-
9	TRS	L	312	-	-	9/9/9/9	-
8	EDO	H	311	-	-	0/1/1/1	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	303	BPH	C1D-C2D	8.18	1.48	1.39
12	M	404	BPH	C1D-C2D	8.11	1.48	1.39
12	M	402	BPH	C1D-C2D	7.59	1.47	1.39
4	M	408	LDA	O1-N1	-6.80	1.25	1.42
4	M	410	LDA	O1-N1	-6.78	1.25	1.42
4	M	411	LDA	O1-N1	-6.75	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	LDA	O1-N1	-6.64	1.25	1.42
4	M	412	LDA	O1-N1	-6.64	1.25	1.42
4	M	409	LDA	O1-N1	-6.64	1.25	1.42
13	M	406	U10	C23-C24	6.57	1.48	1.33
13	M	406	U10	C13-C14	6.51	1.48	1.33
13	L	304	U10	C13-C14	6.42	1.47	1.33
13	M	406	U10	C33-C34	6.42	1.47	1.33
13	M	406	U10	C18-C19	6.29	1.47	1.33
13	L	304	U10	C18-C19	6.28	1.47	1.33
13	M	406	U10	C28-C29	6.23	1.47	1.33
13	L	304	U10	C33-C34	6.22	1.47	1.33
13	L	304	U10	C23-C24	6.09	1.47	1.33
13	L	304	U10	C28-C29	6.00	1.46	1.33
11	L	302	BCL	MG-ND	-5.95	1.94	2.05
13	M	406	U10	C8-C9	5.84	1.46	1.33
11	L	301	BCL	MG-ND	-5.72	1.94	2.05
13	L	304	U10	C38-C39	5.53	1.49	1.32
13	L	304	U10	C8-C9	5.47	1.45	1.33
11	M	403	BCL	MG-ND	-5.47	1.94	2.05
11	L	301	BCL	MG-NB	-5.28	1.95	2.05
13	M	406	U10	O4-C4	-5.01	1.24	1.36
4	M	410	LDA	C1-N1	-4.96	1.46	1.51
4	M	412	LDA	C1-N1	-4.92	1.46	1.51
4	H	301	LDA	C1-N1	-4.90	1.46	1.51
13	M	406	U10	C38-C39	4.90	1.47	1.32
4	M	408	LDA	C1-N1	-4.88	1.46	1.51
4	M	411	LDA	C1-N1	-4.87	1.46	1.51
11	L	302	BCL	MG-NB	-4.82	1.96	2.05
13	L	304	U10	O4-C4	-4.79	1.25	1.36
4	M	409	LDA	C1-N1	-4.70	1.46	1.51
13	L	304	U10	O3-C3	-4.68	1.25	1.36
13	M	406	U10	O3-C3	-4.62	1.25	1.36
11	M	403	BCL	MG-NB	-4.34	1.97	2.05
12	M	402	BPH	C4D-CHA	-3.96	1.33	1.39
11	L	301	BCL	C1D-C2D	-3.95	1.37	1.45
11	L	302	BCL	C1D-C2D	-3.90	1.37	1.45
12	M	404	BPH	C4D-CHA	-3.79	1.33	1.39
12	L	303	BPH	C4D-CHA	-3.48	1.34	1.39
11	M	403	BCL	C1D-C2D	-3.42	1.38	1.45
14	M	401	CDL	OB8-CB7	3.39	1.43	1.33
16	M	407	SPN	C1-C2	-3.33	1.50	1.53
11	L	302	BCL	C1B-C2B	-3.00	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	407	SPN	C25-C26	3.00	1.40	1.33
13	M	406	U10	C6-C1	2.97	1.40	1.35
14	M	401	CDL	OA8-CA7	2.94	1.41	1.33
12	L	303	BPH	CBD-CGD	-2.91	1.48	1.52
13	L	304	U10	C6-C1	2.90	1.40	1.35
12	L	303	BPH	C4D-ND	-2.90	1.34	1.38
13	L	304	U10	C4-C5	-2.84	1.40	1.48
14	M	401	CDL	OB6-CB5	2.81	1.42	1.34
16	M	407	SPN	C8-C9	2.75	1.39	1.33
12	M	402	BPH	C4D-ND	-2.67	1.34	1.38
16	M	407	SPN	C19-C18	2.66	1.39	1.33
11	M	403	BCL	C4B-NB	2.65	1.41	1.37
12	M	404	BPH	C4D-ND	-2.64	1.34	1.38
11	M	403	BCL	MG-NA	-2.56	2.00	2.06
12	L	303	BPH	C3D-C2D	-2.54	1.35	1.39
13	M	406	U10	C4-C5	-2.51	1.41	1.48
12	M	402	BPH	C3D-C2D	-2.49	1.35	1.39
13	L	304	U10	C3-C2	-2.49	1.41	1.48
11	M	403	BCL	MG-NC	-2.48	2.00	2.06
11	L	302	BCL	C4B-NB	2.44	1.41	1.37
12	M	402	BPH	CBD-CGD	-2.43	1.49	1.52
12	M	404	BPH	C3D-C2D	-2.43	1.35	1.39
12	M	404	BPH	C2C-C3C	-2.42	1.52	1.54
12	L	303	BPH	C3D-C4D	2.39	1.44	1.41
12	M	404	BPH	CBD-CGD	-2.35	1.49	1.52
11	L	301	BCL	C1B-C2B	-2.34	1.37	1.43
11	L	302	BCL	MG-NA	-2.28	2.00	2.06
13	L	304	U10	C6-C5	-2.24	1.40	1.46
12	L	303	BPH	C3B-CAB	-2.22	1.43	1.49
14	M	401	CDL	OA6-CA5	2.22	1.40	1.34
13	M	406	U10	C1-C2	-2.21	1.39	1.47
16	M	407	SPN	C29-C30	2.19	1.39	1.32
12	M	402	BPH	C1B-C2B	-2.18	1.37	1.39
16	M	407	SPN	C3-C2	-2.15	1.50	1.52
12	M	402	BPH	C3B-C2B	2.12	1.43	1.39
13	M	406	U10	C3-C2	-2.12	1.42	1.48
16	M	407	SPN	C12-C13	2.11	1.37	1.33
13	M	406	U10	C6-C5	-2.11	1.40	1.46
11	M	403	BCL	C1B-C2B	-2.08	1.38	1.43
11	L	301	BCL	C4B-NB	2.08	1.40	1.37
16	M	407	SPN	C4-C5	2.05	1.37	1.33
14	M	401	CDL	OA6-CA4	-2.03	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	402	BPH	C3D-C4D	2.03	1.44	1.41
11	L	301	BCL	C3D-C4D	-2.03	1.39	1.44
12	M	404	BPH	C3B-CAB	-2.03	1.43	1.49

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C1D-ND-C4D	-9.38	99.73	106.31
11	L	301	BCL	C1D-ND-C4D	-8.56	100.31	106.31
11	L	302	BCL	C1D-ND-C4D	-7.83	100.82	106.31
11	M	403	BCL	C1C-NC-C4C	6.45	109.62	106.68
12	M	404	BPH	C4D-CHA-CBD	6.04	111.35	108.45
11	L	301	BCL	C1C-NC-C4C	5.92	109.38	106.68
13	L	304	U10	C7-C8-C9	-5.52	117.32	126.83
12	M	402	BPH	C2D-C1D-ND	-5.32	105.58	109.43
12	L	303	BPH	C2D-C1D-ND	-5.31	105.59	109.43
12	L	303	BPH	C2B-C1B-NB	-5.13	105.72	109.43
12	M	404	BPH	C2D-C1D-ND	-5.03	105.80	109.43
11	L	301	BCL	O2D-CGD-CBD	4.99	119.96	111.23
11	M	403	BCL	O2D-CGD-CBD	4.99	119.95	111.23
12	M	402	BPH	C4D-CHA-CBD	4.96	110.83	108.45
13	M	406	U10	C30-C29-C31	4.47	123.00	115.23
11	M	403	BCL	C2D-C1D-ND	4.44	114.52	110.13
11	M	403	BCL	CHD-C1D-ND	-4.39	118.63	124.80
12	L	303	BPH	C4D-CHA-CBD	4.09	110.42	108.45
14	M	401	CDL	OB8-CB6-CB4	4.06	120.09	108.40
11	L	302	BCL	C1C-NC-C4C	3.95	108.48	106.68
11	L	302	BCL	CHD-C1D-ND	-3.90	119.31	124.80
13	L	304	U10	C17-C18-C19	-3.88	118.75	127.62
11	L	302	BCL	C2D-C1D-ND	3.83	113.92	110.13
13	L	304	U10	C10-C9-C11	3.75	121.74	115.23
13	M	406	U10	C22-C23-C24	-3.74	119.06	127.62
14	M	401	CDL	OB6-CB5-C51	3.70	119.49	111.48
11	L	301	BCL	C1-C2-C3	-3.70	120.14	126.20
16	M	407	SPN	C24-C25-C26	-3.59	119.40	127.62
13	M	406	U10	C15-C14-C16	3.58	121.44	115.23
13	M	406	U10	C17-C18-C19	-3.50	119.61	127.62
11	M	403	BCL	C1-C2-C3	-3.50	120.46	126.20
12	M	404	BPH	C2B-C1B-NB	-3.48	106.91	109.43
12	M	402	BPH	OBB-CAB-CBB	-3.48	112.77	120.19
14	M	401	CDL	OA8-CA6-CA4	3.46	118.38	108.40
13	M	406	U10	C10-C9-C11	3.46	121.23	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C3D-C4D-ND	3.44	115.57	109.99
16	M	407	SPN	C3-C4-C5	-3.40	120.98	126.83
11	M	403	BCL	CHB-C4A-NA	3.40	129.30	124.40
14	M	401	CDL	OA6-CA5-C11	3.38	118.80	111.48
13	M	406	U10	C27-C28-C29	-3.35	119.96	127.62
13	M	406	U10	C35-C34-C36	3.34	121.02	115.23
12	M	404	BPH	C4-C3-C5	-3.32	109.47	115.23
16	M	407	SPN	C7-C8-C9	-3.31	120.04	127.62
11	L	302	BCL	O2A-CGA-CBA	3.31	121.91	111.83
12	M	402	BPH	CMB-C2B-C3B	3.28	131.23	124.68
13	L	304	U10	C22-C23-C24	-3.25	120.18	127.62
11	L	301	BCL	C2D-C1D-ND	3.23	113.32	110.13
12	M	404	BPH	CMD-C2D-C3D	3.21	131.11	124.68
13	M	406	U10	C32-C33-C34	-3.20	120.30	127.62
13	L	304	U10	C32-C33-C34	-3.15	120.42	127.62
12	M	402	BPH	C1-C2-C3	3.14	131.34	126.20
13	M	406	U10	C41-C39-C40	3.11	121.76	114.59
13	L	304	U10	C12-C13-C14	-3.10	120.52	127.62
11	L	301	BCL	CHD-C1D-ND	-3.09	120.46	124.80
13	L	304	U10	C25-C24-C26	3.09	120.59	115.23
14	M	401	CDL	CB4-OB6-CB5	3.08	125.17	117.80
14	M	401	CDL	OB8-CB7-C71	3.07	121.20	111.83
11	L	302	BCL	CMB-C2B-C1B	-3.03	120.80	125.42
16	M	407	SPN	C20-C19-C18	-3.03	120.69	127.62
13	L	304	U10	C20-C19-C21	2.98	120.40	115.23
12	M	404	BPH	C1-C2-C3	2.98	131.07	126.20
11	L	302	BCL	CHC-C4B-NB	-2.98	119.58	124.05
11	L	302	BCL	CED-O2D-CGD	2.97	122.65	115.92
11	L	301	BCL	O1D-CGD-CBD	-2.96	118.68	124.52
16	M	407	SPN	C6-C5-C4	-2.96	114.53	121.17
11	L	301	BCL	C3D-C4D-ND	2.94	114.77	109.99
12	M	404	BPH	C5-C3-C2	2.93	127.74	121.17
11	L	302	BCL	C4-C3-C5	2.90	120.27	115.23
13	L	304	U10	C27-C28-C29	-2.90	120.99	127.62
13	L	304	U10	C30-C29-C31	2.89	120.25	115.23
12	L	303	BPH	C4C-C3C-C2C	-2.88	100.10	102.84
16	M	407	SPN	CM3-C5-C6	2.86	120.20	115.23
11	L	301	BCL	CED-O2D-CGD	2.86	122.39	115.92
11	L	301	BCL	CHB-C1B-NB	-2.85	119.77	124.05
12	M	404	BPH	C1A-C2A-C3A	-2.84	100.13	102.84
12	M	402	BPH	CMA-C3A-C4A	-2.83	108.51	114.61
13	L	304	U10	C35-C34-C36	2.83	120.14	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	303	BPH	C4D-ND-C1D	2.81	112.24	108.87
16	M	407	SPN	C11-C12-C13	-2.76	121.31	127.62
13	M	406	U10	C20-C19-C21	2.74	119.99	115.23
11	M	403	BCL	CHC-C4B-NB	-2.72	119.97	124.05
12	M	402	BPH	C4C-C3C-C2C	-2.69	100.28	102.84
11	L	301	BCL	C6-C5-C3	-2.68	106.94	113.47
11	L	302	BCL	C4D-CHA-C1A	-2.67	118.06	121.24
11	M	403	BCL	C4D-CHA-C1A	-2.66	118.08	121.24
12	M	402	BPH	C6-C5-C3	2.63	119.88	113.47
12	L	303	BPH	O2D-CGD-O1D	2.62	128.94	123.85
12	L	303	BPH	C6-C5-C3	2.62	119.84	113.47
11	M	403	BCL	C4-C3-C5	2.61	119.76	115.23
11	L	301	BCL	C4D-CHA-C1A	-2.60	118.14	121.24
12	L	303	BPH	OBB-CAB-C3B	2.60	124.33	119.99
11	L	301	BCL	C4-C3-C5	2.59	119.73	115.23
11	L	302	BCL	C3D-C4D-ND	2.56	114.15	109.99
11	M	403	BCL	C3C-C4C-CHD	-2.54	118.03	123.39
11	M	403	BCL	O1D-CGD-CBD	-2.54	119.52	124.52
11	M	403	BCL	C2A-C1A-CHA	-2.53	119.47	123.87
12	L	303	BPH	CMD-C2D-C3D	2.53	129.73	124.68
14	M	401	CDL	OA8-CA7-C31	2.52	119.53	111.83
11	M	403	BCL	C2B-C1B-NB	2.52	112.94	110.33
12	M	402	BPH	CMD-C2D-C3D	2.51	129.71	124.68
12	M	404	BPH	OBB-CAB-C3B	2.49	124.16	119.99
13	M	406	U10	C37-C38-C39	-2.49	119.36	127.64
11	L	302	BCL	O2D-CGD-CBD	2.48	115.57	111.23
11	M	403	BCL	CHB-C1B-NB	-2.46	120.36	124.05
12	M	402	BPH	C4D-ND-C1D	2.46	111.82	108.87
16	M	407	SPN	CM8-C26-C27	2.43	119.45	115.23
12	L	303	BPH	CMA-C3A-C4A	-2.42	109.39	114.61
12	M	402	BPH	OBB-CAB-C3B	2.42	124.04	119.99
13	L	304	U10	C35-C34-C33	-2.39	117.48	123.63
13	L	304	U10	C7-C6-C1	-2.39	120.79	124.89
16	M	407	SPN	CM6-C18-C17	2.37	119.35	115.23
11	L	302	BCL	CBB-CAB-C3B	2.36	125.39	120.40
11	L	302	BCL	CHB-C4A-NA	2.36	127.81	124.40
13	M	406	U10	C7-C8-C9	-2.36	122.76	126.83
13	M	406	U10	C25-C24-C26	2.36	119.33	115.23
11	L	301	BCL	CHC-C4B-NB	-2.36	120.51	124.05
12	L	303	BPH	C3B-C4B-NB	-2.35	104.63	108.05
12	M	404	BPH	CMA-C3A-C4A	-2.35	109.55	114.61
11	L	302	BCL	C3C-C4C-CHD	-2.34	118.47	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	404	BPH	C4D-ND-C1D	2.31	111.64	108.87
11	L	302	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
13	L	304	U10	C15-C14-C16	2.28	119.19	115.23
13	M	406	U10	C7-C6-C1	-2.26	121.02	124.89
16	M	407	SPN	CMA-O1-C1	2.25	125.61	114.23
11	M	403	BCL	CBB-CAB-C3B	2.24	125.12	120.40
12	L	303	BPH	OBB-CAB-CBB	-2.19	115.51	120.19
11	M	403	BCL	CHC-C1C-NC	2.18	127.54	124.40
11	L	302	BCL	C2B-C1B-NB	2.16	112.57	110.33
16	M	407	SPN	C7-C6-C5	2.15	120.32	113.19
12	L	303	BPH	C1B-NB-C4B	2.13	111.92	108.82
11	M	403	BCL	O2A-CGA-CBA	2.11	118.26	111.83
13	L	304	U10	C10-C9-C8	-2.09	118.25	123.63
16	M	407	SPN	CM5-C13-C14	2.08	118.83	115.23
16	M	407	SPN	CM4-C9-C10	2.07	118.81	115.23
11	L	302	BCL	O2A-CGA-O1A	-2.05	118.49	123.63
11	M	403	BCL	C6-C5-C3	-2.05	108.47	113.47
12	L	303	BPH	C1A-C2A-C3A	-2.05	100.89	102.84
12	M	404	BPH	OBB-CAB-CBB	-2.04	115.83	120.19
13	L	304	U10	C1M-C1-C6	-2.04	121.10	124.45
16	M	407	SPN	C15-C14-C13	2.04	118.43	113.47
12	M	404	BPH	OBD-CAD-C3D	-2.02	124.74	127.89
12	M	402	BPH	C2B-C1B-NB	-2.02	107.97	109.43

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	303	BPH	C8
12	L	303	BPH	C13
12	M	402	BPH	C8
12	M	402	BPH	C13
12	M	404	BPH	C8
12	M	404	BPH	C13

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-O1
4	H	301	LDA	C2-C1-N1-CM1
4	H	301	LDA	C2-C1-N1-CM2
4	M	409	LDA	N1-C1-C2-C3
9	H	312	TRS	C2-C-C1-O1

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Mol	Chain	Res	Type	Atoms
9	H	312	TRS	C3-C-C1-O1
9	H	312	TRS	N-C-C1-O1
9	H	312	TRS	C1-C-C2-O2
9	H	312	TRS	N-C-C2-O2
9	L	312	TRS	N-C-C2-O2
11	M	403	BCL	CHA-CBD-CGD-O1D
11	M	403	BCL	CHA-CBD-CGD-O2D
12	M	402	BPH	C4C-C3C-CAC-CBC
12	M	402	BPH	C2C-C3C-CAC-CBC
13	L	304	U10	C14-C16-C17-C18
14	M	401	CDL	O1-C1-CB2-OB2
14	M	401	CDL	CA2-OA2-PA1-OA3
14	M	401	CDL	CA2-OA2-PA1-OA5
16	M	407	SPN	C7-C8-C9-C10
16	M	407	SPN	C11-C10-C9-C8
11	M	403	BCL	CBD-CGD-O2D-CED
11	L	302	BCL	C4-C3-C5-C6
16	M	407	SPN	CM3-C5-C6-C7
16	M	407	SPN	C12-C13-C14-C15
14	M	401	CDL	C31-CA7-OA8-CA6
14	M	401	CDL	OA9-CA7-OA8-CA6
13	M	406	U10	C37-C38-C39-C40
14	M	401	CDL	O1-C1-CA2-OA2
14	M	401	CDL	OB9-CB7-OB8-CB6
14	M	401	CDL	C71-CB7-OB8-CB6
11	L	302	BCL	C2-C3-C5-C6
13	M	406	U10	C14-C16-C17-C18
13	M	406	U10	C29-C31-C32-C33
16	M	407	SPN	C14-C15-C16-C17
16	M	407	SPN	C16-C17-C18-C19
12	L	303	BPH	C14-C13-C15-C16
11	M	403	BCL	O1D-CGD-O2D-CED
13	M	406	U10	C37-C38-C39-C41
13	M	406	U10	C32-C33-C34-C35
11	L	302	BCL	C15-C16-C17-C18
12	M	402	BPH	C15-C16-C17-C18
16	M	407	SPN	C26-C27-C28-C29
11	L	301	BCL	C10-C11-C12-C13
16	M	407	SPN	C28-C29-C30-CM9
14	M	401	CDL	CB7-C71-C72-C73
14	M	401	CDL	C39-C40-C41-C42
14	M	401	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
4	M	411	LDA	C5-C6-C7-C8
14	M	401	CDL	C37-C38-C39-C40
12	L	303	BPH	C10-C11-C12-C13
9	L	312	TRS	C1-C-C2-O2
4	M	411	LDA	C7-C8-C9-C10
4	M	409	LDA	C2-C3-C4-C5
14	M	401	CDL	C72-C73-C74-C75
14	M	401	CDL	C79-C80-C81-C82
4	H	301	LDA	C1-C2-C3-C4
4	M	409	LDA	C1-C2-C3-C4
4	M	412	LDA	C1-C2-C3-C4
12	L	303	BPH	C8-C10-C11-C12
4	M	412	LDA	C4-C5-C6-C7
14	M	401	CDL	C14-C15-C16-C17
14	M	401	CDL	C35-C36-C37-C38
14	M	401	CDL	CA2-C1-CB2-OB2
12	M	404	BPH	C5-C6-C7-C8
14	M	401	CDL	C20-C21-C22-C23
13	M	406	U10	C25-C24-C26-C27
11	L	301	BCL	C11-C10-C8-C9
4	M	412	LDA	C7-C8-C9-C10
14	M	401	CDL	C17-C18-C19-C20
4	M	412	LDA	C3-C4-C5-C6
14	M	401	CDL	CB3-CB4-CB6-OB8
4	M	411	LDA	C4-C5-C6-C7
14	M	401	CDL	C36-C37-C38-C39
13	L	304	U10	C18-C19-C21-C22
13	M	406	U10	C23-C24-C26-C27
4	M	410	LDA	C4-C5-C6-C7
13	L	304	U10	C20-C19-C21-C22
14	M	401	CDL	C80-C81-C82-C83
4	M	412	LDA	C2-C3-C4-C5
4	M	411	LDA	C2-C3-C4-C5
14	M	401	CDL	C13-C14-C15-C16
12	M	402	BPH	C13-C15-C16-C17
4	M	409	LDA	C4-C5-C6-C7
4	M	411	LDA	C9-C10-C11-C12
4	M	411	LDA	C1-C2-C3-C4
13	M	406	U10	C32-C33-C34-C36
14	M	401	CDL	OA5-CA3-CA4-CA6
14	M	401	CDL	OB5-CB3-CB4-CB6
12	M	404	BPH	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
16	M	407	SPN	CM1-C1-C2-O2
16	M	407	SPN	CM1-C1-C2-C3
9	H	312	TRS	C3-C-C2-O2
9	L	312	TRS	C3-C-C1-O1
9	L	312	TRS	N-C-C1-O1
9	L	312	TRS	N-C-C3-O3
4	H	301	LDA	C9-C10-C11-C12
4	H	301	LDA	C7-C8-C9-C10
14	M	401	CDL	C78-C79-C80-C81
16	M	407	SPN	C28-C29-C30-CMB
12	M	404	BPH	C15-C16-C17-C18
14	M	401	CDL	CB5-C51-C52-C53
16	M	407	SPN	C9-C10-C11-C12
16	M	407	SPN	O1-C1-C2-O2
14	M	401	CDL	CB2-C1-CA2-OA2
11	L	301	BCL	CBA-CGA-O2A-C1
11	L	301	BCL	C11-C12-C13-C15
12	L	303	BPH	C12-C13-C15-C16
16	M	407	SPN	C21-C22-C23-C24
14	M	401	CDL	C38-C39-C40-C41
13	L	304	U10	C5-C4-O4-C4M
13	L	304	U10	C9-C11-C12-C13
13	L	304	U10	C24-C26-C27-C28
12	L	303	BPH	C3-C5-C6-C7
14	M	401	CDL	C18-C19-C20-C21
11	L	301	BCL	O1A-CGA-O2A-C1
14	M	401	CDL	C73-C74-C75-C76
16	M	407	SPN	CM7-C22-C23-C24
9	L	312	TRS	C1-C-C3-O3
9	L	312	TRS	C2-C-C3-O3
13	M	406	U10	C30-C29-C31-C32
12	M	402	BPH	CAD-CBD-CGD-O2D
12	M	402	BPH	O1A-CGA-O2A-C1
11	L	302	BCL	C16-C17-C18-C19
4	M	412	LDA	C9-C10-C11-C12
12	M	402	BPH	CAD-CBD-CGD-O1D
14	M	401	CDL	CA2-OA2-PA1-OA4
14	M	401	CDL	C76-C77-C78-C79
4	H	301	LDA	C4-C5-C6-C7
14	M	401	CDL	C11-C12-C13-C14
14	M	401	CDL	OA5-CA3-CA4-OA6
14	M	401	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	M	402	BPH	CBA-CGA-O2A-C1
16	M	407	SPN	C16-C17-C18-CM6
13	M	406	U10	C28-C29-C31-C32
11	L	302	BCL	C16-C17-C18-C20
14	M	401	CDL	C53-C54-C55-C56
11	M	403	BCL	C15-C16-C17-C18
14	M	401	CDL	OB6-CB4-CB6-OB8
13	M	406	U10	C5-C4-O4-C4M
11	L	301	BCL	C6-C7-C8-C9
4	M	408	LDA	C4-C5-C6-C7
12	L	303	BPH	C11-C12-C13-C14
9	L	312	TRS	C2-C-C1-O1
9	L	312	TRS	C3-C-C2-O2
13	L	304	U10	C34-C36-C37-C38
11	L	301	BCL	C5-C6-C7-C8
8	M	419	EDO	O1-C1-C2-O2
8	M	420	EDO	O1-C1-C2-O2
14	M	401	CDL	OA6-CA4-CA6-OA8
12	M	404	BPH	C11-C12-C13-C14
13	L	304	U10	C3-C4-O4-C4M
11	M	403	BCL	CBA-CGA-O2A-C1
11	L	301	BCL	C6-C7-C8-C10
16	M	407	SPN	C13-C14-C15-C16
4	M	408	LDA	C9-C10-C11-C12
4	H	301	LDA	C6-C7-C8-C9
12	L	303	BPH	C2-C1-O2A-CGA
14	M	401	CDL	C40-C41-C42-C43
4	M	409	LDA	C9-C10-C11-C12
14	M	401	CDL	C81-C82-C83-C84
13	L	304	U10	C28-C29-C31-C32
4	M	411	LDA	C11-C10-C9-C8
11	M	403	BCL	O1A-CGA-O2A-C1
14	M	401	CDL	C52-C51-CB5-OB7
8	H	309	EDO	O1-C1-C2-O2
16	M	407	SPN	C24-C25-C26-C27

There are no ring outliers.

21 monomers are involved in 65 short contacts:

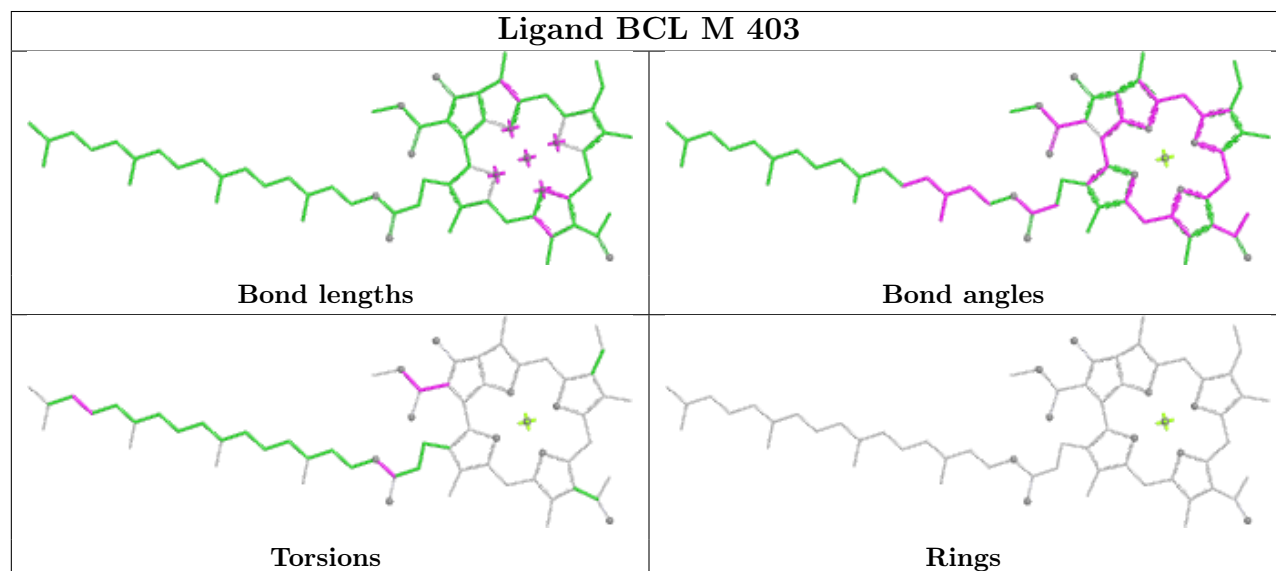
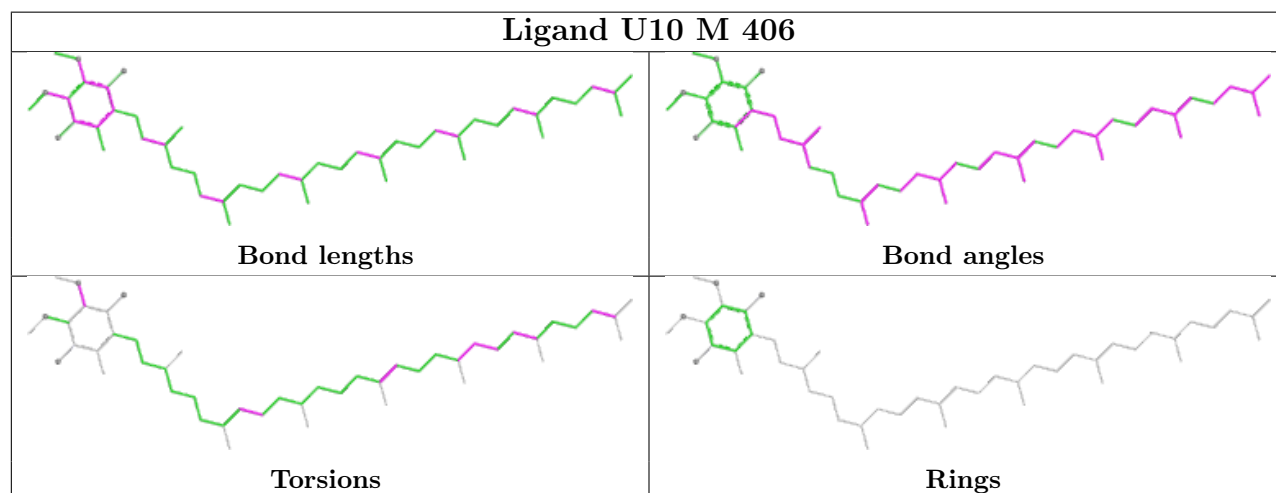
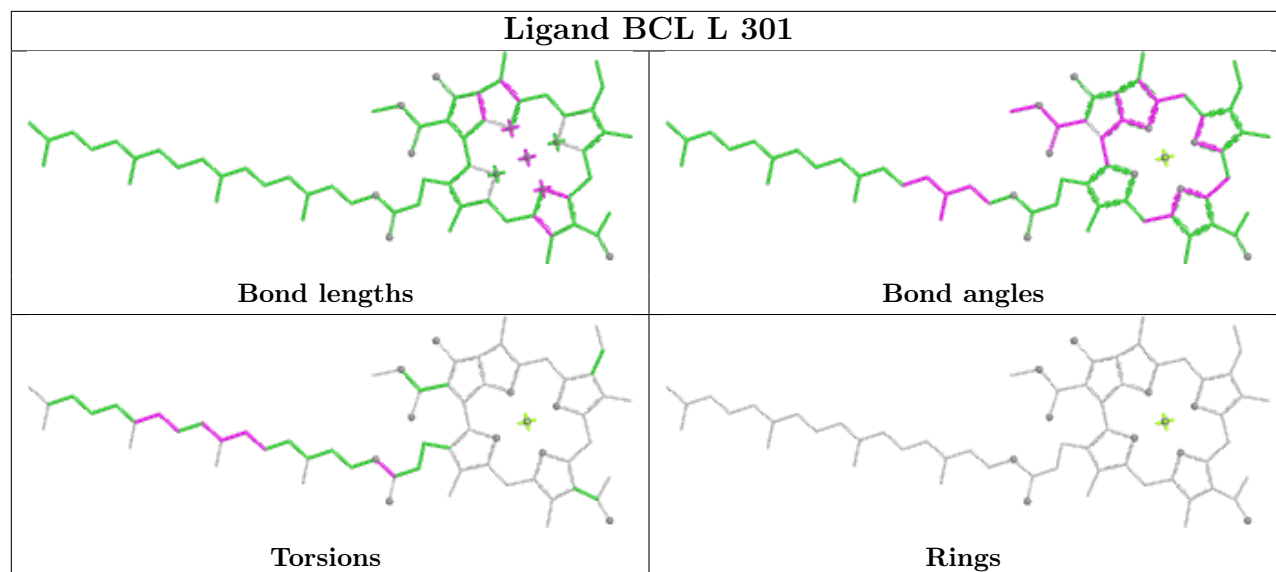
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	309	DIO	3	0
11	L	301	BCL	4	0

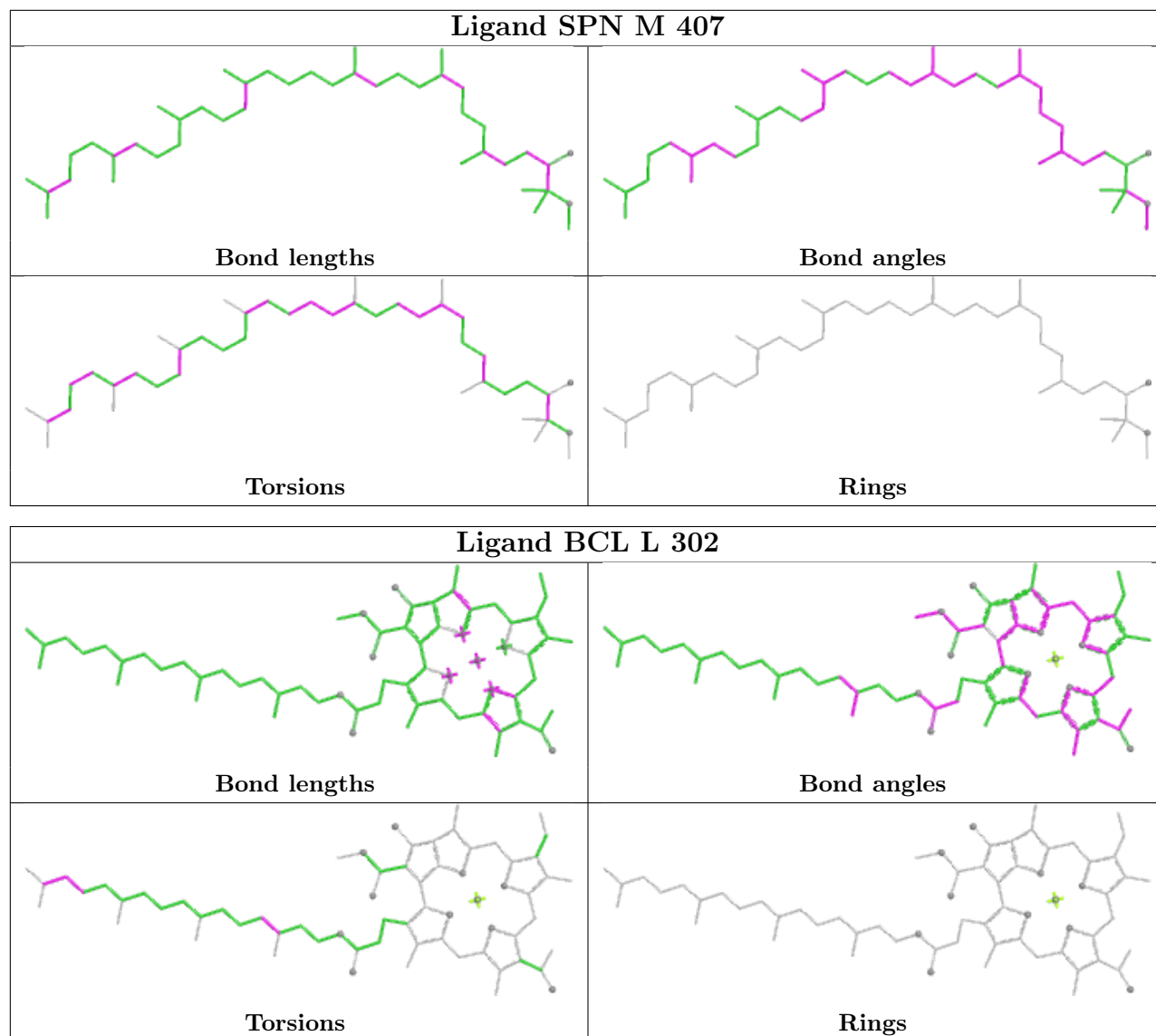
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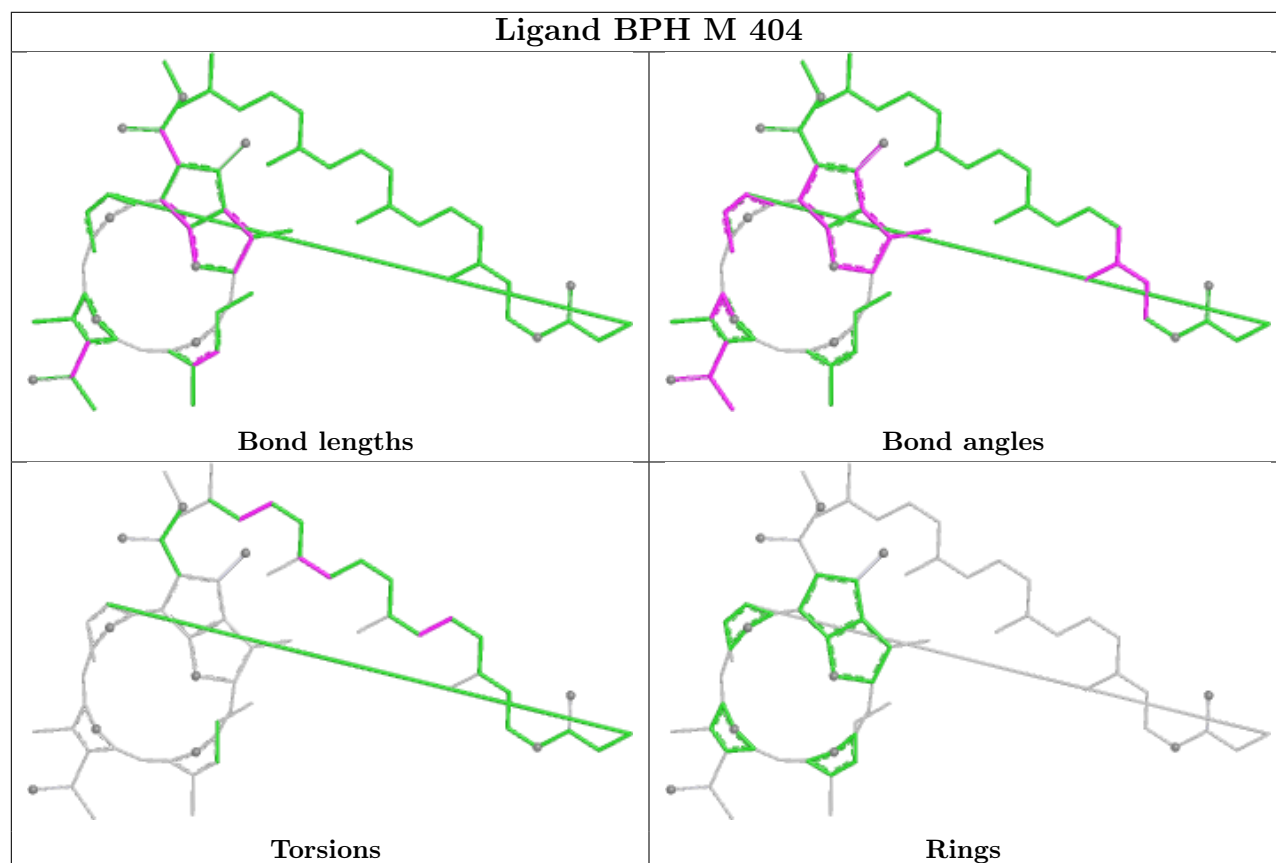
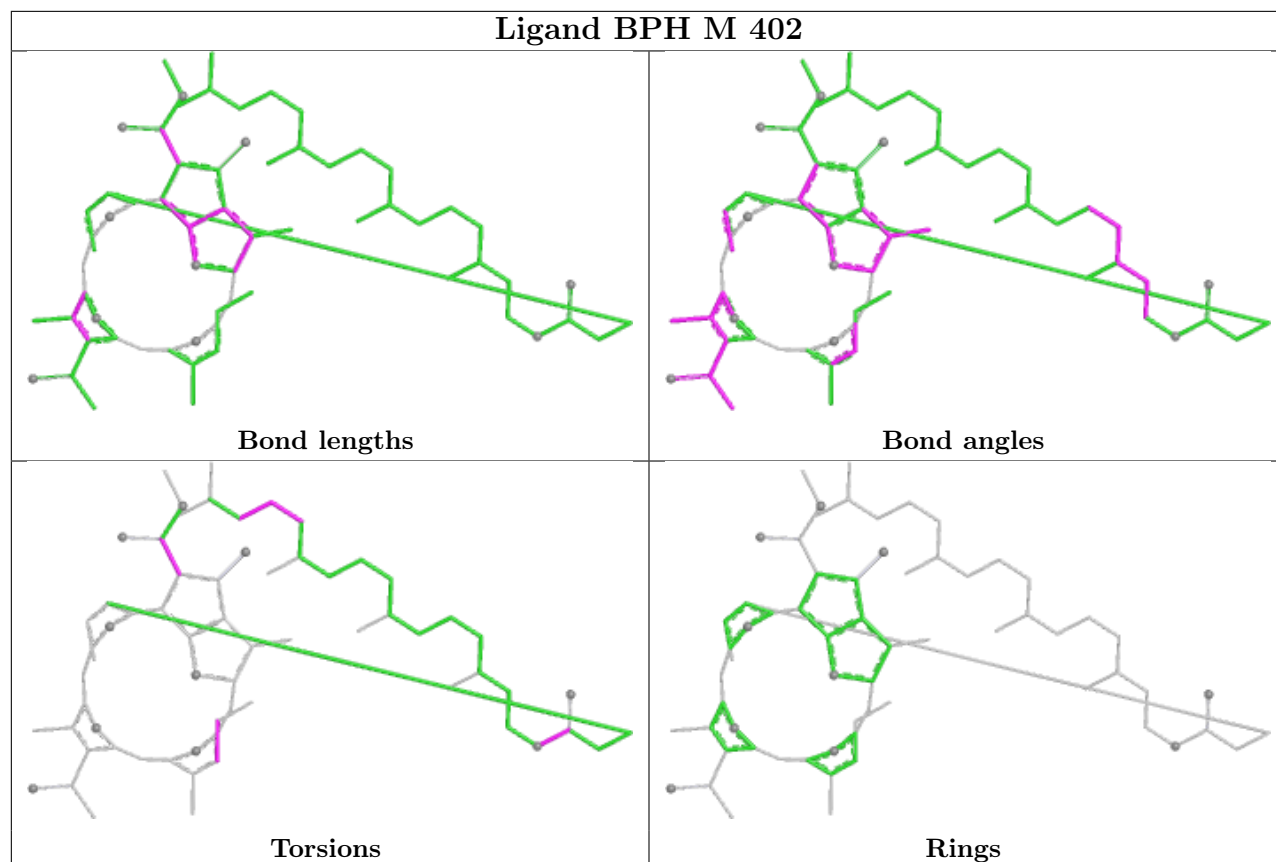
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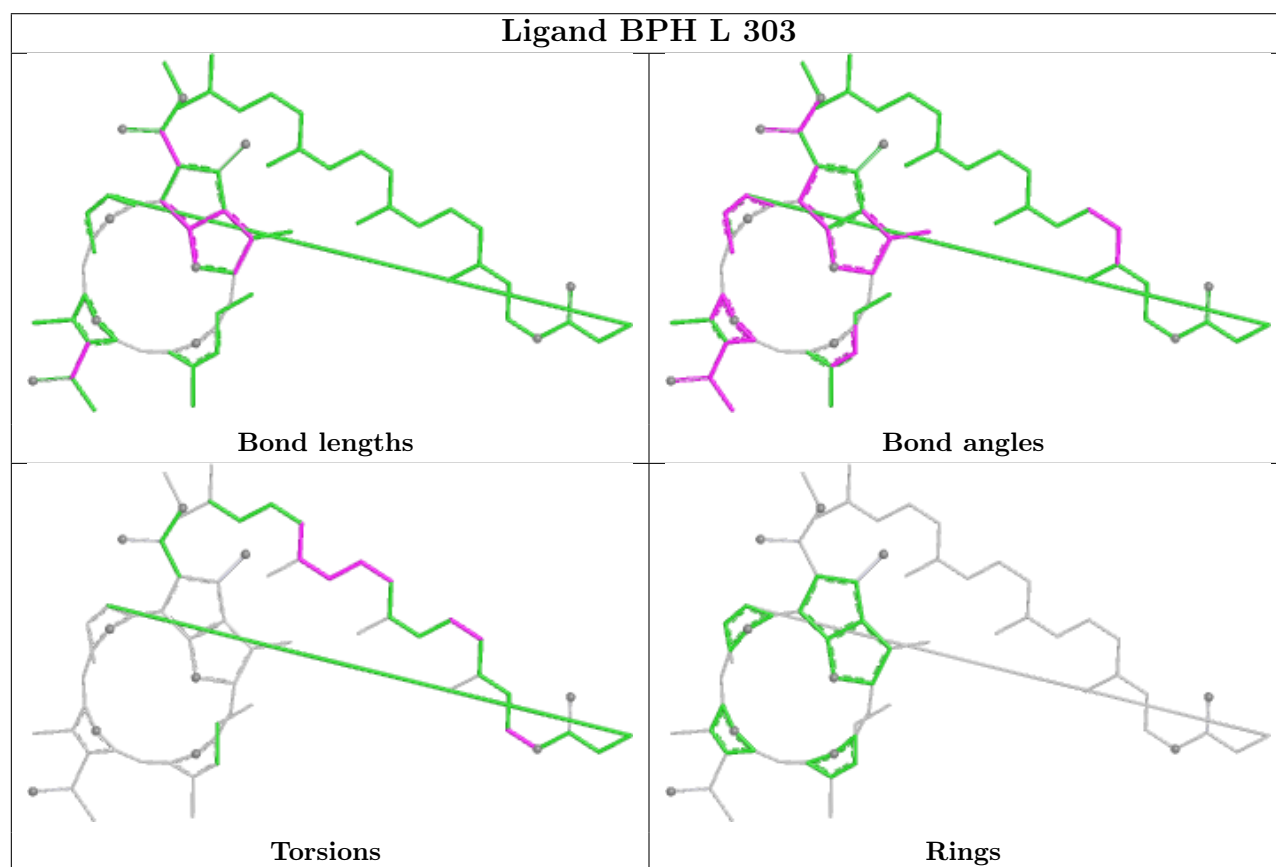
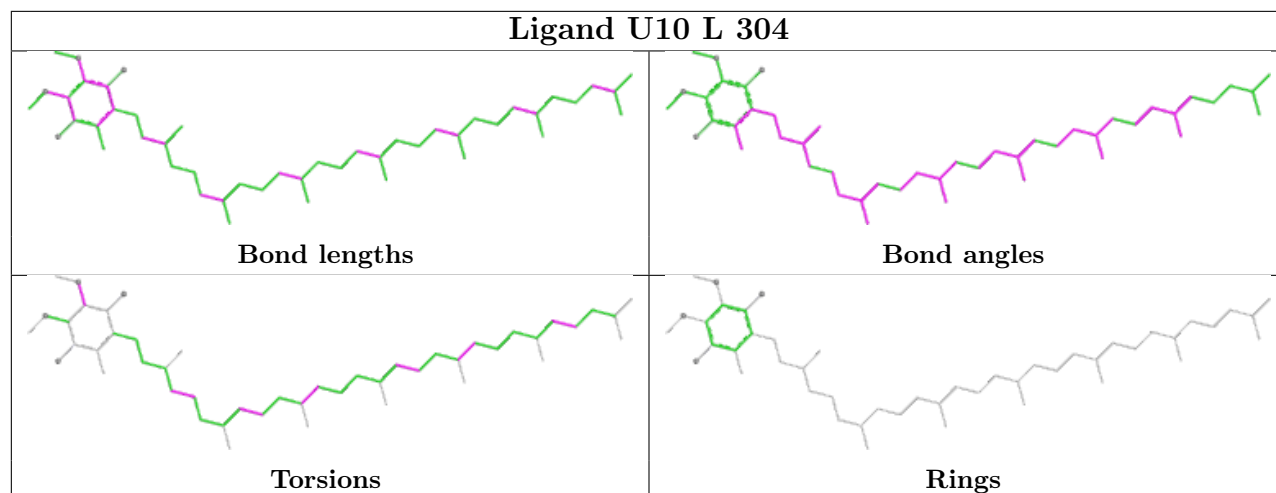
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	406	U10	5	0
4	M	408	LDA	4	0
7	M	418	DIO	1	0
9	H	312	TRS	1	0
11	M	403	BCL	3	0
8	H	310	EDO	2	0
16	M	407	SPN	5	0
4	M	410	LDA	1	0
8	L	311	EDO	1	0
11	L	302	BCL	6	0
12	M	402	BPH	6	0
12	M	404	BPH	7	0
13	L	304	U10	1	0
12	L	303	BPH	10	0
8	M	419	EDO	1	0
4	M	412	LDA	4	0
14	M	401	CDL	7	0
4	H	301	LDA	2	0
8	H	311	EDO	1	0

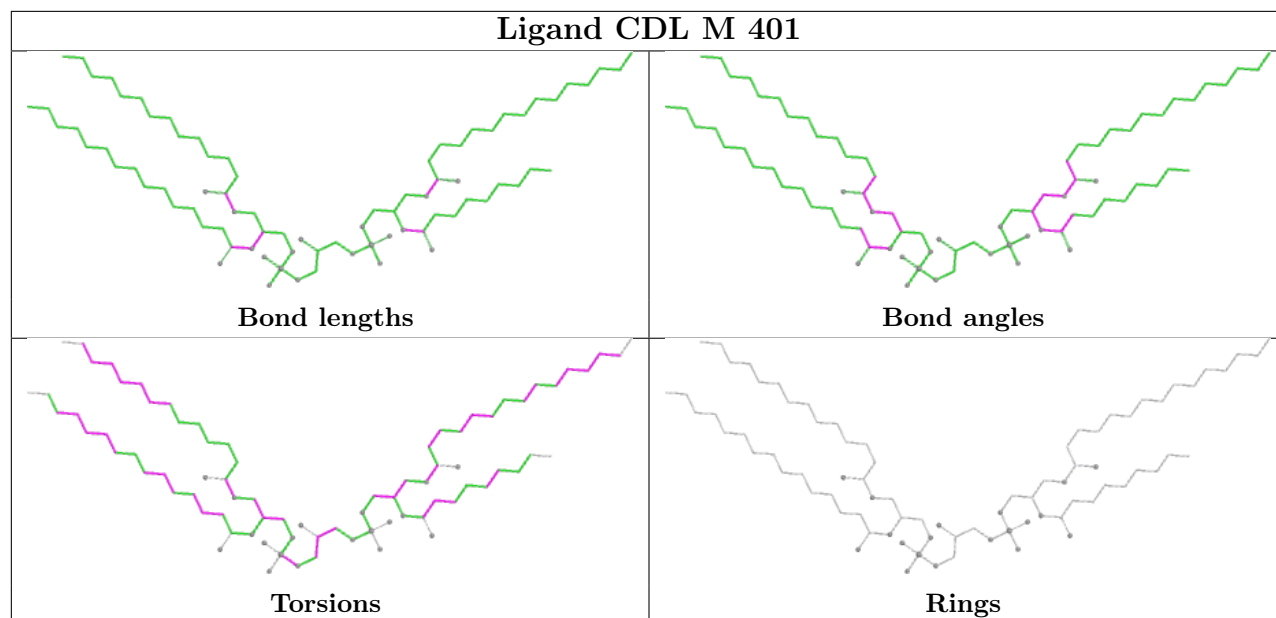
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	240/260 (92%)	-0.44	1 (0%) 88 85	19, 45, 74, 127	0
2	L	281/282 (99%)	-0.39	1 (0%) 88 85	13, 42, 83, 130	0
3	M	302/303 (99%)	-0.43	3 (0%) 79 73	18, 45, 84, 118	0
All	All	823/845 (97%)	-0.42	5 (0%) 85 81	13, 44, 82, 130	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	302	GLY	3.3
3	M	1	ALA	3.1
1	H	249	LYS	2.5
3	M	2	GLU	2.4
2	L	82	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

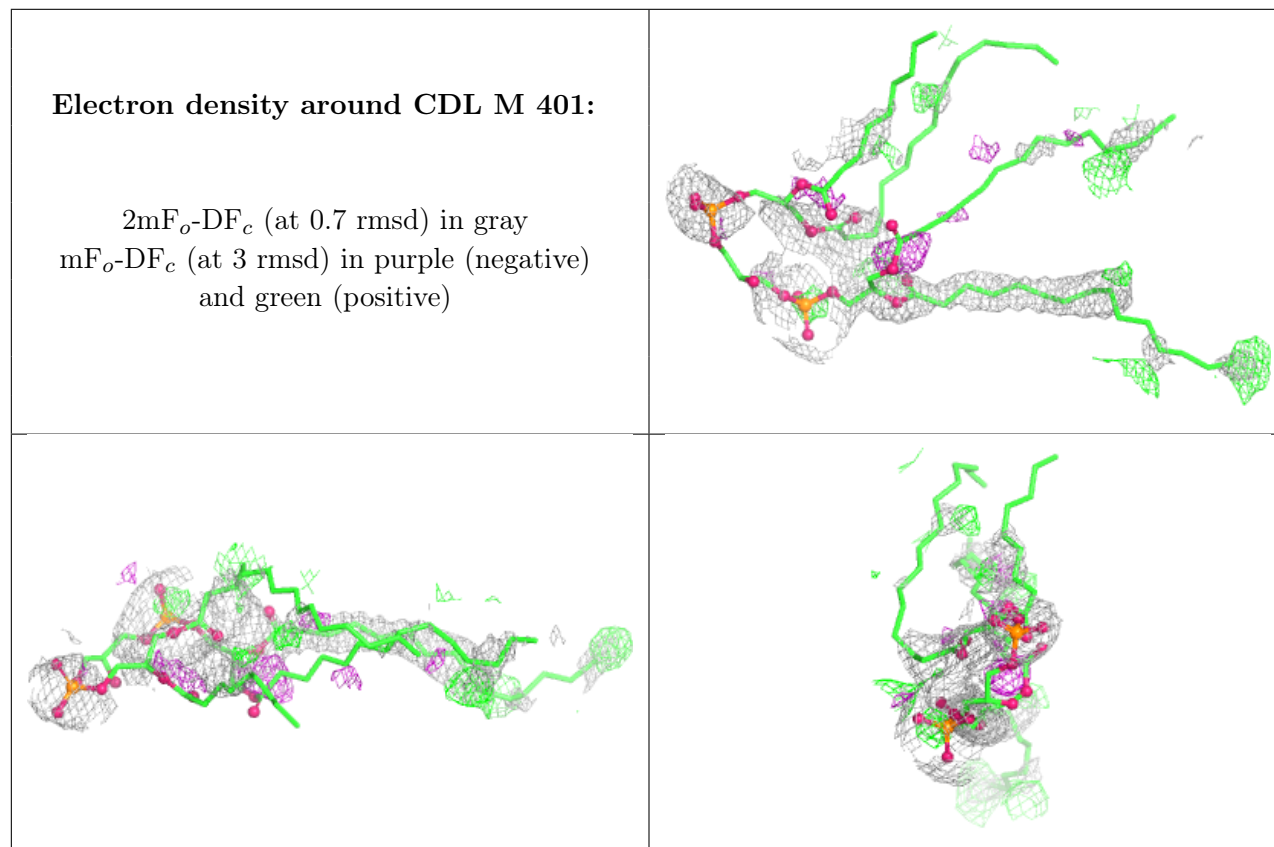
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	UNL	L	308	12/-	0.66	0.37	39,70,76,79	0
8	EDO	H	308	4/4	0.73	0.28	79,79,82,86	0
6	PO4	M	416	5/5	0.74	0.09	95,108,121,134	0
8	EDO	L	311	4/4	0.74	0.28	68,73,73,81	0
9	TRS	H	312	8/8	0.75	0.10	76,84,92,102	0
4	LDA	M	412	16/16	0.76	0.28	63,87,99,105	0
5	UNL	M	413	12/-	0.77	0.25	32,47,55,58	0
7	DIO	L	310	6/6	0.78	0.27	64,68,73,82	0
5	UNL	L	305	12/-	0.80	0.35	67,78,91,94	0
4	LDA	M	409	16/16	0.80	0.18	34,45,80,83	0
5	UNL	H	303	12/-	0.81	0.20	43,54,70,73	0
6	PO4	H	306	5/5	0.82	0.12	94,105,115,120	0
4	LDA	M	410	16/16	0.82	0.21	48,66,88,98	0
5	UNL	L	306	12/-	0.82	0.27	35,54,67,68	0
6	PO4	M	417	5/5	0.83	0.12	94,102,115,118	0
14	CDL	M	401	81/100	0.83	0.26	58,97,140,158	0
7	DIO	M	418	6/6	0.84	0.28	99,104,105,112	0
5	UNL	H	305	12/-	0.84	0.25	54,66,81,82	0
5	UNL	H	302	12/-	0.84	0.22	53,59,78,82	0
7	DIO	H	307	6/6	0.84	0.24	100,102,102,102	0
4	LDA	M	411	16/16	0.84	0.34	63,106,135,139	0
8	EDO	H	311	4/4	0.86	0.18	58,60,62,63	0
7	DIO	L	309	6/6	0.87	0.21	34,36,40,46	6
9	TRS	L	312	8/8	0.87	0.16	73,77,88,89	0
13	U10	L	304	48/63	0.87	0.24	53,70,84,90	0
5	UNL	H	304	12/-	0.87	0.21	39,53,80,83	0
10	K	H	313	1/1	0.88	0.11	64,64,64,64	0
5	UNL	L	307	10/-	0.88	0.34	53,79,104,107	0
5	UNL	M	415	12/-	0.88	0.28	70,82,90,92	0
5	UNL	M	414	12/-	0.90	0.24	45,66,80,85	0
8	EDO	M	419	4/4	0.91	0.21	60,73,77,78	0
8	EDO	H	310	4/4	0.92	0.15	61,65,68,70	0
4	LDA	H	301	16/16	0.94	0.13	48,58,63,69	0
12	BPH	L	303	65/65	0.95	0.09	25,31,44,51	0
12	BPH	M	404	65/65	0.95	0.12	39,54,101,113	0
8	EDO	H	309	4/4	0.95	0.16	55,56,59,61	0
13	U10	M	406	48/63	0.95	0.12	28,39,57,64	0
4	LDA	M	408	16/16	0.95	0.15	45,55,64,66	0
16	SPN	M	407	43/43	0.96	0.12	30,52,74,78	0
11	BCL	L	301	66/66	0.97	0.09	21,34,65,72	0
11	BCL	L	302	66/66	0.97	0.07	24,32,42,46	0
11	BCL	M	403	66/66	0.97	0.08	19,24,37,41	0
8	EDO	M	420	4/4	0.97	0.12	37,40,46,47	0

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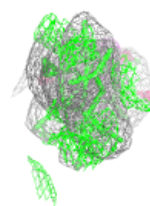
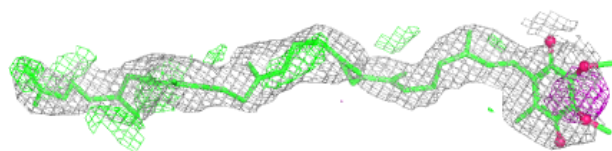
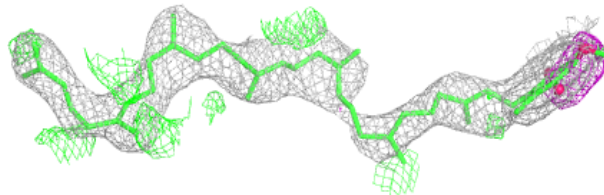
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	BPH	M	402	65/65	0.97	0.08	27,33,55,67	0
15	FE	M	405	1/1	1.00	0.01	25,25,25,25	0

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.



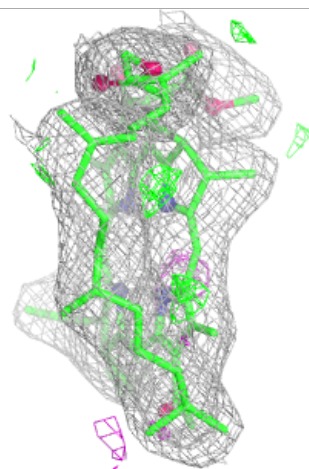
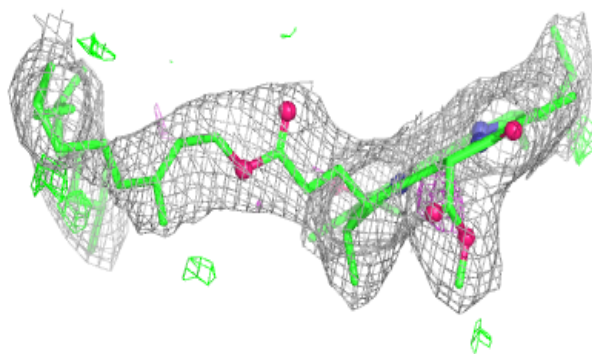
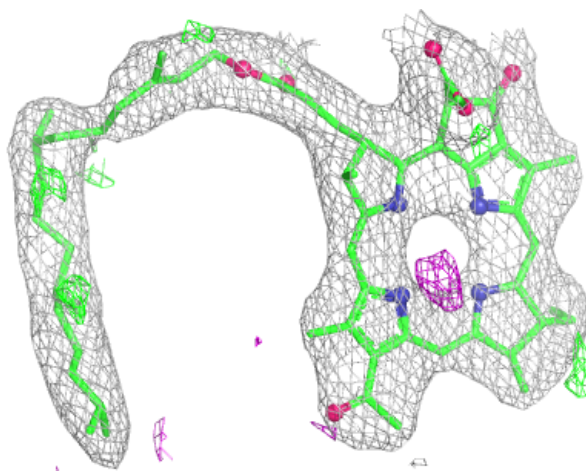
Electron density around U10 L 304:

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



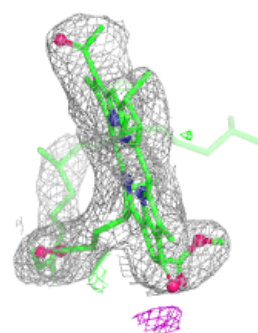
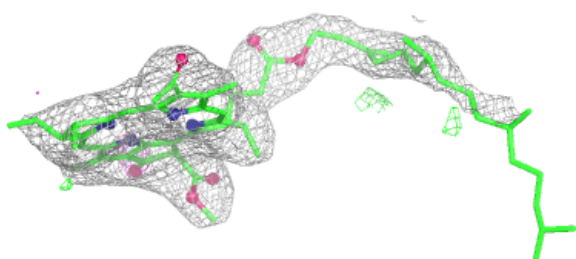
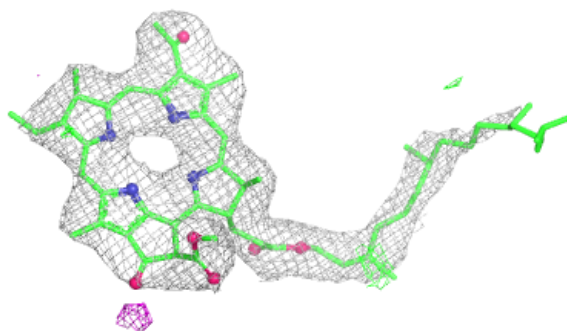
Electron density around BPH L 303:

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

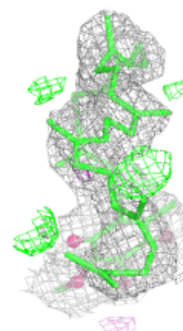
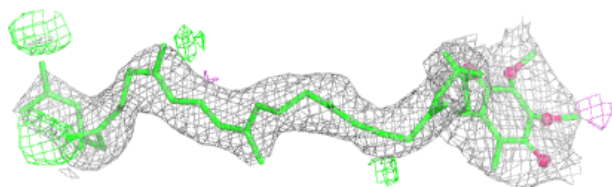
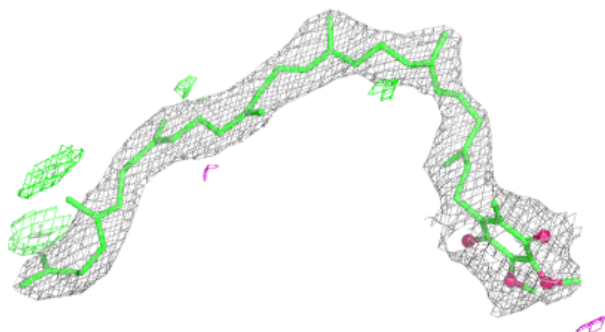


Electron density around BPH M 404:

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

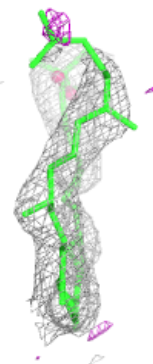
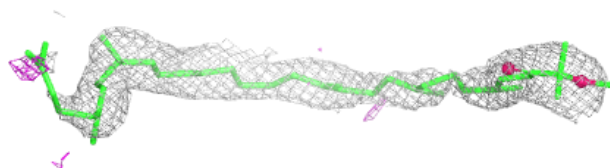
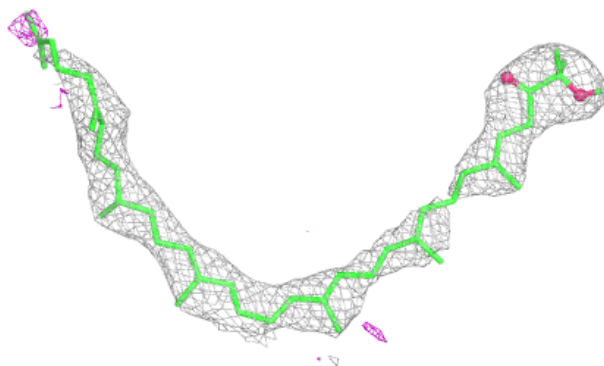
**Electron density around U10 M 406:**

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



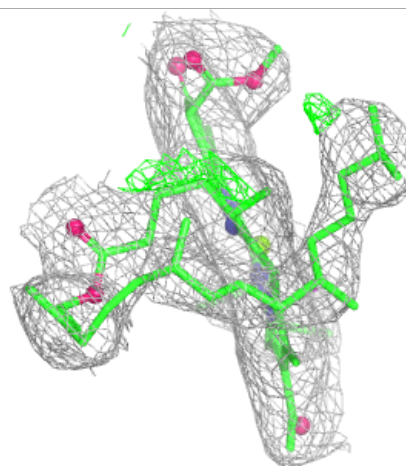
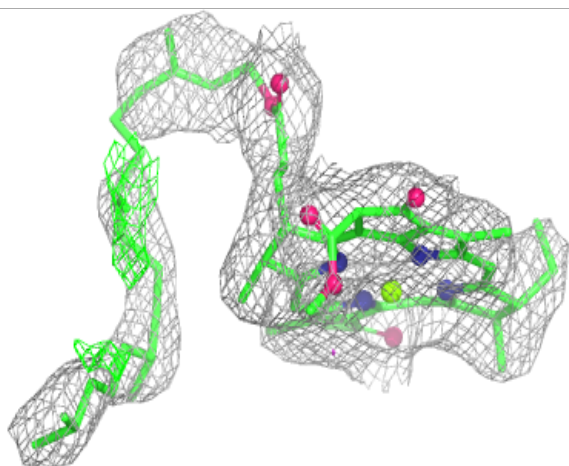
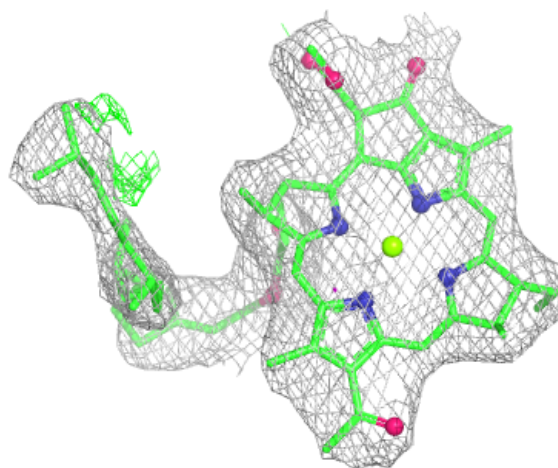
Electron density around SPN M 407:

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



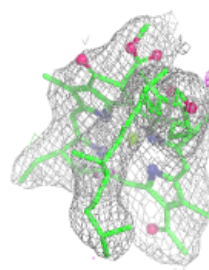
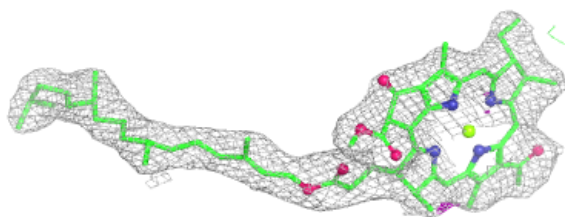
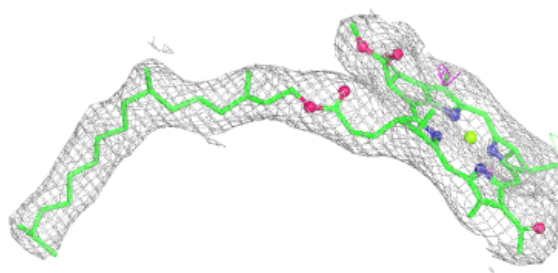
Electron density around BCL L 301:

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



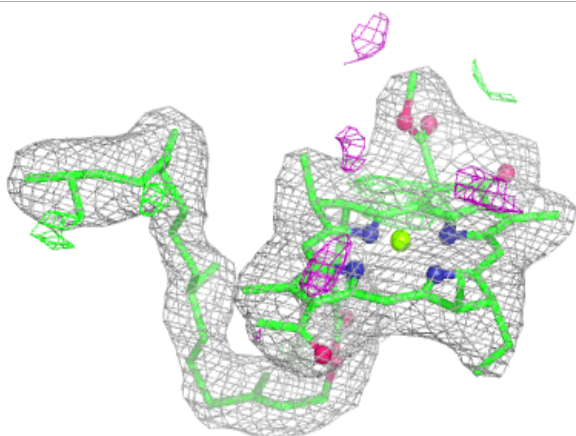
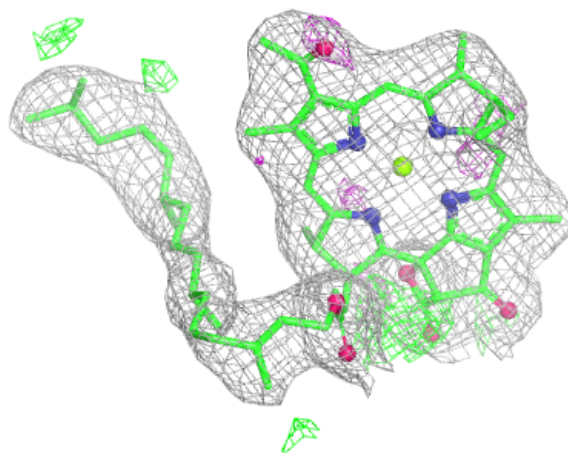
Electron density around BCL L 302:

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



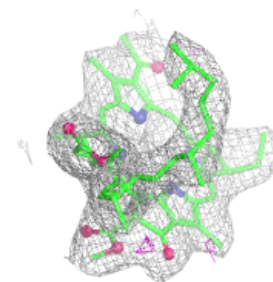
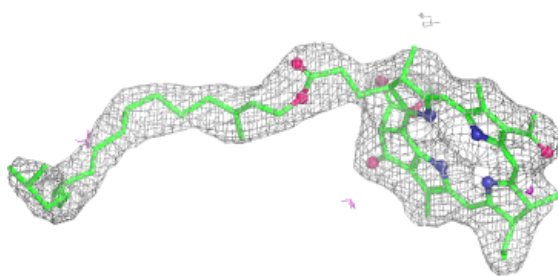
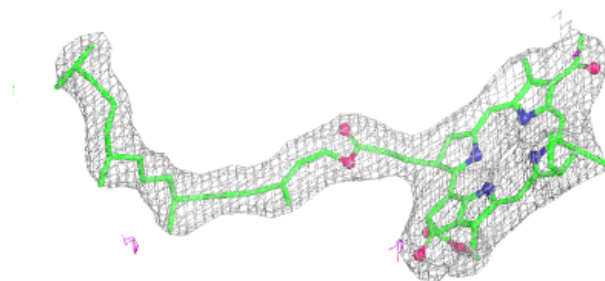
Electron density around BCL M 403:

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



Electron density around BPH M 402:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.