



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 10:43 PM EDT

PDB ID : 2HJ6 / pdb_00002hj6
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylserine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-30
Resolution : 3.00 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

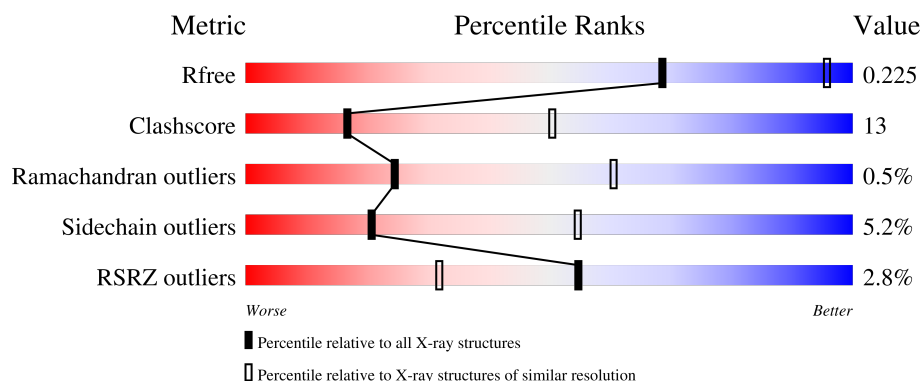
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	4% 74% 23% .
2	M	307	2% 75% 21% ..
3	H	260	2% 68% 23% . 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	LDA	M	920	-	-	X	-
13	GOL	M	704	-	-	-	X
9	HTO	M	703	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7685 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	3	0
			2249	1520	357	364	8			

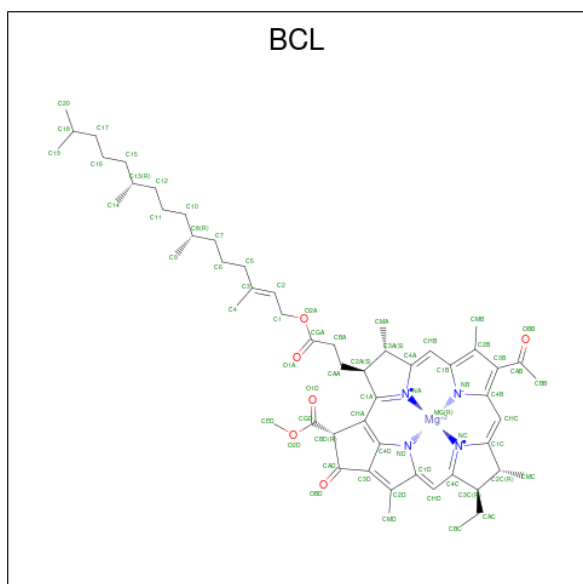
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	5	0
			2452	1637	403	402	10			

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

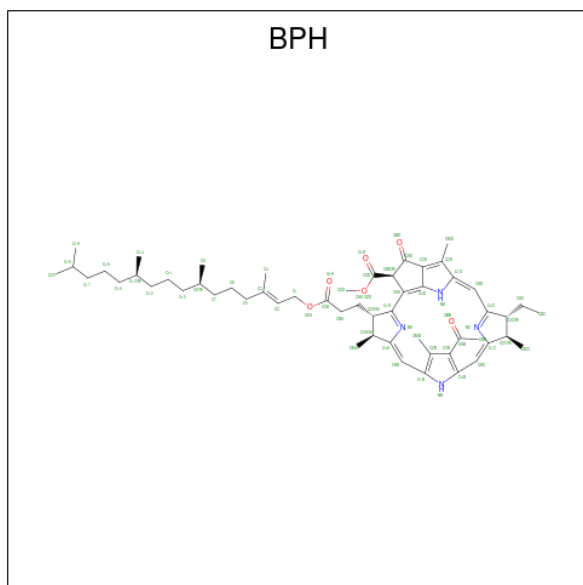
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	5	0
			1846	1180	316	339	11			

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



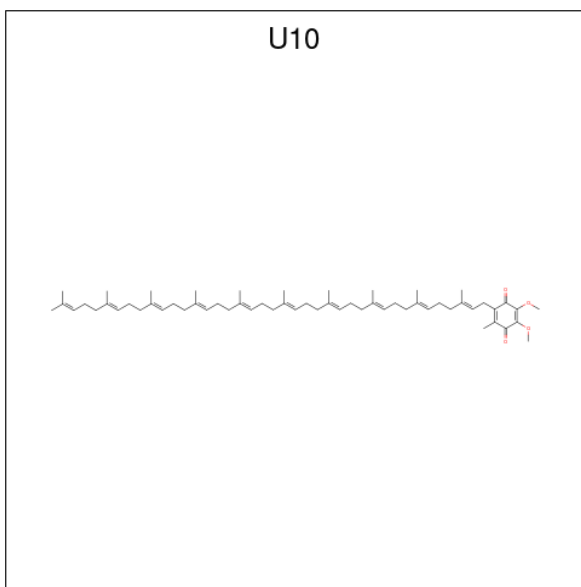
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- 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: $C_{59}H_{90}O_4$).

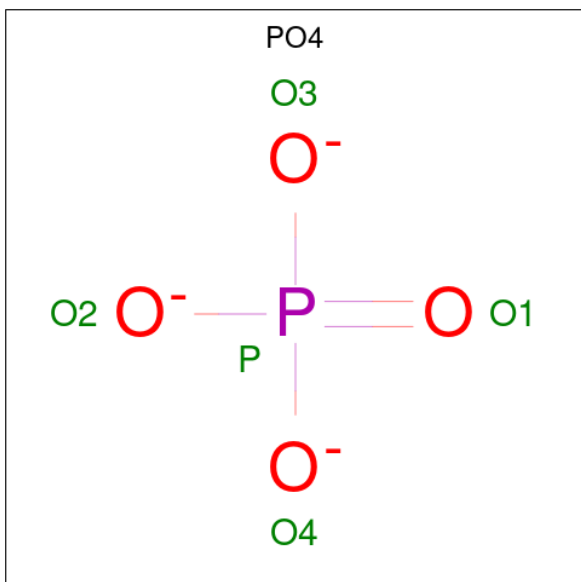


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

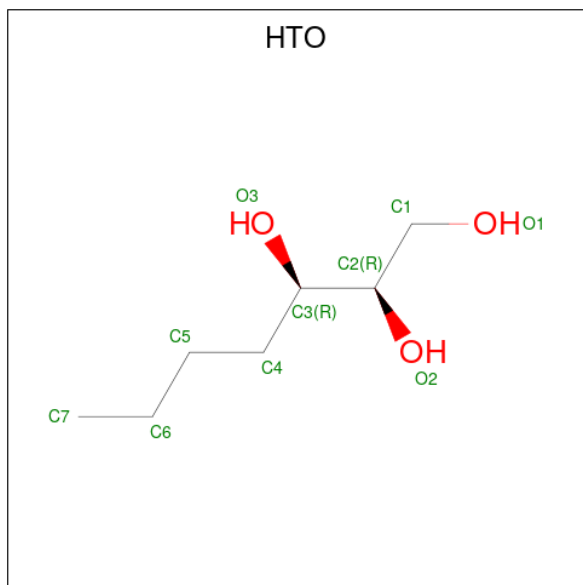
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



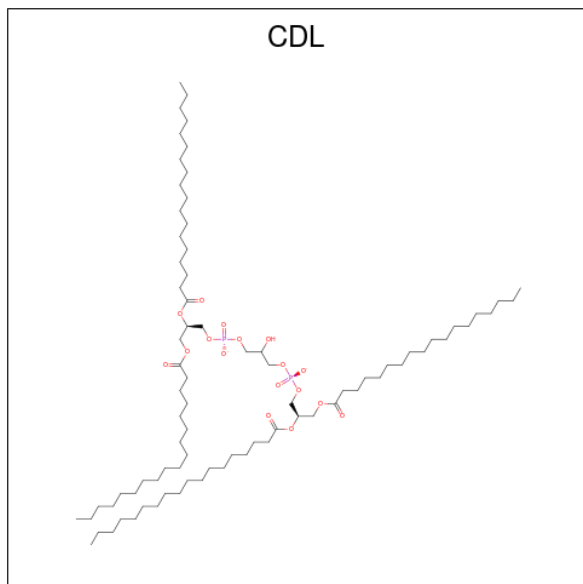
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		

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



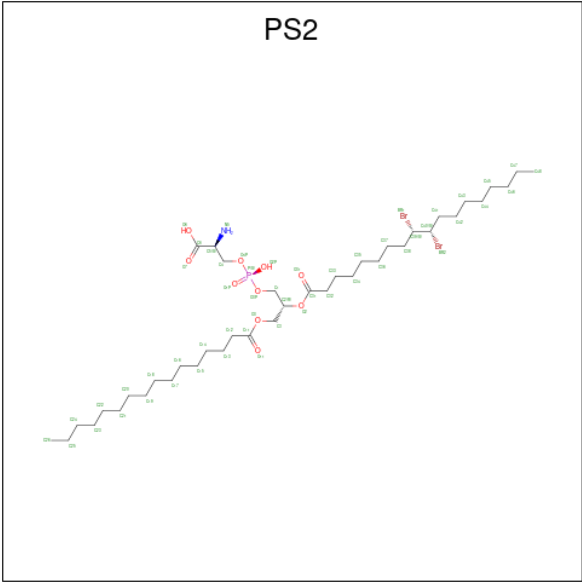
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



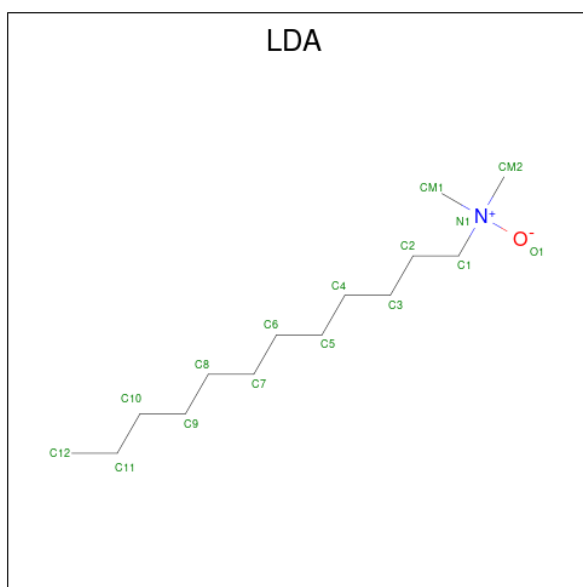
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is O-[[{(2R)-2-{{(9S,10S)-9,10-DIBROMOOCTADECANOYL}OXY}-3-(PALMITOYLOXY)PROPYL}OXY}{(HYDROXY)PHOSPHORYL]-L-SERINE (CCD ID: PS2) (formula: C₄₀H₇₆Br₂NO₁₀P).



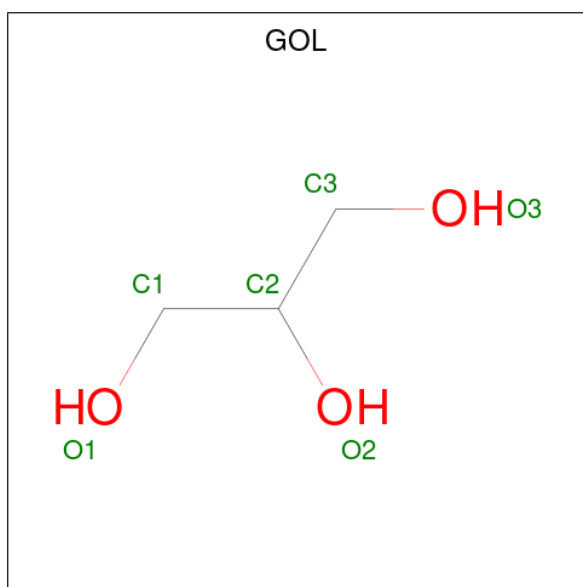
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	M	1	Total	Br	C	N	O	P	0	0
			54	2	40	1	10	1		

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			6	3	3		
13	H	1	Total	C	O	0	0
			6	3	3		

- 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		

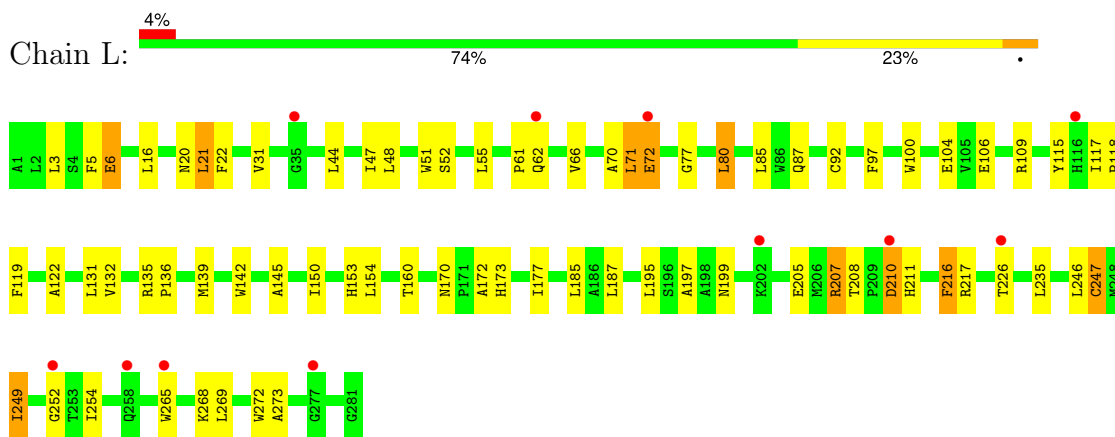
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	78	Total	O	0	0
			78	78		
15	M	108	Total	O	0	0
			108	108		
15	H	165	Total	O	0	0
			165	165		

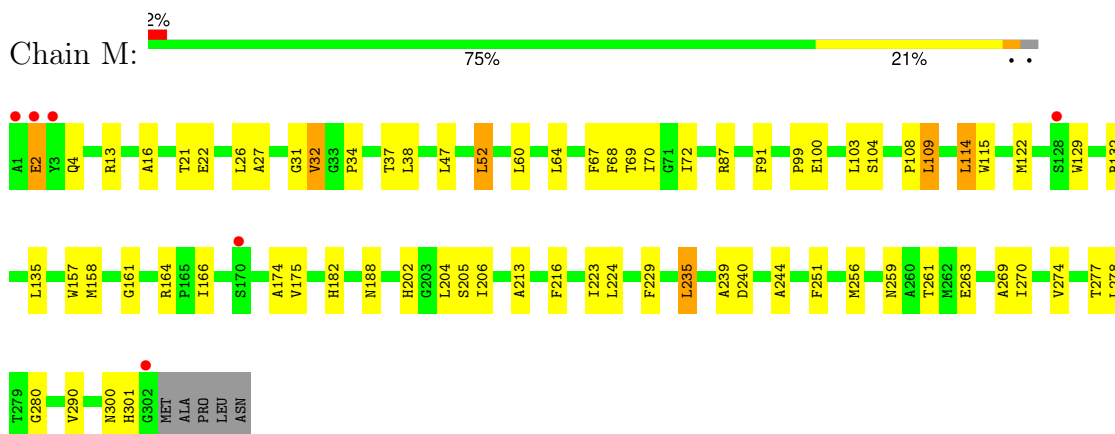
3 Residue-property plots

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.

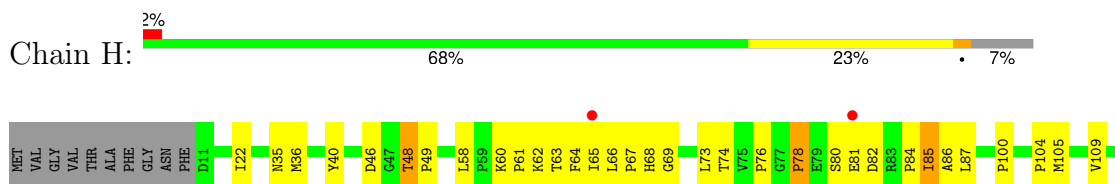
- Molecule 1: Reaction center protein L chain

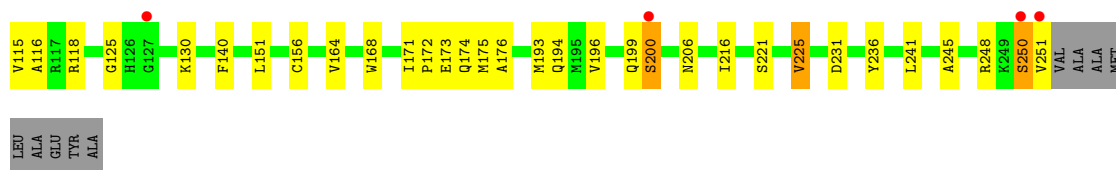


- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.35Å 139.35Å 183.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.29 – 3.00 39.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.29-3.00) 99.4 (39.29-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.227 0.178 , 0.225	Depositor DCC
R_{free} test set	2083 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: BCL, BPH, GOL, PS2, K, PO4, U10, CDL, HTO, FE, LDA

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	1.05	1/2350 (0.0%)	1.06	2/3216 (0.1%)
2	M	1.06	1/2552 (0.0%)	1.09	5/3482 (0.1%)
3	H	1.12	2/1921 (0.1%)	1.17	6/2612 (0.2%)
All	All	1.07	4/6823 (0.1%)	1.10	13/9310 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	132	VAL	C-N	7.42	1.43	1.33
3	H	64	PHE	C-O	-6.95	1.15	1.23
3	H	22	ILE	CA-CB	6.04	1.60	1.54
2	M	235	LEU	CA-C	5.45	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	259	ASN	N-CA-C	8.31	120.77	108.14
3	H	216	ILE	CA-C-N	6.76	126.80	119.90
3	H	216	ILE	C-N-CA	6.76	126.80	119.90
2	M	2	GLU	N-CA-C	-5.81	102.45	110.35
2	M	290	VAL	CB-CA-C	-5.73	104.96	111.55
1	L	160	THR	N-CA-C	-5.68	105.00	111.14
3	H	85	ILE	N-CA-C	5.60	114.80	106.85
3	H	48	THR	CA-C-N	5.55	125.82	119.83
3	H	48	THR	C-N-CA	5.55	125.82	119.83
1	L	6	GLU	N-CA-C	5.39	118.32	111.69
3	H	250	SER	O-C-N	5.19	128.71	122.79
2	M	164	ARG	CA-C-N	-5.11	113.66	119.28
2	M	164	ARG	C-N-CA	-5.11	113.66	119.28

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	2249	0	2210	55	0
2	M	2452	0	2357	68	0
3	H	1846	0	1866	48	0
4	L	132	0	148	12	0
4	M	132	0	148	15	0
5	L	65	0	76	4	0
5	M	65	0	76	3	0
6	L	48	0	63	3	0
6	M	48	0	63	4	0
7	M	1	0	0	0	0
8	M	10	0	0	0	0
9	M	10	0	16	0	0
10	M	81	0	106	3	0
11	M	54	0	72	4	0
12	H	48	0	93	0	0
12	M	80	0	155	22	0
13	H	6	0	8	0	0
13	M	6	0	8	2	0
14	H	1	0	0	0	0
15	H	165	0	0	9	0
15	L	78	0	0	1	0
15	M	108	0	0	3	0
All	All	7685	0	7465	189	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 13.

All (189) 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:H:250:SER:O	3:H:251:VAL:CG2	2.11	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.46	0.97
3:H:250:SER:O	3:H:251:VAL:HG23	1.64	0.97
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.54	0.88
4:M:311:BCL:HMB3	4:M:311:BCL:HBB2	1.63	0.81
2:M:174:ALA:HB1	12:M:920:LDA:C12	2.13	0.77
2:M:135:LEU:HD13	15:M:1331:HOH:O	1.86	0.75
2:M:115:TRP:HZ2	12:M:920:LDA:H121	1.52	0.74
3:H:250:SER:C	3:H:251:VAL:HG23	2.13	0.72
2:M:70:ILE:HG21	12:M:920:LDA:HM21	1.73	0.71
3:H:250:SER:O	3:H:251:VAL:HG22	1.92	0.69
2:M:31:GLY:H	11:M:802:PS2:H11	1.58	0.68
1:L:80:LEU:O	1:L:85:LEU:HD12	1.93	0.68
4:L:312:BCL:HMB3	4:L:312:BCL:CBB	2.25	0.67
2:M:122:MET:HE1	4:M:311:BCL:CBB	2.24	0.67
2:M:174:ALA:HB1	12:M:920:LDA:H121	1.76	0.66
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.30	0.66
12:M:901:LDA:H121	12:M:903:LDA:C8	2.26	0.65
2:M:47:LEU:HD22	11:M:802:PS2:BR2	2.52	0.64
4:M:311:BCL:H92	4:M:313:BCL:H161	1.81	0.62
3:H:250:SER:C	3:H:251:VAL:CG2	2.73	0.62
2:M:175:VAL:N	12:M:920:LDA:H122	2.15	0.62
3:H:175:MET:CE	3:H:176:ALA:O	2.49	0.61
4:L:314:BCL:HBB3	5:L:402:BPH:H141	1.83	0.60
1:L:197:ALA:HB1	2:M:235:LEU:HD11	1.83	0.60
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.82	0.60
2:M:67[A]:PHE:HD2	2:M:68[A]:PHE:CE1	2.19	0.59
2:M:69:THR:HG23	2:M:114:LEU:HD12	1.84	0.59
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.37	0.58
2:M:122:MET:HE1	4:M:311:BCL:HBB1	1.85	0.58
2:M:2:GLU:O	2:M:4:GLN:NE2	2.36	0.58
4:L:314:BCL:HBB2	4:L:314:BCL:HMB3	1.84	0.58
1:L:51:TRP:NE1	1:L:55:LEU:HD11	2.19	0.57
4:L:312:BCL:NA	4:M:313:BCL:HBB2	2.19	0.57
1:L:100:TRP:CH2	6:M:501:U10:H251	2.40	0.57
1:L:216:PHE:CD2	6:L:502:U10:H102	2.39	0.57
2:M:175:VAL:O	12:M:920:LDA:H122	2.04	0.57
4:L:312:BCL:HMB3	4:L:312:BCL:HBB2	1.89	0.55
4:L:312:BCL:CGA	4:L:314:BCL:HBC1	2.36	0.55
5:L:402:BPH:HMC1	2:M:213:ALA:HB3	1.89	0.55
3:H:140:PHE:CE1	3:H:171:ILE:HG23	2.42	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:240:ASP:OD2	3:H:118:ARG:HG3	2.07	0.54
3:H:46:ASP:OD1	3:H:48:THR:HG23	2.07	0.54
3:H:193:MET:O	3:H:196:VAL:HG22	2.08	0.54
2:M:67[B]:PHE:O	2:M:68[B]:PHE:C	2.50	0.54
2:M:16:ALA:HB1	2:M:32:VAL:CG1	2.31	0.53
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.53
4:M:311:BCL:CAB	12:M:920:LDA:H82	2.38	0.53
12:M:901:LDA:H122	12:M:903:LDA:H102	1.89	0.53
2:M:175:VAL:H	12:M:920:LDA:H122	1.73	0.53
4:M:311:BCL:HMB3	4:M:311:BCL:CBB	2.36	0.53
2:M:67[A]:PHE:HD2	2:M:68[A]:PHE:CD1	2.27	0.52
2:M:52:LEU:HD21	2:M:60:LEU:CD1	2.39	0.52
2:M:161:GLY:HA2	12:M:920:LDA:H123	1.89	0.52
1:L:197:ALA:CB	2:M:235:LEU:HD11	2.40	0.52
2:M:34:PRO:HG2	2:M:47:LEU:HD12	1.91	0.52
2:M:64:LEU:HD21	5:M:401:BPH:H112	1.90	0.52
2:M:67[A]:PHE:CD2	2:M:68[A]:PHE:CE1	2.97	0.52
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.28	0.51
2:M:27:ALA:HB2	15:M:1216:HOH:O	2.09	0.51
2:M:31:GLY:N	11:M:802:PS2:H11	2.22	0.51
1:L:136:PRO:HG2	1:L:145:ALA:HB2	1.92	0.51
10:M:800:CDL:OA8	10:M:800:CDL:CA5	2.59	0.51
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.46	0.51
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.91	0.51
4:M:311:BCL:CBB	4:M:311:BCL:CMB	2.89	0.50
1:L:216:PHE:CE2	6:L:502:U10:H102	2.45	0.50
1:L:52:SER:CB	1:L:66:VAL:HG22	2.41	0.50
1:L:135:ARG:NH1	1:L:139:MET:HE1	2.27	0.50
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.47	0.50
6:M:501:U10:H4M2	6:M:501:U10:O3	2.12	0.50
3:H:36:MET:HE2	3:H:58:LEU:HD23	1.94	0.50
4:L:312:BCL:CBB	4:L:312:BCL:CMB	2.91	0.49
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.93	0.49
1:L:199:ASN:HB3	10:M:800:CDL:HA22	1.95	0.49
3:H:105[B]:MET:HE2	3:H:236:TYR:CZ	2.48	0.49
1:L:97:PHE:CZ	4:L:312:BCL:H112	2.48	0.49
2:M:21:THR:O	2:M:22:GLU:C	2.55	0.49
3:H:199:GLN:O	3:H:200:SER:C	2.53	0.49
3:H:84:PRO:O	3:H:85:ILE:HD13	2.13	0.49
2:M:280:GLY:O	4:M:313:BCL:HED3	2.13	0.48
1:L:208:THR:HG21	3:H:125:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:TYR:HB2	12:M:906:LDA:HM13	1.96	0.48
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	1.94	0.48
1:L:172:ALA:HB3	1:L:247:CYS:CB	2.44	0.48
1:L:265:TRP:CZ3	1:L:269:LEU:HD11	2.48	0.48
1:L:187:LEU:HD13	2:M:216:PHE:CD2	2.48	0.48
12:M:901:LDA:H121	12:M:903:LDA:H82	1.95	0.48
3:H:105[B]:MET:CE	3:H:236:TYR:CZ	2.96	0.48
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.48
1:L:226:THR:HG22	6:L:502:U10:H4M3	1.95	0.48
4:L:312:BCL:HMB3	4:L:312:BCL:HBB3	1.96	0.48
1:L:44:LEU:HA	1:L:47:ILE:HD12	1.95	0.47
2:M:52:LEU:HD21	2:M:60:LEU:HD11	1.96	0.47
3:H:241:LEU:HB2	15:H:1089:HOH:O	2.14	0.47
2:M:223:ILE:O	2:M:224:LEU:C	2.54	0.47
1:L:16:LEU:N	1:L:106:GLU:OE2	2.35	0.47
5:L:402:BPH:HMB3	5:L:402:BPH:HBB3	1.95	0.47
2:M:263:GLU:OE1	3:H:62:LYS:NZ	2.46	0.47
4:M:311:BCL:HBB2	4:M:311:BCL:CMB	2.39	0.47
12:M:901:LDA:H121	12:M:903:LDA:C9	2.45	0.47
2:M:108:PRO:O	2:M:109:LEU:C	2.58	0.47
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.46
1:L:210:ASP:OD1	1:L:210:ASP:N	2.47	0.46
1:L:272:TRP:HB2	2:M:87:ARG:HD3	1.98	0.46
2:M:175:VAL:HB	12:M:920:LDA:H101	1.97	0.46
2:M:256:MET:CE	6:M:501:U10:H102	2.45	0.46
3:H:69:GLY:N	15:H:1165:HOH:O	2.41	0.46
3:H:115:VAL:CG1	3:H:116:ALA:N	2.77	0.46
2:M:239:ALA:HA	3:H:73:LEU:HD23	1.98	0.46
2:M:277:THR:CG2	5:M:401:BPH:HAC2	2.46	0.46
4:L:312:BCL:H52	5:L:402:BPH:HBB2	1.98	0.45
1:L:139:MET:CE	1:L:252:GLY:HA3	2.46	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.16	0.45
1:L:20:ASN:C	1:L:20:ASN:ND2	2.74	0.45
12:M:901:LDA:O1	3:H:40:TYR:OH	2.34	0.45
1:L:48:LEU:HD22	1:L:85:LEU:CD2	2.47	0.45
1:L:268:LYS:O	1:L:269:LEU:C	2.59	0.45
1:L:131:LEU:HD21	4:L:312:BCL:CED	2.47	0.45
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.98	0.45
1:L:119:PHE:O	1:L:122:ALA:HB3	2.17	0.45
2:M:269:ALA:O	2:M:270:ILE:C	2.58	0.45
10:M:800:CDL:OB7	10:M:800:CDL:C31	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:139:MET:HE2	1:L:252:GLY:C	2.43	0.44
1:L:172:ALA:HB3	1:L:247:CYS:HB2	1.99	0.44
2:M:4:GLN:CD	12:M:906:LDA:HM23	2.42	0.44
2:M:175:VAL:H	12:M:920:LDA:C12	2.30	0.44
2:M:300:ASN:O	2:M:301[B]:HIS:CG	2.69	0.44
1:L:217:ARG:NH2	15:L:1047:HOH:O	2.50	0.44
3:H:60:LYS:N	15:H:1285:HOH:O	2.46	0.44
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.86	0.44
1:L:195:LEU:O	1:L:199:ASN:HB2	2.17	0.44
2:M:261:THR:HG23	3:H:35:ASN:O	2.18	0.44
4:M:311:BCL:H72	4:M:311:BCL:H41	1.99	0.44
2:M:13:ARG:NH2	15:M:1107:HOH:O	2.49	0.43
1:L:3:LEU:HB2	1:L:6:GLU:HB2	1.99	0.43
12:M:907:LDA:H71	12:M:907:LDA:H101	1.84	0.43
3:H:200:SER:HB3	15:H:1280:HOH:O	2.19	0.43
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.18	0.43
2:M:300:ASN:C	2:M:301[B]:HIS:CG	2.96	0.43
2:M:70:ILE:HG21	12:M:920:LDA:CM2	2.42	0.43
1:L:5:PHE:HA	3:H:81:GLU:OE2	2.19	0.43
1:L:117:ILE:N	1:L:118:PRO:HD2	2.34	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.00	0.43
12:M:901:LDA:C12	12:M:903:LDA:H102	2.48	0.43
3:H:49:PRO:HD3	15:H:1324:HOH:O	2.18	0.43
4:M:311:BCL:H41	4:M:311:BCL:C7	2.48	0.43
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.53	0.42
4:M:311:BCL:H3A	4:M:311:BCL:HBA1	1.85	0.42
1:L:71:LEU:H	1:L:71:LEU:HD12	1.84	0.42
3:H:82:ASP:N	15:H:1348:HOH:O	2.52	0.42
1:L:61:PRO:O	1:L:150:ILE:HD12	2.19	0.42
3:H:63:THR:OG1	3:H:74:THR:HG23	2.19	0.42
3:H:46:ASP:CG	15:H:1254:HOH:O	2.63	0.42
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.34	0.42
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.59	0.42
2:M:99:PRO:HD2	2:M:100:GLU:OE2	2.19	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.20	0.42
1:L:70:ALA:HB1	1:L:72:GLU:HG3	2.02	0.42
2:M:2:GLU:HG3	13:M:704:GOL:H31	2.02	0.41
2:M:60:LEU:HA	5:M:401:BPH:H4C1	2.02	0.41
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.03	0.41
2:M:2:GLU:HG3	13:M:704:GOL:C3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:129:TRP:CZ2	11:M:802:PS2:H263	2.56	0.41
3:H:173:GLU:O	3:H:174:GLN:C	2.62	0.41
2:M:204:LEU:O	2:M:205:SER:C	2.62	0.41
3:H:104:PRO:HA	3:H:109:VAL:HG22	2.02	0.41
3:H:175:MET:HE3	3:H:176:ALA:O	2.21	0.41
1:L:269:LEU:O	1:L:273:ALA:HB2	2.21	0.41
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.55	0.41
4:L:312:BCL:CMB	4:L:312:BCL:HBB3	2.51	0.41
2:M:91:PHE:N	2:M:91:PHE:CD2	2.89	0.41
1:L:3:LEU:HD13	1:L:5:PHE:CZ	2.55	0.41
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.03	0.40
2:M:122:MET:HE1	4:M:311:BCL:HBB3	2.02	0.40
2:M:239:ALA:C	3:H:73:LEU:HD22	2.46	0.40
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.21	0.40
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.21	0.40
6:M:501:U10:H202	12:M:901:LDA:H111	2.04	0.40
1:L:100:TRP:O	1:L:104:GLU:HG3	2.21	0.40
3:H:194:GLN:NE2	15:H:1050:HOH:O	2.54	0.40
1:L:153:HIS:CE1	1:L:154:LEU:CD1	3.04	0.40
2:M:239:ALA:O	3:H:73:LEU:HD22	2.21	0.40
3:H:130:LYS:HZ2	3:H:172:PRO:HG2	1.86	0.40
1:L:16:LEU:HD23	1:L:109:ARG:CZ	2.52	0.40
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	282/281 (100%)	263 (93%)	18 (6%)	1 (0%)	30	65
2	M	305/307 (99%)	283 (93%)	21 (7%)	1 (0%)	36	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	244/260 (94%)	237 (97%)	5 (2%)	2 (1%)	16	50
All	All	831/848 (98%)	783 (94%)	44 (5%)	4 (0%)	24	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	109	LEU
1	L	31	VAL
3	H	86	ALA
3	H	78	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	223/220 (101%)	209 (94%)	14 (6%)	16	48
2	M	241/240 (100%)	229 (95%)	12 (5%)	22	56
3	H	201/208 (97%)	192 (96%)	9 (4%)	24	59
All	All	665/668 (100%)	630 (95%)	35 (5%)	21	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	62	GLN
1	L	71	LEU
1	L	72	GLU
1	L	80	LEU
1	L	185	LEU
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU

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Mol	Chain	Res	Type
1	L	247	CYS
1	L	249	ILE
1	L	254	ILE
2	M	32	VAL
2	M	37	THR
2	M	38	LEU
2	M	52	LEU
2	M	72	ILE
2	M	104	SER
2	M	114	LEU
2	M	132	ARG
2	M	182	HIS
2	M	188	ASN
2	M	274	VAL
2	M	278	LEU
3	H	65	ILE
3	H	66	LEU
3	H	78	PRO
3	H	80	SER
3	H	200	SER
3	H	221[A]	SER
3	H	221[B]	SER
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	62	GLN
1	L	258	GLN
1	L	274	ASN
2	M	202	HIS
2	M	300	ASN
3	H	68	HIS
3	H	129	ASN
3	H	141	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 2 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	1.33	7 (10%)	79,115,115	1.69	19 (24%)
4	BCL	L	312	1	69,74,74	1.35	5 (7%)	79,115,115	1.27	10 (12%)
11	PS2	M	802	-	52,53,53	1.17	4 (7%)	54,62,62	2.39	11 (20%)
8	PO4	M	701	-	4,4,4	0.57	0	6,6,6	1.10	0
12	LDA	M	906	-	13,15,15	1.61	2 (15%)	14,17,17	0.79	1 (7%)
12	LDA	M	907	-	13,15,15	1.78	2 (15%)	14,17,17	0.66	0
4	BCL	M	313	2	69,74,74	1.08	3 (4%)	79,115,115	1.43	15 (18%)
6	U10	M	501	-	48,48,63	1.16	6 (12%)	60,61,79	1.32	6 (10%)
9	HTO	M	703	-	9,9,9	0.94	0	10,10,10	2.39	4 (40%)
12	LDA	M	903	-	13,15,15	1.95	1 (7%)	14,17,17	1.15	1 (7%)
4	BCL	M	311	2	69,74,74	1.34	6 (8%)	79,115,115	1.62	15 (18%)
5	BPH	L	402	-	59,70,70	1.41	7 (11%)	59,101,101	1.76	13 (22%)
12	LDA	M	901	-	13,15,15	2.18	2 (15%)	14,17,17	0.54	0
12	LDA	H	904	-	13,15,15	2.07	2 (15%)	14,17,17	0.56	0
13	GOL	M	704	-	5,5,5	0.54	0	5,5,5	0.43	0
13	GOL	H	705	-	5,5,5	0.40	0	5,5,5	0.31	0
8	PO4	M	702	-	4,4,4	0.79	0	6,6,6	1.02	0
10	CDL	M	800	-	80,80,99	1.28	5 (6%)	86,92,111	1.35	11 (12%)
12	LDA	M	920	-	13,15,15	1.72	2 (15%)	14,17,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BPH	M	401	-	59,70,70	1.20	3 (5%)	59,101,101	2.20	17 (28%)
12	LDA	H	902	-	13,15,15	1.95	2 (15%)	14,17,17	0.87	1 (7%)
6	U10	L	502	-	48,48,63	1.17	2 (4%)	60,61,79	1.55	9 (15%)
12	LDA	H	905	-	13,15,15	2.20	2 (15%)	14,17,17	0.50	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	-
4	BCL	L	312	1	-	0/41/137/137	-
11	PS2	M	802	-	-	40/62/62/62	-
12	LDA	M	906	-	-	9/13/13/13	-
12	LDA	M	907	-	-	6/13/13/13	-
4	BCL	M	313	2	-	5/41/137/137	-
6	U10	M	501	-	-	2/45/69/87	0/1/1/1
9	HTO	M	703	-	-	6/10/10/10	-
12	LDA	M	903	-	-	10/13/13/13	-
4	BCL	M	311	2	-	7/41/137/137	-
5	BPH	L	402	-	-	8/37/105/105	0/5/6/6
12	LDA	M	901	-	-	4/13/13/13	-
12	LDA	H	904	-	-	5/13/13/13	-
13	GOL	M	704	-	-	4/4/4/4	-
13	GOL	H	705	-	-	3/4/4/4	-
10	CDL	M	800	-	-	43/91/91/110	-
12	LDA	M	920	-	-	7/13/13/13	-
5	BPH	M	401	-	-	7/37/105/105	0/5/6/6
12	LDA	H	902	-	-	6/13/13/13	-
6	U10	L	502	-	-	12/45/69/87	0/1/1/1
12	LDA	H	905	-	-	7/13/13/13	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	901	LDA	O1-N1	-7.12	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	905	LDA	O1-N1	-6.68	1.25	1.42
12	H	904	LDA	O1-N1	-6.42	1.26	1.42
12	M	903	LDA	O1-N1	-6.19	1.27	1.42
4	L	312	BCL	MG-NB	6.16	2.18	2.05
12	H	902	LDA	O1-N1	-6.14	1.27	1.42
5	L	402	BPH	C1B-C2B	5.72	1.45	1.39
12	M	920	LDA	O1-N1	-5.66	1.28	1.42
10	M	800	CDL	OA6-CA5	5.53	1.49	1.34
12	M	907	LDA	O1-N1	-5.42	1.28	1.42
10	M	800	CDL	OA8-CA7	5.24	1.48	1.33
5	M	401	BPH	C1B-C2B	5.22	1.45	1.39
4	M	311	BCL	MG-ND	-5.02	1.95	2.05
12	M	906	LDA	O1-N1	-4.92	1.30	1.42
4	L	314	BCL	MG-NA	4.53	2.17	2.06
10	M	800	CDL	OB6-CB5	4.51	1.47	1.34
4	L	312	BCL	MG-NA	4.45	2.16	2.06
6	L	502	U10	O3-C3	4.43	1.47	1.36
11	M	802	PS2	P-O1P	4.40	1.66	1.50
12	H	905	LDA	C1-N1	-4.08	1.47	1.51
5	L	402	BPH	C1D-C2D	4.01	1.44	1.39
4	M	311	BCL	MG-NA	3.81	2.15	2.06
4	L	314	BCL	MG-NB	3.79	2.13	2.05
6	L	502	U10	O4-C4	3.57	1.45	1.36
5	M	401	BPH	C1D-C2D	3.49	1.43	1.39
12	H	904	LDA	C1-N1	-3.48	1.47	1.51
10	M	800	CDL	OB8-CB7	3.46	1.43	1.33
6	M	501	U10	O3-C3	3.45	1.45	1.36
4	M	311	BCL	C3B-C4B	3.38	1.47	1.41
5	L	402	BPH	C3B-C4B	3.37	1.46	1.41
4	L	312	BCL	C3B-C4B	3.16	1.47	1.41
11	M	802	PS2	C32-C31	3.11	1.59	1.50
5	L	402	BPH	C2C-C3C	3.06	1.57	1.54
4	L	314	BCL	C3C-C4C	-3.06	1.47	1.51
4	M	313	BCL	C3B-C4B	3.02	1.47	1.41
12	M	901	LDA	C1-N1	-3.01	1.48	1.51
6	M	501	U10	O4-C4	3.00	1.44	1.36
4	M	313	BCL	MG-NA	3.00	2.13	2.06
5	M	401	BPH	C3B-C4B	2.98	1.46	1.41
5	L	402	BPH	C3A-C2A	-2.96	1.52	1.54
12	H	902	LDA	C1-N1	-2.92	1.48	1.51
4	L	312	BCL	MG-ND	-2.86	2.00	2.05
12	M	907	LDA	C1-N1	-2.80	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	402	BPH	C4D-ND	-2.70	1.34	1.38
4	M	313	BCL	MG-NB	2.70	2.11	2.05
5	L	402	BPH	CBD-CGD	2.70	1.55	1.52
4	L	314	BCL	MG-ND	-2.69	2.00	2.05
4	M	311	BCL	C1D-ND	2.65	1.41	1.37
11	M	802	PS2	BR2-C40	-2.64	1.90	1.97
4	L	314	BCL	C1D-ND	2.57	1.41	1.37
4	L	314	BCL	C1-C2	2.56	1.56	1.49
12	M	906	LDA	C1-N1	-2.47	1.49	1.51
4	M	311	BCL	C1A-CHA	-2.41	1.33	1.43
11	M	802	PS2	P-O4P	2.41	1.68	1.59
6	M	501	U10	C31-C29	2.31	1.56	1.51
12	M	920	LDA	C1-N1	-2.31	1.49	1.51
6	M	501	U10	C18-C19	2.28	1.38	1.33
4	M	311	BCL	OBD-CAD	2.19	1.26	1.22
4	L	314	BCL	C3B-C4B	2.19	1.45	1.41
4	L	312	BCL	C1B-NB	2.12	1.40	1.37
6	M	501	U10	C13-C14	2.05	1.37	1.33
6	M	501	U10	C23-C24	2.04	1.37	1.33
10	M	800	CDL	CB2-C1	2.03	1.57	1.51

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	802	PS2	O4P-C4-C5	9.03	115.94	108.06
5	M	401	BPH	O2D-CGD-CBD	7.77	119.48	110.95
5	M	401	BPH	C4D-CHA-CBD	-6.55	105.31	108.45
11	M	802	PS2	C3-C2-C1	-6.42	96.81	111.78
11	M	802	PS2	BR1-C39-C40	-6.13	98.40	110.27
10	M	800	CDL	OA6-CA5-C11	6.04	124.54	111.48
11	M	802	PS2	O2-C31-C32	5.83	124.09	111.48
5	L	402	BPH	O2D-CGD-CBD	5.43	116.91	110.95
11	M	802	PS2	BR1-C39-C38	5.35	118.17	108.87
5	M	401	BPH	OBD-CAD-CBD	-4.93	118.58	125.82
9	M	703	HTO	C1-C2-C3	4.55	122.26	113.00
5	M	401	BPH	C1-O2A-CGA	4.54	127.65	116.65
6	L	502	U10	C25-C24-C26	4.52	123.07	115.23
5	L	402	BPH	OBD-CAD-CBD	-4.43	119.32	125.82
4	M	311	BCL	C1-O2A-CGA	4.42	127.35	116.65
4	M	311	BCL	O2D-CGD-CBD	4.40	118.92	111.23
6	M	501	U10	C17-C18-C19	-4.21	117.98	127.62
5	M	401	BPH	CMA-C3A-C4A	-4.10	105.78	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	800	CDL	OB6-CB5-C51	4.02	120.17	111.48
4	M	313	BCL	CHD-C1D-ND	-3.96	119.23	124.80
4	L	314	BCL	CAA-C2A-C3A	-3.96	102.30	113.00
4	L	314	BCL	O1D-CGD-CBD	-3.92	116.79	124.52
4	L	314	BCL	O2D-CGD-CBD	3.75	117.78	111.23
6	L	502	U10	C7-C8-C9	-3.70	120.46	126.83
4	M	311	BCL	CED-O2D-CGD	-3.67	107.58	115.92
5	M	401	BPH	C2B-C1B-NB	-3.61	106.82	109.43
4	L	312	BCL	C4-C3-C5	3.60	121.48	115.23
4	L	314	BCL	CBC-CAC-C3C	3.59	121.02	113.41
5	L	402	BPH	C1-C2-C3	-3.58	120.33	126.20
4	M	313	BCL	CMD-C2D-C1D	3.51	130.90	124.73
4	L	314	BCL	C2C-C3C-C4C	3.50	106.57	101.34
6	L	502	U10	C30-C29-C31	3.46	121.23	115.23
4	L	314	BCL	C2B-C1B-NB	-3.44	106.75	110.33
4	M	313	BCL	C4D-CHA-C1A	3.44	125.35	121.24
11	M	802	PS2	C3-O3-C11	-3.42	104.62	117.12
11	M	802	PS2	O2-C31-O31	-3.41	115.74	123.70
9	M	703	HTO	O2-C2-C1	-3.40	101.29	109.03
4	L	314	BCL	C4D-CHA-C1A	3.38	125.28	121.24
11	M	802	PS2	O3-C11-C12	3.35	122.04	111.83
5	L	402	BPH	C4D-CHA-CBD	-3.34	106.85	108.45
4	L	314	BCL	CAC-C3C-C4C	-3.33	105.19	112.58
9	M	703	HTO	C4-C3-C2	3.32	121.72	113.73
4	M	311	BCL	C5-C3-C2	3.32	128.62	121.17
4	M	313	BCL	O2D-CGD-CBD	3.29	116.98	111.23
10	M	800	CDL	OB8-CB7-OB9	-3.19	115.66	123.63
4	M	311	BCL	CMA-C3A-C4A	-3.18	103.23	111.77
10	M	800	CDL	OA8-CA7-C31	3.14	121.39	111.83
4	L	314	BCL	CAA-CBA-CGA	3.04	121.83	113.21
5	M	401	BPH	OBD-CAD-C3D	3.02	132.60	127.89
5	M	401	BPH	O1D-CGD-CBD	-3.02	120.15	124.72
4	L	312	BCL	CAA-C2A-C3A	-3.00	104.88	113.00
4	M	313	BCL	O2D-CGD-O1D	-2.98	118.04	123.85
4	L	314	BCL	C6-C5-C3	-2.95	106.27	113.47
4	M	313	BCL	CHA-C1A-NA	-2.95	119.71	126.39
4	M	311	BCL	CHA-C1A-NA	-2.93	119.75	126.39
5	M	401	BPH	CMD-C2D-C3D	2.92	130.51	124.68
5	L	402	BPH	CMA-C3A-C4A	-2.90	108.35	114.61
4	M	311	BCL	CAA-C2A-C3A	-2.86	105.26	113.00
4	M	311	BCL	O1D-CGD-CBD	-2.85	118.89	124.52
4	L	314	BCL	C2A-C1A-CHA	2.85	128.82	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	312	BCL	C2B-C1B-NB	-2.85	107.37	110.33
5	L	402	BPH	C2D-C1D-ND	-2.84	107.38	109.43
5	M	401	BPH	C2D-C1D-ND	-2.83	107.39	109.43
5	L	402	BPH	CED-O2D-CGD	2.82	122.32	115.92
5	L	402	BPH	CAA-C2A-C3A	-2.82	105.39	113.00
4	M	311	BCL	C3B-C4B-NB	-2.77	106.10	109.76
4	L	314	BCL	CHA-C1A-NA	-2.76	120.15	126.39
4	M	311	BCL	C2B-C1B-NB	-2.71	107.51	110.33
4	M	313	BCL	CHD-C1D-C2D	2.70	131.10	125.49
12	M	903	LDA	CM1-N1-C1	2.68	115.86	110.23
5	M	401	BPH	CAA-C2A-C3A	-2.67	105.80	113.00
5	M	401	BPH	C1-C2-C3	-2.66	121.83	126.20
4	M	311	BCL	C4D-CHA-C1A	2.66	124.41	121.24
5	L	402	BPH	C1C-C2C-C3C	-2.65	100.31	102.84
6	L	502	U10	C12-C11-C9	-2.65	104.40	113.19
4	L	314	BCL	C5-C3-C2	-2.65	115.22	121.17
11	M	802	PS2	BR2-C40-C39	-2.64	105.16	110.27
5	L	402	BPH	C2B-C1B-NB	-2.63	107.53	109.43
6	M	501	U10	C41-C39-C40	2.63	120.64	114.59
4	M	313	BCL	CMC-C2C-C3C	-2.63	103.82	113.98
10	M	800	CDL	CA4-OA6-CA5	-2.62	111.52	117.80
4	L	314	BCL	C4-C3-C5	2.62	119.77	115.23
5	L	402	BPH	CMD-C2D-C3D	2.61	129.89	124.68
4	M	313	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
6	L	502	U10	C35-C34-C33	-2.60	116.95	123.63
9	M	703	HTO	C5-C4-C3	-2.57	109.89	114.11
5	L	402	BPH	CMB-C2B-C3B	2.57	129.82	124.68
4	M	311	BCL	CBB-CAB-C3B	-2.57	114.99	120.40
4	M	313	BCL	C1C-NC-C4C	2.55	107.84	106.68
10	M	800	CDL	CA6-OA8-CA7	2.54	126.42	117.12
4	L	314	BCL	CHD-C1D-ND	-2.54	121.23	124.80
5	M	401	BPH	C1B-NB-C4B	2.54	112.52	108.82
6	L	502	U10	C15-C14-C13	-2.53	117.12	123.63
4	L	314	BCL	C3A-C2A-C1A	2.49	105.08	101.34
4	M	313	BCL	C2B-C1B-NB	-2.46	107.78	110.33
5	M	401	BPH	C3B-C4B-NB	-2.41	104.54	108.05
4	L	312	BCL	CHA-C1A-NA	-2.40	120.95	126.39
4	L	312	BCL	C5-C3-C2	-2.39	115.79	121.17
4	M	313	BCL	C3B-C4B-NB	-2.37	106.63	109.76
6	M	501	U10	C37-C38-C39	-2.37	119.73	127.64
4	L	314	BCL	CAA-C2A-C1A	-2.35	104.26	111.97
12	H	902	LDA	CM1-N1-C1	-2.34	105.31	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	501	U10	C7-C6-C5	-2.33	115.81	118.52
4	M	313	BCL	O2A-C1-C2	2.33	117.07	108.11
6	L	502	U10	C15-C14-C16	2.33	119.27	115.23
4	L	312	BCL	C1D-ND-C4D	2.33	107.94	106.31
10	M	800	CDL	CB6-CB4-CB3	-2.32	106.37	111.78
5	M	401	BPH	CMC-C2C-C1C	2.31	119.59	114.61
6	L	502	U10	C12-C13-C14	-2.29	122.39	127.62
4	M	311	BCL	CAC-C3C-C4C	-2.29	107.51	112.58
5	M	401	BPH	CMB-C2B-C3B	2.26	129.21	124.68
10	M	800	CDL	OB6-CB5-OB7	-2.22	118.51	123.70
6	L	502	U10	C31-C29-C28	-2.22	116.18	121.17
10	M	800	CDL	OB8-CB7-C71	2.22	118.61	111.83
4	L	314	BCL	O2A-CGA-O1A	-2.21	118.09	123.63
4	L	312	BCL	C6-C7-C8	-2.21	108.62	115.97
4	L	314	BCL	CHD-C1D-C2D	2.19	130.04	125.49
6	M	501	U10	O5-C5-C6	-2.19	117.56	121.79
11	M	802	PS2	O3-C11-O11	-2.19	118.16	123.63
4	M	313	BCL	C1-C2-C3	-2.19	122.62	126.20
4	L	312	BCL	CBC-CAC-C3C	-2.18	108.78	113.41
4	L	312	BCL	O1D-CGD-CBD	-2.17	120.23	124.52
10	M	800	CDL	OA6-CA4-CA3	2.16	116.09	108.34
4	M	311	BCL	C4-C3-C5	-2.16	111.49	115.23
5	L	402	BPH	O2D-CGD-O1D	-2.14	119.68	123.85
4	M	313	BCL	O2A-CGA-O1A	-2.14	118.29	123.63
5	M	401	BPH	CMA-C3A-C2A	-2.12	105.93	114.13
4	M	311	BCL	C6-C5-C3	-2.09	108.37	113.47
6	M	501	U10	C21-C19-C18	2.08	125.84	121.17
11	M	802	PS2	BR2-C40-C41	-2.08	105.26	108.87
12	M	906	LDA	O1-N1-C1	2.05	114.29	109.27
10	M	800	CDL	OA5-PA1-OA3	2.02	116.94	108.94
4	L	312	BCL	OB6-CAB-C3B	2.01	123.99	120.43

There are no chirality outliers.

All (196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C4C-C3C-CAC-CBC
9	M	703	HTO	C1-C2-C3-C4
10	M	800	CDL	CB2-C1-CA2-OA2
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA5
10	M	800	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
10	M	800	CDL	CB3-OB5-PB2-OB3
11	M	802	PS2	C40-C41-C42-C43
11	M	802	PS2	BR1-C39-C40-C41
11	M	802	PS2	C38-C39-C40-C41
11	M	802	PS2	C1-O3P-P-O1P
11	M	802	PS2	C1-O3P-P-O2P
11	M	802	PS2	C1-O3P-P-O4P
11	M	802	PS2	C4-O4P-P-O3P
11	M	802	PS2	C4-O4P-P-O1P
11	M	802	PS2	C4-O4P-P-O2P
12	M	903	LDA	C2-C1-N1-O1
12	M	903	LDA	C2-C1-N1-CM1
12	M	903	LDA	C2-C1-N1-CM2
12	M	903	LDA	N1-C1-C2-C3
12	M	906	LDA	C2-C1-N1-O1
12	M	906	LDA	C2-C1-N1-CM1
13	M	704	GOL	O1-C1-C2-C3
13	H	705	GOL	C1-C2-C3-O3
11	M	802	PS2	O11-C11-O3-C3
5	M	401	BPH	C3-C5-C6-C7
11	M	802	PS2	C12-C11-O3-C3
9	M	703	HTO	O1-C1-C2-O2
10	M	800	CDL	O1-C1-CA2-OA2
6	L	502	U10	C29-C31-C32-C33
10	M	800	CDL	C1-CB2-OB2-PB2
12	H	905	LDA	C1-C2-C3-C4
6	L	502	U10	C35-C34-C36-C37
10	M	800	CDL	CB7-C71-C72-C73
6	M	501	U10	C24-C26-C27-C28
11	M	802	PS2	C11-C12-C13-C14
12	M	907	LDA	C7-C8-C9-C10
11	M	802	PS2	C31-C32-C33-C34
10	M	800	CDL	C11-CA5-OA6-CA4
9	M	703	HTO	O1-C1-C2-C3
10	M	800	CDL	OA7-CA5-OA6-CA4
6	L	502	U10	C33-C34-C36-C37
4	M	313	BCL	C13-C15-C16-C17
13	M	704	GOL	C1-C2-C3-O3
13	H	705	GOL	O1-C1-C2-C3
4	M	311	BCL	C3-C5-C6-C7
12	M	920	LDA	C5-C6-C7-C8
11	M	802	PS2	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
12	H	905	LDA	C4-C5-C6-C7
11	M	802	PS2	C43-C44-C45-C46
12	M	903	LDA	C7-C8-C9-C10
12	M	906	LDA	C7-C8-C9-C10
12	H	904	LDA	C4-C5-C6-C7
13	M	704	GOL	O2-C2-C3-O3
13	H	705	GOL	O2-C2-C3-O3
11	M	802	PS2	C22-C23-C24-C25
11	M	802	PS2	C44-C45-C46-C47
10	M	800	CDL	C51-CB5-OB6-CB4
10	M	800	CDL	C19-C20-C21-C22
12	M	901	LDA	C5-C6-C7-C8
11	M	802	PS2	C15-C16-C17-C18
12	H	905	LDA	C6-C7-C8-C9
11	M	802	PS2	C12-C13-C14-C15
11	M	802	PS2	C21-C22-C23-C24
11	M	802	PS2	C34-C35-C36-C37
10	M	800	CDL	OB7-CB5-OB6-CB4
12	M	903	LDA	C2-C3-C4-C5
10	M	800	CDL	CA5-C11-C12-C13
10	M	800	CDL	C31-CA7-OA8-CA6
12	M	903	LDA	C1-C2-C3-C4
10	M	800	CDL	C11-C12-C13-C14
12	H	904	LDA	C6-C7-C8-C9
11	M	802	PS2	C32-C31-O2-C2
12	M	907	LDA	C4-C5-C6-C7
11	M	802	PS2	C14-C15-C16-C17
11	M	802	PS2	C35-C36-C37-C38
11	M	802	PS2	O4P-C4-C5-C6
10	M	800	CDL	C38-C39-C40-C41
5	M	401	BPH	C2C-C3C-CAC-CBC
12	H	905	LDA	C3-C4-C5-C6
10	M	800	CDL	OA9-CA7-OA8-CA6
10	M	800	CDL	C77-C78-C79-C80
12	M	903	LDA	C4-C5-C6-C7
12	M	920	LDA	C11-C10-C9-C8
5	M	401	BPH	C15-C16-C17-C18
10	M	800	CDL	C18-C19-C20-C21
10	M	800	CDL	OA5-CA3-CA4-CA6
11	M	802	PS2	O3P-C1-C2-C3
5	M	401	BPH	C12-C13-C15-C16
11	M	802	PS2	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C14-C13-C15-C16
10	M	800	CDL	C36-C37-C38-C39
12	H	904	LDA	C1-C2-C3-C4
10	M	800	CDL	C72-C73-C74-C75
11	M	802	PS2	C23-C24-C25-C26
4	M	313	BCL	C16-C17-C18-C20
12	M	920	LDA	C4-C5-C6-C7
9	M	703	HTO	O2-C2-C3-O3
10	M	800	CDL	C13-C14-C15-C16
12	H	904	LDA	C11-C10-C9-C8
12	M	906	LDA	C6-C7-C8-C9
12	M	907	LDA	C11-C10-C9-C8
12	H	905	LDA	C11-C10-C9-C8
12	M	901	LDA	N1-C1-C2-C3
6	L	502	U10	C13-C14-C16-C17
4	M	311	BCL	C11-C10-C8-C9
5	L	402	BPH	C8-C10-C11-C12
12	M	901	LDA	C9-C10-C11-C12
4	M	311	BCL	C11-C10-C8-C7
4	M	311	BCL	C3A-C2A-CAA-CBA
9	M	703	HTO	O2-C2-C3-C4
12	M	920	LDA	C1-C2-C3-C4
5	L	402	BPH	C4-C3-C5-C6
6	L	502	U10	C15-C14-C16-C17
12	M	906	LDA	C2-C3-C4-C5
10	M	800	CDL	OA5-CA3-CA4-OA6
11	M	802	PS2	O3P-C1-C2-O2
4	M	313	BCL	C16-C17-C18-C19
12	M	906	LDA	C3-C4-C5-C6
12	M	906	LDA	C4-C5-C6-C7
11	M	802	PS2	C42-C43-C44-C45
11	M	802	PS2	O31-C31-O2-C2
6	L	502	U10	C20-C19-C21-C22
5	L	402	BPH	C2-C3-C5-C6
5	L	402	BPH	O2A-C1-C2-C3
12	M	907	LDA	C2-C3-C4-C5
9	M	703	HTO	C1-C2-C3-O3
12	M	906	LDA	C2-C1-N1-CM2
12	M	903	LDA	C9-C10-C11-C12
12	H	902	LDA	C1-C2-C3-C4
4	L	314	BCL	C12-C13-C15-C16
12	H	902	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	M	311	BCL	C14-C13-C15-C16
11	M	802	PS2	C1-C2-C3-O3
4	L	314	BCL	C13-C15-C16-C17
12	H	902	LDA	C4-C5-C6-C7
10	M	800	CDL	C53-C54-C55-C56
6	L	502	U10	C5-C4-O4-C4M
4	L	314	BCL	CHA-CBD-CGD-O1D
4	L	314	BCL	CHA-CBD-CGD-O2D
4	M	313	BCL	CAD-CBD-CGD-O1D
10	M	800	CDL	CA3-OA5-PA1-OA4
6	L	502	U10	C18-C19-C21-C22
12	M	907	LDA	C9-C10-C11-C12
12	M	901	LDA	C7-C8-C9-C10
11	M	802	PS2	C33-C34-C35-C36
12	H	905	LDA	C7-C8-C9-C10
12	M	907	LDA	N1-C1-C2-C3
12	M	920	LDA	N1-C1-C2-C3
11	M	802	PS2	O2-C2-C3-O3
11	M	802	PS2	C18-C19-C20-C21
4	L	314	BCL	C14-C13-C15-C16
12	H	904	LDA	C9-C10-C11-C12
4	M	311	BCL	C16-C17-C18-C20
11	M	802	PS2	C38-C39-C40-BR2
10	M	800	CDL	C17-C18-C19-C20
5	M	401	BPH	C2-C1-O2A-CGA
11	M	802	PS2	BR2-C40-C41-C42
6	M	501	U10	C5-C4-O4-C4M
12	M	920	LDA	C2-C3-C4-C5
12	H	902	LDA	C11-C10-C9-C8
12	M	903	LDA	C3-C4-C5-C6
13	M	704	GOL	O1-C1-C2-O2
12	H	905	LDA	C2-C3-C4-C5
10	M	800	CDL	C20-C21-C22-C23
10	M	800	CDL	C78-C79-C80-C81
5	L	402	BPH	C6-C7-C8-C10
10	M	800	CDL	C40-C41-C42-C43
10	M	800	CDL	C33-C34-C35-C36
6	L	502	U10	C3-C4-O4-C4M
12	M	920	LDA	C7-C8-C9-C10
6	L	502	U10	C31-C32-C33-C34
10	M	800	CDL	CB4-CB3-OB5-PB2
4	M	313	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	M	311	BCL	C5-C6-C7-C8
6	L	502	U10	C34-C36-C37-C38
12	M	906	LDA	C5-C6-C7-C8
12	H	902	LDA	N1-C1-C2-C3
10	M	800	CDL	C52-C51-CB5-OB6
10	M	800	CDL	C72-C71-CB7-OB8
5	L	402	BPH	C2C-C3C-CAC-CBC
11	M	802	PS2	C5-C4-O4P-P
10	M	800	CDL	C39-C40-C41-C42
6	L	502	U10	C26-C27-C28-C29
10	M	800	CDL	C32-C31-CA7-OA8
12	H	902	LDA	C9-C10-C11-C12
10	M	800	CDL	C80-C81-C82-C83
10	M	800	CDL	C72-C71-CB7-OB9
5	L	402	BPH	C6-C7-C8-C9
10	M	800	CDL	C52-C51-CB5-OB7
10	M	800	CDL	C32-C31-CA7-OA9
11	M	802	PS2	O2-C31-C32-C33
10	M	800	CDL	C54-C55-C56-C57
5	L	402	BPH	C4C-C3C-CAC-CBC
10	M	800	CDL	C34-C35-C36-C37
11	M	802	PS2	C17-C18-C19-C20

There are no ring outliers.

16 monomers are involved in 67 short contacts:

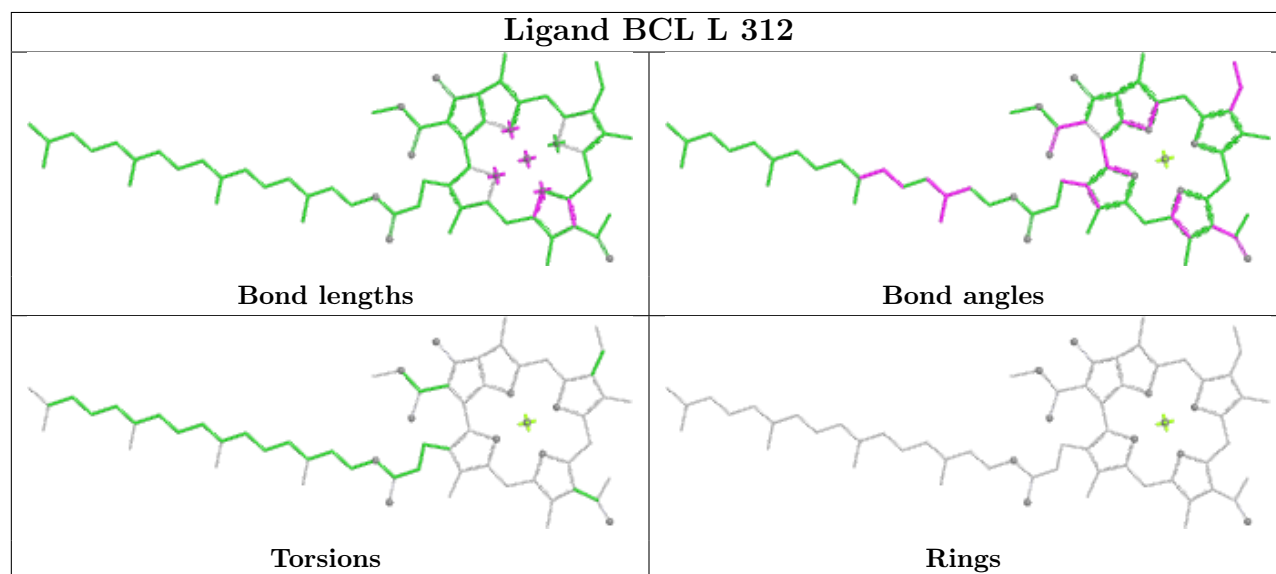
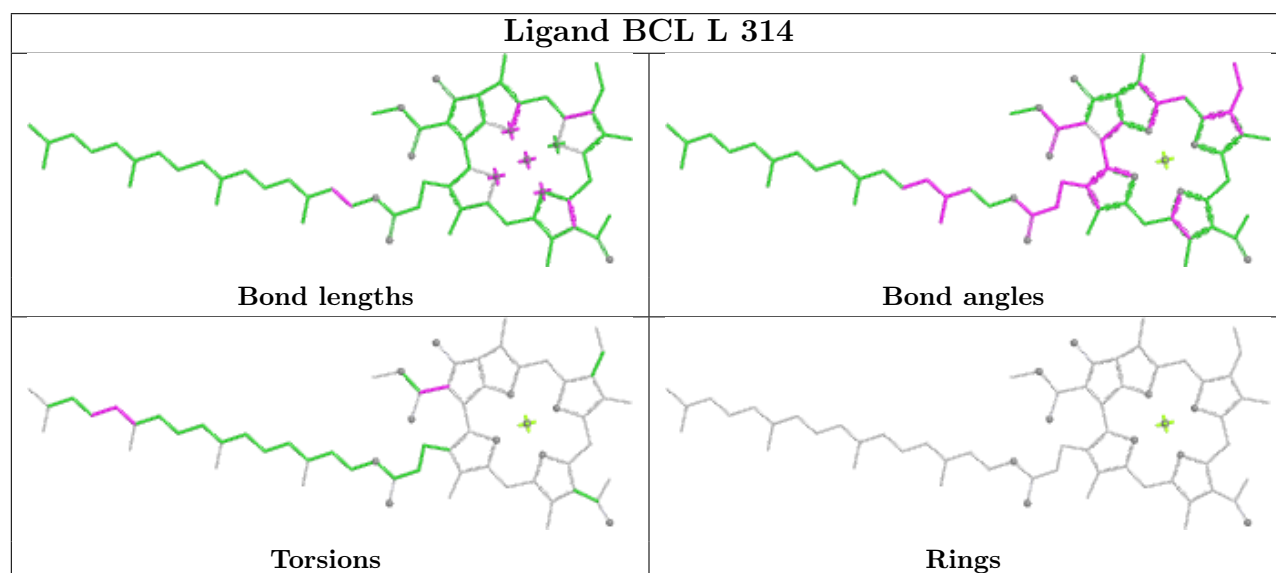
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	314	BCL	3	0
4	L	312	BCL	10	0
11	M	802	PS2	4	0
12	M	906	LDA	2	0
12	M	907	LDA	1	0
4	M	313	BCL	4	0
6	M	501	U10	4	0
12	M	903	LDA	5	0
4	M	311	BCL	12	0
5	L	402	BPH	4	0
12	M	901	LDA	7	0
13	M	704	GOL	2	0
10	M	800	CDL	3	0
12	M	920	LDA	12	0
5	M	401	BPH	3	0

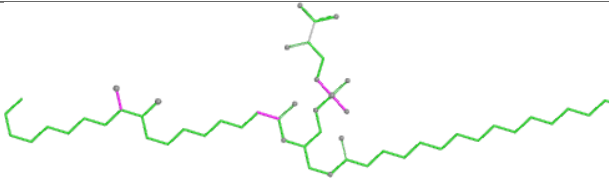
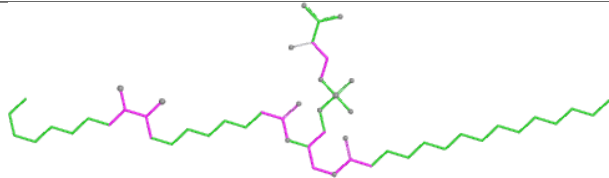
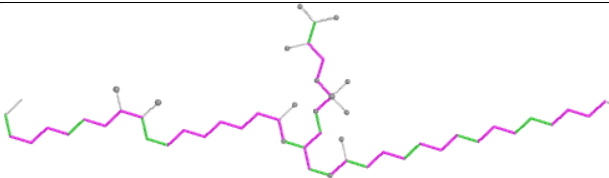
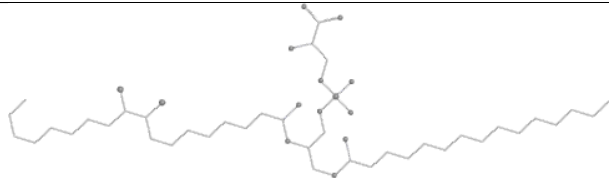
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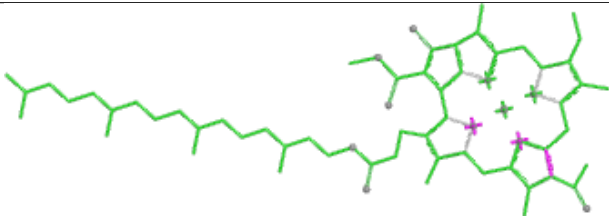
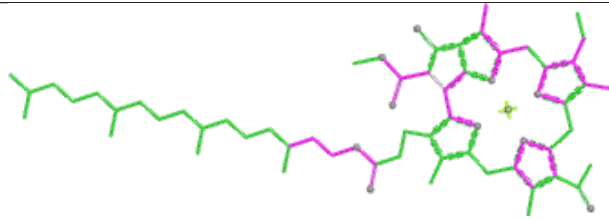
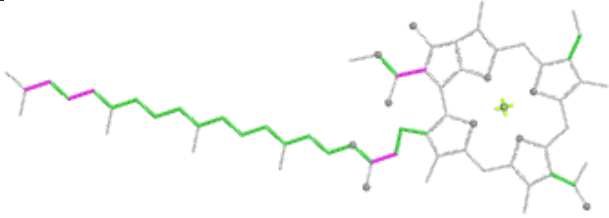
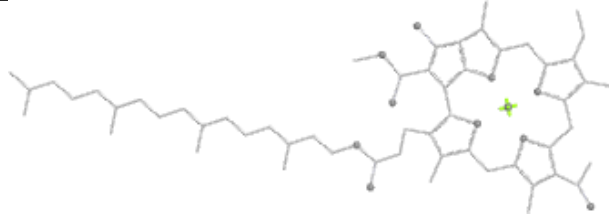
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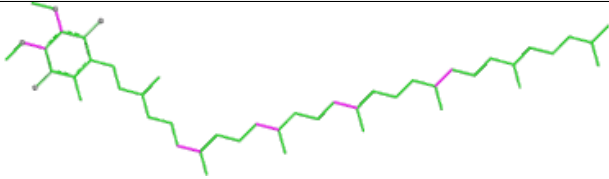
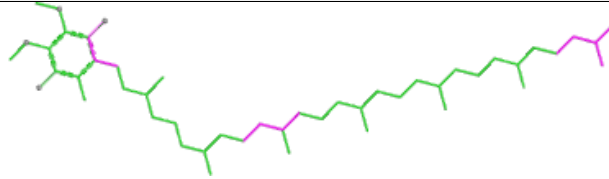
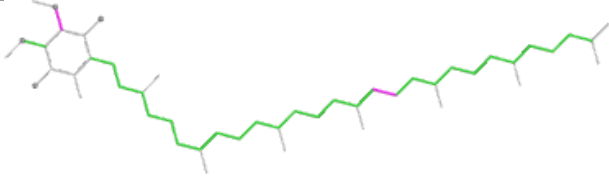
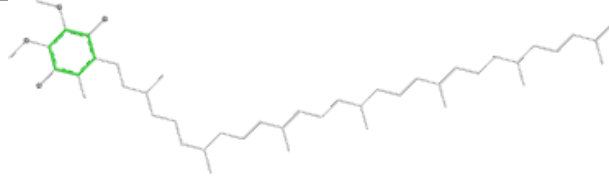
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	502	U10	3	0

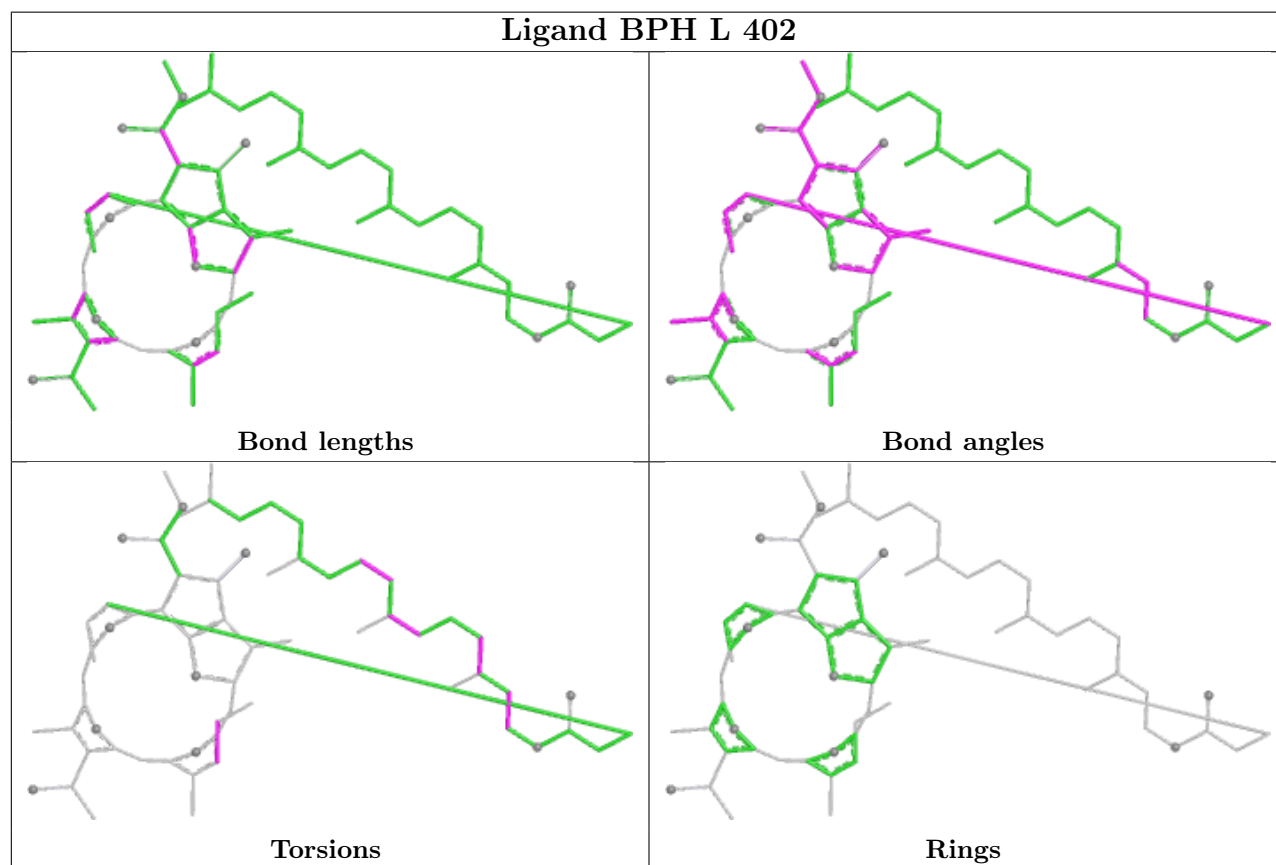
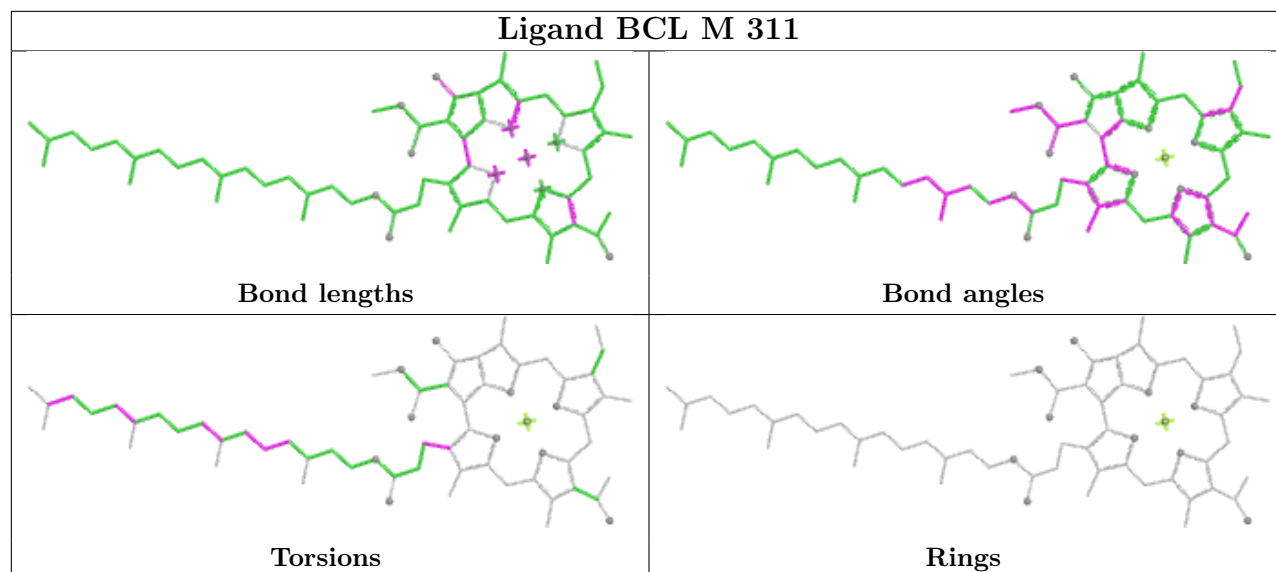
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

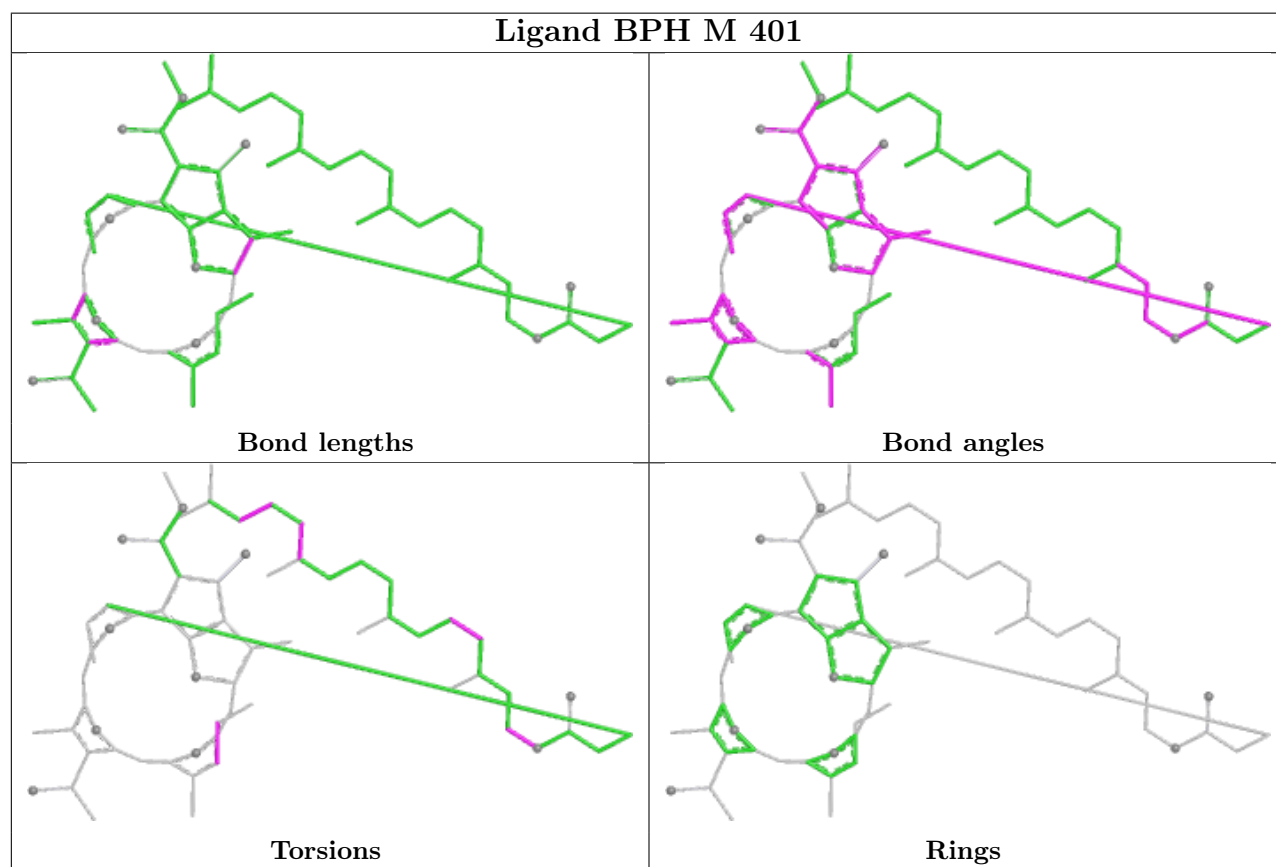
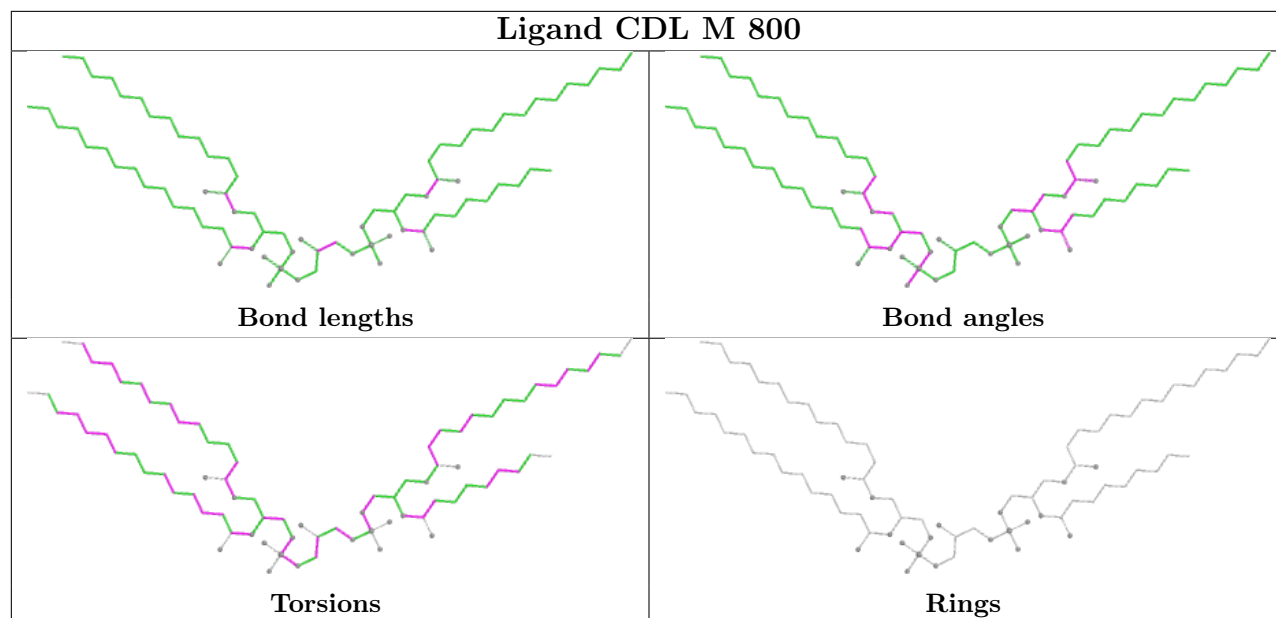


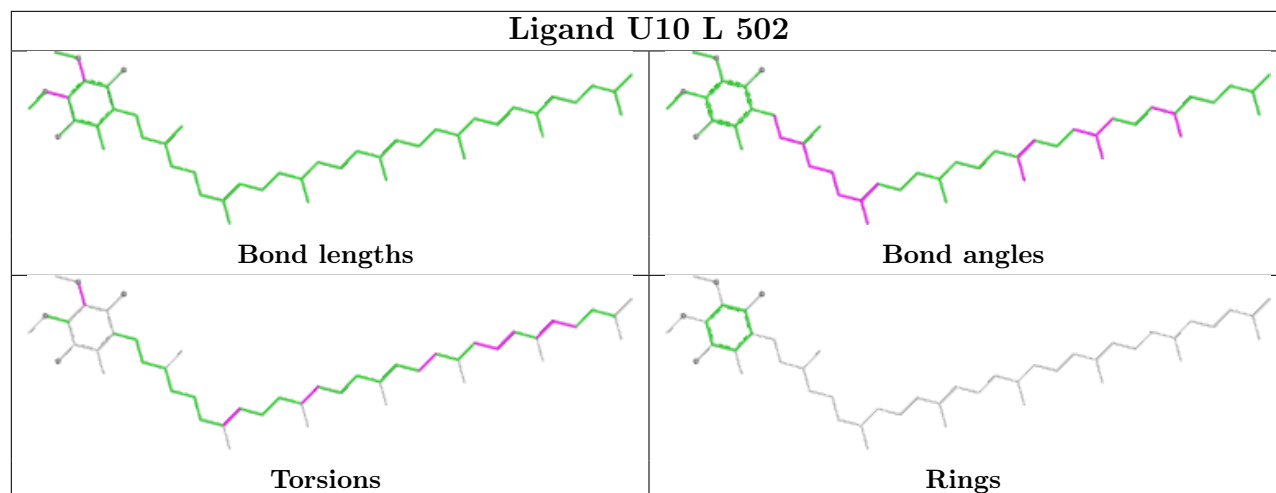
Ligand PS2 M 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL M 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 M 501	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.15	11 (3%) 43 24	32, 70, 78, 86	3 (1%)
2	M	302/307 (98%)	0.01	6 (1%) 65 41	34, 69, 78, 113	5 (1%)
3	H	241/260 (92%)	0.03	6 (2%) 58 35	49, 69, 80, 100	5 (2%)
All	All	824/848 (97%)	0.06	23 (2%) 55 32	32, 69, 78, 113	13 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.0
1	L	202	LYS	4.0
2	M	2	GLU	3.3
2	M	3	TYR	3.3
2	M	302	GLY	2.9
1	L	72	GLU	2.9
1	L	226	THR	2.8
3	H	251	VAL	2.8
3	H	81	GLU	2.8
3	H	250	SER	2.8
1	L	277	GLY	2.8
3	H	127	GLY	2.8
1	L	62	GLN	2.7
2	M	128[A]	SER	2.7
3	H	200	SER	2.5
1	L	252	GLY	2.5
1	L	265	TRP	2.2
3	H	65	ILE	2.2
2	M	170	SER	2.1
1	L	210	ASP	2.1
1	L	35	GLY	2.1
1	L	258	GLN	2.1
1	L	116	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

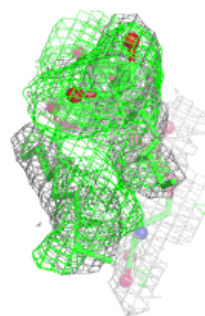
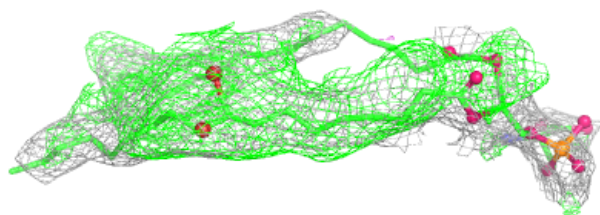
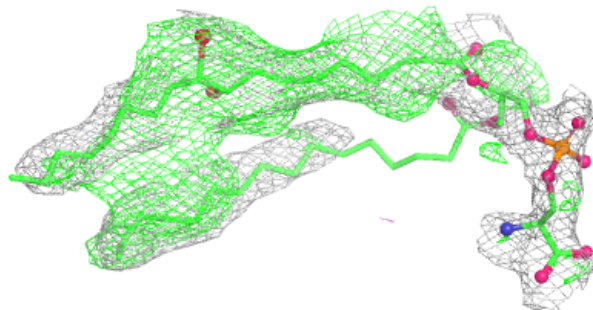
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	HTO	M	703	10/10	0.54	0.55	58,61,63,63	10
13	GOL	H	705	6/6	0.77	0.23	56,58,60,61	6
13	GOL	M	704	6/6	0.78	0.62	68,71,72,74	6
11	PS2	M	802	54/54	0.83	0.36	48,62,75,77	54
12	LDA	H	904	16/16	0.84	0.39	53,57,61,62	16
10	CDL	M	800	81/100	0.86	0.26	57,70,81,82	81
12	LDA	H	902	16/16	0.87	0.35	55,59,73,73	16
12	LDA	M	907	16/16	0.89	0.30	63,67,78,78	16
12	LDA	H	905	16/16	0.89	0.40	65,69,74,75	16
8	PO4	M	702	5/5	0.90	0.17	64,66,68,68	5
6	U10	L	502	48/63	0.91	0.31	52,57,69,71	48
6	U10	M	501	48/63	0.91	0.17	64,72,91,92	0
12	LDA	M	906	16/16	0.92	0.29	57,61,68,70	16
12	LDA	M	901	16/16	0.92	0.18	67,70,73,74	16
12	LDA	M	920	16/16	0.92	0.29	65,70,85,87	16
12	LDA	M	903	16/16	0.92	0.22	41,60,71,72	16
4	BCL	M	311	66/66	0.93	0.14	52,66,113,114	0
8	PO4	M	701	5/5	0.93	0.08	61,62,63,64	5
5	BPH	M	401	65/65	0.94	0.12	61,71,110,111	0
4	BCL	L	312	66/66	0.96	0.11	60,66,77,82	0
4	BCL	M	313	66/66	0.96	0.11	55,65,80,84	0
5	BPH	L	402	65/65	0.96	0.11	61,71,74,75	0
4	BCL	L	314	66/66	0.97	0.08	62,69,74,78	0
14	K	H	700	1/1	0.97	0.05	63,63,63,63	0
7	FE	M	500	1/1	1.00	0.03	70,70,70,70	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.

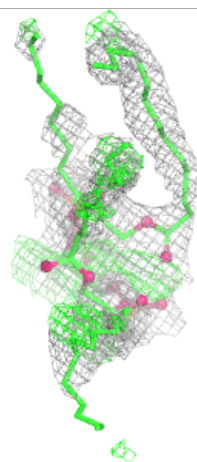
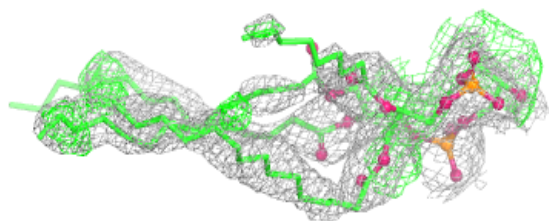
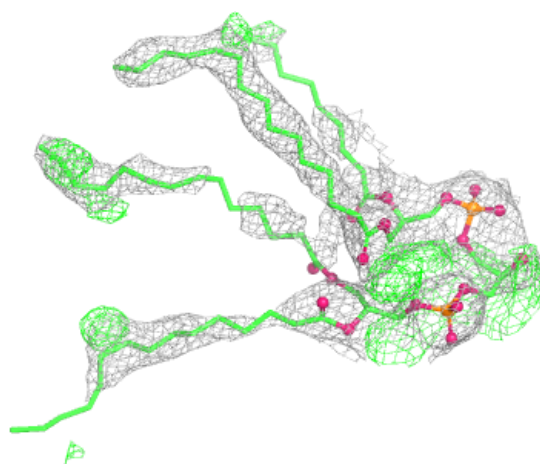
Electron density around PS2 M 802:

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



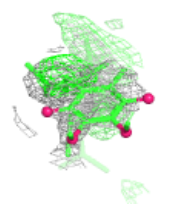
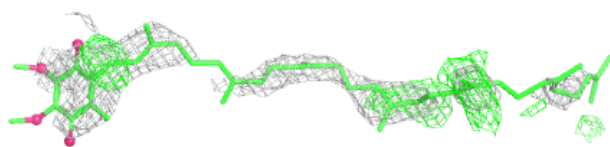
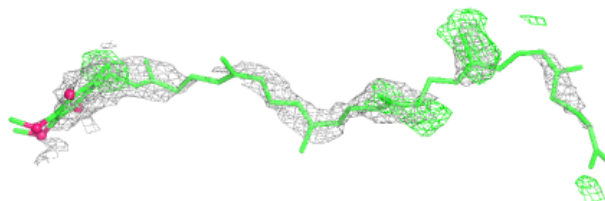
Electron density around CDL M 800:

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

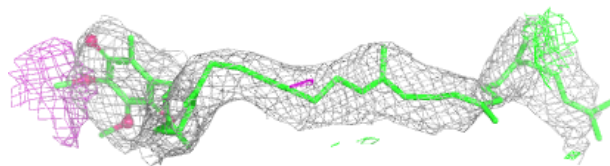
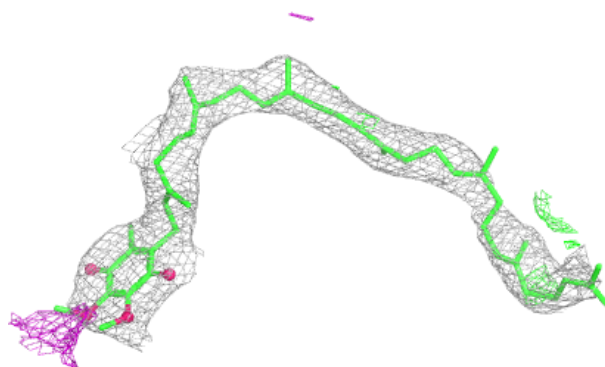


Electron density around U10 L 502:

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

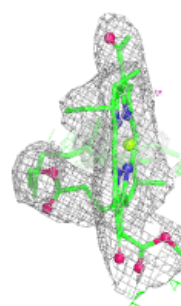
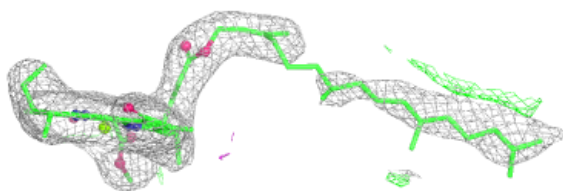
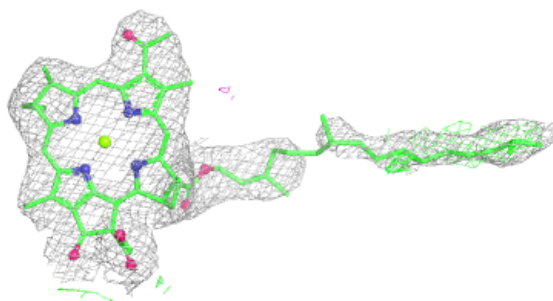
**Electron density around U10 M 501:**

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

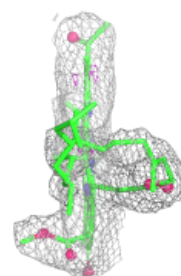
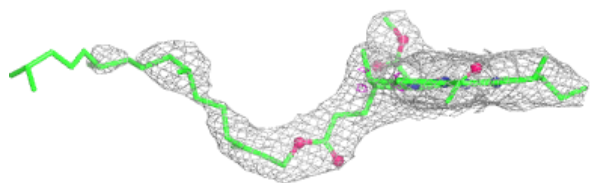
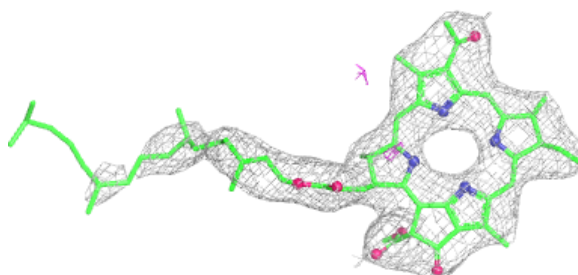


Electron density around BCL M 311:

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and green (positive)

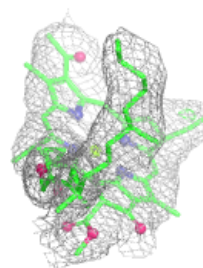
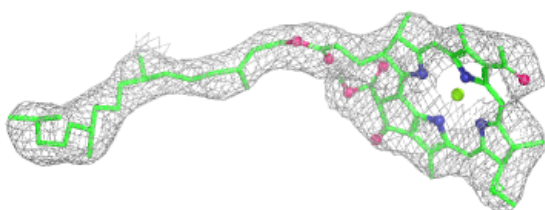
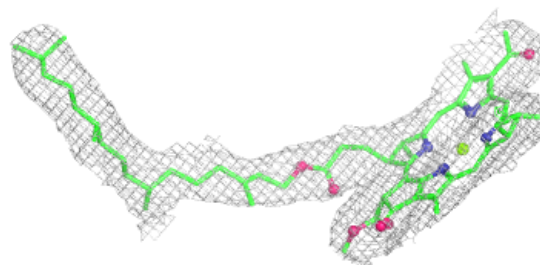
**Electron density around BPH M 401:**

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

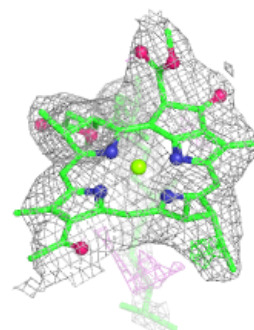
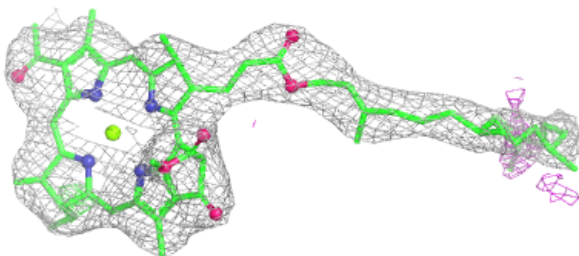
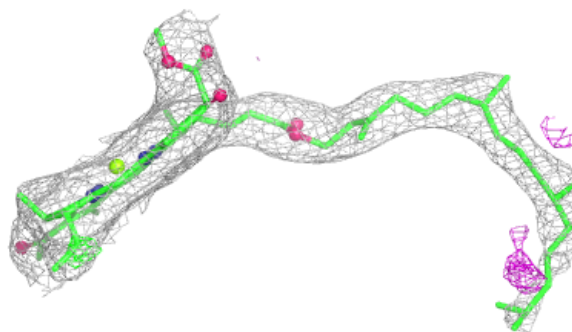


Electron density around BCL L 312:

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

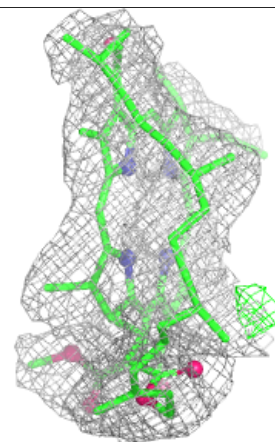
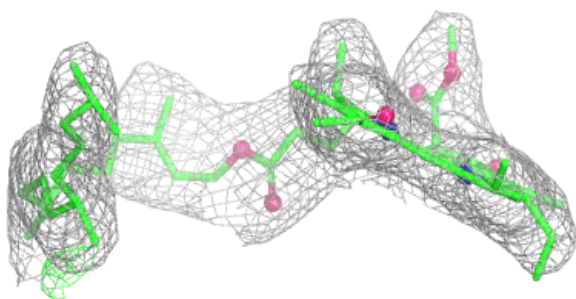
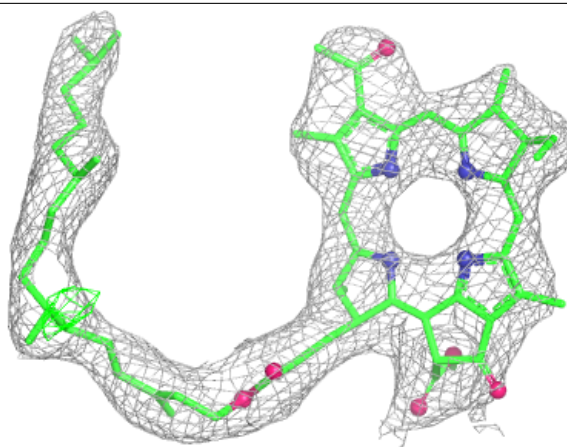
**Electron density around BCL M 313:**

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



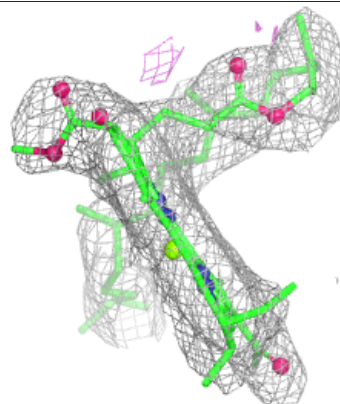
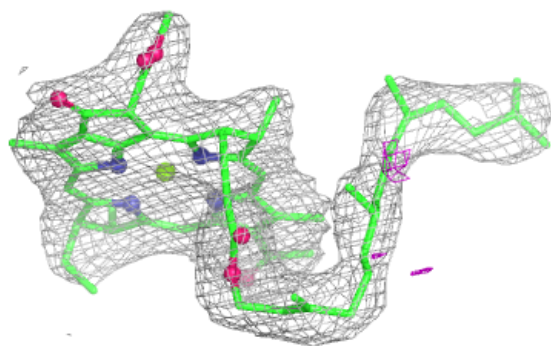
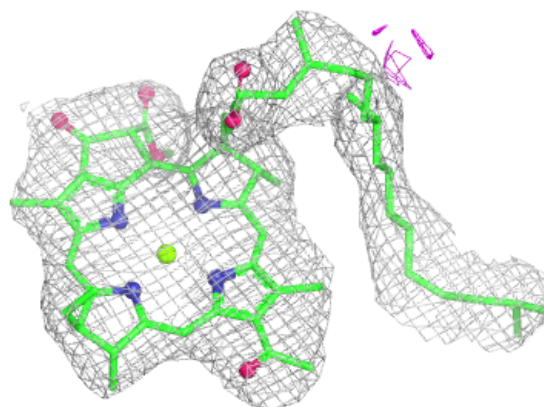
Electron density around BPH L 402:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.