



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:11 AM EDT

PDB ID : 2HHK / pdb_00002hhk
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-28
Resolution : 2.50 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

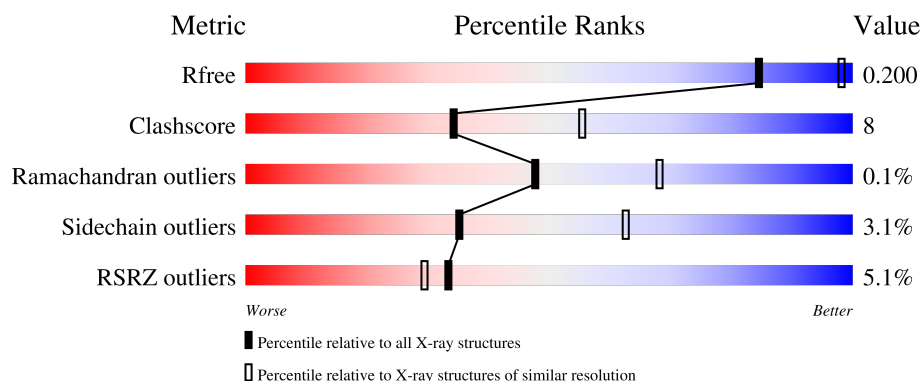
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

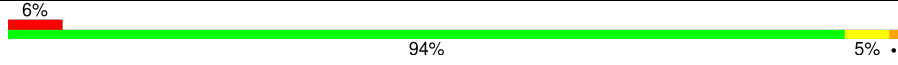
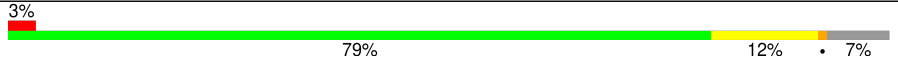
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

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
10	PO4	H	704	-	-	-	X
10	PO4	M	705	-	-	-	X
13	LDA	H	901	-	-	X	-
7	GOL	L	709	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7824 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	1	0
			2235	1510	356	361	8			

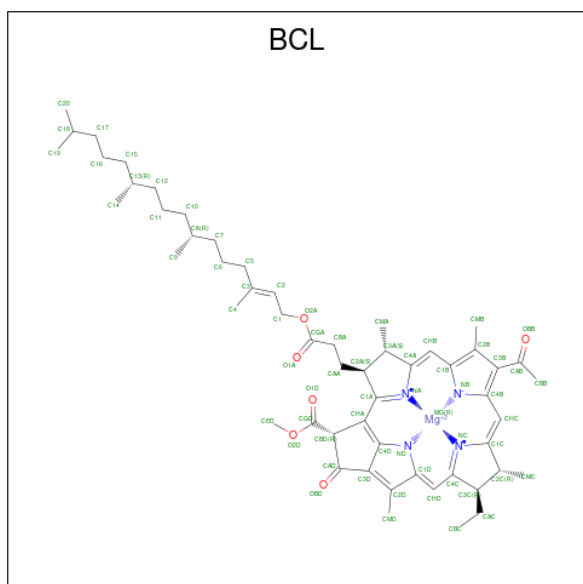
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	10	0
			2448	1633	402	402	11			

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

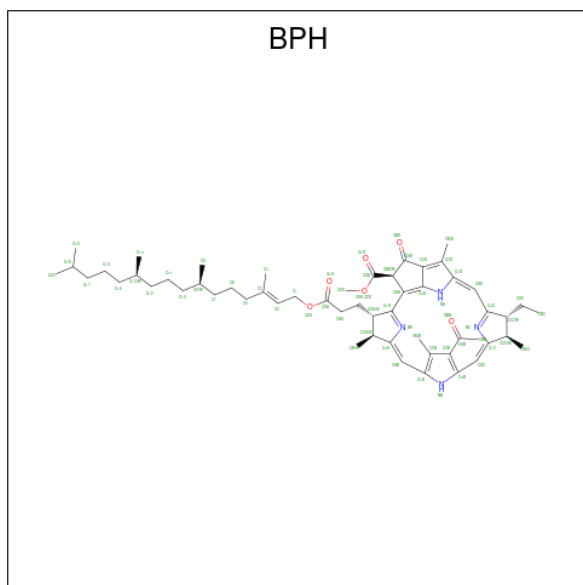
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1862	1189	323	339	11			

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



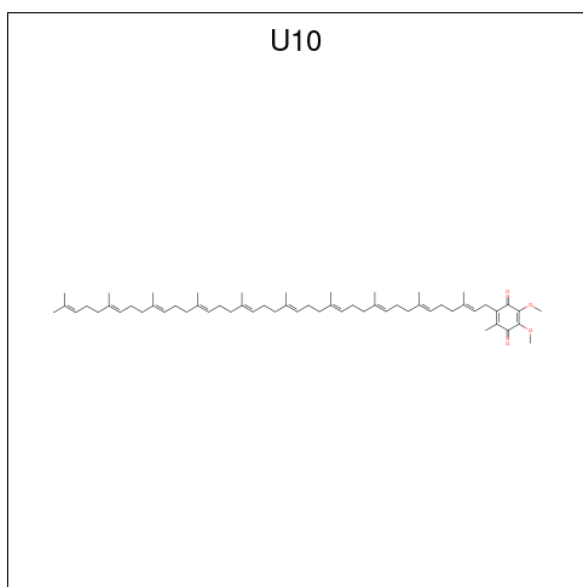
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- 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 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	L	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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		

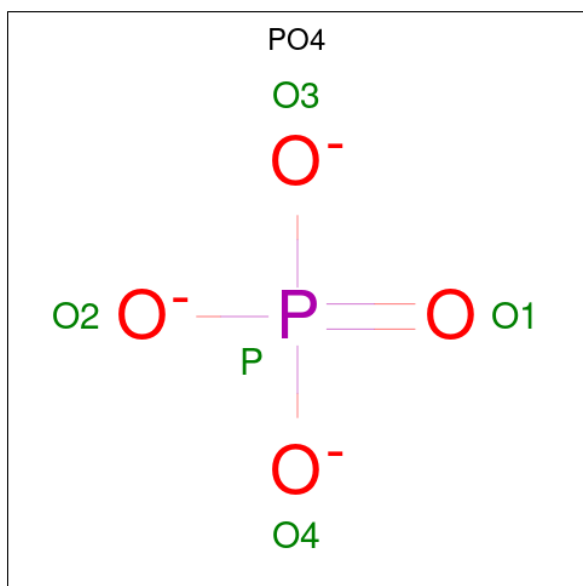
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

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	1	Total	Cl	0	0
			1	1		

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



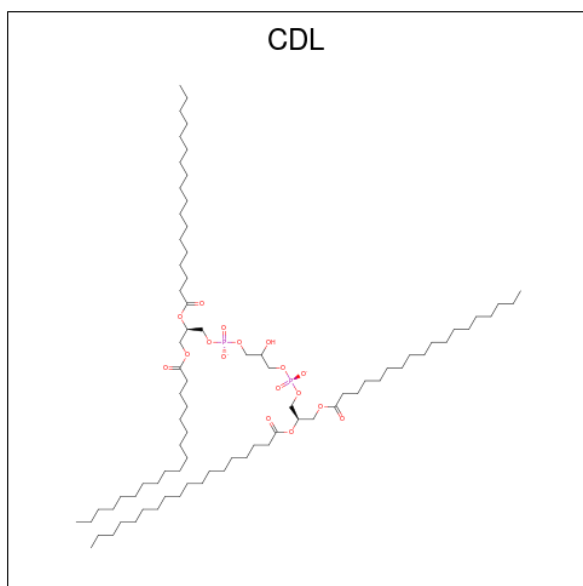
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

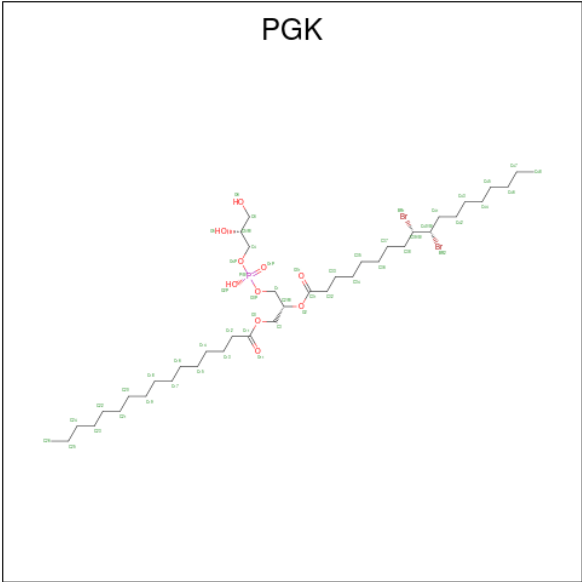
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



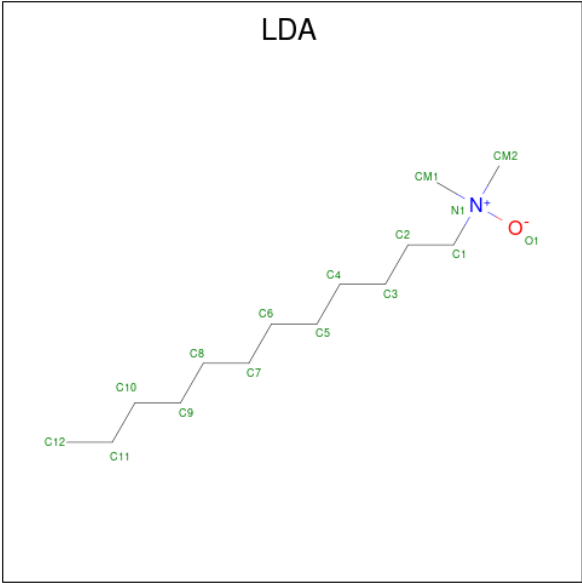
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 12 is (1R)-2-{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (9S,10S)-9,10-DIBROMOOCTADECANOATE (CCD ID: PGK) (formula: $C_{40}H_{77}Br_2O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	O	P		
12	M	1	53	2	40	10	1	0	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

Continued on next page...

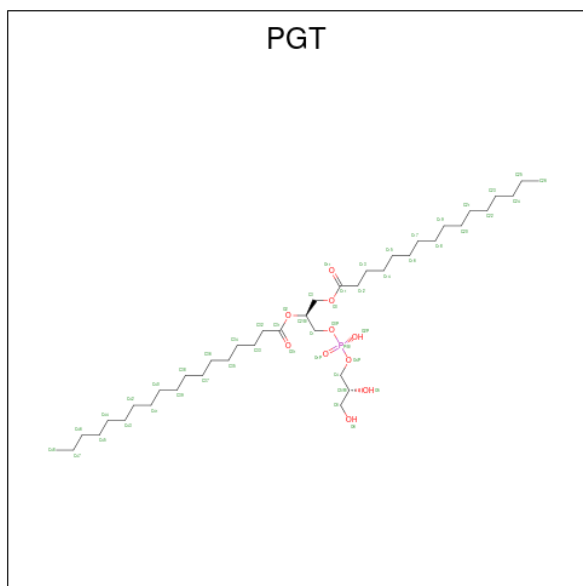
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	O	P	0	1
			102	80	20	2		

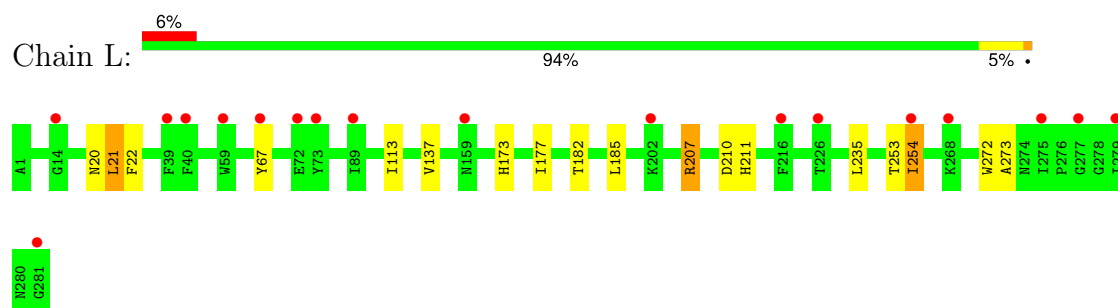
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	92	Total 92	O 92	0	0
16	M	119	Total 119	O 119	0	0
16	H	199	Total 199	O 199	0	0

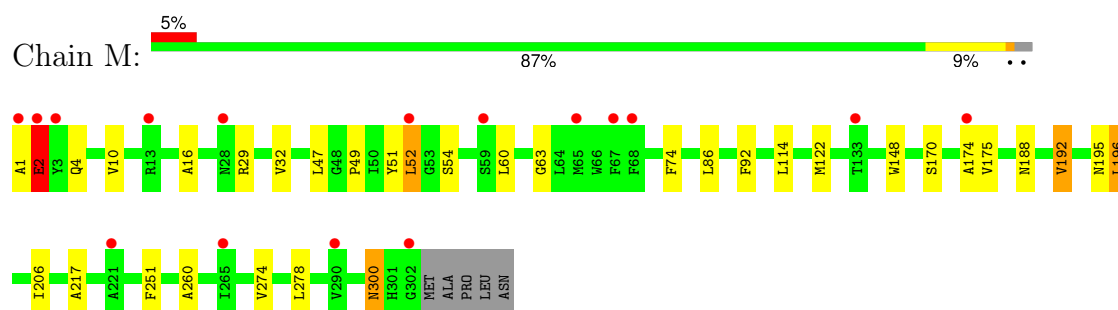
3 Residue-property plots [i](#)

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.

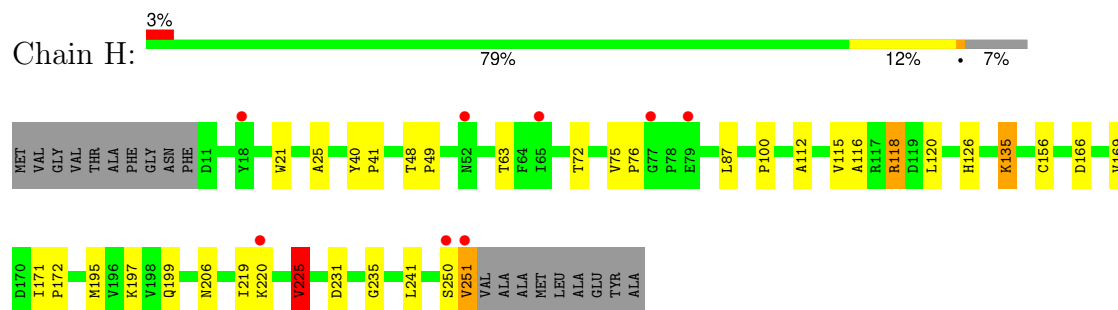
- Molecule 1: Reaction center protein L chain



- 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	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 46.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (46.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.197 0.177 , 0.200	Depositor DCC
R_{free} test set	3548 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 100.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: PO4, BPH, BCL, CL, FE, U10, LDA, K, PGT, PGK, GOL, CDL

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	1.08	1/2328 (0.0%)	0.96	0/3186
2	M	1.08	3/2592 (0.1%)	0.99	2/3536 (0.1%)
3	H	1.12	1/1953 (0.1%)	0.99	1/2652 (0.0%)
All	All	1.09	5/6873 (0.1%)	0.98	3/9374 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	126	HIS	C-O	-6.96	1.15	1.24
2	M	260	ALA	CA-CB	5.75	1.62	1.53
2	M	217	ALA	CA-C	5.72	1.60	1.52
2	M	192	VAL	CA-CB	5.58	1.62	1.54
1	L	137	VAL	CA-CB	5.12	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	225	VAL	CB-CA-C	-6.44	100.90	110.82
2	M	2	GLU	O-C-N	5.30	129.47	123.12
2	M	170	SER	N-CA-C	5.10	116.81	108.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	Peptide

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	2235	0	2196	11	0
2	M	2448	0	2367	28	0
3	H	1862	0	1883	26	0
4	L	132	0	148	5	0
4	M	132	0	148	21	0
5	L	65	0	75	2	0
5	M	65	0	76	4	0
6	L	48	0	63	4	0
6	M	48	0	63	1	0
7	H	6	0	8	0	0
7	L	18	0	24	5	0
8	M	1	0	0	0	0
9	M	1	0	0	0	0
10	H	5	0	0	0	0
10	M	15	0	0	1	0
11	M	81	0	106	3	0
12	M	53	0	74	10	0
13	H	48	0	93	14	0
13	M	48	0	93	5	0
14	H	1	0	0	0	0
15	H	102	0	156	16	0
16	H	199	0	0	2	0
16	L	92	0	0	2	0
16	M	119	0	0	1	0
All	All	7824	0	7573	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (114) 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)
4:M:311:BCL:H41	4:M:311:BCL:C9	1.91	0.99
4:M:311:BCL:H41	4:M:311:BCL:C7	1.92	0.98
4:M:311:BCL:C4	4:M:311:BCL:H92	1.98	0.94
4:M:311:BCL:H41	4:M:311:BCL:H92	1.48	0.92
7:L:709:GOL:H2	3:H:241:LEU:HD13	1.54	0.89
15:H:801[A]:PGT:C44	13:H:901:LDA:H121	2.05	0.86
15:H:801[A]:PGT:C43	13:H:901:LDA:H121	2.05	0.85
4:M:313:BCL:H201	12:M:802:PGK:H252	1.59	0.84
4:M:311:BCL:H41	4:M:311:BCL:H71	1.64	0.77
3:H:250:SER:O	3:H:251:VAL:HG23	1.85	0.76
4:M:311:BCL:HMB3	4:M:311:BCL:HBB2	1.66	0.75
6:L:502:U10:H153	12:M:802:PGK:H482	1.69	0.74
1:L:254:ILE:C	1:L:254:ILE:HD12	2.13	0.73
15:H:801[A]:PGT:H442	13:H:901:LDA:C12	2.20	0.71
4:M:311:BCL:H41	4:M:311:BCL:C8	2.20	0.71
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.73	0.69
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:H321	1.75	0.68
15:H:801[B]:PGT:H12	15:H:801[B]:PGT:C32	2.22	0.68
1:L:182:THR:OG1	4:M:311:BCL:H2	1.94	0.68
15:H:801[A]:PGT:H442	13:H:901:LDA:H121	1.72	0.68
6:L:502:U10:H153	12:M:802:PGK:C48	2.25	0.66
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.78	0.66
15:H:801[B]:PGT:C43	13:H:901:LDA:H121	2.24	0.66
15:H:801[B]:PGT:C44	13:H:901:LDA:H121	2.26	0.65
4:M:313:BCL:C20	12:M:802:PGK:H252	2.26	0.64
4:M:311:BCL:C9	4:M:311:BCL:C4	2.63	0.64
15:H:801[A]:PGT:H432	13:H:901:LDA:H121	1.81	0.62
2:M:122:MET:HE1	4:M:311:BCL:CBB	2.29	0.61
11:M:800:CDL:H231	13:H:904:LDA:HM12	1.82	0.60
2:M:174:ALA:HB1	13:M:920:LDA:H121	1.83	0.60
2:M:175:VAL:H	13:M:920:LDA:H123	1.66	0.60
4:M:311:BCL:H191	12:M:802:PGK:BR2	2.57	0.60
4:M:311:BCL:H92	4:M:311:BCL:H42	1.84	0.60
4:M:311:BCL:HMB3	4:M:311:BCL:CBB	2.32	0.59
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.68	0.57
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.40	0.57
4:M:311:BCL:C4	4:M:311:BCL:H71	2.33	0.57
3:H:21:TRP:CD1	15:H:801[B]:PGT:H5	2.41	0.56
11:M:800:CDL:C23	13:H:904:LDA:HM12	2.37	0.54
3:H:220[B]:LYS:NZ	16:H:1209:HOH:O	2.25	0.53
5:L:402:BPH:HMB3	5:L:402:BPH:HBB3	1.91	0.52
4:M:311:BCL:H8	12:M:802:PGK:H471	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:60[A]:LEU:HD23	5:M:401:BPH:H4C1	1.92	0.52
15:H:801[B]:PGT:H12	15:H:801[B]:PGT:H322	1.92	0.52
7:L:709:GOL:H2	3:H:241:LEU:CD1	2.35	0.51
3:H:220[B]:LYS:NZ	16:H:1100:HOH:O	2.41	0.51
2:M:278[B]:LEU:HD11	11:M:800:CDL:H811	1.91	0.51
3:H:197[A]:LYS:NZ	3:H:199:GLN:HE21	2.09	0.51
6:L:502:U10:C15	12:M:802:PGK:H482	2.41	0.50
15:H:801[B]:PGT:H431	13:H:901:LDA:H121	1.90	0.50
2:M:175:VAL:N	13:M:920:LDA:H123	2.26	0.50
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.93	0.50
2:M:51:TYR:O	2:M:52:LEU:HD23	2.11	0.50
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.93	0.50
4:M:311:BCL:CBB	4:M:311:BCL:CMB	2.90	0.50
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.47	0.50
2:M:188[B]:ASN:ND2	16:M:1077:HOH:O	2.43	0.48
4:L:314:BCL:CBB	4:L:314:BCL:HMB1	2.44	0.48
2:M:54:SER:OG	10:M:703:PO4:O2	2.32	0.47
2:M:175:VAL:H	13:M:920:LDA:C12	2.27	0.47
4:L:314:BCL:HMB1	4:L:314:BCL:HBB2	1.95	0.47
15:H:801[A]:PGT:H442	13:H:901:LDA:H123	1.96	0.47
6:L:502:U10:H4M3	6:L:502:U10:H3M2	1.96	0.47
5:L:402:BPH:HMB3	5:L:402:BPH:CBB	2.44	0.47
2:M:122:MET:HE1	4:M:311:BCL:HBB3	1.95	0.47
1:L:113:ILE:O	7:L:709:GOL:H11	2.15	0.47
2:M:29:ARG:O	12:M:802:PGK:H42	2.15	0.47
2:M:175:VAL:HB	13:M:920:LDA:H123	1.97	0.47
1:L:113:ILE:O	7:L:709:GOL:C1	2.63	0.46
4:L:312:BCL:OBB	4:L:312:BCL:HHC	2.15	0.46
3:H:63:THR:CG2	3:H:72:THR:HB	2.46	0.46
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.51	0.46
7:L:709:GOL:C2	3:H:241:LEU:HD13	2.36	0.46
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.46
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	1.99	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.81	0.45
5:M:401:BPH:HHD	5:M:401:BPH:CBC	2.47	0.45
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.52	0.44
3:H:135:LYS:HB3	3:H:135:LYS:HE3	1.57	0.44
15:H:801[A]:PGT:H362	15:H:801[A]:PGT:C32	2.46	0.44
2:M:63:GLY:HA3	5:M:401:BPH:H5C2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:LEU:HD22	12:M:802:PGK:BR2	2.73	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.43	0.43
15:H:801[B]:PGT:H322	15:H:801[B]:PGT:H351	1.58	0.43
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.91	0.43
3:H:40:TYR:HA	3:H:41:PRO:C	2.42	0.43
1:L:67:TYR:HB3	16:L:1167:HOH:O	2.19	0.42
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
4:M:313:BCL:H201	12:M:802:PGK:C25	2.40	0.42
3:H:135:LYS:HB3	3:H:166:ASP:OD2	2.20	0.42
3:H:48:THR:HB	3:H:49:PRO:HD2	2.02	0.42
3:H:25:ALA:HB2	13:H:903:LDA:H52	2.01	0.42
2:M:2:GLU:H	2:M:2:GLU:HG3	1.53	0.42
2:M:2:GLU:O	2:M:4:GLN:NE2	2.52	0.42
15:H:801[A]:PGT:C44	13:H:901:LDA:C12	2.81	0.42
2:M:32:VAL:HG12	2:M:49:PRO:HD3	2.02	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
13:H:901:LDA:HM11	13:H:901:LDA:H22	1.80	0.42
3:H:195:MET:HE1	3:H:241:LEU:HD11	2.02	0.41
6:M:501:U10:H28	6:M:501:U10:H322	1.80	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
1:L:20:ASN:ND2	16:L:1300:HOH:O	2.52	0.41
4:L:312:BCL:CGA	4:L:314:BCL:HBC1	2.51	0.41
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.35	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.01	0.41
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD12	2.02	0.41
1:L:272:TRP:O	1:L:273:ALA:C	2.63	0.40
4:L:314:BCL:HMD2	2:M:206:ILE:HD13	2.03	0.40
5:M:401:BPH:HHH	5:M:401:BPH:HBC3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	36	55
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

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	221/220 (100%)	215 (97%)	6 (3%)	39	67
2	M	246/240 (102%)	236 (96%)	10 (4%)	27	53
3	H	204/208 (98%)	198 (97%)	6 (3%)	37	65
All	All	671/668 (100%)	649 (97%)	22 (3%)	35	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	254	ILE
2	M	2	GLU
2	M	10	VAL
2	M	52	LEU
2	M	86	LEU
2	M	114	LEU
2	M	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	196	LEU
2	M	274	VAL
2	M	300[A]	ASN
2	M	300[B]	ASN
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	135	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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	183	ASN
2	M	28	ASN
3	H	44	ASN
3	H	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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
15	PGT	H	801[B]	-	50,50,50	0.84	1 (2%)	53,56,56	1.11	5 (9%)
7	GOL	H	706	-	5,5,5	0.28	0	5,5,5	0.92	0
6	U10	L	502	-	48,48,63	1.12	4 (8%)	60,61,79	1.63	10 (16%)
4	BCL	M	311	2	69,74,74	1.10	4 (5%)	79,115,115	1.79	20 (25%)
13	LDA	H	901	-	13,15,15	2.18	2 (15%)	14,17,17	0.85	0
10	PO4	M	705	-	4,4,4	0.89	0	6,6,6	0.82	0
7	GOL	L	707	-	5,5,5	0.39	0	5,5,5	0.52	0
13	LDA	M	907	-	13,15,15	2.10	2 (15%)	14,17,17	0.61	0
7	GOL	L	708	-	5,5,5	0.50	0	5,5,5	0.59	0
12	PGK	M	802	-	52,52,52	0.90	3 (5%)	55,60,60	1.49	5 (9%)
4	BCL	L	312	1	69,74,74	1.27	4 (5%)	79,115,115	1.39	15 (18%)
4	BCL	M	313	2	69,74,74	1.21	5 (7%)	79,115,115	1.61	20 (25%)
7	GOL	L	709	-	5,5,5	0.68	0	5,5,5	0.68	0
6	U10	M	501	-	48,48,63	1.17	2 (4%)	60,61,79	1.43	8 (13%)
13	LDA	H	903	-	13,15,15	2.12	2 (15%)	14,17,17	0.53	0
15	PGT	H	801[A]	-	50,50,50	0.72	0	53,56,56	0.98	3 (5%)
5	BPH	L	402	-	59,70,70	1.40	8 (13%)	59,101,101	1.68	13 (22%)
13	LDA	H	904	-	13,15,15	2.25	2 (15%)	14,17,17	0.52	0
13	LDA	M	920	-	13,15,15	2.12	2 (15%)	14,17,17	0.81	0
10	PO4	M	703	-	4,4,4	0.95	0	6,6,6	1.48	2 (33%)
5	BPH	M	401	-	59,70,70	1.52	6 (10%)	59,101,101	2.04	13 (22%)
13	LDA	M	902	-	13,15,15	2.04	2 (15%)	14,17,17	0.54	0
10	PO4	M	702	-	4,4,4	0.66	0	6,6,6	0.69	0
11	CDL	M	800	-	80,80,99	1.26	5 (6%)	86,92,111	1.46	13 (15%)
10	PO4	H	704	-	4,4,4	0.95	0	6,6,6	0.71	0
4	BCL	L	314	1	69,74,74	1.17	4 (5%)	79,115,115	1.56	16 (20%)

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
15	PGT	H	801[B]	-	-	23/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	H	706	-	-	1/4/4/4	-
6	U10	L	502	-	-	9/45/69/87	0/1/1/1
4	BCL	M	311	2	-	9/41/137/137	-
13	LDA	H	901	-	-	4/13/13/13	-
7	GOL	L	707	-	-	4/4/4/4	-
13	LDA	M	907	-	-	7/13/13/13	-
7	GOL	L	708	-	-	4/4/4/4	-
12	PGK	M	802	-	-	24/60/60/60	-
4	BCL	L	312	1	-	1/41/137/137	-
4	BCL	M	313	2	-	2/41/137/137	-
7	GOL	L	709	-	-	2/4/4/4	-
6	U10	M	501	-	-	6/45/69/87	0/1/1/1
13	LDA	H	903	-	-	5/13/13/13	-
15	PGT	H	801[A]	-	-	30/55/55/55	-
5	BPH	L	402	-	-	4/37/105/105	0/5/6/6
13	LDA	H	904	-	-	7/13/13/13	-
13	LDA	M	920	-	-	7/13/13/13	-
5	BPH	M	401	-	-	7/37/105/105	0/5/6/6
13	LDA	M	902	-	-	1/13/13/13	-
11	CDL	M	800	-	-	37/91/91/110	-
4	BCL	L	314	1	-	3/41/137/137	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BPH	C1B-C2B	6.72	1.46	1.39
13	M	907	LDA	O1-N1	-6.64	1.25	1.42
13	H	904	LDA	O1-N1	-6.58	1.26	1.42
13	M	902	LDA	O1-N1	-6.28	1.26	1.42
13	H	903	LDA	O1-N1	-6.22	1.26	1.42
13	M	920	LDA	O1-N1	-6.05	1.27	1.42
13	H	901	LDA	O1-N1	-5.82	1.27	1.42
4	M	313	BCL	MG-NA	5.74	2.19	2.06
5	L	402	BPH	C1B-C2B	5.62	1.45	1.39
4	L	312	BCL	MG-NA	5.47	2.19	2.06
11	M	800	CDL	OA8-CA7	5.43	1.49	1.33
13	H	901	LDA	C1-N1	-5.23	1.46	1.51
4	M	311	BCL	MG-NA	4.98	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	312	BCL	MG-NB	4.79	2.15	2.05
11	M	800	CDL	OB6-CB5	4.62	1.47	1.34
5	M	401	BPH	C1D-C2D	4.59	1.44	1.39
13	H	904	LDA	C1-N1	-4.58	1.46	1.51
13	M	920	LDA	C1-N1	-4.49	1.46	1.51
4	L	314	BCL	MG-NA	4.45	2.16	2.06
11	M	800	CDL	OA6-CA5	4.36	1.46	1.34
11	M	800	CDL	OB8-CB7	4.34	1.46	1.33
13	H	903	LDA	C1-N1	-4.34	1.47	1.51
6	M	501	U10	O3-C3	4.31	1.47	1.36
6	L	502	U10	O3-C3	4.25	1.47	1.36
5	L	402	BPH	C1D-C2D	3.94	1.43	1.39
5	M	401	BPH	C3A-C2A	-3.87	1.51	1.54
13	M	902	LDA	C1-N1	-3.67	1.47	1.51
12	M	802	PGK	P-O1P	3.45	1.62	1.50
13	M	907	LDA	C1-N1	-3.22	1.48	1.51
6	M	501	U10	O4-C4	3.14	1.44	1.36
4	M	311	BCL	MG-NB	3.13	2.12	2.05
5	L	402	BPH	C3B-C4B	3.12	1.46	1.41
4	L	312	BCL	C4-C3	3.03	1.58	1.50
6	L	502	U10	C13-C14	2.94	1.39	1.33
4	L	314	BCL	MG-NB	2.81	2.11	2.05
4	L	314	BCL	MG-NC	-2.78	1.99	2.06
5	M	401	BPH	C3B-C4B	2.76	1.45	1.41
4	M	311	BCL	C3B-C4B	2.75	1.46	1.41
15	H	801[B]	PGT	C1-C2	2.73	1.59	1.50
5	L	402	BPH	C2C-C3C	2.67	1.57	1.54
6	L	502	U10	O4-C4	2.65	1.43	1.36
4	L	312	BCL	C3B-C4B	2.62	1.46	1.41
4	M	313	BCL	C3B-C4B	2.59	1.46	1.41
4	M	311	BCL	MG-NC	2.47	2.12	2.06
12	M	802	PGK	O2-C2	-2.29	1.41	1.46
6	L	502	U10	C33-C34	2.27	1.38	1.33
5	M	401	BPH	C3D-CAD	-2.25	1.43	1.47
5	M	401	BPH	C2C-C3C	2.22	1.56	1.54
4	M	313	BCL	C1B-NB	-2.20	1.35	1.37
4	M	313	BCL	MG-ND	2.19	2.10	2.05
4	M	313	BCL	C5-C3	2.14	1.55	1.51
5	L	402	BPH	C4D-ND	-2.14	1.35	1.38
5	L	402	BPH	C3A-C2A	-2.12	1.52	1.54
5	L	402	BPH	C3B-C2B	-2.10	1.36	1.39
4	L	314	BCL	C3B-C4B	2.08	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	802	PGK	BR1-C39	-2.03	1.92	1.97
5	L	402	BPH	C3D-CAD	-2.02	1.43	1.47
11	M	800	CDL	PA1-OA3	-2.02	1.43	1.50

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	O2D-CGD-CBD	7.87	119.59	110.95
5	L	402	BPH	C4D-CHA-CBD	-6.56	105.31	108.45
5	M	401	BPH	C4D-CHA-CBD	-5.42	105.85	108.45
11	M	800	CDL	OB6-CB5-C51	5.37	123.09	111.48
12	M	802	PGK	BR1-C39-C40	-5.10	100.39	110.27
5	L	402	BPH	O2D-CGD-CBD	5.04	116.48	110.95
5	M	401	BPH	C1-C2-C3	-4.73	118.45	126.20
12	M	802	PGK	C3-C2-C1	-4.67	100.90	111.78
6	L	502	U10	C25-C24-C26	4.52	123.07	115.23
4	M	311	BCL	C2B-C1B-NB	-4.43	105.73	110.33
11	M	800	CDL	CA4-OA6-CA5	-4.28	107.55	117.80
4	M	311	BCL	C1-O2A-CGA	4.26	126.97	116.65
4	M	313	BCL	C1C-NC-C4C	4.24	108.61	106.68
6	L	502	U10	O2-C2-C3	-4.23	112.07	121.03
4	M	311	BCL	O2D-CGD-CBD	4.19	118.56	111.23
15	H	801[A]	PGT	O2-C31-C32	4.16	120.47	111.48
12	M	802	PGK	O2-C31-C32	4.15	120.45	111.48
4	M	311	BCL	OB6-CAB-C3B	4.13	127.73	120.43
5	M	401	BPH	C2B-C1B-NB	-4.06	106.49	109.43
4	M	311	BCL	C4-C3-C2	-4.01	113.32	123.63
11	M	800	CDL	OB8-CB6-CB4	3.99	119.91	108.40
4	L	314	BCL	CAA-C2A-C3A	-3.99	102.21	113.00
15	H	801[B]	PGT	O2-C31-C32	3.98	120.08	111.48
4	M	313	BCL	CMB-C2B-C1B	-3.97	119.38	125.42
4	M	313	BCL	C3B-C4B-NB	-3.96	104.53	109.76
11	M	800	CDL	OA6-CA5-C11	3.93	119.98	111.48
6	M	501	U10	C17-C18-C19	-3.87	118.77	127.62
4	M	311	BCL	C4D-CHA-C1A	3.71	125.66	121.24
4	M	311	BCL	CED-O2D-CGD	-3.61	107.73	115.92
4	L	314	BCL	O2D-CGD-CBD	3.60	117.53	111.23
6	M	501	U10	C22-C23-C24	-3.59	119.41	127.62
6	L	502	U10	C12-C13-C14	-3.57	119.44	127.62
15	H	801[B]	PGT	C2-O2-C31	-3.55	109.30	117.80
4	L	314	BCL	CHD-C1D-ND	-3.54	119.82	124.80
4	L	314	BCL	C2B-C1B-NB	-3.41	106.79	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	CAA-C2A-C3A	-3.40	103.80	113.00
4	L	314	BCL	C4D-CHA-C1A	3.33	125.22	121.24
5	M	401	BPH	OBD-CAD-CBD	-3.28	121.02	125.82
5	L	402	BPH	C1-C2-C3	-3.27	120.84	126.20
6	L	502	U10	C3M-O3-C3	3.26	127.91	116.47
11	M	800	CDL	OA8-CA7-C31	3.24	121.72	111.83
4	L	312	BCL	CAA-C2A-C3A	-3.23	104.27	113.00
4	L	314	BCL	CAA-CBA-CGA	3.14	122.13	113.21
6	L	502	U10	C30-C29-C31	3.14	120.68	115.23
4	M	313	BCL	C1D-ND-C4D	3.13	108.51	106.31
6	M	501	U10	C32-C33-C34	-3.11	120.50	127.62
6	M	501	U10	C7-C6-C5	-3.11	114.90	118.52
6	M	501	U10	C15-C14-C16	3.10	120.61	115.23
11	M	800	CDL	OB8-CB7-C71	3.04	121.12	111.83
6	M	501	U10	C30-C29-C31	3.04	120.50	115.23
6	L	502	U10	C22-C23-C24	-3.00	120.75	127.62
4	L	312	BCL	C1D-ND-C4D	3.00	108.42	106.31
4	L	312	BCL	CHA-C1A-NA	-2.92	119.78	126.39
4	M	311	BCL	C5-C3-C2	2.91	127.70	121.17
6	L	502	U10	C25-C24-C23	-2.91	116.15	123.63
5	L	402	BPH	C2B-C1B-NB	-2.91	107.33	109.43
12	M	802	PGK	C2-O2-C31	-2.90	110.85	117.80
6	L	502	U10	C7-C6-C5	-2.90	115.15	118.52
4	M	313	BCL	C4D-CHA-C1A	2.89	124.69	121.24
6	M	501	U10	C41-C39-C40	2.87	121.20	114.59
5	M	401	BPH	C2D-C1D-ND	-2.86	107.36	109.43
4	M	311	BCL	C3B-C4B-NB	-2.84	106.02	109.76
4	M	313	BCL	O2D-CGD-O1D	-2.83	118.34	123.85
4	M	313	BCL	C4-C3-C5	2.79	120.06	115.23
4	L	314	BCL	C5-C3-C2	-2.79	114.92	121.17
5	M	401	BPH	O2D-CGD-O1D	-2.78	118.44	123.85
6	L	502	U10	C1M-C1-C6	-2.78	119.88	124.45
4	L	314	BCL	C1C-NC-C4C	2.77	107.94	106.68
4	L	312	BCL	C3B-C4B-NB	-2.75	106.12	109.76
15	H	801[B]	PGT	O3-C11-C12	2.71	120.11	111.83
4	M	311	BCL	CAA-CBA-CGA	2.68	120.82	113.21
4	M	311	BCL	CHA-C1A-NA	-2.67	120.33	126.39
4	M	313	BCL	C2B-C1B-NB	-2.67	107.56	110.33
4	L	312	BCL	C2C-C3C-C4C	2.65	105.31	101.34
4	M	313	BCL	CHB-C1B-NB	2.64	128.01	124.05
4	L	312	BCL	CMB-C2B-C1B	-2.63	121.41	125.42
5	L	402	BPH	CMA-C3A-C2A	-2.62	104.01	114.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	314	BCL	O1D-CGD-CBD	-2.61	119.38	124.52
4	L	314	BCL	CHD-C1D-C2D	2.58	130.86	125.49
11	M	800	CDL	OB8-CB7-OB9	-2.56	117.23	123.63
4	M	313	BCL	CHA-C1A-NA	-2.55	120.61	126.39
4	M	313	BCL	C1-C2-C3	-2.54	122.04	126.20
4	L	314	BCL	CMC-C2C-C3C	-2.50	104.31	113.98
11	M	800	CDL	C72-C71-CB7	-2.50	104.53	113.69
4	M	311	BCL	CHD-C1D-ND	-2.50	121.29	124.80
4	L	314	BCL	C2C-C3C-C4C	2.49	105.08	101.34
4	L	314	BCL	C4-C3-C5	2.47	119.52	115.23
4	M	313	BCL	CMA-C3A-C4A	2.47	118.41	111.77
15	H	801[B]	PGT	O2-C31-O31	-2.47	117.94	123.70
5	L	402	BPH	CMA-C3A-C4A	-2.47	109.30	114.61
15	H	801[A]	PGT	O3-C3-C2	2.46	115.50	108.40
4	M	311	BCL	CAA-C2A-C3A	-2.45	106.38	113.00
4	L	312	BCL	CHD-C1D-ND	-2.44	121.37	124.80
12	M	802	PGK	BR2-C40-C39	-2.44	105.55	110.27
11	M	800	CDL	OA6-CA5-OA7	-2.44	118.01	123.70
5	M	401	BPH	CMA-C3A-C4A	-2.43	109.37	114.61
11	M	800	CDL	C74-C73-C72	-2.43	102.08	114.37
5	M	401	BPH	C4-C3-C2	-2.41	117.43	123.63
5	L	402	BPH	O2D-CGD-O1D	-2.41	119.17	123.85
4	L	312	BCL	C1-O2A-CGA	2.40	122.46	116.65
10	M	703	PO4	O4-P-O3	2.40	115.36	107.91
5	M	401	BPH	CMA-C3A-C2A	-2.39	104.88	114.13
4	M	311	BCL	C6-C5-C3	-2.39	107.65	113.47
5	M	401	BPH	C1-O2A-CGA	2.38	122.41	116.65
15	H	801[A]	PGT	O3-C11-C12	2.36	119.05	111.83
5	L	402	BPH	CMB-C2B-C3B	2.36	129.41	124.68
5	L	402	BPH	C2D-C1D-ND	-2.36	107.72	109.43
4	L	312	BCL	C4-C3-C5	2.35	119.30	115.23
4	L	314	BCL	CAC-C3C-C4C	-2.32	107.43	112.58
4	L	312	BCL	CMA-C3A-C2A	-2.30	105.08	113.98
4	L	312	BCL	C2B-C1B-NB	-2.27	107.97	110.33
5	M	401	BPH	CMB-C2B-C3B	2.25	129.18	124.68
4	M	313	BCL	C2C-C3C-C4C	2.25	104.70	101.34
4	L	314	BCL	CMA-C3A-C2A	-2.24	105.33	113.98
5	L	402	BPH	CAA-C2A-C3A	-2.21	107.02	113.00
4	M	311	BCL	CBB-CAB-C3B	-2.20	115.75	120.40
4	M	311	BCL	C4A-NA-C1A	2.20	107.68	106.68
4	M	313	BCL	C16-C15-C13	-2.19	108.70	115.97
6	L	502	U10	O2-C2-C1	2.18	126.82	120.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	313	BCL	CMB-C2B-C3B	2.16	132.48	125.67
4	M	311	BCL	C4-C3-C5	2.16	118.97	115.23
4	L	312	BCL	C4A-NA-C1A	-2.15	105.70	106.68
4	M	313	BCL	O2A-C1-C2	2.15	116.36	108.11
4	L	314	BCL	C4A-NA-C1A	2.14	107.66	106.68
15	H	801[B]	PGT	O3-C3-C2	2.14	114.58	108.40
4	M	311	BCL	CMA-C3A-C4A	-2.13	106.04	111.77
5	L	402	BPH	C3B-C4B-NB	-2.13	104.95	108.05
5	L	402	BPH	CBC-CAC-C3C	2.11	117.93	113.78
4	M	313	BCL	O2D-CGD-CBD	2.10	114.89	111.23
11	M	800	CDL	OB6-CB5-OB7	-2.09	118.82	123.70
6	M	501	U10	C26-C27-C28	-2.08	101.73	112.02
5	L	402	BPH	C7-C6-C5	-2.08	107.72	113.26
4	L	312	BCL	CMB-C2B-C3B	2.06	132.16	125.67
4	L	312	BCL	CMA-C3A-C4A	-2.05	106.25	111.77
4	L	312	BCL	C1C-NC-C4C	2.05	107.61	106.68
4	M	311	BCL	C2A-C1A-CHA	2.05	127.43	123.87
11	M	800	CDL	CA6-OA8-CA7	2.04	124.57	117.12
4	M	313	BCL	C1-O2A-CGA	2.03	121.56	116.65
4	M	313	BCL	CHC-C1C-NC	2.02	127.32	124.40
4	M	313	BCL	CAA-CBA-CGA	2.01	118.92	113.21
4	M	311	BCL	C1D-ND-C4D	2.01	107.72	106.31
11	M	800	CDL	CB6-CB4-CB3	-2.01	107.10	111.78
10	M	703	PO4	O4-P-O1	-2.01	103.86	110.95

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	707	GOL	O1-C1-C2-C3
7	L	708	GOL	O1-C1-C2-C3
7	L	708	GOL	C1-C2-C3-O3
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	CA3-OA5-PA1-OA4
11	M	800	CDL	CB2-OB2-PB2-OB4
11	M	800	CDL	CB3-OB5-PB2-OB3
11	M	800	CDL	CB3-OB5-PB2-OB4
12	M	802	PGK	C1-O3P-P-O1P
12	M	802	PGK	C1-O3P-P-O2P
12	M	802	PGK	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	M	802	PGK	C4-O4P-P-O3P
12	M	802	PGK	C4-O4P-P-O1P
12	M	802	PGK	C4-O4P-P-O2P
12	M	802	PGK	C5-C4-O4P-P
13	M	902	LDA	C2-C1-N1-CM1
13	M	907	LDA	C2-C1-N1-CM2
13	M	920	LDA	N1-C1-C2-C3
13	H	904	LDA	N1-C1-C2-C3
15	H	801[A]	PGT	C32-C31-O2-C2
15	H	801[A]	PGT	C4-O4P-P-O3P
15	H	801[A]	PGT	C4-O4P-P-O1P
15	H	801[A]	PGT	C4-O4P-P-O2P
15	H	801[A]	PGT	C4-C5-C6-O6
15	H	801[B]	PGT	C32-C31-O2-C2
15	H	801[B]	PGT	C1-O3P-P-O1P
12	M	802	PGK	O11-C11-O3-C3
12	M	802	PGK	C12-C11-O3-C3
15	H	801[A]	PGT	O31-C31-O2-C2
15	H	801[B]	PGT	O31-C31-O2-C2
4	M	311	BCL	C4-C3-C5-C6
4	M	311	BCL	C2-C3-C5-C6
15	H	801[B]	PGT	C12-C11-O3-C3
6	L	502	U10	C23-C24-C26-C27
15	H	801[B]	PGT	O11-C11-O3-C3
6	M	501	U10	C29-C31-C32-C33
6	L	502	U10	C25-C24-C26-C27
7	L	708	GOL	O2-C2-C3-O3
15	H	801[B]	PGT	C32-C33-C34-C35
6	L	502	U10	C34-C36-C37-C38
4	M	311	BCL	C10-C11-C12-C13
15	H	801[A]	PGT	C11-C12-C13-C14
15	H	801[A]	PGT	O4P-C4-C5-O5
15	H	801[A]	PGT	C12-C11-O3-C3
15	H	801[A]	PGT	C31-C32-C33-C34
15	H	801[A]	PGT	O4P-C4-C5-C6
6	L	502	U10	C19-C21-C22-C23
15	H	801[A]	PGT	O11-C11-O3-C3
7	L	707	GOL	C1-C2-C3-O3
12	M	802	PGK	C4-C5-C6-O6
11	M	800	CDL	C11-CA5-OA6-CA4
13	H	903	LDA	C2-C3-C4-C5
13	H	904	LDA	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	H	801[B]	PGT	C14-C15-C16-C17
7	L	707	GOL	O2-C2-C3-O3
12	M	802	PGK	O5-C5-C6-O6
15	H	801[A]	PGT	O5-C5-C6-O6
11	M	800	CDL	C38-C39-C40-C41
11	M	800	CDL	CB7-C71-C72-C73
13	M	920	LDA	C3-C4-C5-C6
5	M	401	BPH	C13-C15-C16-C17
11	M	800	CDL	OA7-CA5-OA6-CA4
13	H	904	LDA	C2-C3-C4-C5
11	M	800	CDL	CA3-CA4-CA6-OA8
12	M	802	PGK	C32-C33-C34-C35
15	H	801[B]	PGT	C11-C12-C13-C14
12	M	802	PGK	C21-C22-C23-C24
11	M	800	CDL	C51-CB5-OB6-CB4
15	H	801[A]	PGT	C20-C21-C22-C23
15	H	801[B]	PGT	C42-C43-C44-C45
15	H	801[B]	PGT	C33-C34-C35-C36
15	H	801[B]	PGT	C17-C18-C19-C20
11	M	800	CDL	C11-C12-C13-C14
13	M	920	LDA	C11-C10-C9-C8
12	M	802	PGK	C16-C17-C18-C19
13	H	901	LDA	C5-C6-C7-C8
13	M	907	LDA	C4-C5-C6-C7
15	H	801[B]	PGT	C37-C38-C39-C40
13	H	901	LDA	C11-C10-C9-C8
15	H	801[A]	PGT	C14-C15-C16-C17
5	M	401	BPH	C16-C17-C18-C19
15	H	801[A]	PGT	C17-C18-C19-C20
12	M	802	PGK	C32-C31-O2-C2
4	M	311	BCL	C5-C6-C7-C8
12	M	802	PGK	C23-C24-C25-C26
13	H	904	LDA	C1-C2-C3-C4
15	H	801[B]	PGT	C20-C21-C22-C23
6	M	501	U10	C30-C29-C31-C32
12	M	802	PGK	C34-C35-C36-C37
11	M	800	CDL	CA5-C11-C12-C13
15	H	801[B]	PGT	C39-C40-C41-C42
6	M	501	U10	C28-C29-C31-C32
7	L	709	GOL	O2-C2-C3-O3
11	M	800	CDL	OA5-CA3-CA4-CA6
11	M	800	CDL	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	502	U10	C15-C14-C16-C17
11	M	800	CDL	OB7-CB5-OB6-CB4
15	H	801[A]	PGT	C34-C35-C36-C37
6	L	502	U10	C13-C14-C16-C17
15	H	801[B]	PGT	C1-C2-O2-C31
13	M	907	LDA	C11-C10-C9-C8
11	M	800	CDL	C17-C18-C19-C20
15	H	801[A]	PGT	C2-C3-O3-C11
11	M	800	CDL	C19-C20-C21-C22
13	M	907	LDA	C9-C10-C11-C12
13	M	920	LDA	C9-C10-C11-C12
4	M	311	BCL	C15-C16-C17-C18
13	H	903	LDA	C6-C7-C8-C9
7	H	706	GOL	O2-C2-C3-O3
13	H	904	LDA	C9-C10-C11-C12
5	M	401	BPH	C16-C17-C18-C20
13	M	920	LDA	C5-C6-C7-C8
12	M	802	PGK	O31-C31-O2-C2
15	H	801[A]	PGT	C1-C2-C3-O3
11	M	800	CDL	C20-C21-C22-C23
11	M	800	CDL	C75-C76-C77-C78
12	M	802	PGK	C44-C45-C46-C47
13	H	904	LDA	C6-C7-C8-C9
11	M	800	CDL	OA5-CA3-CA4-OA6
12	M	802	PGK	C18-C19-C20-C21
5	L	402	BPH	C8-C10-C11-C12
5	L	402	BPH	C4-C3-C5-C6
5	L	402	BPH	C2-C3-C5-C6
13	H	901	LDA	C3-C4-C5-C6
15	H	801[B]	PGT	O5-C5-C6-O6
11	M	800	CDL	C18-C19-C20-C21
13	H	903	LDA	C11-C10-C9-C8
11	M	800	CDL	OA6-CA4-CA6-OA8
15	H	801[B]	PGT	C44-C45-C46-C47
13	M	920	LDA	C4-C5-C6-C7
15	H	801[A]	PGT	C42-C43-C44-C45
13	H	901	LDA	C4-C5-C6-C7
4	M	311	BCL	C2-C1-O2A-CGA
7	L	707	GOL	O1-C1-C2-O2
7	L	708	GOL	O1-C1-C2-O2
13	M	907	LDA	C7-C8-C9-C10
4	L	314	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	311	BCL	C6-C7-C8-C10
15	H	801[A]	PGT	C2-C1-O3P-P
11	M	800	CDL	C39-C40-C41-C42
15	H	801[B]	PGT	O3P-C1-C2-O2
15	H	801[A]	PGT	O2-C2-C3-O3
5	M	401	BPH	C10-C11-C12-C13
11	M	800	CDL	CA3-OA5-PA1-OA3
11	M	800	CDL	CB2-OB2-PB2-OB5
11	M	800	CDL	CB3-OB5-PB2-OB2
15	H	801[A]	PGT	C1-O3P-P-O1P
11	M	800	CDL	C1-CB2-OB2-PB2
15	H	801[A]	PGT	C37-C38-C39-C40
11	M	800	CDL	CB3-CB4-OB6-CB5
15	H	801[A]	PGT	C1-C2-O2-C31
13	H	903	LDA	N1-C1-C2-C3
15	H	801[B]	PGT	C5-C4-O4P-P
11	M	800	CDL	OB6-CB4-CB6-OB8
11	M	800	CDL	O1-C1-CA2-OA2
15	H	801[B]	PGT	C12-C13-C14-C15
4	L	314	BCL	C14-C13-C15-C16
5	M	401	BPH	C15-C16-C17-C18
15	H	801[B]	PGT	C4-C5-C6-O6
11	M	800	CDL	CB6-CB4-OB6-CB5
12	M	802	PGK	C1-C2-O2-C31
4	M	313	BCL	C16-C17-C18-C19
15	H	801[A]	PGT	C12-C13-C14-C15
6	M	501	U10	C5-C4-O4-C4M
15	H	801[A]	PGT	C22-C23-C24-C25
15	H	801[B]	PGT	C22-C23-C24-C25
13	M	907	LDA	C2-C3-C4-C5
15	H	801[A]	PGT	O2-C31-C32-C33
12	M	802	PGK	C1-C2-C3-O3
15	H	801[A]	PGT	C33-C34-C35-C36
4	M	313	BCL	CAA-CBA-CGA-O2A
12	M	802	PGK	O4P-C4-C5-C6
4	M	311	BCL	C11-C10-C8-C9
7	L	709	GOL	C1-C2-C3-O3
12	M	802	PGK	C41-C42-C43-C44
4	L	312	BCL	C16-C17-C18-C19
13	H	903	LDA	C5-C6-C7-C8
15	H	801[A]	PGT	C35-C36-C37-C38
13	M	907	LDA	C2-C1-N1-CM1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	M	920	LDA	C7-C8-C9-C10
6	L	502	U10	C30-C29-C31-C32
11	M	800	CDL	C72-C71-CB7-OB8
11	M	800	CDL	C36-C37-C38-C39
5	M	401	BPH	C6-C7-C8-C10
6	L	502	U10	C3-C4-O4-C4M
15	H	801[B]	PGT	C2-C1-O3P-P
6	L	502	U10	C5-C4-O4-C4M
4	M	311	BCL	C6-C7-C8-C9
6	M	501	U10	C25-C24-C26-C27
13	H	904	LDA	C2-C1-N1-O1
11	M	800	CDL	C72-C71-CB7-OB9
6	M	501	U10	C24-C26-C27-C28
4	L	314	BCL	C15-C16-C17-C18
5	L	402	BPH	CAD-CBD-CGD-O2D
5	M	401	BPH	C4C-C3C-CAC-CBC

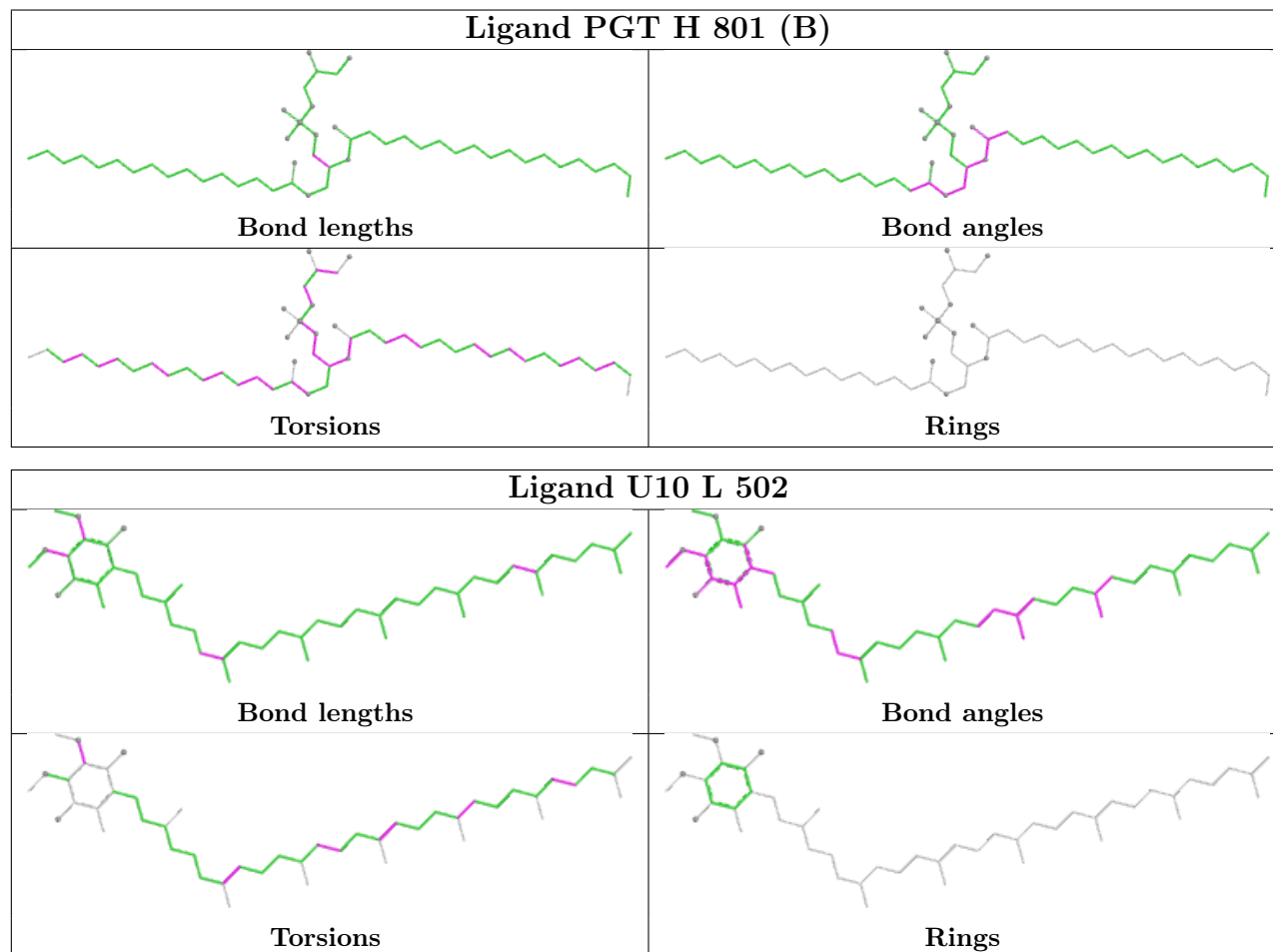
There are no ring outliers.

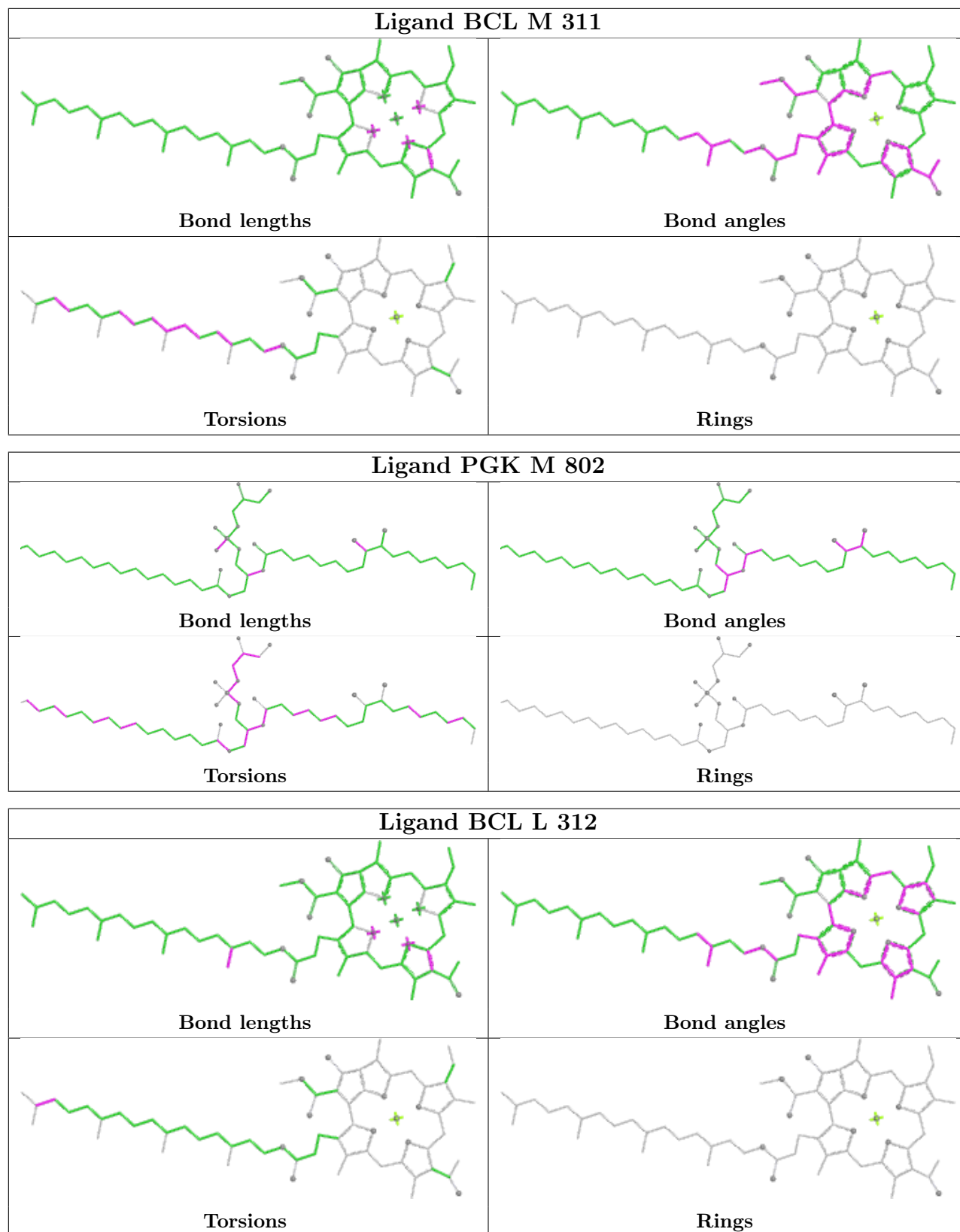
18 monomers are involved in 71 short contacts:

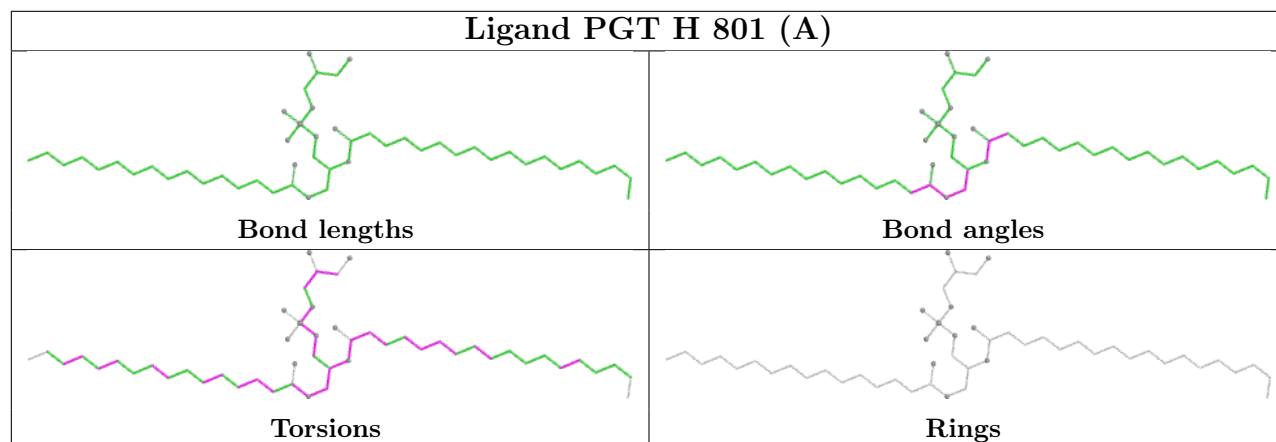
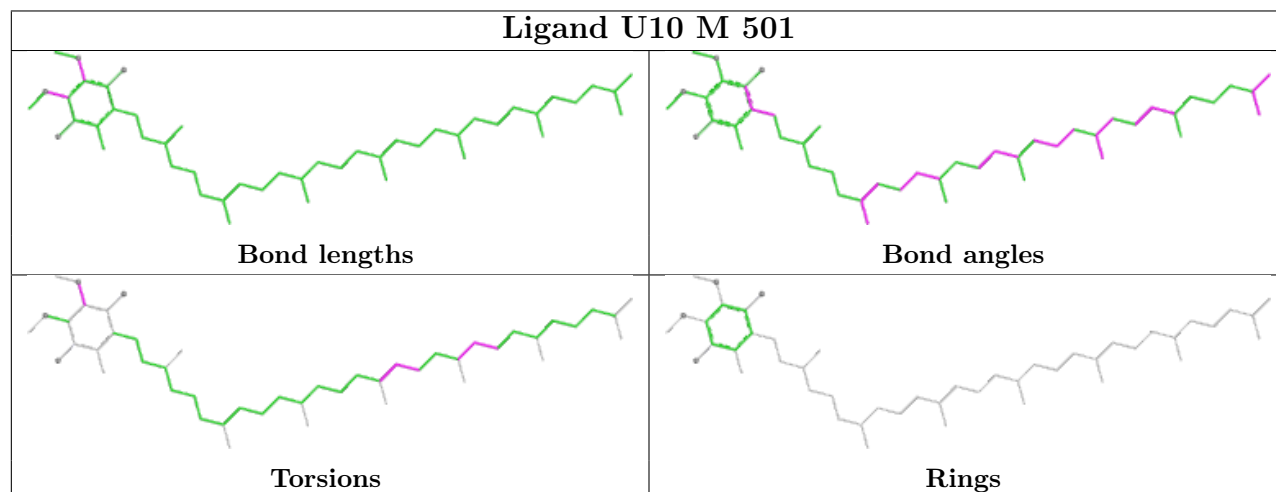
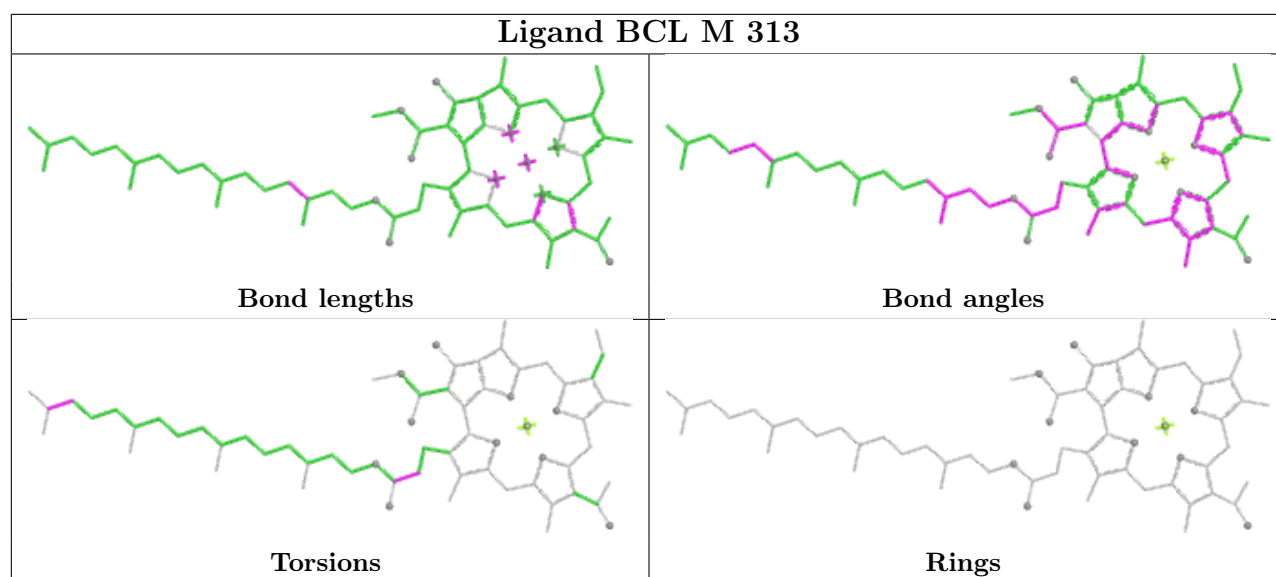
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	801[B]	PGT	7	0
6	L	502	U10	4	0
4	M	311	BCL	17	0
13	H	901	LDA	11	0
12	M	802	PGK	10	0
4	L	312	BCL	2	0
4	M	313	BCL	4	0
7	L	709	GOL	5	0
6	M	501	U10	1	0
13	H	903	LDA	1	0
15	H	801[A]	PGT	9	0
5	L	402	BPH	2	0
13	H	904	LDA	2	0
13	M	920	LDA	5	0
10	M	703	PO4	1	0
5	M	401	BPH	4	0
11	M	800	CDL	3	0
4	L	314	BCL	4	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

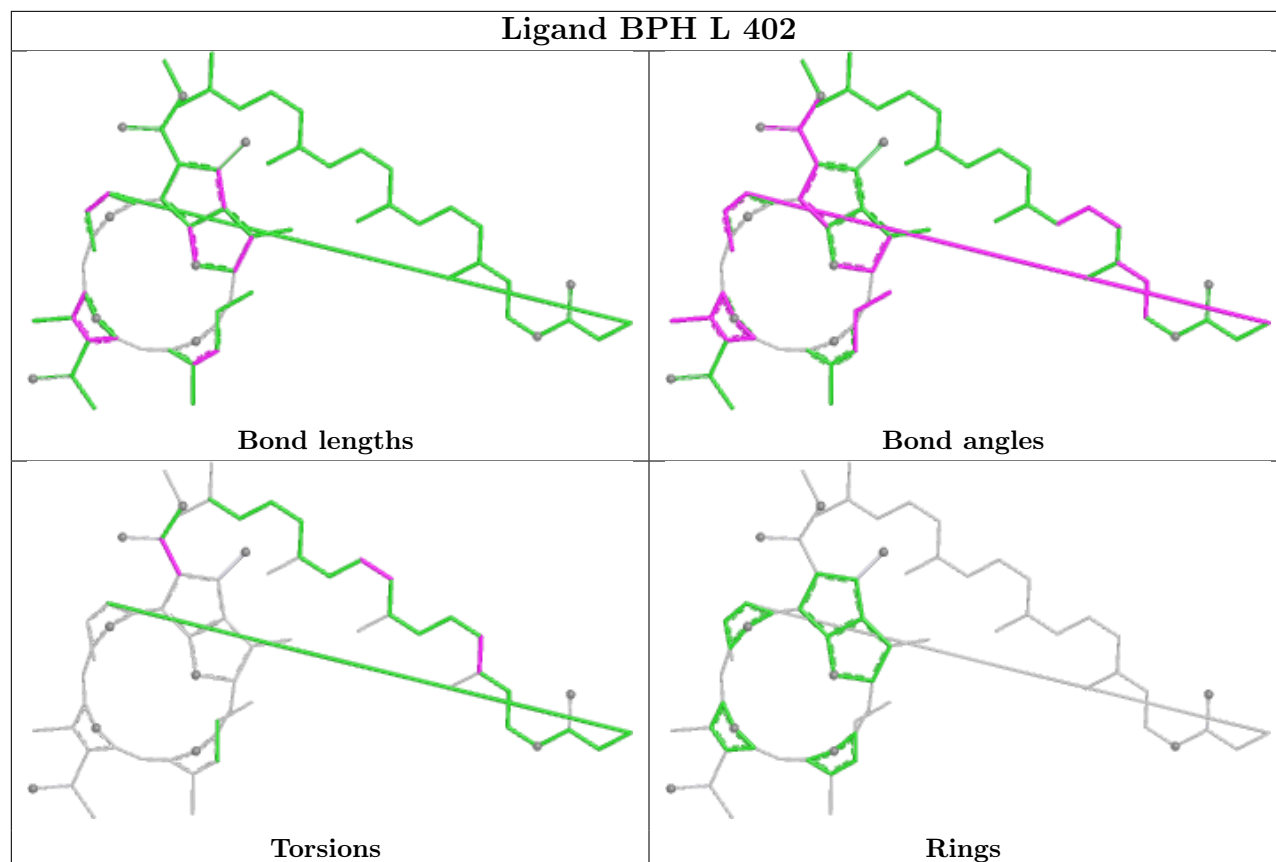
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



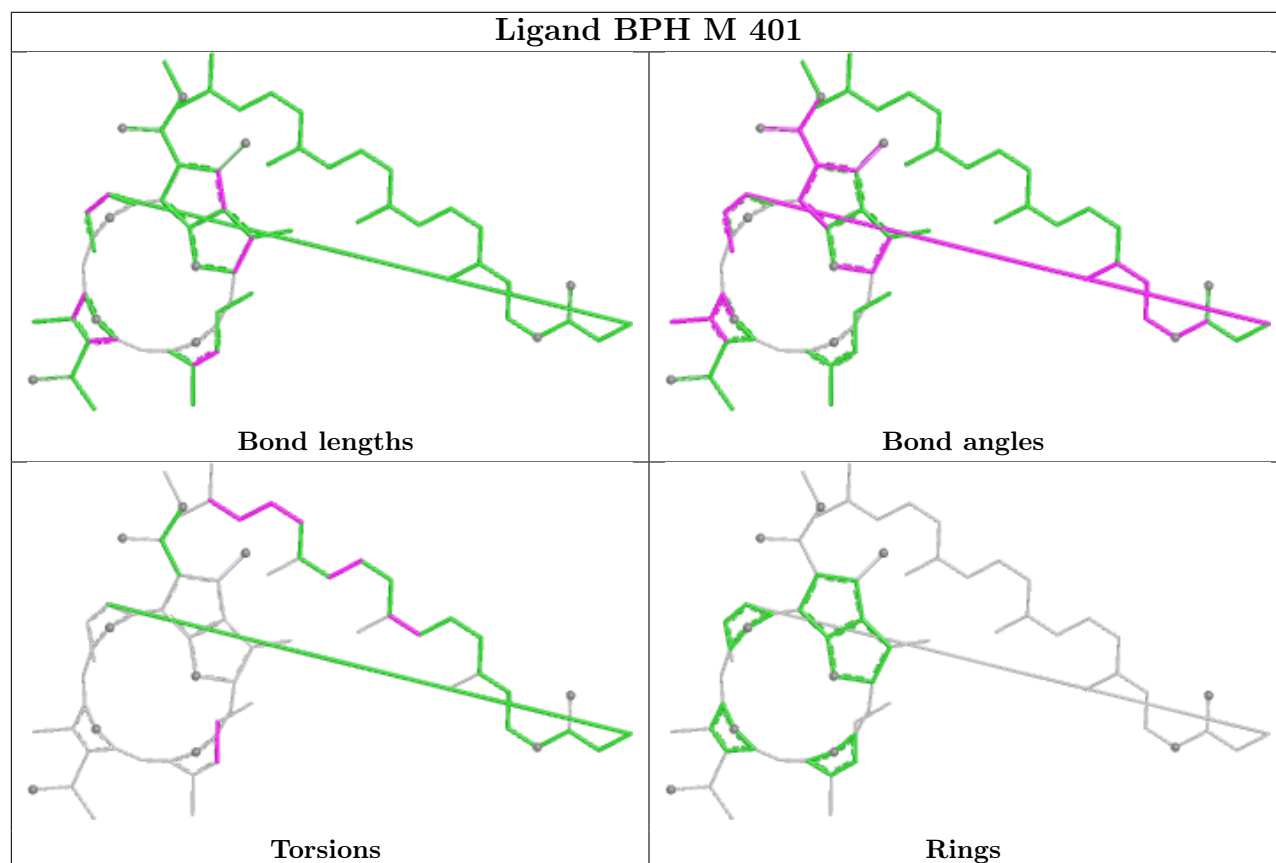


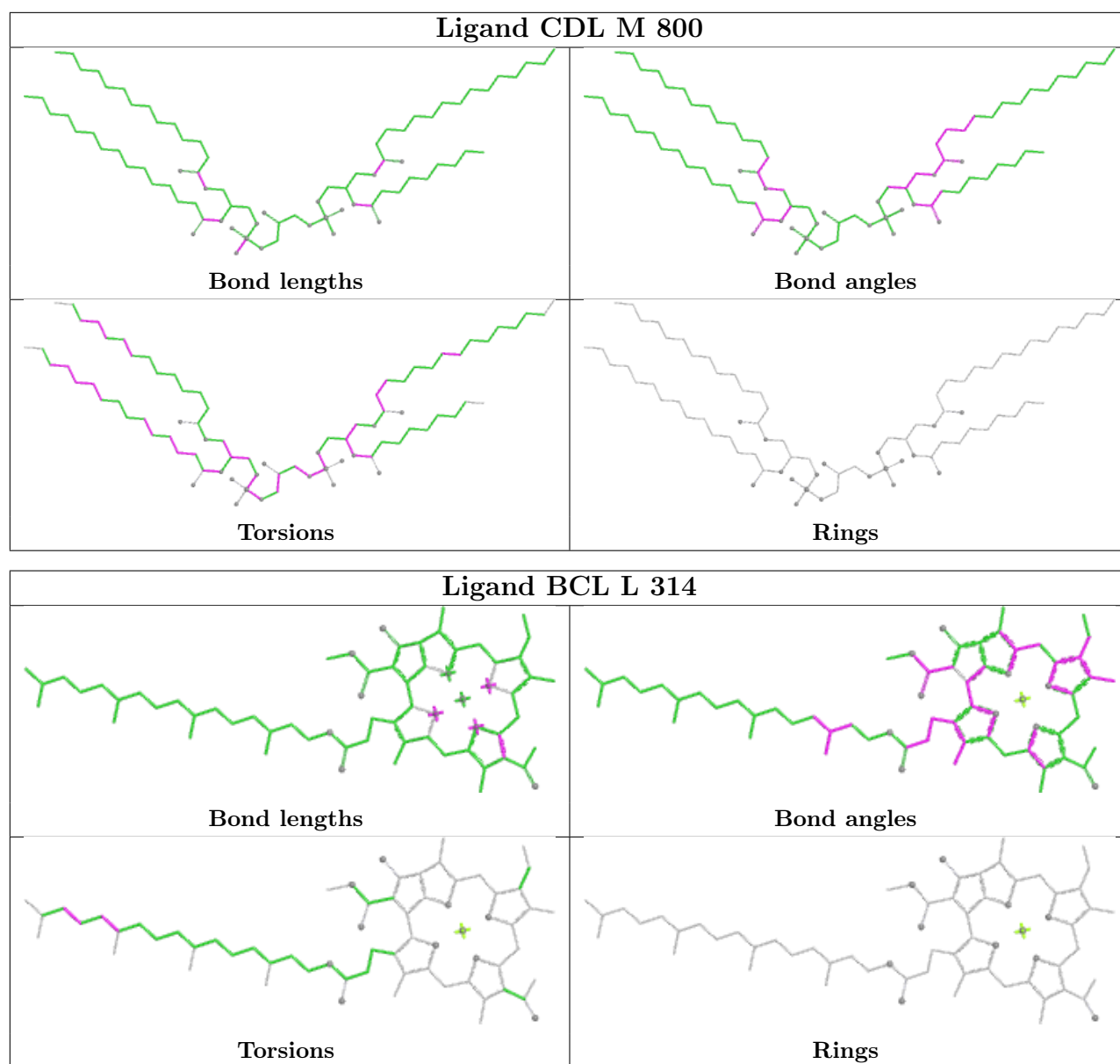


Ligand BPH L 402



Ligand BPH M 401





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%)	0.59	18 (6%)	25	22	43, 62, 73, 80	1 (0%)
2	M	302/307 (98%)	0.54	16 (5%)	32	28	37, 62, 72, 94	10 (3%)
3	H	241/260 (92%)	0.41	8 (3%)	49	45	42, 62, 73, 100	8 (3%)
All	All	824/848 (97%)	0.52	42 (5%)	33	29	37, 62, 73, 100	19 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	8.1
3	H	251	VAL	6.5
2	M	68[A]	PHE	5.3
2	M	2	GLU	4.5
2	M	302	GLY	4.0
1	L	67	TYR	3.3
1	L	277	GLY	3.3
1	L	281	GLY	3.3
1	L	226	THR	3.2
2	M	67	PHE	3.1
1	L	202	LYS	3.0
3	H	65	ILE	2.9
3	H	79	GLU	2.9
3	H	220[A]	LYS	2.8
1	L	268	LYS	2.8
2	M	52	LEU	2.7
3	H	250	SER	2.7
3	H	18	TYR	2.7
2	M	265	ILE	2.6
2	M	59	SER	2.6
2	M	133	THR	2.6
1	L	40	PHE	2.5
1	L	59	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	13	ARG	2.5
1	L	216	PHE	2.5
2	M	65[A]	MET	2.4
2	M	221	ALA	2.4
2	M	28	ASN	2.3
1	L	14	GLY	2.3
2	M	3	TYR	2.3
1	L	72	GLU	2.2
2	M	290	VAL	2.2
3	H	52	ASN	2.2
1	L	279	ILE	2.2
1	L	254	ILE	2.1
1	L	39	PHE	2.1
2	M	174	ALA	2.1
1	L	73	TYR	2.1
1	L	89	ILE	2.1
3	H	77	GLY	2.0
1	L	159	ASN	2.0
1	L	275	ILE	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
10	PO4	H	704	5/5	0.19	0.65	61,61,63,63	5
10	PO4	M	705	5/5	0.76	0.57	63,64,65,65	5
12	PGK	M	802	53/53	0.82	0.45	61,67,76,77	53
15	PGT	H	801[A]	51/51	0.83	0.39	45,73,81,82	51

Continued on next page...

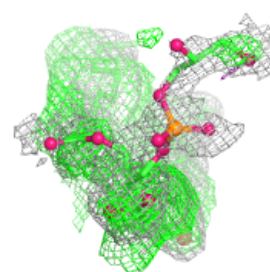
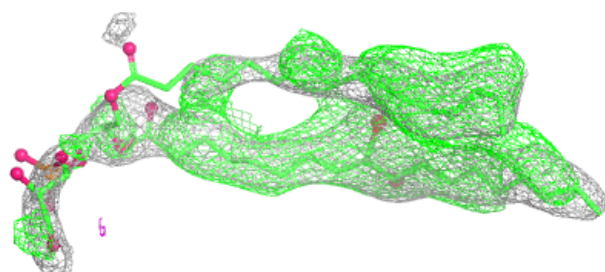
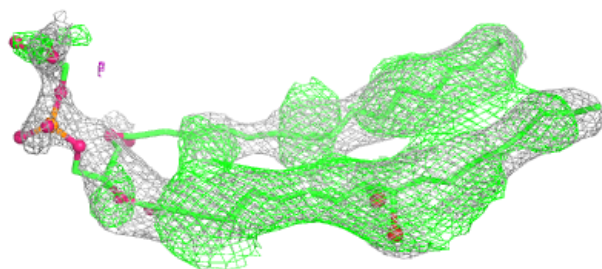
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	PGT	H	801[B]	51/51	0.83	0.39	47,76,84,85	51
11	CDL	M	800	81/100	0.84	0.35	49,74,88,90	81
7	GOL	L	707	6/6	0.84	0.44	65,67,68,68	6
7	GOL	L	709	6/6	0.86	0.30	65,66,68,70	6
13	LDA	H	904	16/16	0.87	0.36	76,79,86,86	16
13	LDA	M	907	16/16	0.88	0.32	69,72,77,77	16
13	LDA	M	902	16/16	0.88	0.31	66,71,75,79	16
5	BPH	M	401	65/65	0.89	0.17	56,62,116,118	0
6	U10	L	502	48/63	0.90	0.29	53,68,86,90	48
7	GOL	H	706	6/6	0.90	0.27	72,72,73,74	6
13	LDA	H	903	16/16	0.90	0.37	73,75,78,78	16
13	LDA	M	920	16/16	0.91	0.29	41,60,78,80	16
13	LDA	H	901	16/16	0.91	0.21	72,77,86,88	16
9	CL	M	701	1/1	0.91	0.47	73,73,73,73	1
10	PO4	M	702	5/5	0.92	0.20	69,71,74,77	5
6	U10	M	501	48/63	0.94	0.14	56,69,90,93	0
4	BCL	M	313	66/66	0.95	0.10	51,59,84,95	0
7	GOL	L	708	6/6	0.95	0.15	60,66,68,68	6
4	BCL	M	311	66/66	0.95	0.13	55,62,119,120	0
5	BPH	L	402	65/65	0.96	0.10	50,62,66,68	0
4	BCL	L	312	66/66	0.96	0.10	49,59,70,78	0
10	PO4	M	703	5/5	0.96	0.08	59,59,63,64	5
4	BCL	L	314	66/66	0.97	0.08	50,59,75,80	0
14	K	H	700	1/1	0.98	0.05	58,58,58,58	0
8	FE	M	500	1/1	1.00	0.02	59,59,59,59	0

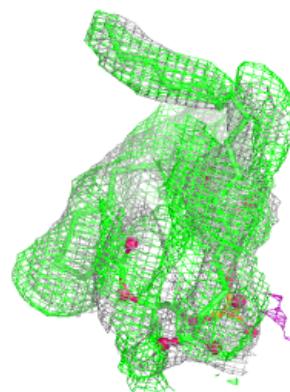
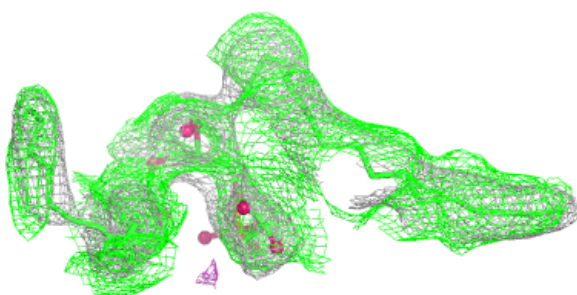
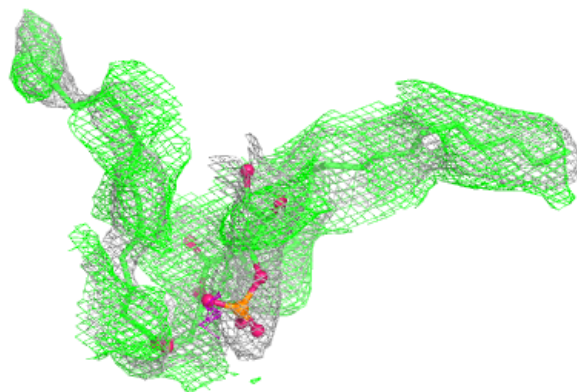
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGK 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)

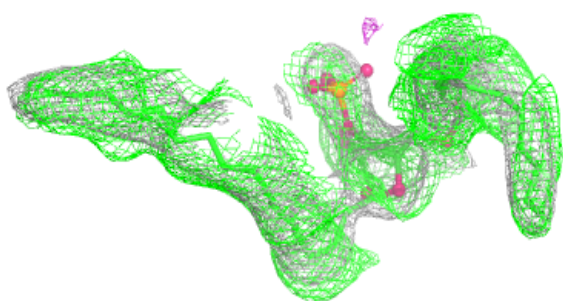
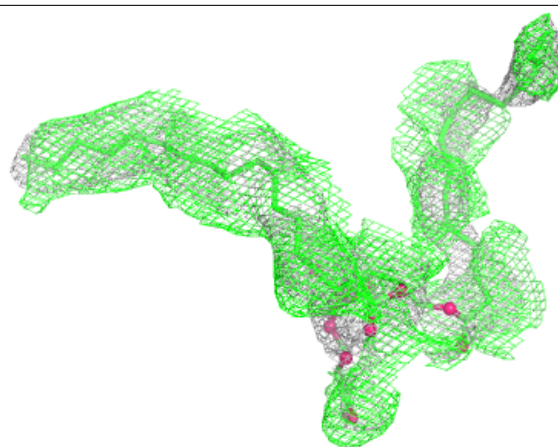
**Electron density around PGT H 801 (A):**

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



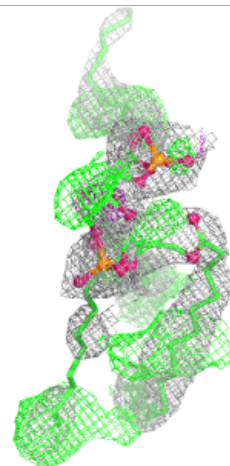
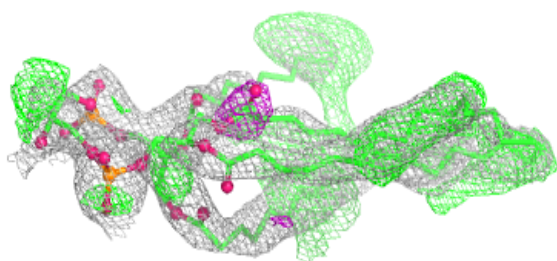
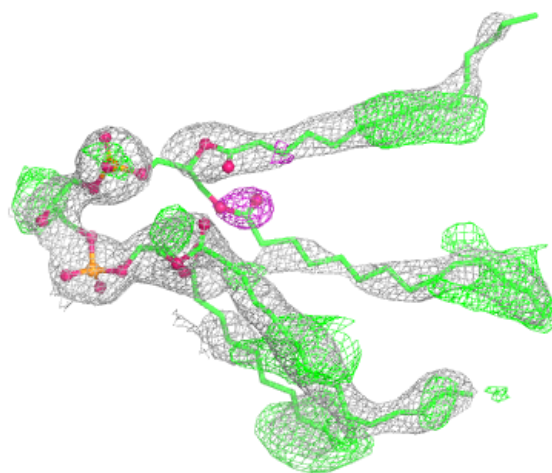
Electron density around PGT H 801 (B):

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



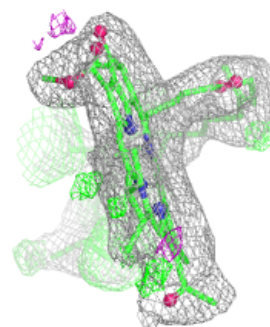
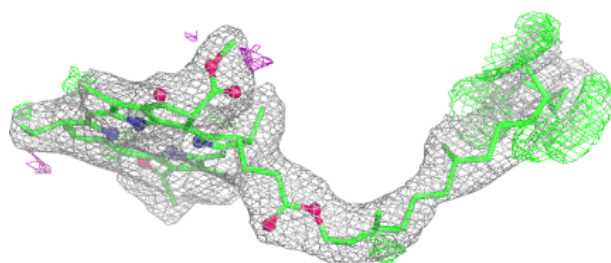
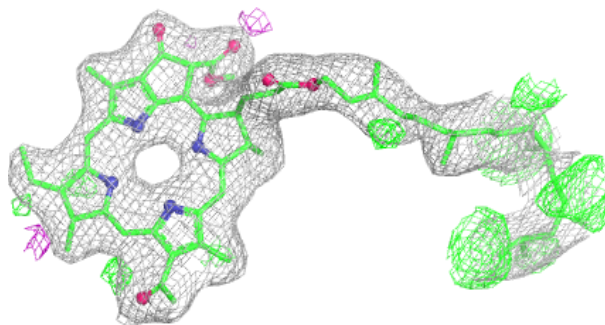
Electron density around CDL M 800:

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

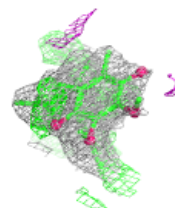
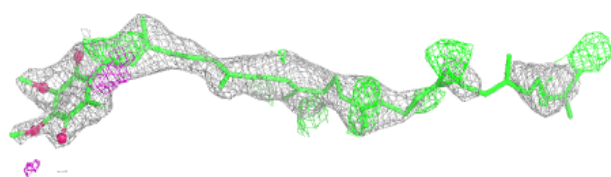
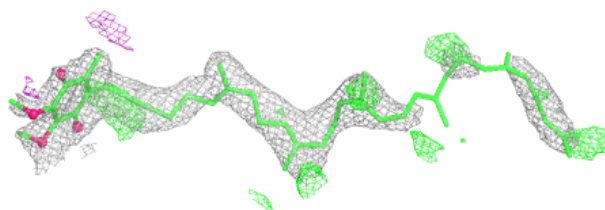


Electron density around BPH M 401:

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

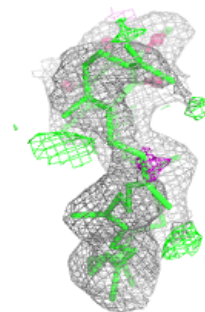
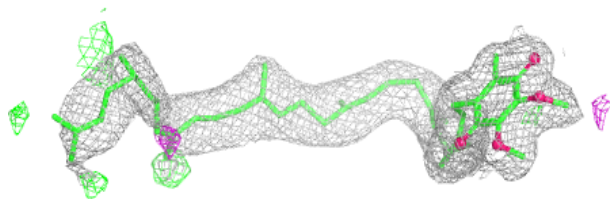
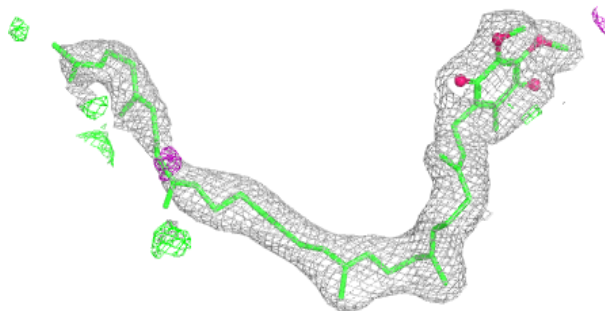
**Electron density around U10 L 502:**

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

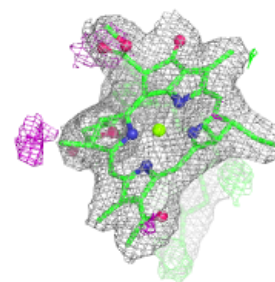
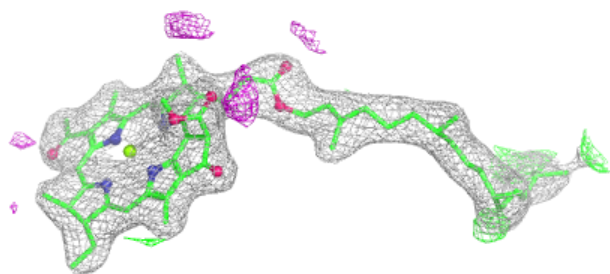
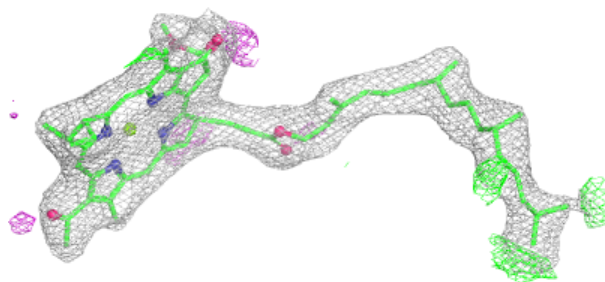


Electron density around U10 M 501:

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

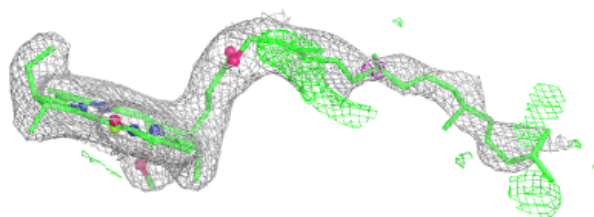
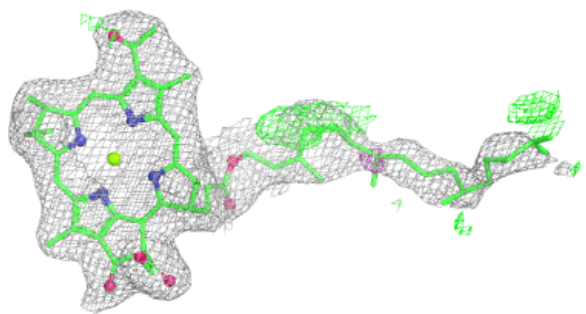
**Electron density around BCL M 313:**

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



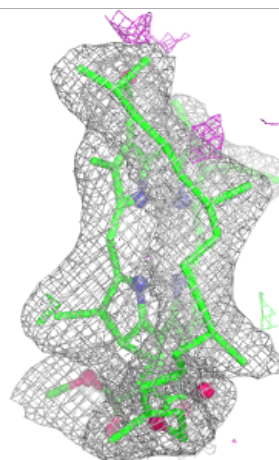
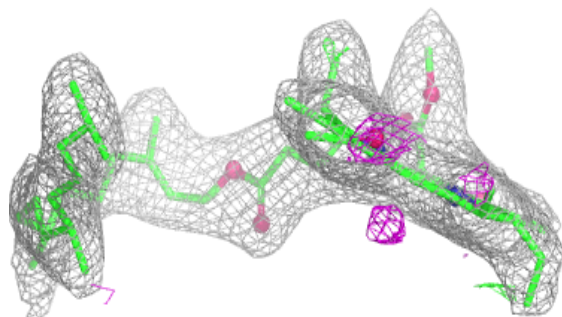
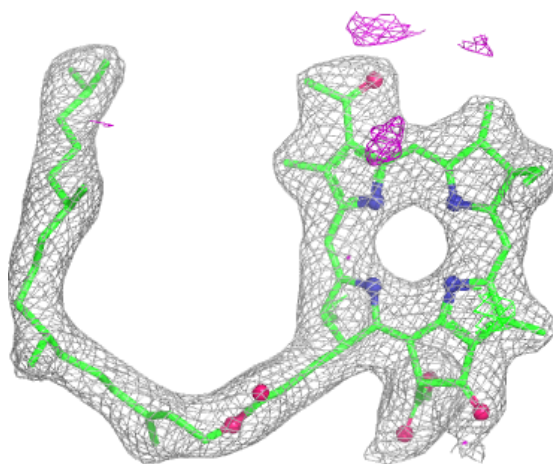
Electron density around BCL M 311:

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



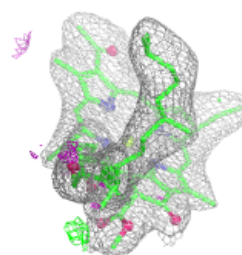
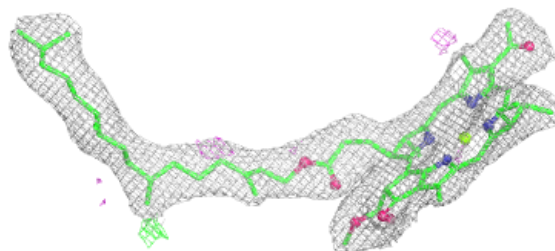
Electron density around BPH L 402:

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



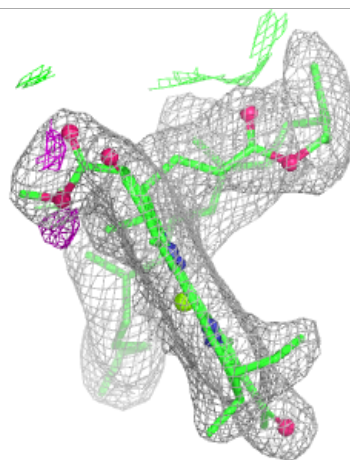
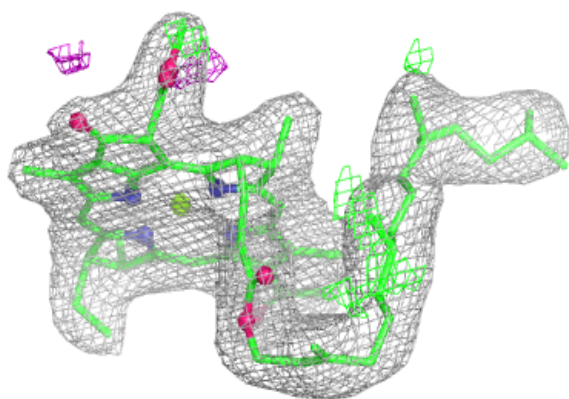
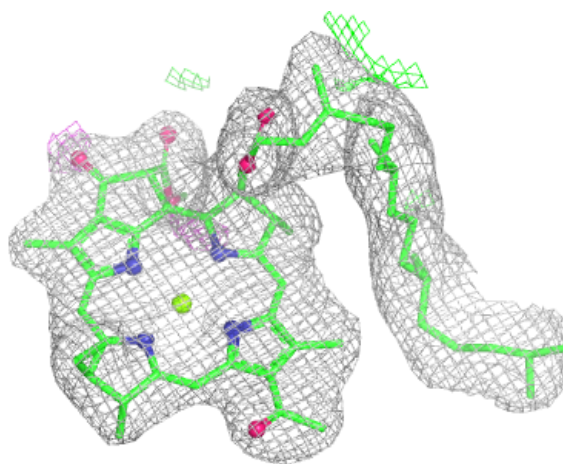
Electron density around BCL L 312:

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



Electron density around BCL 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.