



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 02:31 AM EDT

PDB ID : 2HIT / pdb_00002hit
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylethanolamine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-29
Resolution : 2.75 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

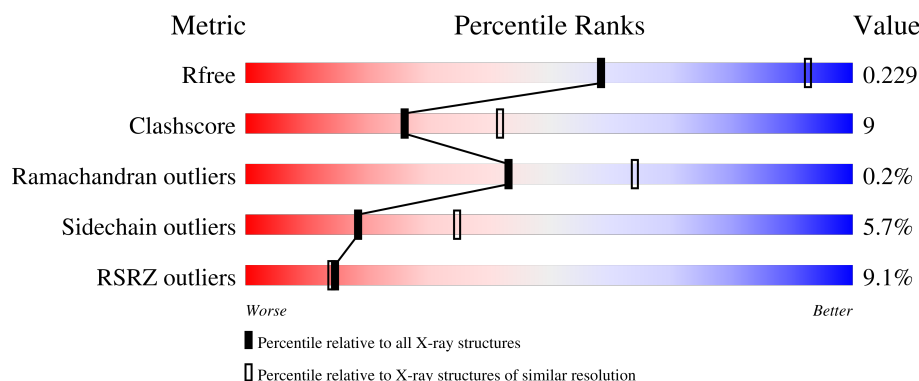
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	L	281	9% 86% 13% .
2	M	307	10% 76% 21% ..
3	H	260	7% 73% 17% • 7%

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	PEW	M	802	-	-	-	X
13	LDA	M	920	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7851 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	4	0
			2256	1523	360	365	8			

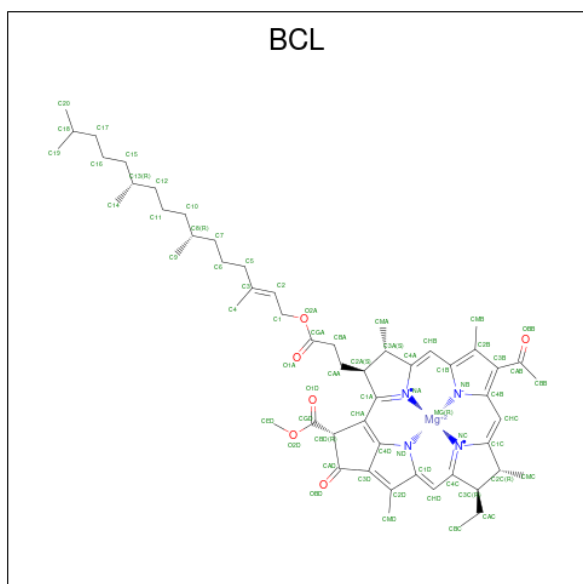
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	12	0
			2477	1650	405	411	11			

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

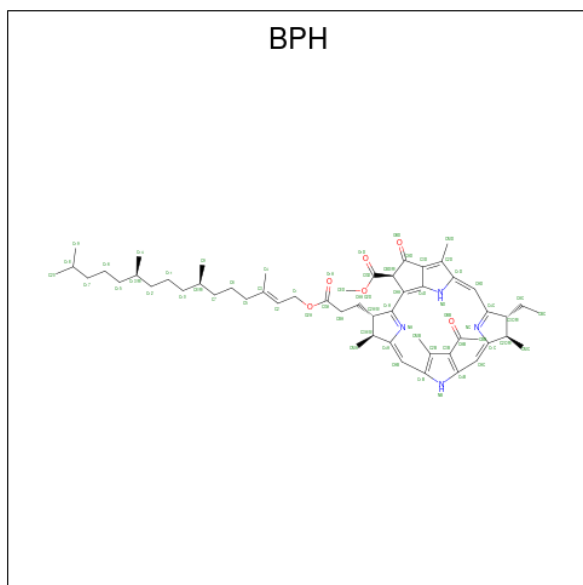
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	243	Total	C	N	O	S	0	6	0
			1876	1199	323	343	11			

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



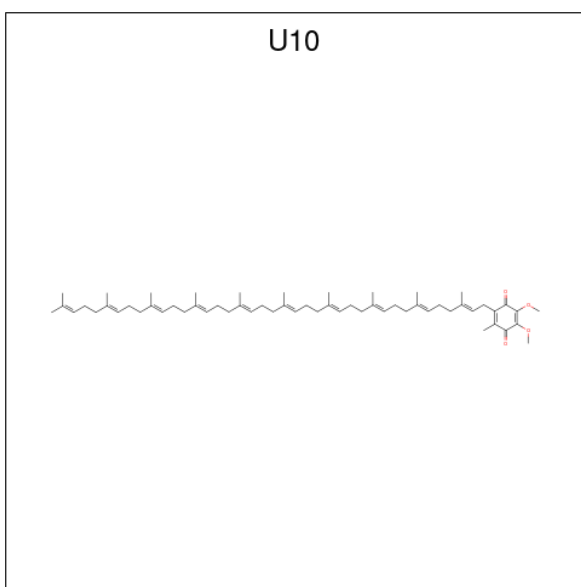
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



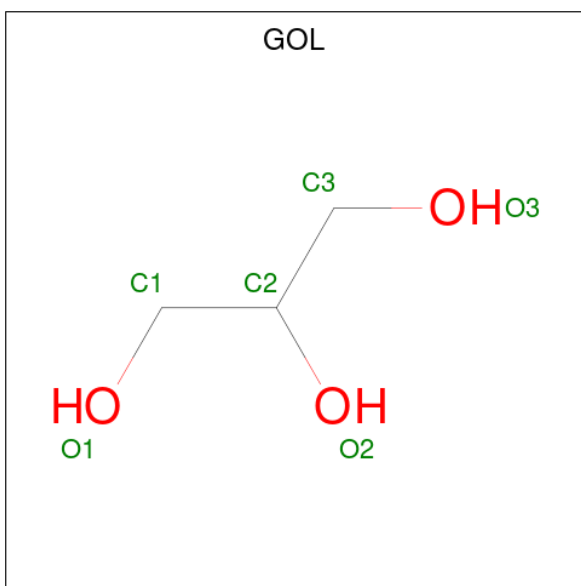
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

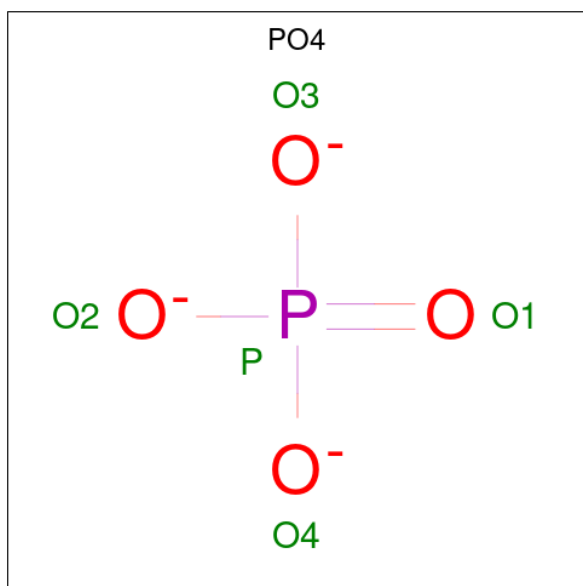
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

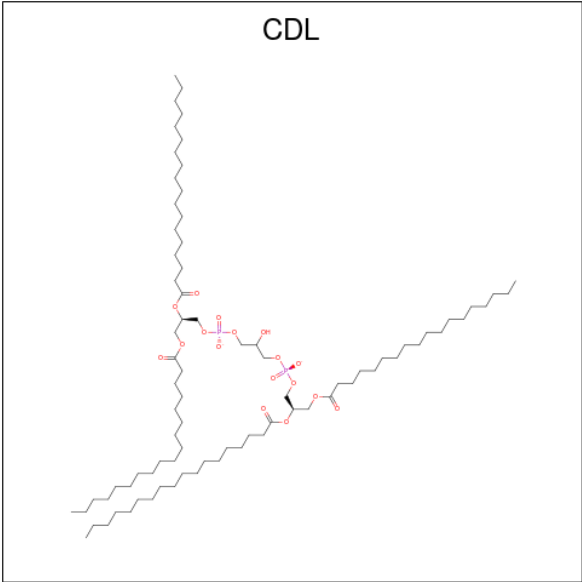
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	2	Total	Cl	0	0
			2	2		
9	H	1	Total	Cl	0	0
			1	1		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



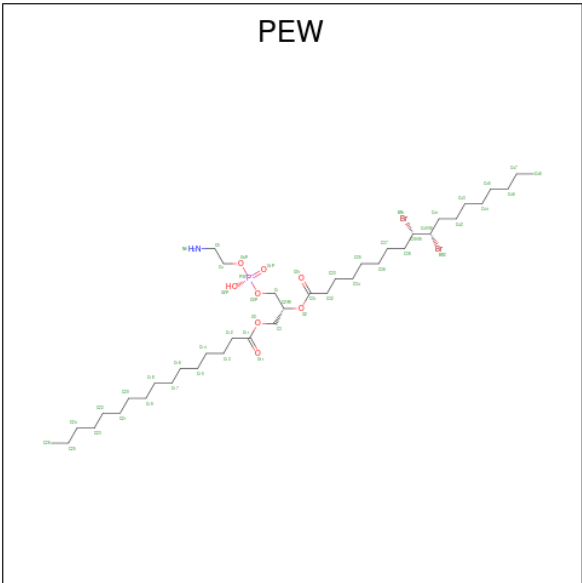
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

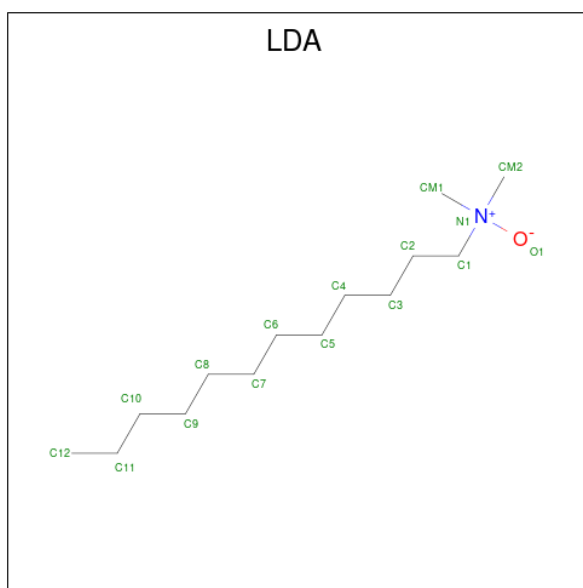
- Molecule 12 is (1R)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (CCD ID: PEW) (formula: C₃₉H₇₆Br₂NO₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	M	1	Total	Br	C	N	O	P	0	0
			51	2	39	1	8	1		

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:

C₁₄H₃₁NO).

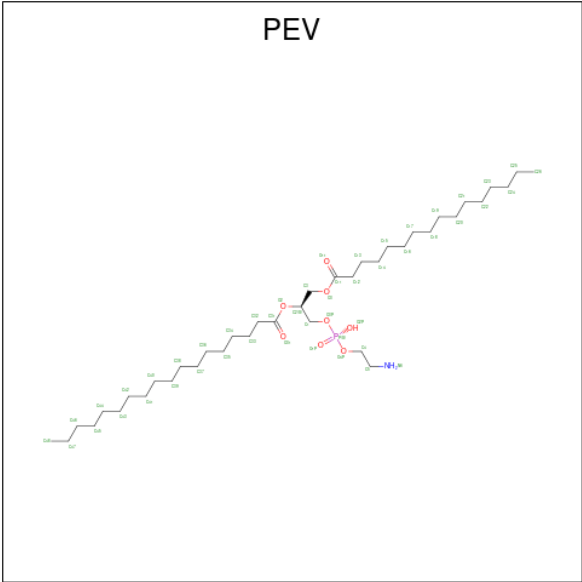


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 14 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 15 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	N	O	P	0	1
			98	78	2	16	2		

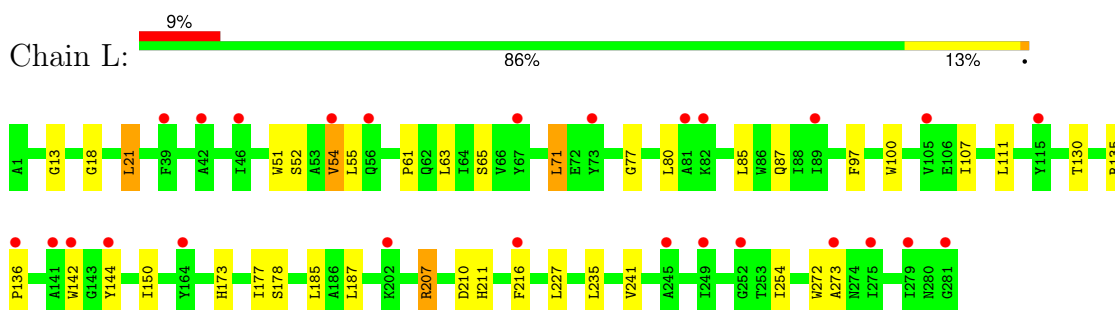
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	91	Total	O	0	0
			91	91		
16	M	118	Total	O	0	0
			118	118		
16	H	185	Total	O	0	0
			185	185		

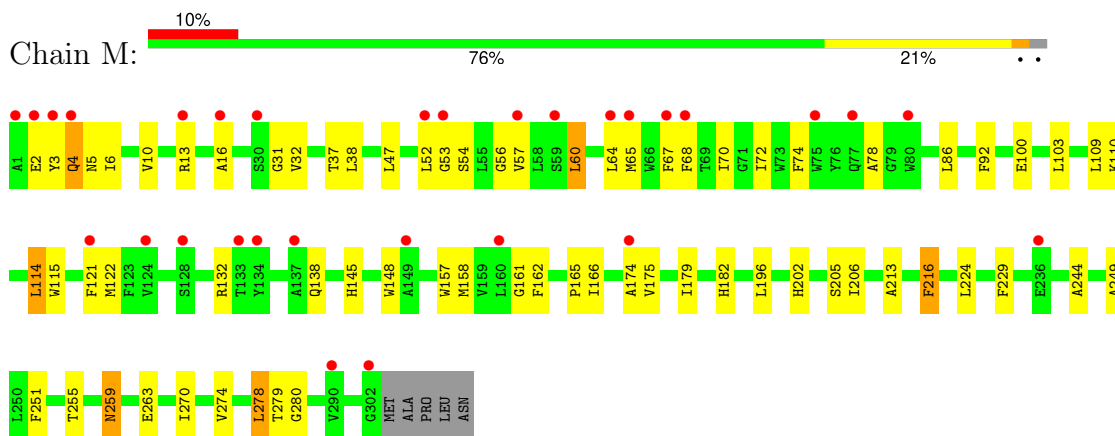
3 Residue-property plots [i](#)

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

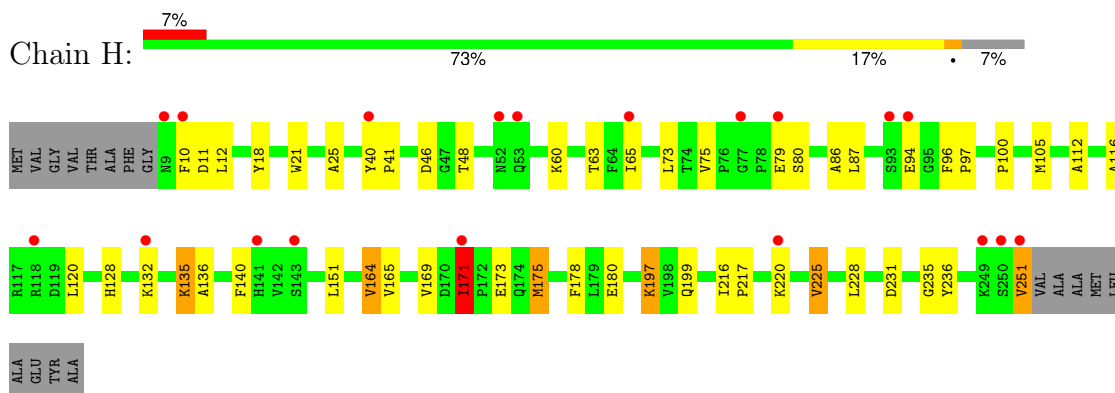
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.29Å 139.29Å 183.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.01 – 2.75 46.01 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-2.75) 99.9 (46.01-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.222 0.186 , 0.229	Depositor DCC
R_{free} test set	2689 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 121.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: GOL, BCL, FE, PEW, CDL, U10, PO4, LDA, CL, BPH, K, PEV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.09	0/2357	1.03	2/3228 (0.1%)
2	M	1.12	2/2617 (0.1%)	1.08	6/3569 (0.2%)
3	H	1.15	3/1952 (0.2%)	1.10	7/2653 (0.3%)
All	All	1.12	5/6926 (0.1%)	1.07	15/9450 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	217	PRO	C-N	-7.40	1.23	1.33
2	M	145	HIS	C-O	-6.38	1.16	1.24
3	H	171	ILE	CA-CB	6.36	1.62	1.54
3	H	120	LEU	N-CA	6.14	1.50	1.45
2	M	216	PHE	N-CA	-5.09	1.39	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	164	VAL	CB-CA-C	-6.37	103.63	111.08
2	M	279	THR	N-CA-C	-6.16	104.57	111.28
3	H	225	VAL	CB-CA-C	-5.97	101.62	110.82
2	M	263	GLU	N-CA-C	-5.86	104.25	111.40
2	M	216	PHE	N-CA-C	-5.61	105.16	112.23
2	M	4	GLN	N-CA-C	5.59	119.83	112.89
3	H	216	ILE	CA-C-N	5.59	125.52	119.76
3	H	216	ILE	C-N-CA	5.59	125.52	119.76
2	M	259	ASN	N-CA-C	5.56	115.72	107.88
1	L	227	LEU	N-CA-C	-5.45	104.99	111.69
3	H	216	ILE	N-CA-CB	5.43	116.19	110.17
1	L	13	GLY	N-CA-C	5.25	116.94	111.95
3	H	217	PRO	O-C-N	-5.25	116.68	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	278	LEU	CB-CA-C	-5.18	102.99	110.96
3	H	63	THR	N-CA-C	5.12	117.31	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2256	0	2215	34	0
2	M	2477	0	2381	53	0
3	H	1876	0	1893	30	0
4	L	132	0	148	8	0
4	M	132	0	148	16	0
5	L	65	0	76	5	0
5	M	65	0	76	9	0
6	L	48	0	63	3	0
6	M	48	0	63	0	0
7	H	6	0	8	1	0
7	L	6	0	8	0	0
8	M	1	0	0	0	0
9	H	1	0	0	0	0
9	M	2	0	0	0	0
10	H	5	0	0	1	0
10	M	10	0	0	2	0
11	M	81	0	106	1	0
12	M	51	0	73	11	0
13	H	48	0	93	3	0
13	M	48	0	93	12	0
14	H	1	0	0	0	0
15	H	98	0	154	3	0
16	H	185	0	0	5	0
16	L	91	0	0	1	0
16	M	118	0	0	1	0
All	All	7851	0	7598	142	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 9.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135[B]:ARG:HB3	1:L:136:PRO:HD3	1.18	1.16
1:L:135[B]:ARG:HB3	1:L:136:PRO:CD	1.87	1.02
1:L:135[B]:ARG:HG3	1:L:135[B]:ARG:HH21	1.28	0.95
2:M:31:GLY:H	12:M:802:PEW:H11	1.31	0.91
2:M:175:VAL:H	13:M:920:LDA:H122	1.32	0.90
2:M:47:LEU:HD22	12:M:802:PEW:BR2	2.30	0.86
1:L:135[B]:ARG:HH21	1:L:135[B]:ARG:CG	1.90	0.83
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.58	0.83
2:M:67[B]:PHE:HD2	2:M:68[B]:PHE:CE1	2.00	0.80
2:M:70:ILE:HG21	13:M:920:LDA:HM23	1.70	0.74
2:M:67[B]:PHE:HD2	2:M:68[B]:PHE:CD1	2.07	0.73
4:M:313:BCL:C20	12:M:802:PEW:H263	2.19	0.73
3:H:46:ASP:OD1	3:H:48:THR:HG23	1.90	0.72
2:M:122:MET:HE1	4:M:311:BCL:HBB3	1.76	0.68
2:M:70:ILE:HD13	13:M:920:LDA:HM22	1.76	0.67
10:H:705:PO4:P	16:H:1354:HOH:O	2.53	0.67
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.78	0.66
4:L:314:BCL:HBB3	5:L:402:BPH:H141	1.79	0.65
2:M:31:GLY:N	12:M:802:PEW:H11	2.10	0.65
4:M:313:BCL:H203	12:M:802:PEW:H263	1.79	0.64
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:CE1	2.84	0.64
2:M:122:MET:HE1	4:M:311:BCL:CBB	2.29	0.63
1:L:135[B]:ARG:CB	1:L:136:PRO:CD	2.69	0.62
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.00	0.62
1:L:71:LEU:HD21	1:L:144:TYR:CZ	2.34	0.61
1:L:61:PRO:O	1:L:150:ILE:HD12	2.00	0.61
3:H:46:ASP:OD1	3:H:46:ASP:C	2.42	0.61
1:L:135[B]:ARG:CG	1:L:135[B]:ARG:NH2	2.56	0.60
1:L:135[B]:ARG:CB	1:L:136:PRO:HD3	2.13	0.60
2:M:70:ILE:HD13	13:M:920:LDA:CM2	2.32	0.59
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.84	0.59
1:L:71:LEU:HD13	1:L:71:LEU:O	2.03	0.58
4:M:313:BCL:H201	12:M:802:PEW:H263	1.85	0.58
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:HE1	2.21	0.58
1:L:97:PHE:CZ	4:L:312:BCL:H112	2.38	0.58
2:M:175:VAL:H	13:M:920:LDA:C12	2.11	0.57
4:M:311:BCL:HMB3	4:M:311:BCL:HBB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:311:BCL:H192	12:M:802:PEW:H191	1.85	0.57
3:H:128:HIS:HD2	16:H:1245:HOH:O	1.86	0.57
1:L:135[A]:ARG:HB3	1:L:136:PRO:HD3	1.85	0.57
2:M:53:GLY:O	2:M:57:VAL:HG23	2.04	0.57
3:H:18:TYR:CD1	13:H:903:LDA:HM12	2.39	0.57
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.73	0.57
1:L:216:PHE:CD2	6:L:502:U10:H102	2.40	0.57
3:H:135:LYS:HG2	3:H:136:ALA:N	2.20	0.56
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.41	0.56
2:M:70:ILE:HG21	13:M:920:LDA:CM2	2.37	0.55
2:M:138:GLN:NE2	10:M:706:PO4:O2	2.40	0.55
2:M:65[A]:MET:HE2	2:M:121:PHE:CE2	2.43	0.54
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.43	0.54
2:M:60[A]:LEU:HD12	5:M:401:BPH:H4C1	1.89	0.54
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.44	0.52
5:L:402:BPH:HBB3	5:L:402:BPH:HMB1	1.91	0.52
1:L:178:SER:HB3	6:L:502:U10:H251	1.92	0.52
2:M:67[B]:PHE:CD2	2:M:68[B]:PHE:CD1	2.95	0.52
5:M:401:BPH:HHD	5:M:401:BPH:CBC	2.39	0.52
4:M:313:BCL:H203	12:M:802:PEW:C26	2.40	0.52
5:M:401:BPH:HHD	5:M:401:BPH:HBC2	1.92	0.51
2:M:56:GLY:O	2:M:60[A]:LEU:HD22	2.10	0.51
2:M:174:ALA:HB1	13:M:920:LDA:C12	2.39	0.51
4:M:311:BCL:H141	5:M:401:BPH:H9C1	1.92	0.51
3:H:135:LYS:CG	3:H:136:ALA:N	2.74	0.51
1:L:52:SER:HA	1:L:55:LEU:CD1	2.41	0.50
1:L:135[B]:ARG:O	1:L:136:PRO:C	2.54	0.50
2:M:205[A]:SER:HB3	4:M:313:BCL:HMA3	1.94	0.50
1:L:65:SER:O	16:L:1324:HOH:O	2.20	0.49
1:L:241:VAL:HG21	5:L:402:BPH:H2C	1.93	0.49
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.48	0.49
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.49
5:M:401:BPH:CBC	5:M:401:BPH:CHD	2.90	0.49
2:M:179:ILE:HG12	13:M:920:LDA:HM13	1.95	0.49
2:M:205[B]:SER:HB3	4:M:313:BCL:HMA3	1.94	0.49
2:M:280:GLY:O	4:M:313:BCL:HED3	2.13	0.48
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.48	0.47
3:H:135:LYS:HE3	3:H:135:LYS:HB3	1.24	0.47
3:H:105[B]:MET:HE2	3:H:236:TYR:CZ	2.49	0.47
4:M:313:BCL:OBB	4:M:313:BCL:HHC	2.14	0.47
1:L:80:LEU:HD22	1:L:85:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:109:LEU:HB3	2:M:114:LEU:HD22	1.97	0.46
3:H:135:LYS:HG2	3:H:136:ALA:H	1.80	0.46
5:M:401:BPH:C14	12:M:802:PEW:H182	2.45	0.46
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.46
4:L:314:BCL:HBB2	4:L:314:BCL:HMB3	1.98	0.45
3:H:79:GLU:HB2	16:H:1235:HOH:O	2.15	0.45
2:M:249:ALA:HB1	2:M:259:ASN:ND2	2.31	0.45
5:M:401:BPH:CHD	5:M:401:BPH:HBC3	2.47	0.45
3:H:132:LYS:HG3	3:H:171:ILE:HD11	1.98	0.45
1:L:272:TRP:O	1:L:273:ALA:C	2.59	0.45
3:H:21:TRP:NE1	15:H:801[B]:PEV:HN61	2.14	0.45
4:L:312:BCL:NA	4:M:313:BCL:HBB2	2.33	0.44
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.99	0.44
1:L:52:SER:HA	1:L:55:LEU:HD12	1.99	0.44
2:M:13:ARG:O	3:H:140:PHE:HA	2.18	0.44
3:H:112:ALA:HA	3:H:235:GLY:O	2.18	0.44
2:M:175:VAL:N	13:M:920:LDA:H122	2.15	0.44
1:L:51:TRP:O	1:L:54:VAL:HB	2.18	0.44
4:L:312:BCL:H52	5:L:402:BPH:HBB2	1.99	0.43
2:M:2[B]:GLU:O	2:M:4:GLN:NE2	2.51	0.43
4:L:312:BCL:HMB3	4:L:312:BCL:CBB	2.48	0.43
5:L:402:BPH:HMC3	2:M:213:ALA:CB	2.49	0.43
3:H:175:MET:HE3	16:H:1139:HOH:O	2.18	0.43
15:H:801[A]:PEV:O31	15:H:801[A]:PEV:H32	2.18	0.43
15:H:801[A]:PEV:O31	15:H:801[A]:PEV:C3	2.66	0.43
2:M:115:TRP:HZ2	13:M:920:LDA:H121	1.84	0.43
3:H:18:TYR:HD1	13:H:903:LDA:HM12	1.82	0.43
2:M:157:TRP:CZ3	2:M:158:MET:HG2	2.54	0.43
5:M:401:BPH:H142	12:M:802:PEW:H202	2.01	0.43
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.37	0.42
3:H:73:LEU:HD11	3:H:75:VAL:HG13	2.02	0.42
2:M:161:GLY:HA2	13:M:920:LDA:H123	2.01	0.42
4:L:312:BCL:OBB	4:L:312:BCL:HHC	2.19	0.42
3:H:116:ALA:HA	3:H:228:LEU:CD1	2.50	0.42
4:L:314:BCL:HBA1	4:L:314:BCL:C4A	2.49	0.42
2:M:6:ILE:HD13	2:M:224:LEU:HD13	2.01	0.42
1:L:130:THR:O	1:L:135[B]:ARG:HB2	2.18	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.55	0.42
2:M:270:ILE:HD13	11:M:800:CDL:C71	2.49	0.42
3:H:94:GLU:HG2	16:H:1242:HOH:O	2.20	0.42
3:H:73:LEU:HD11	3:H:75:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:251:VAL:O	3:H:251:VAL:HG12	2.20	0.42
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.56	0.41
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.00	0.41
1:L:51:TRP:CH2	1:L:80:LEU:HD13	2.54	0.41
1:L:207:ARG:CG	1:L:211:HIS:CG	3.03	0.41
2:M:64:LEU:HD21	5:M:401:BPH:H121	2.02	0.41
13:M:902:LDA:HM13	13:M:902:LDA:H21	1.90	0.41
1:L:216:PHE:CE2	6:L:502:U10:H102	2.55	0.41
2:M:162:PHE:C	2:M:165:PRO:HD2	2.46	0.41
3:H:197[A]:LYS:CD	3:H:199:GLN:CG	2.98	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
2:M:110:LYS:NZ	16:M:1389:HOH:O	2.54	0.41
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	2.02	0.41
3:H:25:ALA:HB1	13:H:904:LDA:HM11	2.03	0.41
3:H:165:VAL:CG2	3:H:180:GLU:HG2	2.51	0.41
4:M:313:BCL:C20	12:M:802:PEW:C26	2.96	0.40
3:H:151:LEU:O	3:H:164:VAL:HG23	2.20	0.40
3:H:178:PHE:CE2	7:H:708:GOL:H11	2.57	0.40
1:L:107:ILE:HG22	1:L:111:LEU:HD12	2.03	0.40
2:M:54:SER:OG	10:M:704:PO4:O2	2.38	0.40
3:H:40:TYR:HA	3:H:41:PRO:C	2.46	0.40
1:L:100:TRP:CZ2	2:M:255:THR:HG22	2.57	0.40
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	283/281 (101%)	268 (95%)	14 (5%)	1 (0%)	30	50
2	M	313/307 (102%)	299 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	H	247/260 (95%)	237 (96%)	9 (4%)	1 (0%)	30 50
All	All	843/848 (99%)	804 (95%)	37 (4%)	2 (0%)	43 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	86	ALA
1	L	54	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	224/220 (102%)	216 (96%)	8 (4%)	31 55
2	M	249/240 (104%)	233 (94%)	16 (6%)	16 29
3	H	204/208 (98%)	188 (92%)	16 (8%)	11 21
All	All	677/668 (101%)	637 (94%)	40 (6%)	18 33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	63	LEU
1	L	71	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	254	ILE
2	M	10	VAL
2	M	37	THR
2	M	38	LEU
2	M	52	LEU
2	M	60[A]	LEU

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Mol	Chain	Res	Type
2	M	60[B]	LEU
2	M	72	ILE
2	M	86	LEU
2	M	100[A]	GLU
2	M	100[B]	GLU
2	M	114	LEU
2	M	132	ARG
2	M	182	HIS
2	M	196	LEU
2	M	274	VAL
2	M	278	LEU
3	H	10	PHE
3	H	11	ASP
3	H	12	LEU
3	H	60	LYS
3	H	65	ILE
3	H	80	SER
3	H	135	LYS
3	H	171	ILE
3	H	173	GLU
3	H	175	MET
3	H	197[A]	LYS
3	H	197[B]	LYS
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP
3	H	251	VAL

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

Mol	Chain	Res	Type
1	L	274	ASN
2	M	4	GLN
2	M	28	ASN
2	M	202	HIS
3	H	9	ASN

5.3.3 RNA ⓘ

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 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	BCL	L	314	1	69,74,74	1.18	4 (5%)	79,115,115	1.81	18 (22%)
7	GOL	L	707	-	5,5,5	0.48	0	5,5,5	0.60	0
13	LDA	H	904	-	13,15,15	2.21	2 (15%)	14,17,17	0.56	0
13	LDA	H	901	-	13,15,15	2.17	2 (15%)	14,17,17	0.55	0
12	PEW	M	802	-	50,50,50	0.98	3 (6%)	53,57,57	1.33	5 (9%)
13	LDA	H	903	-	13,15,15	2.13	2 (15%)	14,17,17	0.56	0
4	BCL	M	311	2	69,74,74	1.19	5 (7%)	79,115,115	1.45	16 (20%)
4	BCL	L	312	1	69,74,74	1.23	5 (7%)	79,115,115	1.26	9 (11%)
6	U10	L	502	-	48,48,63	1.24	3 (6%)	60,61,79	1.71	13 (21%)
10	PO4	M	704	-	4,4,4	0.68	0	6,6,6	1.77	2 (33%)
7	GOL	H	708	-	5,5,5	0.31	0	5,5,5	0.74	0
15	PEV	H	801[B]	-	48,48,48	0.97	2 (4%)	51,53,53	1.06	4 (7%)
11	CDL	M	800	-	80,80,99	1.31	5 (6%)	86,92,111	1.26	9 (10%)
10	PO4	H	705	-	4,4,4	1.11	0	6,6,6	0.69	0
5	BPH	L	402	-	59,70,70	1.51	8 (13%)	59,101,101	1.86	16 (27%)
10	PO4	M	706	-	4,4,4	0.95	0	6,6,6	0.94	1 (16%)
6	U10	M	501	-	48,48,63	1.19	4 (8%)	60,61,79	1.44	9 (15%)
13	LDA	M	902	-	13,15,15	1.97	2 (15%)	14,17,17	0.58	0
4	BCL	M	313	2	69,74,74	1.42	8 (11%)	79,115,115	1.61	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEV	H	801[A]	-	48,48,48	0.93	1 (2%)	51,53,53	1.05	4 (7%)
13	LDA	M	920	-	13,15,15	2.01	2 (15%)	14,17,17	1.10	1 (7%)
5	BPH	M	401	-	59,70,70	1.25	5 (8%)	59,101,101	2.33	19 (32%)
13	LDA	M	907	-	13,15,15	2.16	2 (15%)	14,17,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	314	1	-	5/41/137/137	-
7	GOL	L	707	-	-	3/4/4/4	-
13	LDA	H	904	-	-	6/13/13/13	-
13	LDA	H	901	-	-	6/13/13/13	-
12	PEW	M	802	-	-	27/57/57/57	-
13	LDA	H	903	-	-	2/13/13/13	-
4	BCL	M	311	2	-	9/41/137/137	-
4	BCL	L	312	1	-	3/41/137/137	-
6	U10	L	502	-	-	14/45/69/87	0/1/1/1
7	GOL	H	708	-	-	2/4/4/4	-
15	PEV	H	801[B]	-	-	26/52/52/52	-
11	CDL	M	800	-	-	36/91/91/110	-
5	BPH	L	402	-	-	4/37/105/105	0/5/6/6
6	U10	M	501	-	-	6/45/69/87	0/1/1/1
13	LDA	M	902	-	-	3/13/13/13	-
4	BCL	M	313	2	-	5/41/137/137	-
15	PEV	H	801[A]	-	-	20/52/52/52	-
13	LDA	M	920	-	-	7/13/13/13	-
5	BPH	M	401	-	-	14/37/105/105	0/5/6/6
13	LDA	M	907	-	-	7/13/13/13	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	901	LDA	O1-N1	-6.62	1.25	1.42
13	M	907	LDA	O1-N1	-6.51	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	904	LDA	O1-N1	-6.49	1.26	1.42
13	H	903	LDA	O1-N1	-6.44	1.26	1.42
13	M	920	LDA	O1-N1	-6.32	1.26	1.42
13	M	902	LDA	O1-N1	-6.02	1.27	1.42
4	L	312	BCL	MG-NA	5.77	2.20	2.06
4	M	313	BCL	MG-NB	5.68	2.17	2.05
11	M	800	CDL	OA8-CA7	5.50	1.49	1.33
4	M	313	BCL	MG-NA	5.38	2.19	2.06
6	L	502	U10	O3-C3	5.03	1.48	1.36
11	M	800	CDL	OA6-CA5	4.79	1.47	1.34
5	M	401	BPH	C1B-C2B	4.69	1.44	1.39
4	L	314	BCL	MG-NB	4.57	2.14	2.05
11	M	800	CDL	OB6-CB5	4.43	1.46	1.34
13	H	904	LDA	C1-N1	-4.38	1.47	1.51
5	L	402	BPH	C1B-C2B	4.30	1.44	1.39
11	M	800	CDL	OB8-CB7	4.27	1.45	1.33
5	M	401	BPH	C1D-C2D	4.27	1.44	1.39
5	L	402	BPH	C1D-C2D	4.18	1.44	1.39
13	H	903	LDA	C1-N1	-4.11	1.47	1.51
13	M	907	LDA	C1-N1	-4.04	1.47	1.51
6	M	501	U10	O3-C3	3.99	1.46	1.36
4	M	311	BCL	MG-NA	3.96	2.15	2.06
13	H	901	LDA	C1-N1	-3.94	1.47	1.51
5	L	402	BPH	C3B-C4B	3.94	1.47	1.41
4	M	311	BCL	C3B-C4B	3.89	1.48	1.41
15	H	801[B]	PEV	P-O1P	3.85	1.64	1.50
5	L	402	BPH	CBD-CGD	3.77	1.57	1.52
4	M	313	BCL	C3C-C4C	-3.54	1.47	1.51
12	M	802	PEW	P-O1P	3.53	1.63	1.50
13	M	902	LDA	C1-N1	-3.49	1.47	1.51
13	M	920	LDA	C1-N1	-3.43	1.48	1.51
6	M	501	U10	O4-C4	3.29	1.44	1.36
6	L	502	U10	O4-C4	3.27	1.44	1.36
5	L	402	BPH	C3A-C2A	-3.25	1.51	1.54
15	H	801[A]	PEV	P-O1P	3.15	1.61	1.50
4	M	311	BCL	MG-NB	3.00	2.11	2.05
6	M	501	U10	C31-C29	2.86	1.57	1.51
4	M	313	BCL	CHD-C1D	2.86	1.44	1.38
4	L	312	BCL	C3B-C4B	2.82	1.46	1.41
4	L	312	BCL	MG-NB	2.74	2.11	2.05
4	L	312	BCL	C4-C3	2.62	1.57	1.50
4	L	314	BCL	MG-NA	2.54	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	C13-C14	2.42	1.38	1.33
4	M	313	BCL	C3B-C4B	2.36	1.45	1.41
5	M	401	BPH	C3A-C2A	-2.29	1.52	1.54
5	L	402	BPH	C2C-C3C	2.27	1.56	1.54
5	M	401	BPH	C3B-C4B	2.24	1.45	1.41
5	L	402	BPH	C4D-ND	-2.23	1.35	1.38
12	M	802	PEW	BR1-C39	-2.19	1.92	1.97
4	M	313	BCL	CHB-C4A	2.19	1.43	1.37
4	M	313	BCL	CBB-CAB	2.17	1.54	1.50
5	L	402	BPH	C3B-C2B	-2.11	1.36	1.39
4	L	314	BCL	C2A-C1A	-2.11	1.47	1.52
12	M	802	PEW	P-O4P	2.09	1.67	1.59
5	M	401	BPH	OBD-CAD	-2.09	1.19	1.22
4	M	313	BCL	CHC-C1C	2.09	1.42	1.37
11	M	800	CDL	CA3-CA4	2.07	1.57	1.50
15	H	801[B]	PEV	C3-C2	2.07	1.57	1.50
4	M	311	BCL	OBD-CAD	2.05	1.26	1.22
4	L	314	BCL	O2A-CGA	2.02	1.39	1.33
6	M	501	U10	C13-C14	2.01	1.37	1.33
4	L	312	BCL	MG-NC	2.00	2.11	2.06
4	M	311	BCL	C1-C2	2.00	1.54	1.49

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	O2D-CGD-CBD	7.56	119.25	110.95
5	M	401	BPH	O2D-CGD-CBD	7.53	119.22	110.95
5	M	401	BPH	OBD-CAD-CBD	-7.03	115.51	125.82
6	L	502	U10	C25-C24-C26	6.16	125.93	115.23
12	M	802	PEW	O2-C31-C32	5.36	123.08	111.48
4	M	313	BCL	C4D-CHA-C1A	5.19	127.44	121.24
5	M	401	BPH	C4D-CHA-CBD	-5.02	106.05	108.45
11	M	800	CDL	OA6-CA5-C11	5.00	122.30	111.48
4	L	314	BCL	O2D-CGD-CBD	4.92	119.83	111.23
5	M	401	BPH	C2D-C1D-ND	-4.70	106.03	109.43
4	L	314	BCL	O1D-CGD-CBD	-4.58	115.49	124.52
4	M	313	BCL	C1C-NC-C4C	4.38	108.68	106.68
6	M	501	U10	C17-C18-C19	-4.27	117.84	127.62
4	L	314	BCL	C2B-C1B-NB	-4.22	105.95	110.33
5	M	401	BPH	C2B-C1B-NB	-4.19	106.40	109.43
4	L	314	BCL	CAA-C2A-C3A	-4.15	101.79	113.00
11	M	800	CDL	OB6-CB5-C51	4.09	120.33	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	OBD-CAD-C3D	4.01	134.15	127.89
6	L	502	U10	C25-C24-C23	-3.94	113.51	123.63
15	H	801[A]	PEV	O2-C31-C32	3.88	119.87	111.48
4	L	314	BCL	CAC-C3C-C4C	-3.83	104.08	112.58
5	L	402	BPH	C1-C2-C3	-3.75	120.06	126.20
15	H	801[B]	PEV	O2-C31-C32	3.71	119.50	111.48
5	M	401	BPH	C1-C2-C3	-3.70	120.13	126.20
4	L	312	BCL	C2B-C1B-NB	-3.53	106.66	110.33
5	M	401	BPH	CAA-C2A-C3A	-3.53	103.46	113.00
4	M	311	BCL	C4D-CHA-C1A	3.53	125.45	121.24
12	M	802	PEW	BR1-C39-C40	-3.53	103.44	110.27
4	M	311	BCL	C1-O2A-CGA	3.51	125.14	116.65
6	M	501	U10	C30-C29-C31	3.45	121.22	115.23
4	M	313	BCL	CHD-C1D-ND	-3.45	119.95	124.80
4	M	313	BCL	CAC-C3C-C4C	-3.44	104.96	112.58
5	M	401	BPH	CMA-C3A-C4A	-3.42	107.25	114.61
4	M	313	BCL	C1D-ND-C4D	3.40	108.70	106.31
4	L	314	BCL	C2C-C3C-C4C	3.39	106.42	101.34
5	L	402	BPH	CMD-C2D-C3D	3.36	131.40	124.68
4	M	311	BCL	C2B-C1B-NB	-3.30	106.90	110.33
6	M	501	U10	C22-C23-C24	-3.26	120.16	127.62
5	L	402	BPH	CMA-C3A-C4A	-3.23	107.65	114.61
12	M	802	PEW	BR2-C40-C39	-3.23	104.02	110.27
11	M	800	CDL	OB8-CB7-C71	3.20	121.59	111.83
6	L	502	U10	C22-C23-C24	-3.19	120.31	127.62
4	M	311	BCL	O2D-CGD-CBD	3.15	116.73	111.23
4	L	314	BCL	C4A-NA-C1A	3.14	108.11	106.68
4	M	311	BCL	OB8-CAB-C3B	3.12	125.96	120.43
4	L	314	BCL	CAA-CBA-CGA	3.12	122.06	113.21
10	M	704	PO4	O4-P-O1	-3.09	100.03	110.95
11	M	800	CDL	CA6-OA8-CA7	3.08	128.39	117.12
15	H	801[B]	PEV	O3-C3-C2	3.07	117.24	108.40
4	L	312	BCL	CAA-C2A-C3A	-3.06	104.74	113.00
5	L	402	BPH	CMA-C3A-C2A	-3.00	102.53	114.13
5	L	402	BPH	C2D-C1D-ND	-2.99	107.27	109.43
4	M	313	BCL	CHD-C1D-C2D	2.97	131.67	125.49
5	L	402	BPH	C4D-CHA-CBD	-2.94	107.04	108.45
5	L	402	BPH	CMB-C2B-C3B	2.94	130.56	124.68
4	M	313	BCL	CHA-C1A-NA	-2.94	119.74	126.39
4	L	314	BCL	C16-C15-C13	-2.92	106.24	115.97
4	M	311	BCL	CAA-C2A-C3A	-2.92	105.10	113.00
4	L	314	BCL	OB8-CAB-C3B	2.91	125.58	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	U10	C30-C29-C31	2.91	120.28	115.23
6	L	502	U10	O2-C2-C3	-2.91	114.87	121.03
4	M	313	BCL	C2C-C3C-C4C	2.90	105.68	101.34
4	M	313	BCL	C3B-C4B-NB	-2.90	105.93	109.76
11	M	800	CDL	O1-C1-CB2	2.89	119.67	109.70
4	L	314	BCL	C4D-CHA-C1A	2.87	124.67	121.24
15	H	801[A]	PEV	O2-C2-C3	2.87	118.65	108.34
13	M	920	LDA	CM1-N1-C1	2.84	116.21	110.23
6	L	502	U10	C1-C6-C5	-2.83	116.87	119.62
4	L	312	BCL	C5-C3-C2	-2.83	114.82	121.17
4	M	313	BCL	C4-C3-C5	2.79	120.07	115.23
6	M	501	U10	C16-C14-C13	-2.74	115.01	121.17
15	H	801[B]	PEV	O3-C11-C12	2.73	120.16	111.83
5	M	401	BPH	C1-O2A-CGA	2.73	123.26	116.65
6	M	501	U10	C41-C39-C40	2.72	120.85	114.59
5	L	402	BPH	C3B-C4B-NB	-2.70	104.13	108.05
10	M	704	PO4	O4-P-O3	2.68	116.24	107.91
15	H	801[A]	PEV	O3-C3-C2	2.67	116.11	108.40
4	L	314	BCL	C5-C3-C2	-2.66	115.20	121.17
5	M	401	BPH	O2D-CGD-O1D	-2.62	118.75	123.85
4	M	311	BCL	C4A-NA-C1A	2.60	107.87	106.68
5	M	401	BPH	CMC-C2C-C1C	2.57	120.16	114.61
5	L	402	BPH	O2D-CGD-O1D	-2.56	118.87	123.85
12	M	802	PEW	O2-C31-O31	-2.55	117.75	123.70
6	L	502	U10	C3M-O3-C3	2.54	125.41	116.47
5	M	401	BPH	CMB-C2B-C3B	2.53	129.74	124.68
6	L	502	U10	C12-C13-C14	-2.52	121.85	127.62
6	M	501	U10	C7-C6-C5	-2.52	115.59	118.52
15	H	801[A]	PEV	O3-C11-C12	2.49	119.43	111.83
4	L	314	BCL	CHD-C1D-ND	-2.49	121.30	124.80
4	M	313	BCL	C2B-C1B-NB	-2.46	107.77	110.33
6	M	501	U10	C15-C14-C16	2.46	119.50	115.23
4	L	314	BCL	OBb-CAB-CBB	-2.45	114.27	119.77
4	M	313	BCL	C1-C2-C3	-2.44	122.20	126.20
11	M	800	CDL	OA8-CA7-C31	2.43	119.26	111.83
5	L	402	BPH	C2B-C1B-NB	-2.41	107.69	109.43
4	L	312	BCL	C4-C3-C5	2.41	119.41	115.23
4	M	311	BCL	CMB-C2B-C1B	-2.41	121.76	125.42
4	L	312	BCL	C3B-C4B-NB	-2.40	106.60	109.76
4	M	311	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
4	L	312	BCL	CHA-C1A-NA	-2.39	120.98	126.39
5	L	402	BPH	CBC-CAC-C3C	2.38	118.45	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	CMA-C3A-C2A	-2.37	104.96	114.13
6	M	501	U10	C31-C32-C33	2.34	123.61	112.02
5	M	401	BPH	C1C-C2C-C3C	-2.34	100.61	102.84
4	M	311	BCL	CED-O2D-CGD	-2.33	110.62	115.92
4	L	314	BCL	C16-C17-C18	-2.33	105.54	115.94
4	M	311	BCL	CHA-C1A-NA	-2.32	121.14	126.39
4	M	311	BCL	C3B-C4B-NB	-2.32	106.70	109.76
4	L	312	BCL	CMB-C2B-C1B	-2.31	121.90	125.42
4	L	312	BCL	C6-C7-C8	-2.30	108.31	115.97
6	L	502	U10	C7-C8-C9	-2.28	122.90	126.83
5	L	402	BPH	CMC-C2C-C3C	2.26	122.86	114.13
4	M	313	BCL	O2D-CGD-O1D	-2.25	119.46	123.85
12	M	802	PEW	C2-O2-C31	-2.25	112.41	117.80
5	L	402	BPH	CED-O2D-CGD	2.21	120.94	115.92
4	L	312	BCL	CAA-C2A-C1A	-2.21	104.73	111.97
6	L	502	U10	C36-C34-C33	2.20	126.10	121.17
5	M	401	BPH	CBC-CAC-C3C	-2.19	109.47	113.78
4	L	314	BCL	CAA-C2A-C1A	-2.18	104.83	111.97
6	L	502	U10	C3-C2-C1	2.16	122.36	118.10
4	M	311	BCL	CHD-C1D-ND	-2.15	121.78	124.80
11	M	800	CDL	OB8-CB7-OB9	-2.13	118.29	123.63
11	M	800	CDL	OA6-CA5-OA7	-2.13	118.72	123.70
15	H	801[B]	PEV	O2-C31-O31	-2.13	118.72	123.70
11	M	800	CDL	PB2-OB2-CB2	2.13	133.56	121.35
4	M	311	BCL	CMC-C2C-C3C	-2.13	105.75	113.98
6	L	502	U10	C7-C6-C5	-2.13	116.04	118.52
4	L	314	BCL	C11-C12-C13	-2.12	108.92	115.97
5	L	402	BPH	OBD-CAD-CBD	-2.11	122.73	125.82
5	M	401	BPH	C4-C3-C2	-2.10	118.23	123.63
4	M	311	BCL	OBD-CAD-C3D	2.07	133.25	128.42
5	M	401	BPH	C3D-CAD-CBD	2.07	110.33	107.61
10	M	706	PO4	O4-P-O3	2.06	114.32	107.91
6	M	501	U10	C10-C9-C11	2.05	118.79	115.23
4	M	313	BCL	CAB-C3B-C2B	2.05	132.00	127.74
6	L	502	U10	C35-C34-C33	-2.04	118.39	123.63
4	M	311	BCL	CMA-C3A-C2A	-2.03	106.14	113.98
5	L	402	BPH	CAA-C2A-C3A	-2.03	107.53	113.00
5	M	401	BPH	C1B-NB-C4B	2.02	111.76	108.82
4	L	314	BCL	CHB-C4A-NA	2.01	127.30	124.40

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	311	BCL	C11-C12-C13-C14
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
7	L	707	GOL	O1-C1-C2-C3
11	M	800	CDL	CA2-C1-CB2-OB2
11	M	800	CDL	CA2-OA2-PA1-OA3
11	M	800	CDL	CA2-OA2-PA1-OA4
11	M	800	CDL	CA2-OA2-PA1-OA5
11	M	800	CDL	C1-CB2-OB2-PB2
11	M	800	CDL	CB3-OB5-PB2-OB2
11	M	800	CDL	CB3-OB5-PB2-OB3
11	M	800	CDL	CB3-OB5-PB2-OB4
11	M	800	CDL	OB6-CB4-CB6-OB8
12	M	802	PEW	C40-C41-C42-C43
12	M	802	PEW	BR1-C39-C40-C41
12	M	802	PEW	C38-C39-C40-C41
12	M	802	PEW	C38-C39-C40-BR2
12	M	802	PEW	C1-O3P-P-O1P
12	M	802	PEW	C1-O3P-P-O2P
12	M	802	PEW	C1-O3P-P-O4P
12	M	802	PEW	C4-O4P-P-O3P
12	M	802	PEW	C4-O4P-P-O1P
12	M	802	PEW	C4-O4P-P-O2P
12	M	802	PEW	O11-C11-O3-C3
13	M	920	LDA	C2-C1-N1-O1
13	M	920	LDA	C2-C1-N1-CM1
13	H	904	LDA	N1-C1-C2-C3
15	H	801[A]	PEV	C1-O3P-P-O1P
15	H	801[A]	PEV	O4P-C4-C5-N6
15	H	801[B]	PEV	C32-C31-O2-C2
15	H	801[B]	PEV	C1-O3P-P-O1P
15	H	801[B]	PEV	C4-O4P-P-O3P
15	H	801[B]	PEV	C4-O4P-P-O1P
15	H	801[B]	PEV	C4-O4P-P-O2P
12	M	802	PEW	C12-C11-O3-C3
15	H	801[B]	PEV	C12-C11-O3-C3
15	H	801[B]	PEV	O31-C31-O2-C2
11	M	800	CDL	O1-C1-CB2-OB2
15	H	801[B]	PEV	O11-C11-O3-C3
5	M	401	BPH	C11-C12-C13-C14
11	M	800	CDL	CB7-C71-C72-C73
5	M	401	BPH	C12-C13-C15-C16
11	M	800	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	H	801[B]	PEV	C31-C32-C33-C34
5	M	401	BPH	C8-C10-C11-C12
11	M	800	CDL	C38-C39-C40-C41
4	M	313	BCL	C13-C15-C16-C17
15	H	801[A]	PEV	C11-C12-C13-C14
4	M	311	BCL	C16-C17-C18-C20
12	M	802	PEW	C32-C31-O2-C2
5	M	401	BPH	C16-C17-C18-C20
5	L	402	BPH	C8-C10-C11-C12
15	H	801[A]	PEV	C19-C20-C21-C22
13	H	901	LDA	C5-C6-C7-C8
13	H	901	LDA	C11-C10-C9-C8
7	L	707	GOL	O1-C1-C2-O2
11	M	800	CDL	C18-C19-C20-C21
12	M	802	PEW	C19-C20-C21-C22
15	H	801[B]	PEV	C21-C22-C23-C24
13	M	920	LDA	C7-C8-C9-C10
11	M	800	CDL	C78-C79-C80-C81
13	M	920	LDA	C4-C5-C6-C7
13	M	920	LDA	C5-C6-C7-C8
15	H	801[A]	PEV	C36-C37-C38-C39
13	H	901	LDA	C6-C7-C8-C9
15	H	801[B]	PEV	C43-C44-C45-C46
15	H	801[B]	PEV	C37-C38-C39-C40
13	H	904	LDA	C7-C8-C9-C10
12	M	802	PEW	C15-C16-C17-C18
15	H	801[A]	PEV	C2-C1-O3P-P
12	M	802	PEW	O31-C31-O2-C2
4	M	311	BCL	C16-C17-C18-C19
15	H	801[A]	PEV	C32-C31-O2-C2
13	M	902	LDA	C1-C2-C3-C4
13	H	901	LDA	C1-C2-C3-C4
15	H	801[A]	PEV	O31-C31-O2-C2
15	H	801[B]	PEV	C11-C12-C13-C14
13	H	904	LDA	C1-C2-C3-C4
15	H	801[A]	PEV	C37-C38-C39-C40
15	H	801[A]	PEV	C32-C33-C34-C35
12	M	802	PEW	C34-C35-C36-C37
11	M	800	CDL	C20-C21-C22-C23
13	H	904	LDA	C2-C3-C4-C5
11	M	800	CDL	C17-C18-C19-C20
15	H	801[B]	PEV	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	H	801[A]	PEV	C15-C16-C17-C18
13	M	907	LDA	C11-C10-C9-C8
11	M	800	CDL	C71-C72-C73-C74
11	M	800	CDL	OA5-CA3-CA4-CA6
5	M	401	BPH	C11-C12-C13-C15
11	M	800	CDL	C13-C14-C15-C16
11	M	800	CDL	CB3-CB4-CB6-OB8
11	M	800	CDL	C72-C73-C74-C75
15	H	801[B]	PEV	C14-C15-C16-C17
15	H	801[B]	PEV	C17-C18-C19-C20
13	H	903	LDA	C7-C8-C9-C10
7	H	708	GOL	O1-C1-C2-C3
15	H	801[A]	PEV	C3-C2-O2-C31
15	H	801[B]	PEV	C1-C2-O2-C31
11	M	800	CDL	C19-C20-C21-C22
15	H	801[B]	PEV	C18-C19-C20-C21
13	H	901	LDA	C9-C10-C11-C12
15	H	801[B]	PEV	C19-C20-C21-C22
13	M	907	LDA	C2-C3-C4-C5
6	L	502	U10	C20-C19-C21-C22
6	M	501	U10	C35-C34-C36-C37
13	M	907	LDA	C9-C10-C11-C12
5	M	401	BPH	C15-C16-C17-C18
13	M	907	LDA	C1-C2-C3-C4
13	M	907	LDA	C6-C7-C8-C9
13	M	920	LDA	C3-C4-C5-C6
12	M	802	PEW	C11-C12-C13-C14
4	M	311	BCL	C11-C12-C13-C15
4	L	312	BCL	C15-C16-C17-C18
15	H	801[A]	PEV	C44-C45-C46-C47
12	M	802	PEW	C39-C40-C41-C42
6	M	501	U10	C33-C34-C36-C37
15	H	801[A]	PEV	C12-C13-C14-C15
11	M	800	CDL	CA3-CA4-CA6-OA8
11	M	800	CDL	OA5-CA3-CA4-OA6
12	M	802	PEW	C12-C13-C14-C15
5	L	402	BPH	C4-C3-C5-C6
11	M	800	CDL	C74-C75-C76-C77
12	M	802	PEW	C14-C15-C16-C17
11	M	800	CDL	C31-CA7-OA8-CA6
5	M	401	BPH	C16-C17-C18-C19
7	L	707	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
11	M	800	CDL	C55-C56-C57-C58
5	L	402	BPH	C2-C3-C5-C6
6	L	502	U10	C18-C19-C21-C22
5	M	401	BPH	C10-C11-C12-C13
13	H	904	LDA	C6-C7-C8-C9
13	M	907	LDA	C7-C8-C9-C10
11	M	800	CDL	OA9-CA7-OA8-CA6
5	M	401	BPH	C6-C7-C8-C10
12	M	802	PEW	O3P-C1-C2-O2
11	M	800	CDL	C79-C80-C81-C82
6	M	501	U10	C24-C26-C27-C28
6	L	502	U10	C15-C14-C16-C17
11	M	800	CDL	OA6-CA4-CA6-OA8
5	M	401	BPH	C6-C7-C8-C9
5	M	401	BPH	C14-C13-C15-C16
15	H	801[A]	PEV	C13-C14-C15-C16
13	M	920	LDA	C2-C1-N1-CM2
12	M	802	PEW	O3P-C1-C2-C3
11	M	800	CDL	C51-C52-C53-C54
13	H	903	LDA	C6-C7-C8-C9
4	L	312	BCL	C4-C3-C5-C6
4	L	314	BCL	CHA-CBD-CGD-O1D
4	L	314	BCL	CHA-CBD-CGD-O2D
15	H	801[A]	PEV	C1-O3P-P-O4P
13	M	902	LDA	C4-C5-C6-C7
15	H	801[B]	PEV	C36-C37-C38-C39
6	L	502	U10	C13-C14-C16-C17
15	H	801[A]	PEV	C18-C19-C20-C21
15	H	801[B]	PEV	C32-C33-C34-C35
12	M	802	PEW	C22-C23-C24-C25
6	L	502	U10	C5-C4-O4-C4M
6	M	501	U10	C31-C32-C33-C34
4	M	311	BCL	C3-C5-C6-C7
5	M	401	BPH	C3-C5-C6-C7
15	H	801[B]	PEV	C12-C13-C14-C15
4	L	314	BCL	C15-C16-C17-C18
4	M	311	BCL	C13-C15-C16-C17
13	M	902	LDA	C5-C6-C7-C8
12	M	802	PEW	BR2-C40-C41-C42
15	H	801[B]	PEV	C1-C2-C3-O3
15	H	801[B]	PEV	C23-C24-C25-C26
11	M	800	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
6	L	502	U10	C12-C11-C9-C10
4	M	311	BCL	C12-C13-C15-C16
11	M	800	CDL	C40-C41-C42-C43
13	H	901	LDA	C2-C3-C4-C5
6	M	501	U10	C5-C4-O4-C4M
11	M	800	CDL	OB7-CB5-OB6-CB4
4	M	313	BCL	C4-C3-C5-C6
6	L	502	U10	C12-C11-C9-C8
12	M	802	PEW	O2-C31-C32-C33
4	M	311	BCL	C4C-C3C-CAC-CBC
4	L	314	BCL	C16-C17-C18-C19
13	M	907	LDA	C4-C5-C6-C7
13	H	904	LDA	C11-C10-C9-C8
6	L	502	U10	C3-C4-O4-C4M
4	L	314	BCL	C14-C13-C15-C16
4	M	313	BCL	C6-C7-C8-C9
4	L	312	BCL	C2-C3-C5-C6
4	M	313	BCL	C2-C3-C5-C6
6	L	502	U10	C28-C29-C31-C32
15	H	801[B]	PEV	C34-C35-C36-C37
11	M	800	CDL	C15-C16-C17-C18
15	H	801[A]	PEV	C16-C17-C18-C19
15	H	801[A]	PEV	O2-C31-C32-C33
6	L	502	U10	C34-C36-C37-C38
4	M	313	BCL	CAA-CBA-CGA-O2A
12	M	802	PEW	O3-C11-C12-C13
6	M	501	U10	C25-C24-C26-C27
4	M	311	BCL	C15-C16-C17-C18
15	H	801[B]	PEV	C41-C42-C43-C44
6	L	502	U10	C11-C12-C13-C14
6	L	502	U10	C9-C11-C12-C13
6	L	502	U10	C30-C29-C31-C32
6	L	502	U10	C31-C32-C33-C34
15	H	801[A]	PEV	O31-C31-C32-C33
7	H	708	GOL	O1-C1-C2-O2
5	L	402	BPH	C4C-C3C-CAC-CBC

There are no ring outliers.

19 monomers are involved in 63 short contacts:

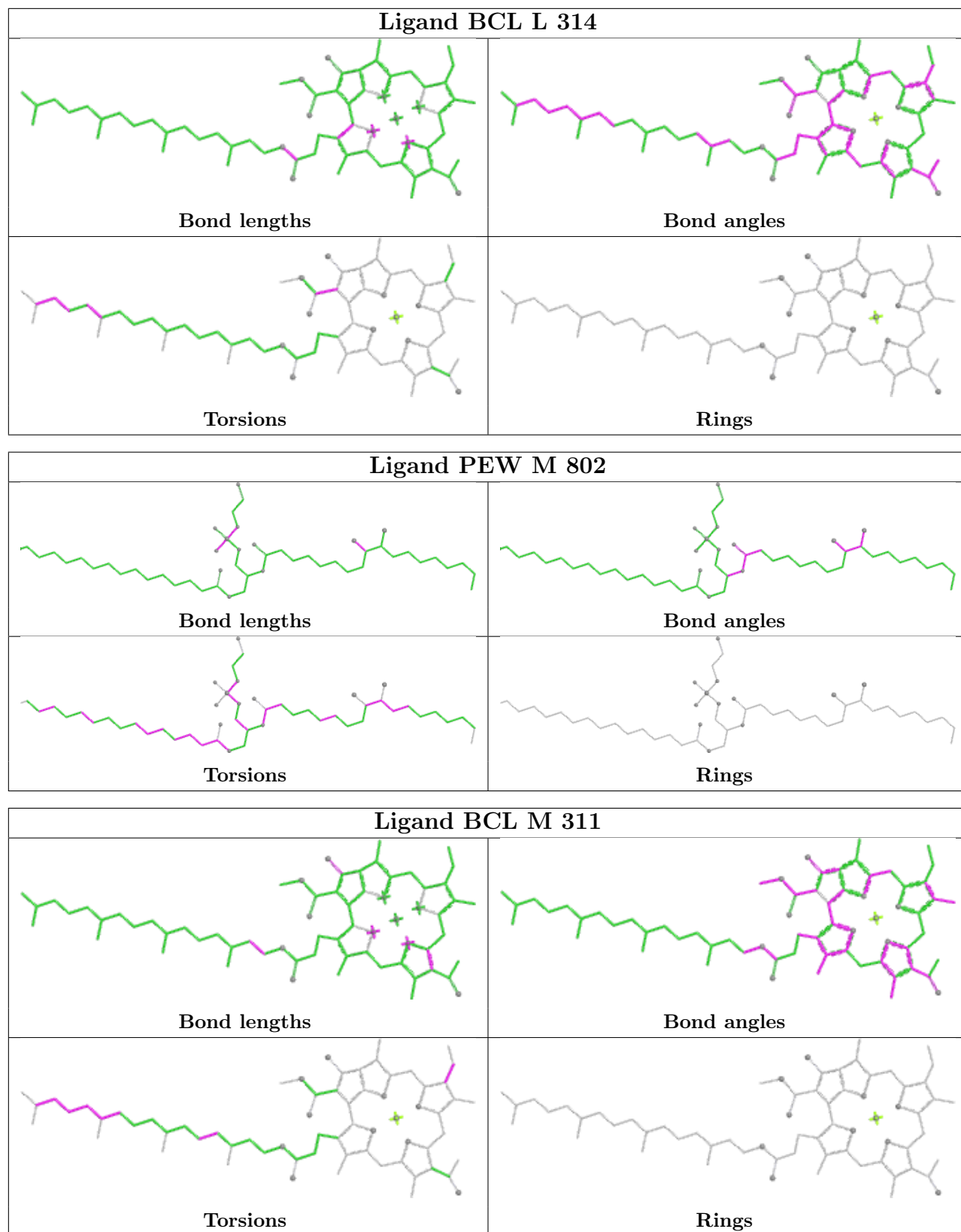
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	314	BCL	3	0

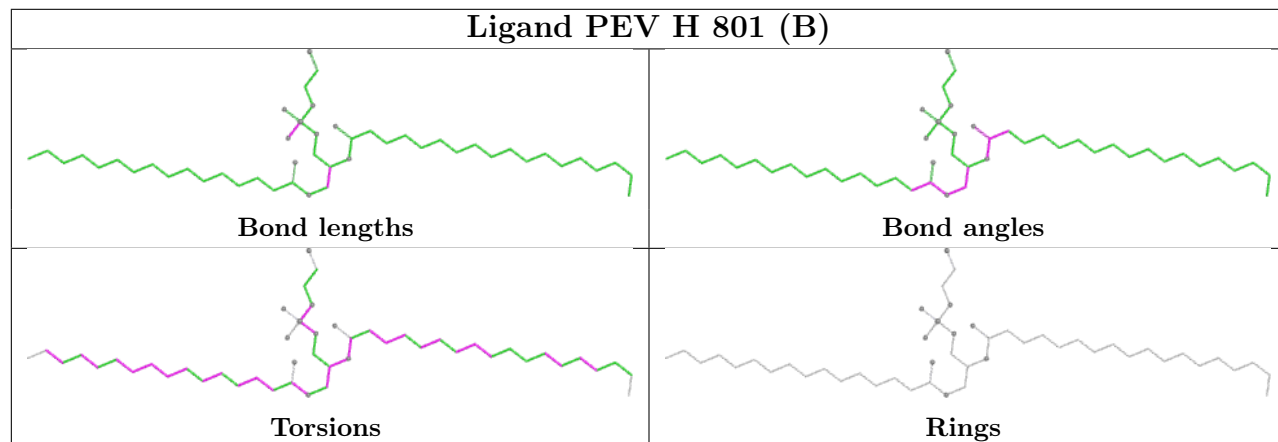
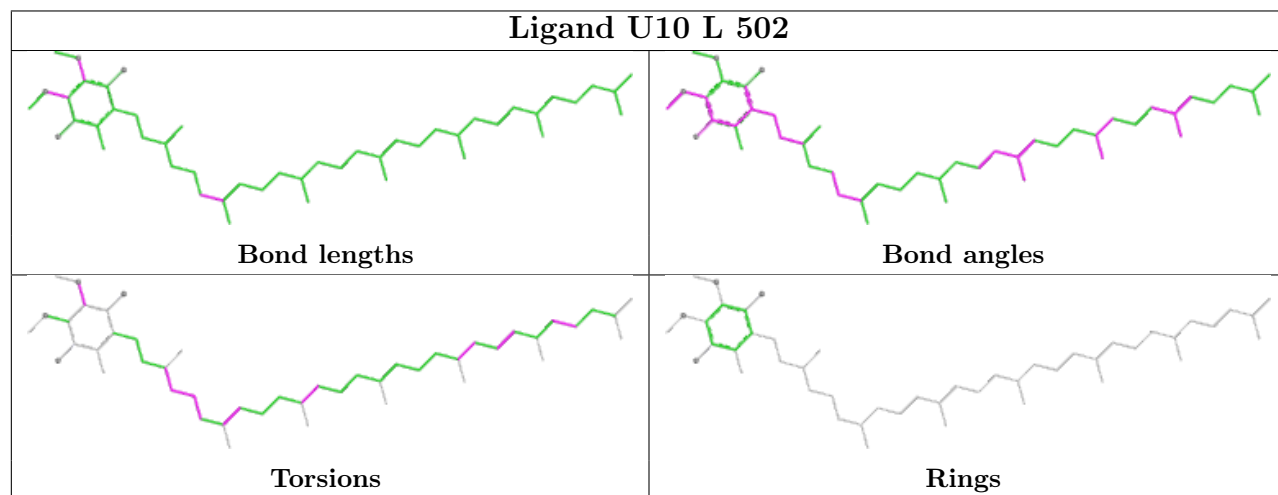
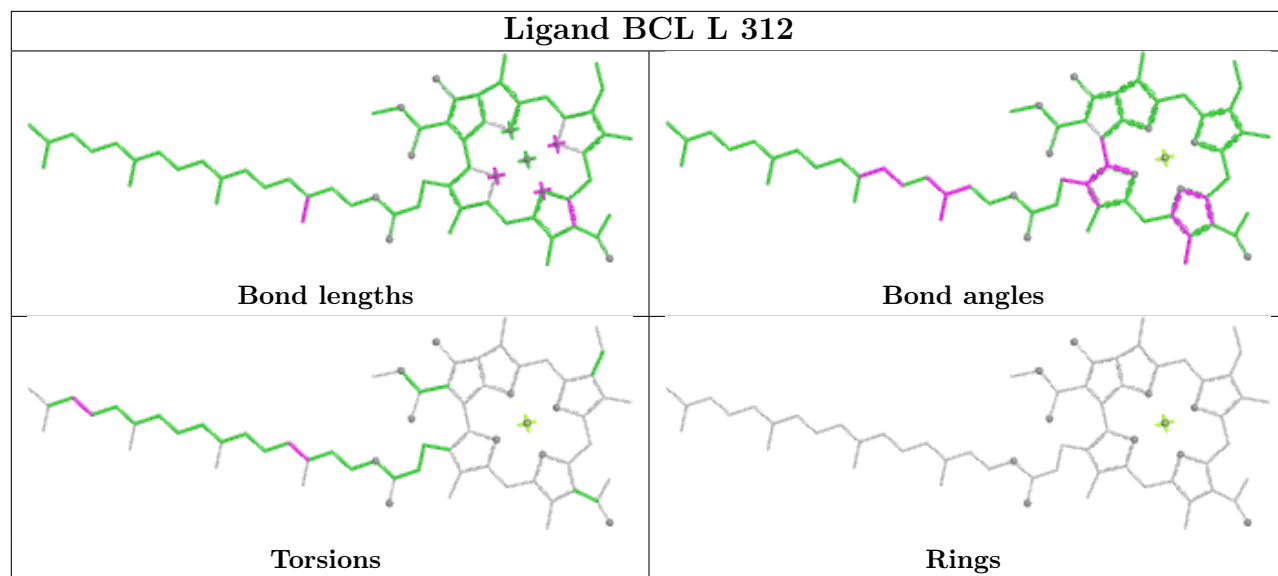
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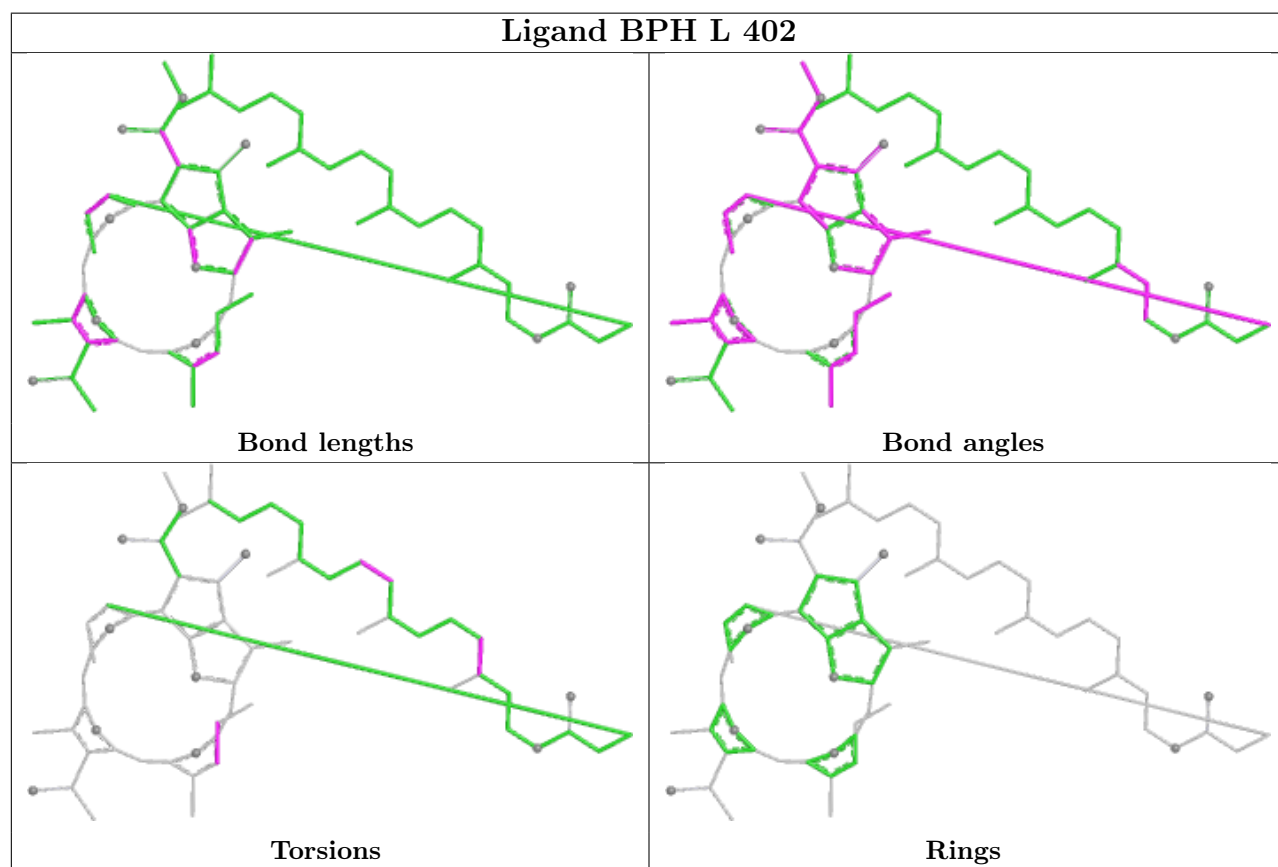
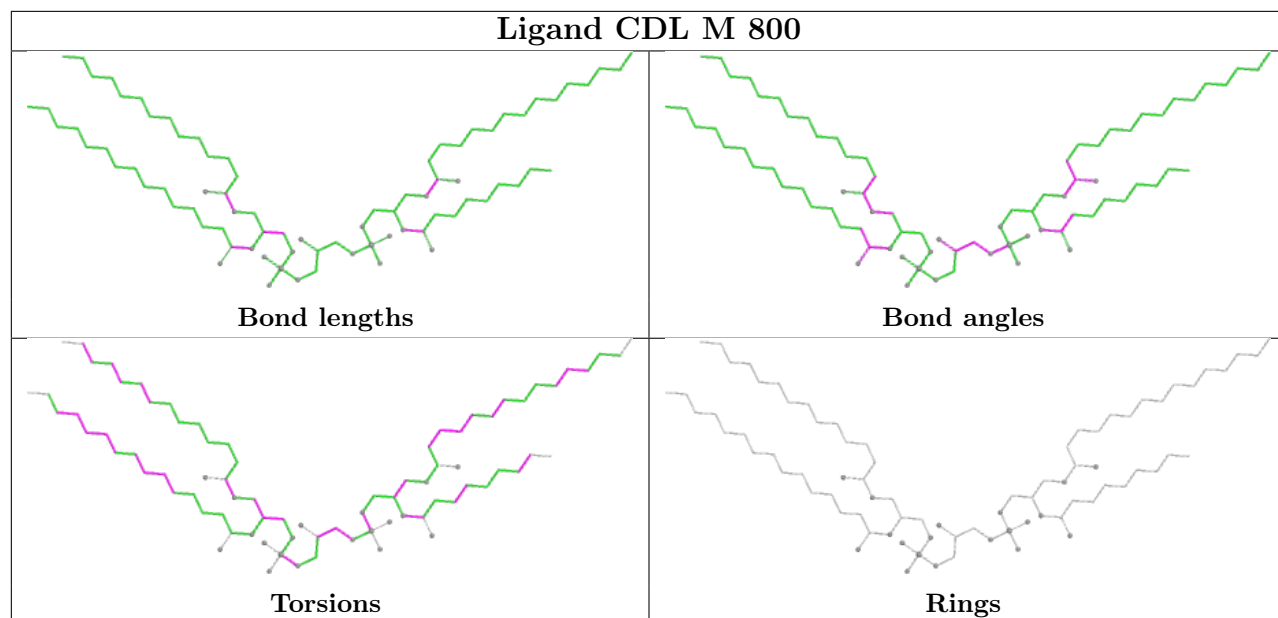
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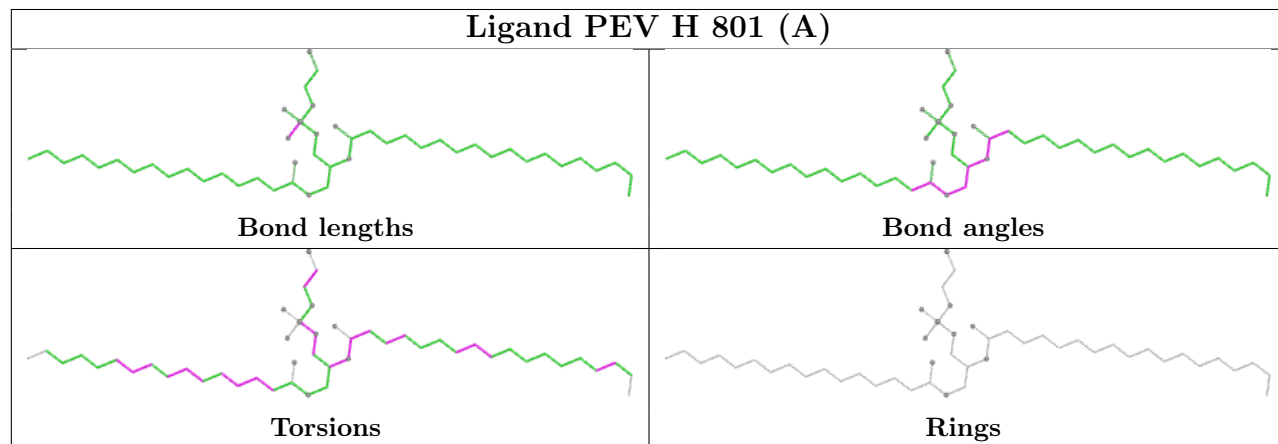
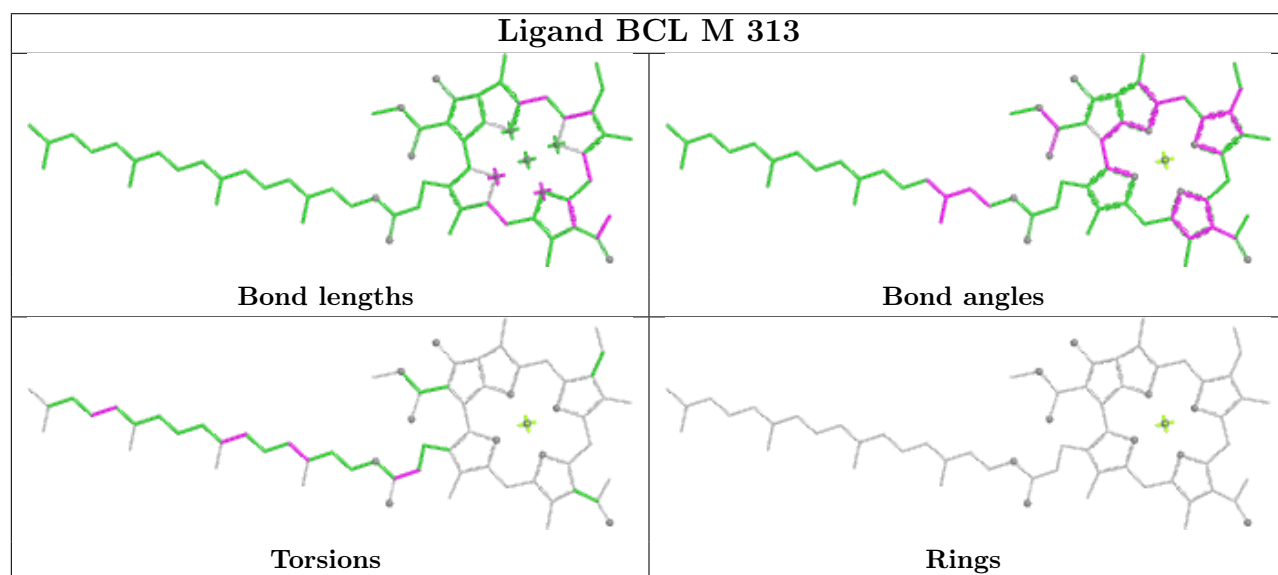
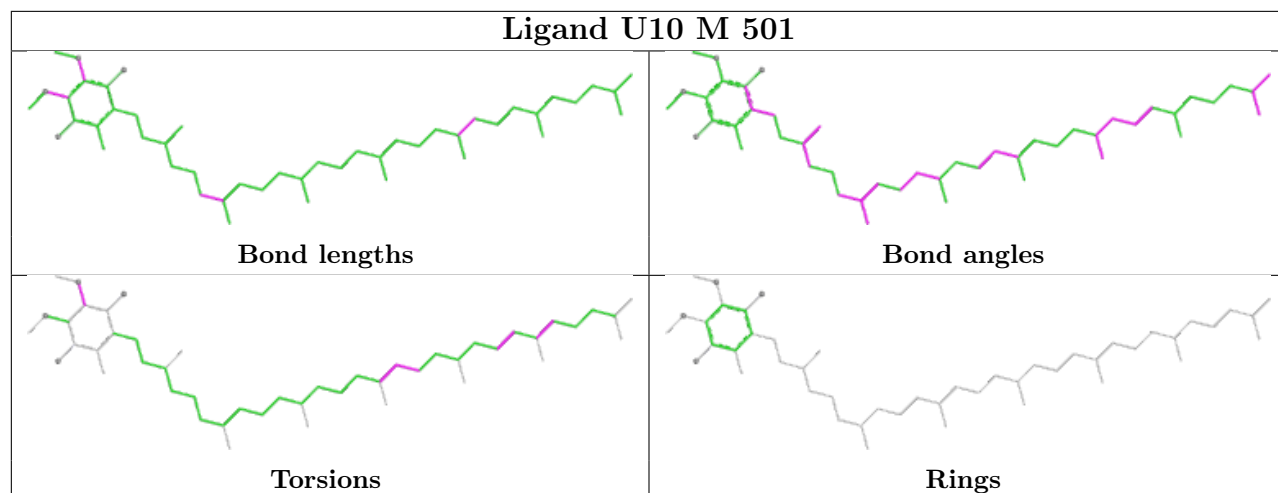
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	904	LDA	1	0
12	M	802	PEW	11	0
13	H	903	LDA	2	0
4	M	311	BCL	5	0
4	L	312	BCL	5	0
6	L	502	U10	3	0
10	M	704	PO4	1	0
7	H	708	GOL	1	0
15	H	801[B]	PEV	1	0
11	M	800	CDL	1	0
10	H	705	PO4	1	0
5	L	402	BPH	5	0
10	M	706	PO4	1	0
13	M	902	LDA	1	0
4	M	313	BCL	11	0
15	H	801[A]	PEV	2	0
13	M	920	LDA	11	0
5	M	401	BPH	9	0

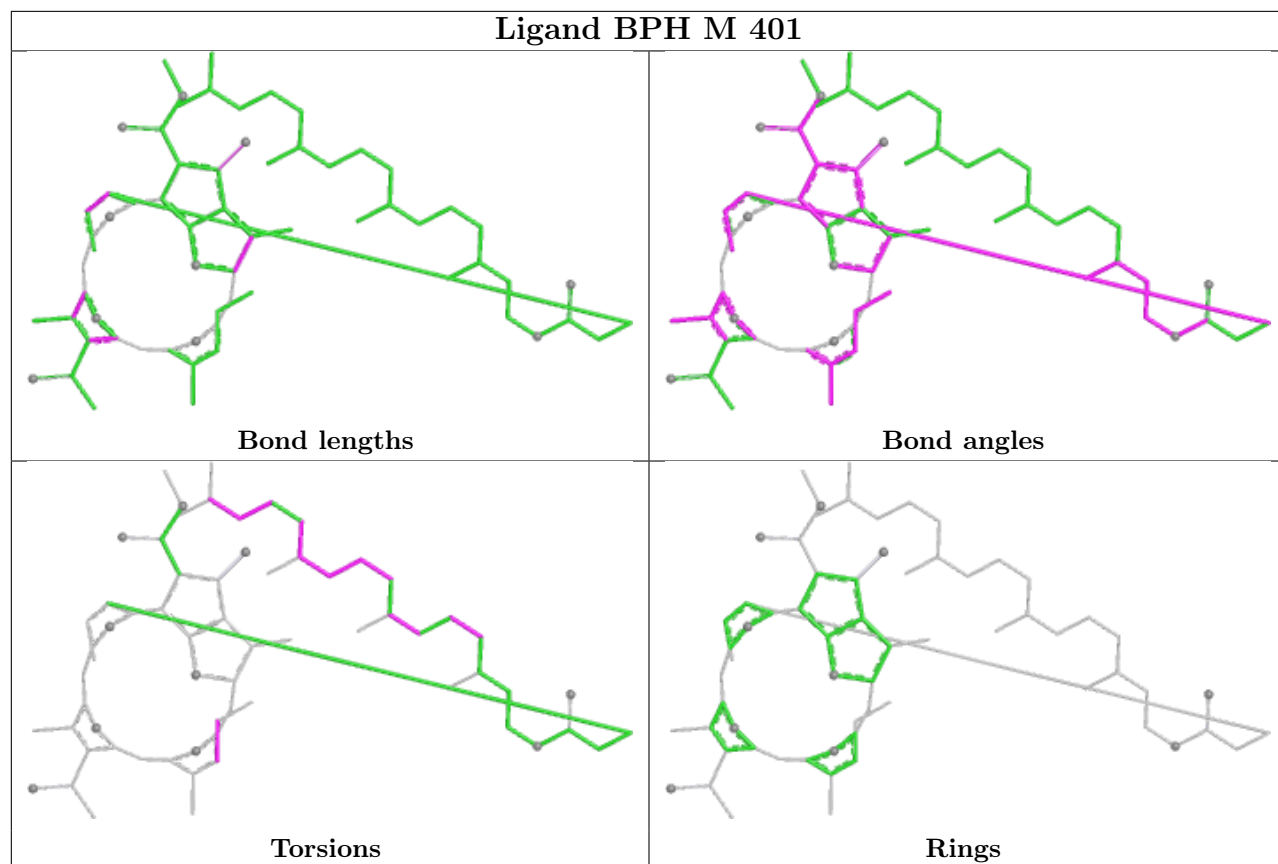
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.76	26 (9%)	14 14	34, 73, 81, 90	4 (1%)
2	M	302/307 (98%)	0.79	30 (9%)	13 12	34, 72, 82, 106	12 (3%)
3	H	243/260 (93%)	0.66	19 (7%)	19 19	36, 72, 86, 111	6 (2%)
All	All	826/848 (97%)	0.74	75 (9%)	15 14	34, 72, 82, 111	22 (2%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	2[A]	GLU	13.7
2	M	1	ALA	6.9
2	M	68[A]	PHE	6.9
3	H	251	VAL	6.3
2	M	3	TYR	5.4
3	H	9	ASN	5.0
1	L	216	PHE	4.2
2	M	52	LEU	3.9
3	H	10	PHE	3.9
2	M	128	SER	3.8
2	M	65[A]	MET	3.5
3	H	53	GLN	3.5
3	H	77	GLY	3.5
2	M	67[A]	PHE	3.4
3	H	65	ILE	3.4
2	M	53	GLY	3.3
2	M	174	ALA	3.3
2	M	134	TYR	3.3
3	H	52	ASN	3.2
1	L	42	ALA	3.2
2	M	160	LEU	3.1
1	L	142	TRP	3.1
2	M	133	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	H	118[A]	ARG	2.9
1	L	273	ALA	2.8
1	L	202	LYS	2.8
1	L	39	PHE	2.8
1	L	105	VAL	2.7
1	L	281	GLY	2.7
1	L	141	ALA	2.7
2	M	75	TRP	2.6
3	H	250	SER	2.6
1	L	56	GLN	2.6
2	M	13	ARG	2.6
3	H	94	GLU	2.5
1	L	46	ILE	2.5
1	L	67[A]	TYR	2.5
3	H	143	SER	2.5
3	H	79	GLU	2.5
2	M	137	ALA	2.5
1	L	89	ILE	2.4
3	H	93	SER	2.4
3	H	132	LYS	2.4
3	H	220	LYS	2.4
2	M	124	VAL	2.3
1	L	249	ILE	2.3
1	L	144	TYR	2.3
1	L	245	ALA	2.3
1	L	252	GLY	2.3
1	L	279	ILE	2.2
2	M	149	ALA	2.2
3	H	40	TYR	2.2
2	M	30	SER	2.2
1	L	54	VAL	2.2
1	L	275	ILE	2.2
2	M	302	GLY	2.2
2	M	57	VAL	2.2
2	M	80	TRP	2.2
2	M	290	VAL	2.2
2	M	121	PHE	2.2
3	H	171	ILE	2.2
1	L	73	TYR	2.2
2	M	59	SER	2.2
1	L	164	TYR	2.2
2	M	77	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	81	ALA	2.1
3	H	141	HIS	2.1
2	M	16	ALA	2.1
2	M	236	GLU	2.1
3	H	249	LYS	2.1
2	M	4	GLN	2.1
1	L	115	TYR	2.1
2	M	64	LEU	2.1
1	L	82	LYS	2.0
1	L	136	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

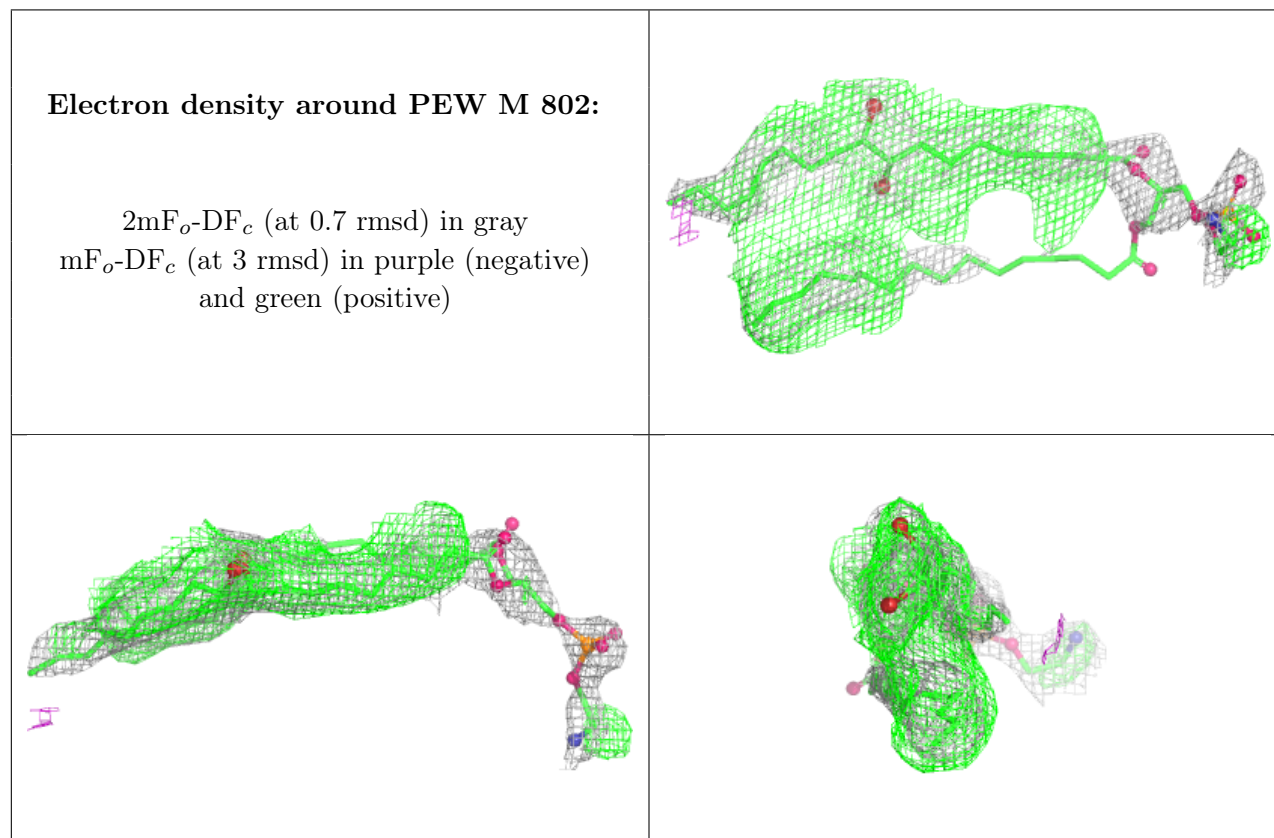
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	PEW	M	802	51/51	0.77	0.53	62,74,82,84	51
10	PO4	H	705	5/5	0.80	0.11	80,80,80,81	5
13	LDA	H	904	16/16	0.81	0.48	75,78,87,87	16
9	CL	H	703	1/1	0.86	0.50	72,72,72,72	1
11	CDL	M	800	81/100	0.86	0.40	51,71,89,91	81
13	LDA	M	902	16/16	0.87	0.36	73,77,87,88	16
10	PO4	M	706	5/5	0.89	0.20	73,73,75,75	5
7	GOL	H	708	6/6	0.89	0.45	75,75,76,76	6
6	U10	L	502	48/63	0.89	0.37	60,69,77,78	48
13	LDA	M	907	16/16	0.90	0.30	74,80,85,87	16
13	LDA	H	903	16/16	0.90	0.37	76,79,84,84	16
5	BPH	M	401	65/65	0.90	0.17	63,75,122,124	0
4	BCL	M	311	66/66	0.91	0.16	64,73,127,128	0

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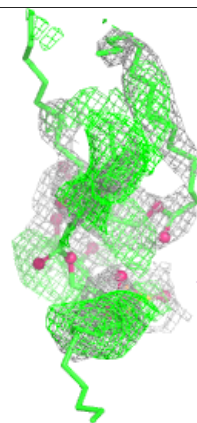
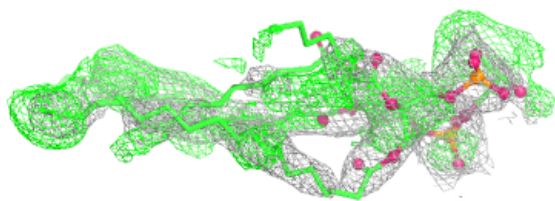
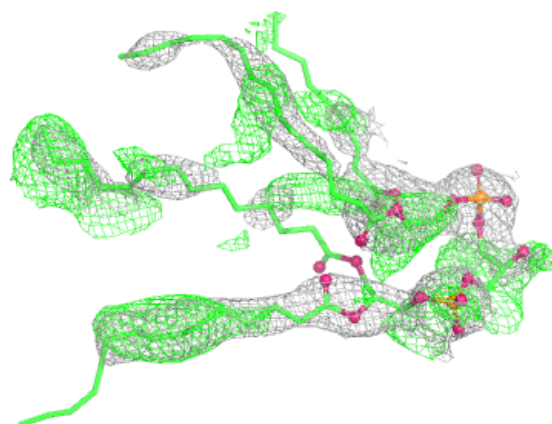
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	U10	M	501	48/63	0.92	0.16	64,76,99,100	0
10	PO4	M	704	5/5	0.92	0.08	69,69,75,76	5
15	PEV	H	801[A]	49/49	0.92	0.31	50,72,79,80	49
15	PEV	H	801[B]	49/49	0.92	0.31	48,75,85,85	49
13	LDA	M	920	16/16	0.93	0.27	52,61,74,75	16
7	GOL	L	707	6/6	0.95	0.17	69,78,79,79	6
5	BPH	L	402	65/65	0.95	0.11	59,71,75,75	0
9	CL	M	702	1/1	0.95	0.12	66,66,66,66	1
13	LDA	H	901	16/16	0.95	0.20	74,77,85,86	16
9	CL	M	701	1/1	0.96	0.10	71,71,71,71	1
4	BCL	L	314	66/66	0.96	0.10	56,68,80,86	0
4	BCL	L	312	66/66	0.96	0.11	58,70,77,84	0
4	BCL	M	313	66/66	0.96	0.11	61,69,90,101	0
14	K	H	700	1/1	0.99	0.03	66,66,66,66	0
8	FE	M	500	1/1	1.00	0.04	72,72,72,72	0

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

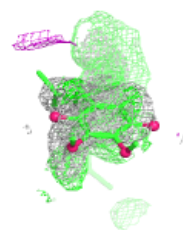
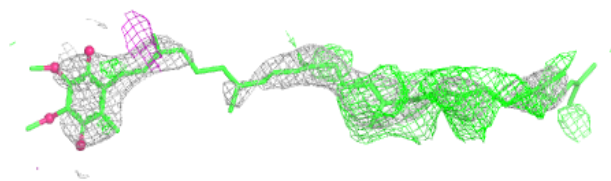
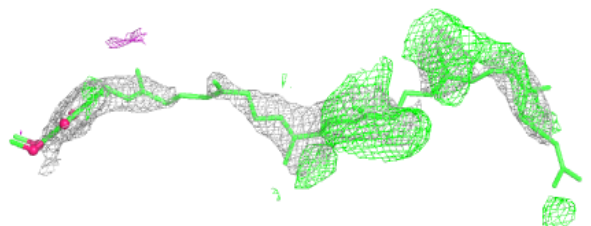


Electron density around CDL M 800:

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

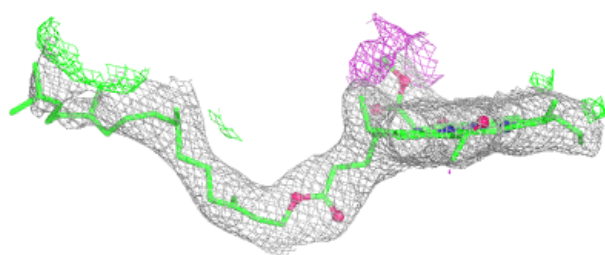
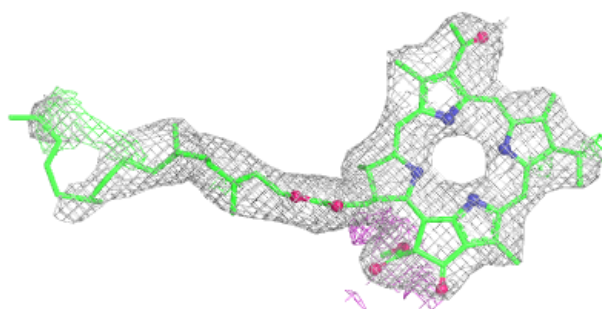
**Electron density around U10 L 502:**

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

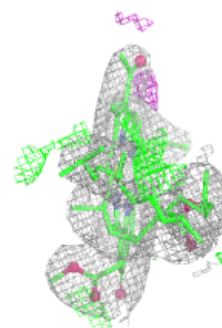
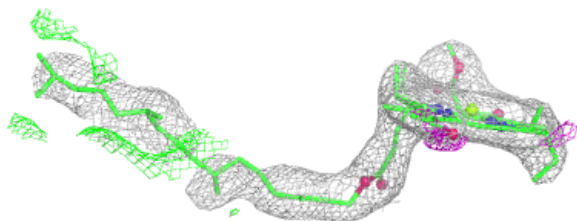
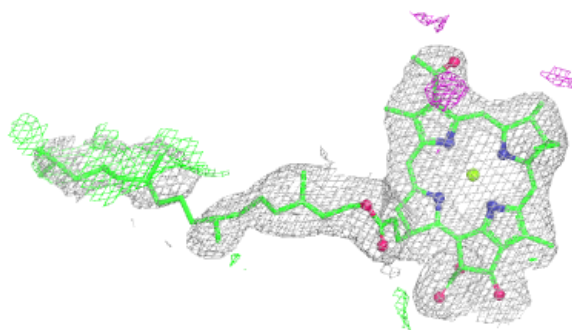


Electron density around BPH M 401:

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

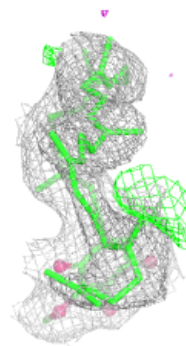
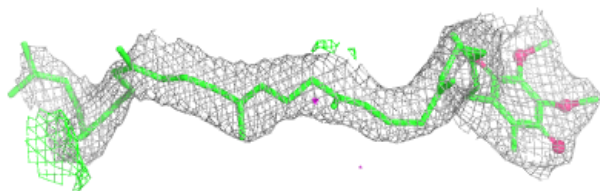
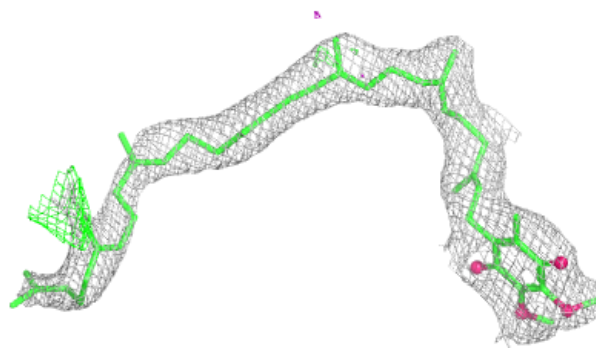
**Electron density around BCL M 311:**

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

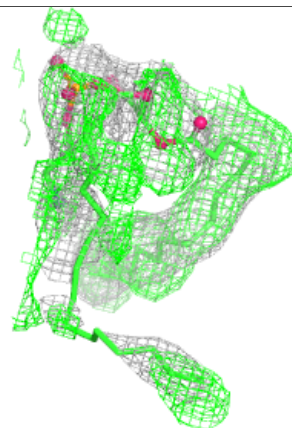
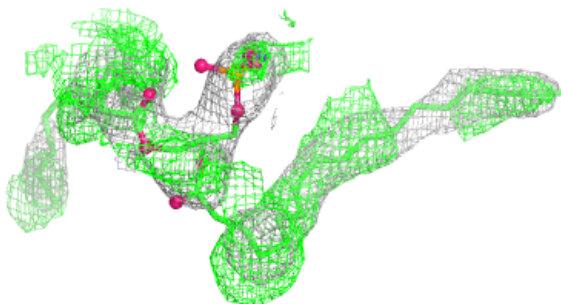
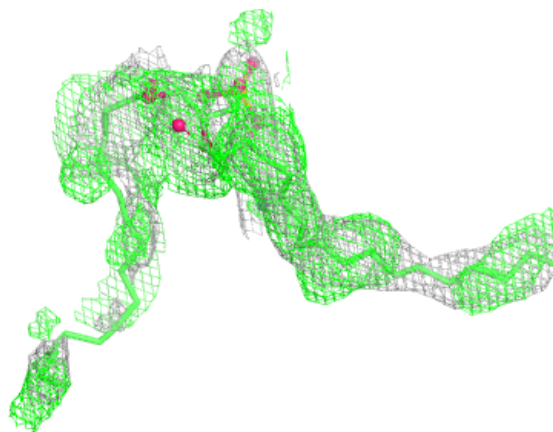


Electron density around U10 M 501:

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

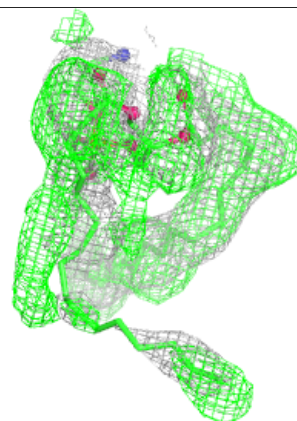
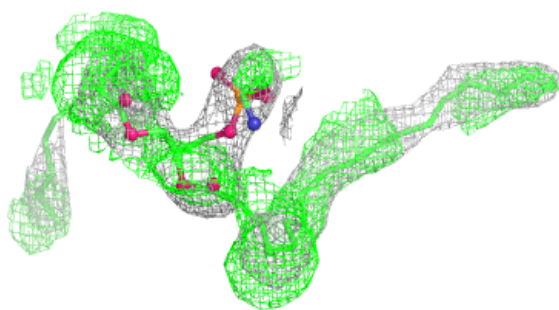
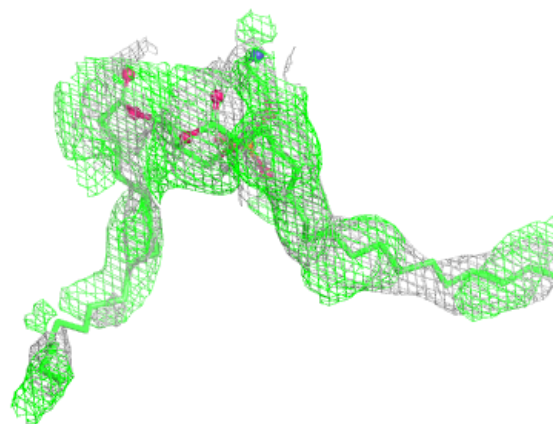
**Electron density around PEV H 801 (A):**

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



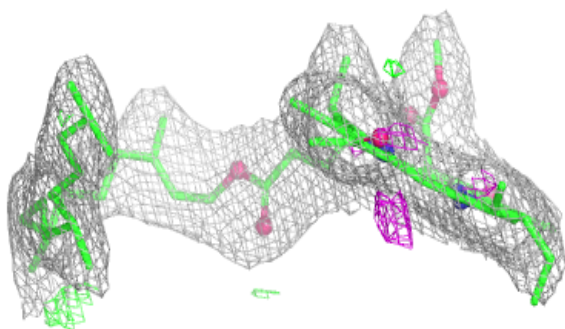
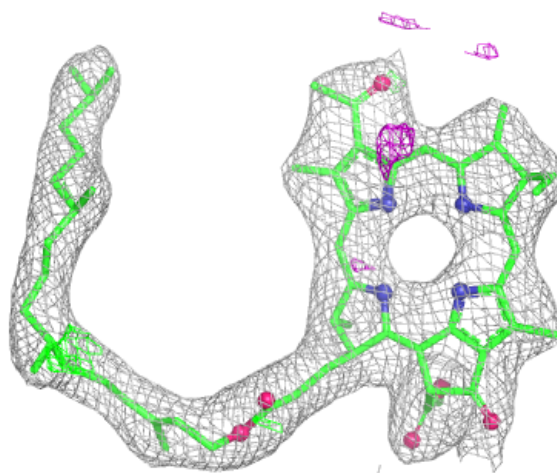
Electron density around PEV H 801 (B):

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



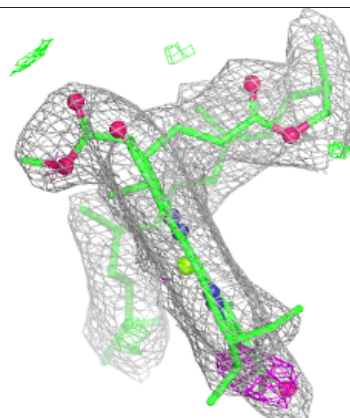
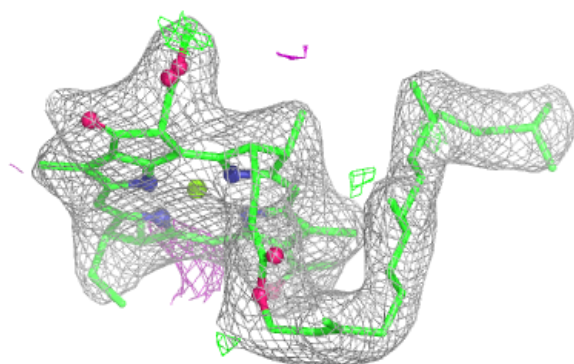
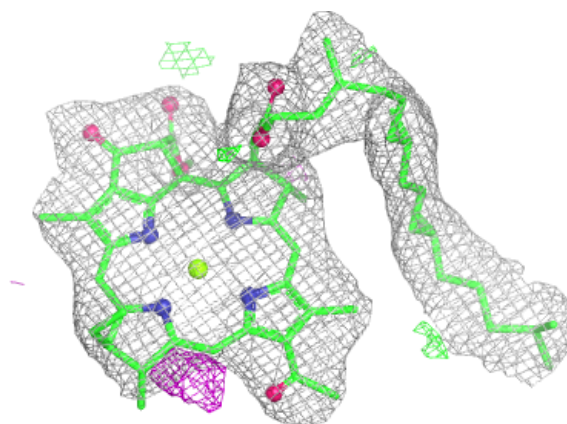
Electron density around BPH L 402:

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

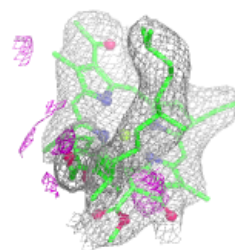
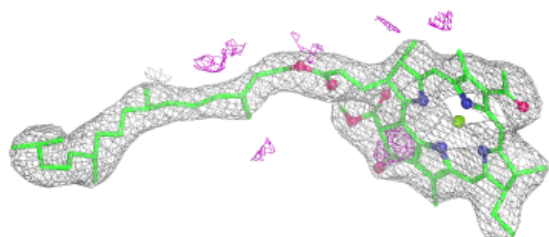
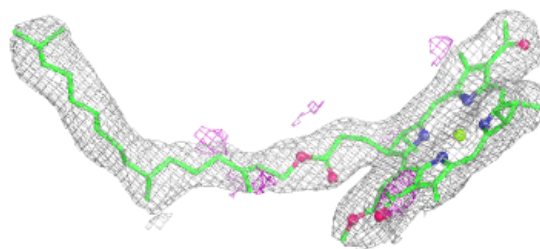


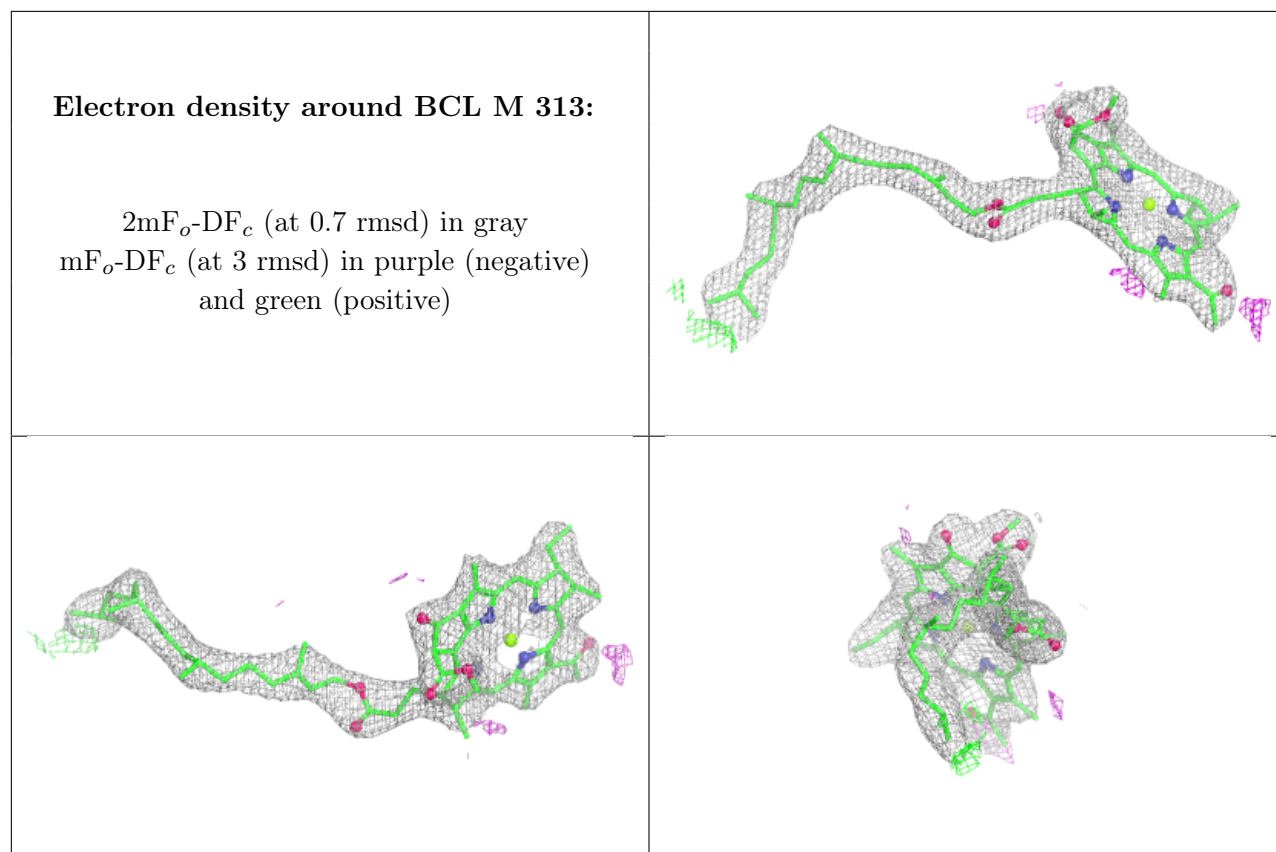
Electron density around BCL L 314:

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

**Electron density around BCL L 312:**

$2mF_o-DF_c$ (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.