



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:14 PM UTC

PDB ID : 2WX5 / pdb_00002wx5
Title : Hexa-coordination of a bacteriochlorophyll cofactor in the Rhodobacter sphaeroides reaction centre
Authors : Marsh, M.; Frolov, D.; Crouch, L.I.; Fyfe, P.K.; Robert, B.; van Grondelle, R.; Jones, M.R.; Hadfield, A.T.
Deposited on : 2009-11-02
Resolution : 2.63 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

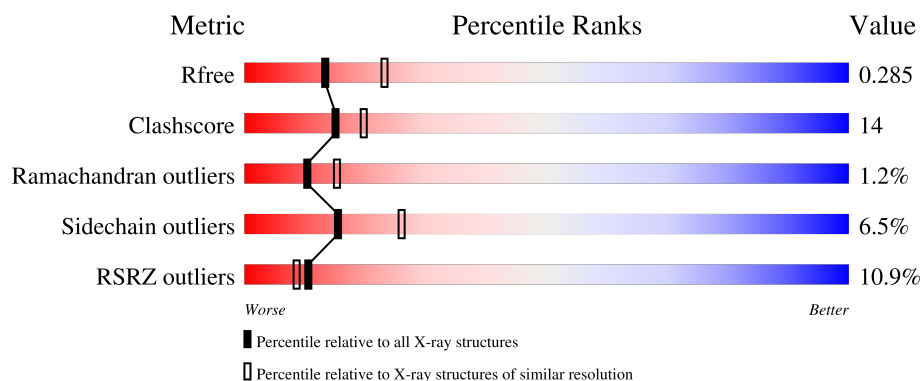
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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

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

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
8	HTO	L	1286	X	-	-	-
8	HTO	L	1287	X	-	-	-
8	HTO	M	1313	X	-	X	-
9	BPH	L	1288	X	-	-	-
9	BPH	M	1314	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 2 is a protein called REACTION CENTRE PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1504	358	362	8			

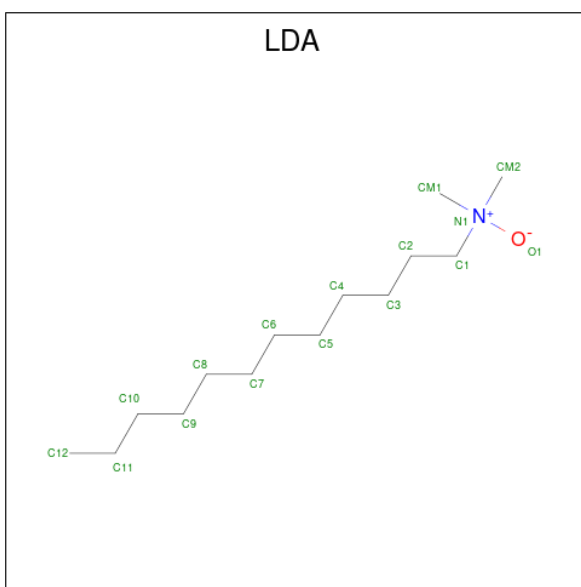
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	181	ARG	PHE	engineered mutation	UNP P0C0Y8

- Molecule 3 is a protein called REACTION CENTRE PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

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

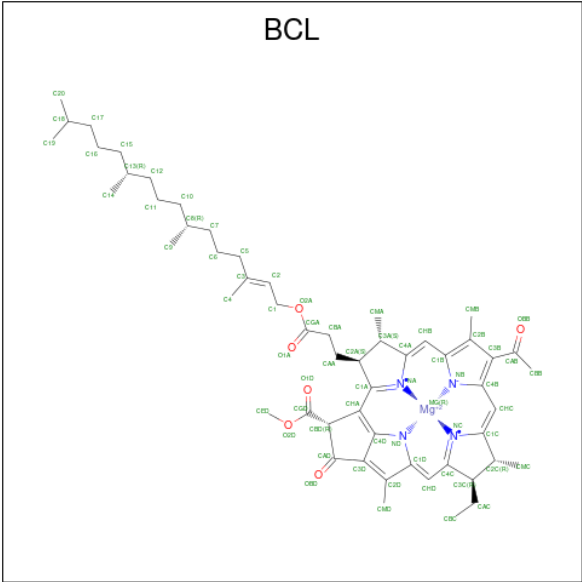


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

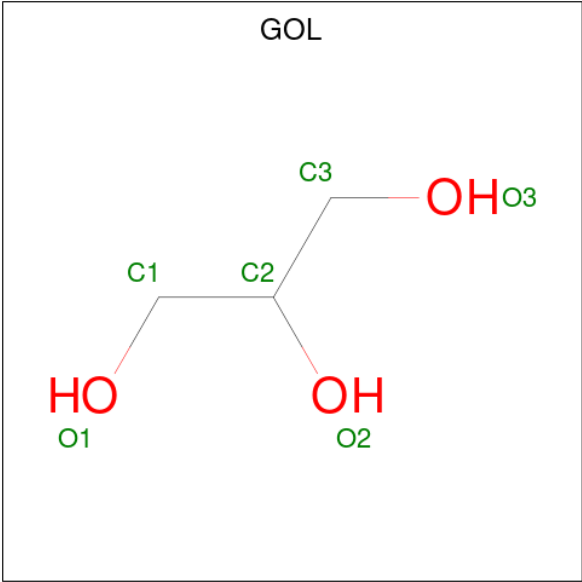
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	M	1	Total	Na	0	0
			1	1		

- Molecule 6 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



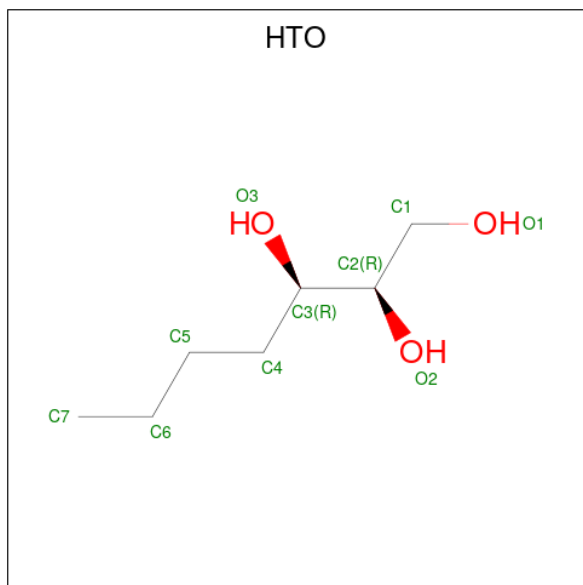
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



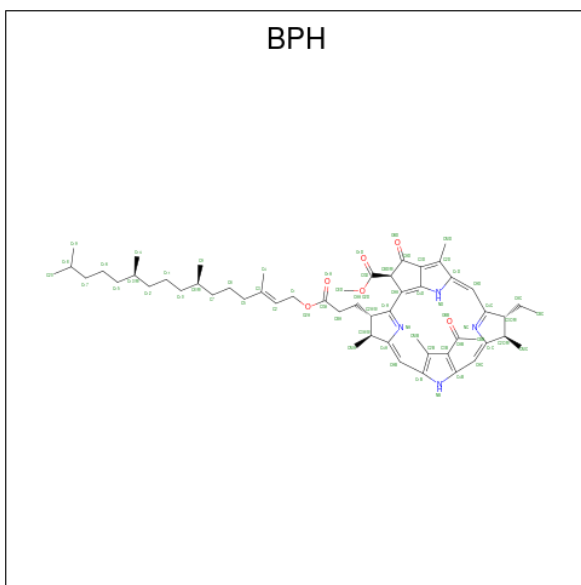
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



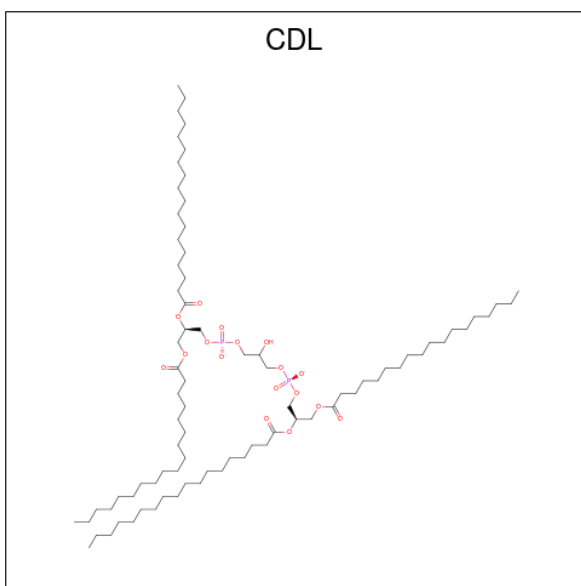
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			10	7	3		
8	L	1	Total	C	O	0	0
			10	7	3		
8	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

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

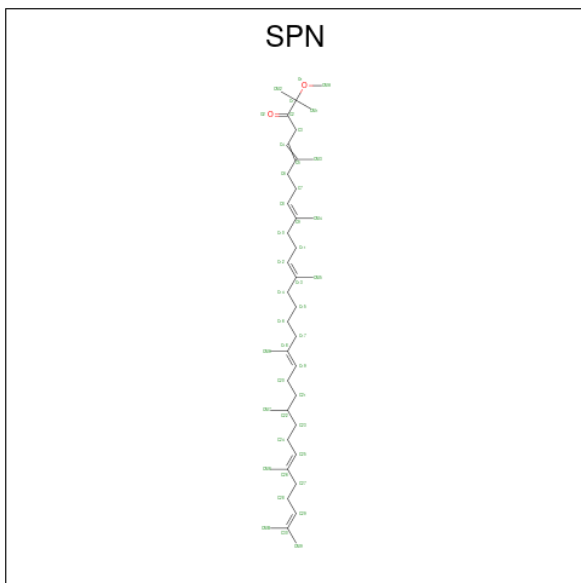


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

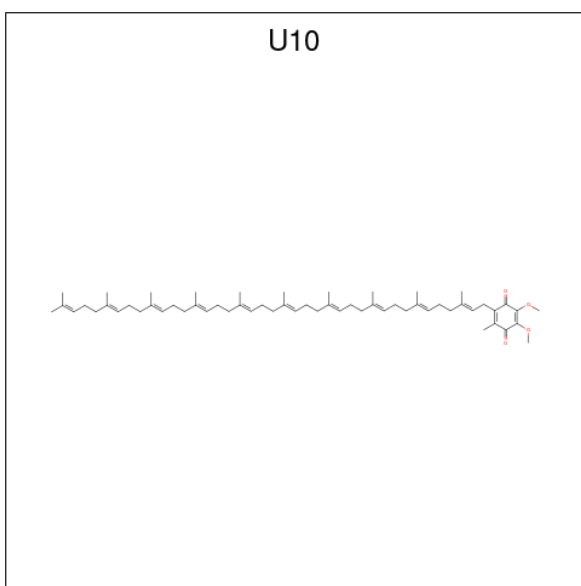
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



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

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



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

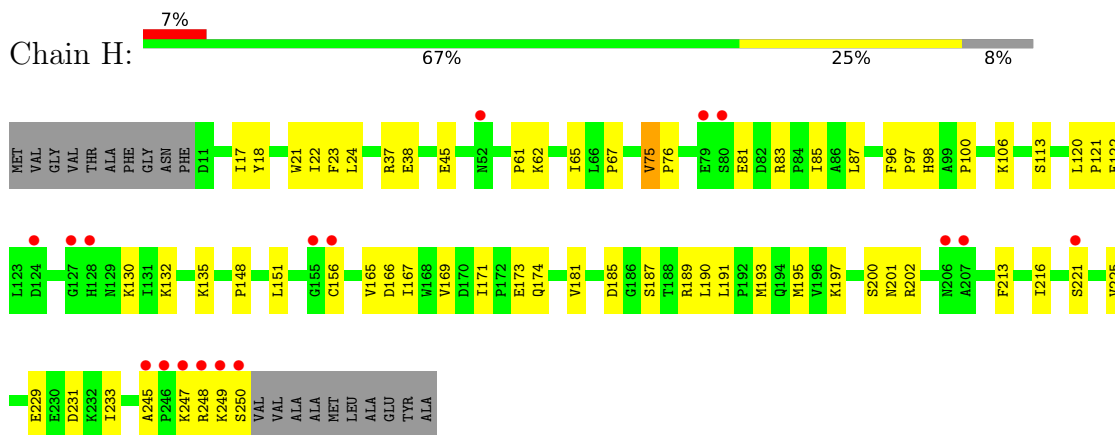
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	111	Total	O	0	0
			111	111		
14	L	99	Total	O	0	0
			99	99		
14	M	82	Total	O	0	0
			82	82		

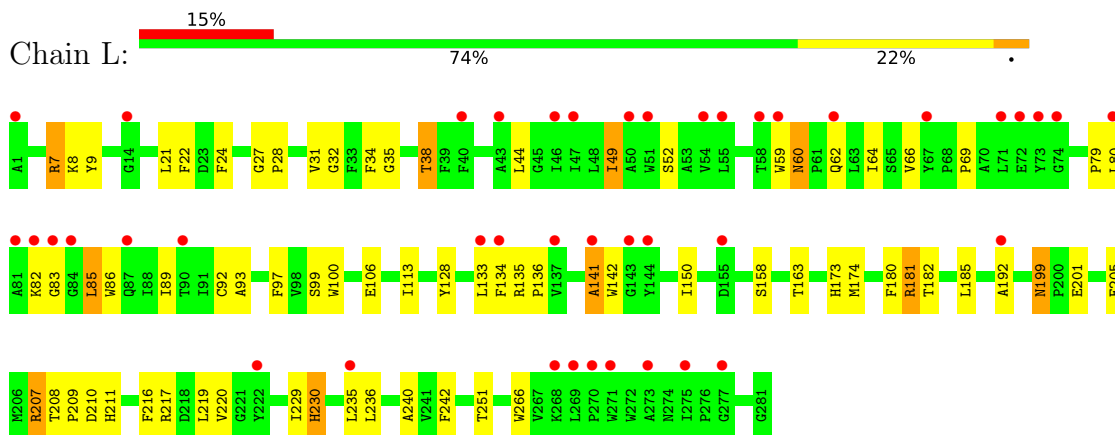
3 Residue-property plots [i](#)

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

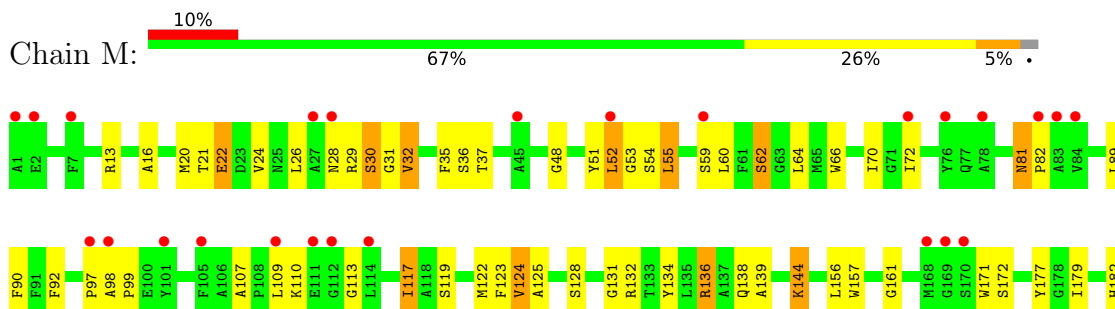
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

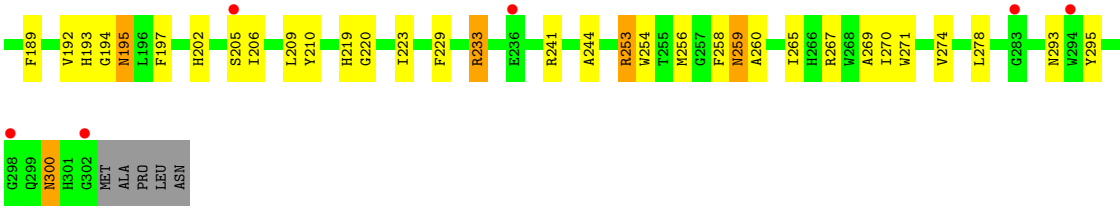


• Molecule 2: REACTION CENTRE PROTEIN L CHAIN



• Molecule 3: REACTION CENTRE PROTEIN M CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.18Å 140.18Å 185.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.40 – 2.63 20.40 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.40-2.63) 95.3 (20.40-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.63Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.279 (Not available) , 0.285	Depositor DCC
R_{free} test set	3047 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: BPH, HTO, BCL, CDL, U10, NA, LDA, SPN, GOL, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	1.11	2/1877 (0.1%)	1.21	7/2553 (0.3%)
2	L	1.13	1/2319 (0.0%)	1.21	14/3173 (0.4%)
3	M	1.07	2/2500 (0.1%)	1.18	7/3413 (0.2%)
All	All	1.10	5/6696 (0.1%)	1.20	28/9139 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	233	ARG	CA-C	-7.12	1.45	1.53
3	M	219	HIS	N-CA	-5.42	1.39	1.46
1	H	130	LYS	C-O	-5.28	1.17	1.24
1	H	65	ILE	CA-CB	5.16	1.58	1.53
2	L	192	ALA	CA-CB	-5.13	1.45	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	221	SER	CA-C-N	-10.58	108.88	120.94
1	H	221	SER	C-N-CA	-10.58	108.88	120.94
2	L	173	HIS	N-CA-C	-9.77	101.49	113.50
3	M	253	ARG	N-CA-C	-7.80	102.85	111.36
2	L	27	GLY	CA-C-N	7.42	127.13	119.64
2	L	27	GLY	C-N-CA	7.42	127.13	119.64
2	L	199	ASN	CA-C-N	7.32	128.99	119.84
2	L	199	ASN	C-N-CA	7.32	128.99	119.84
2	L	150	ILE	N-CA-C	7.06	117.19	110.42
2	L	230	HIS	N-CA-C	-6.77	105.15	113.41
3	M	209	LEU	N-CA-C	-6.35	104.44	111.36
2	L	106	GLU	N-CA-C	-6.33	104.25	112.23
3	M	81	ASN	CA-C-N	6.25	125.99	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	81	ASN	C-N-CA	6.25	125.99	119.05
1	H	245	ALA	N-CA-C	6.14	123.38	109.81
1	H	120	LEU	CA-C-N	-5.91	114.22	120.66
1	H	120	LEU	C-N-CA	-5.91	114.22	120.66
3	M	117	ILE	N-CA-C	-5.81	104.66	110.30
2	L	60	ASN	CA-C-N	5.75	125.22	119.24
2	L	60	ASN	C-N-CA	5.75	125.22	119.24
1	H	18	TYR	N-CA-C	-5.68	105.01	111.14
3	M	131	GLY	N-CA-C	-5.67	105.93	112.73
3	M	220	GLY	N-CA-C	-5.57	106.05	112.73
2	L	242	PHE	N-CA-C	-5.55	105.15	111.14
2	L	35	GLY	N-CA-C	-5.44	105.80	112.77
1	H	24	LEU	N-CA-C	5.17	116.99	111.36
2	L	141	ALA	N-CA-C	5.14	116.87	108.55
2	L	216	PHE	N-CA-C	5.04	116.59	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	35	0
2	L	2232	0	2191	61	0
3	M	2408	0	2321	78	0
4	H	16	0	31	2	0
4	M	80	0	155	8	0
5	H	1	0	0	0	0
5	M	1	0	0	0	0
6	L	132	0	148	18	0
6	M	132	0	148	18	0
7	L	12	0	16	0	0
8	L	20	0	32	4	0
8	M	10	0	16	7	0
9	L	65	0	76	8	0
9	M	65	0	76	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	81	0	106	3	0
11	M	1	0	0	0	0
12	M	43	0	70	10	0
13	M	48	0	63	5	0
14	H	111	0	0	1	0
14	L	99	0	0	6	0
14	M	82	0	0	5	0
All	All	7468	0	7285	197	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 14.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:HD2	1:H:250:SER:HB2	1.46	0.98
4:M:1306:LDA:H91	4:M:1307:LDA:H121	1.43	0.97
2:L:182:THR:HG22	2:L:236:LEU:HD13	1.50	0.91
2:L:34:PHE:O	2:L:38:THR:HG23	1.71	0.89
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.56	0.86
3:M:271:TRP:CD1	14:M:2075:HOH:O	2.28	0.85
2:L:38:THR:HG22	2:L:99:SER:HB3	1.59	0.85
3:M:197:PHE:HZ	6:M:1303:BCL:HBB2	1.42	0.84
2:L:181:ARG:NH2	14:L:2073:HOH:O	2.11	0.83
2:L:219:LEU:O	3:M:132:ARG:NH2	2.13	0.82
1:H:98:HIS:CD2	2:L:7:ARG:HH11	1.98	0.81
3:M:60:LEU:O	3:M:64:LEU:HD12	1.80	0.81
2:L:38:THR:HG22	2:L:99:SER:CB	2.11	0.81
6:M:1303:BCL:HHC	6:M:1303:BCL:CBB	2.12	0.80
3:M:197:PHE:CZ	6:M:1303:BCL:HBB2	2.16	0.79
3:M:300:ASN:HD22	3:M:300:ASN:N	1.81	0.79
2:L:229:ILE:HG13	2:L:229:ILE:O	1.83	0.78
9:L:1288:BPH:HBB3	9:L:1288:BPH:HHC	1.66	0.76
3:M:267:ARG:O	14:M:2075:HOH:O	2.03	0.76
8:L:1287:HTO:H71	4:M:1310:LDA:H121	1.67	0.75
9:M:1314:BPH:HBB3	9:M:1314:BPH:HHC	1.68	0.75
3:M:300:ASN:H	3:M:300:ASN:ND2	1.81	0.74
6:L:1282:BCL:HBB2	6:L:1282:BCL:HHC	1.68	0.74
1:H:248:ARG:HD2	1:H:250:SER:CB	2.19	0.73
2:L:229:ILE:HD13	8:L:1286:HTO:H3	1.71	0.72
3:M:300:ASN:N	3:M:300:ASN:ND2	2.33	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:ILE:HG13	2:L:89:ILE:HD13	1.73	0.71
4:M:1307:LDA:H102	13:M:1316:U10:H202	1.74	0.70
2:L:174:MET:HE2	6:L:1282:BCL:HED3	1.73	0.70
6:L:1282:BCL:HHC	6:L:1282:BCL:CBB	2.22	0.69
2:L:182:THR:HG22	2:L:236:LEU:CD1	2.21	0.69
2:L:82:LYS:NZ	14:L:2044:HOH:O	2.24	0.69
6:M:1303:BCL:HHC	6:M:1303:BCL:HBB3	1.74	0.68
6:L:1283:BCL:HMB3	6:L:1283:BCL:CBB	2.25	0.67
2:L:181:ARG:HG2	9:M:1314:BPH:CBB	2.25	0.67
1:H:121:PRO:HB3	1:H:225:VAL:O	1.95	0.66
2:L:185:LEU:HD13	9:M:1314:BPH:ND	2.10	0.66
3:M:52:LEU:HG	3:M:53:GLY:H	1.61	0.66
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.78	0.66
1:H:165:VAL:O	1:H:166:ASP:HB2	1.95	0.66
1:H:213:PHE:O	1:H:216:ILE:HG13	1.96	0.65
1:H:156:CYS:SG	1:H:248:ARG:HD3	2.36	0.65
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.32	0.64
2:L:128:TYR:HD1	6:M:1304:BCL:HBB1	1.61	0.64
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.80	0.64
6:L:1282:BCL:HBB2	12:M:1315:SPN:H162	1.79	0.64
9:L:1288:BPH:HBB2	3:M:210:TYR:HB3	1.80	0.63
2:L:93:ALA:HA	9:L:1288:BPH:H9C2	1.80	0.62
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.34	0.62
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.82	0.62
2:L:93:ALA:HA	9:L:1288:BPH:C9	2.29	0.61
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.82	0.61
6:M:1303:BCL:HAA2	6:M:1303:BCL:HBD	1.83	0.61
3:M:194:GLY:O	3:M:195:ASN:HB3	2.02	0.60
1:H:62:LYS:NZ	2:L:199:ASN:HD21	2.01	0.59
3:M:21:THR:O	3:M:22:GLU:C	2.46	0.59
4:M:1306:LDA:C9	4:M:1307:LDA:H121	2.27	0.59
3:M:161:GLY:HA3	12:M:1315:SPN:H201	1.83	0.59
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.84	0.59
1:H:229:GLU:O	1:H:233:ILE:HD12	2.02	0.59
6:M:1304:BCL:HBB2	6:M:1304:BCL:HHC	1.86	0.58
2:L:174:MET:HG2	6:L:1282:BCL:O1D	2.04	0.58
3:M:157:TRP:CZ2	12:M:1315:SPN:H22	2.38	0.58
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.86	0.57
2:L:207:ARG:HG2	2:L:211:HIS:CG	2.40	0.57
3:M:89:LEU:HB3	8:M:1313:HTO:H52	1.87	0.57
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:220:VAL:HB	8:L:1287:HTO:H11	1.86	0.56
6:L:1283:BCL:HMB3	6:L:1283:BCL:HBB2	1.87	0.56
9:L:1288:BPH:HBB1	3:M:210:TYR:CD2	2.39	0.56
1:H:189:ARG:HA	14:H:2089:HOH:O	2.06	0.56
6:L:1282:BCL:HBB3	6:M:1303:BCL:H41	1.89	0.54
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.43	0.54
3:M:270:ILE:HG22	14:M:2075:HOH:O	2.07	0.54
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.88	0.54
3:M:89:LEU:HA	3:M:92:PHE:CE2	2.42	0.53
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.44	0.53
10:M:1305:CDL:HA4	10:M:1305:CDL:HB61	1.90	0.52
2:L:185:LEU:HD13	9:M:1314:BPH:C1D	2.39	0.52
8:L:1287:HTO:C7	4:M:1310:LDA:H121	2.38	0.51
3:M:161:GLY:HA3	12:M:1315:SPN:HM72	1.92	0.51
6:M:1303:BCL:HAA2	6:M:1303:BCL:CBD	2.41	0.51
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.93	0.51
1:H:37:ARG:O	1:H:38:GLU:HG2	2.11	0.50
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.37	0.50
2:L:38:THR:HG22	2:L:99:SER:HB2	1.93	0.50
3:M:113:GLY:O	3:M:117:ILE:HG13	2.10	0.50
3:M:256:MET:HE3	3:M:258:PHE:CZ	2.45	0.50
1:H:62:LYS:HZ1	2:L:199:ASN:HD21	1.58	0.50
2:L:31:VAL:HG12	2:L:32:GLY:N	2.27	0.50
3:M:31:GLY:H	4:M:1309:LDA:H92	1.76	0.50
2:L:208:THR:HB	2:L:209:PRO:HD2	1.94	0.50
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.47	0.50
3:M:253:ARG:HB2	3:M:259:ASN:OD1	2.12	0.49
2:L:163:THR:HG22	2:L:163:THR:O	2.12	0.49
6:M:1303:BCL:HBB2	6:M:1303:BCL:HHC	1.90	0.49
6:L:1282:BCL:HBB2	12:M:1315:SPN:HM63	1.95	0.49
6:L:1282:BCL:CBB	12:M:1315:SPN:H162	2.42	0.49
1:H:21:TRP:CD2	4:H:1251:LDA:H12	2.48	0.49
3:M:270:ILE:CG2	14:M:2075:HOH:O	2.60	0.49
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.95	0.48
1:H:122:GLU:OE1	3:M:233:ARG:NH2	2.42	0.48
2:L:128:TYR:CD1	6:M:1304:BCL:HBB1	2.44	0.48
2:L:60:ASN:O	2:L:64:ILE:HG13	2.12	0.48
1:H:21:TRP:CE2	4:H:1251:LDA:H12	2.49	0.48
6:L:1283:BCL:CBB	6:L:1283:BCL:CMB	2.92	0.48
1:H:185:ASP:OD2	1:H:187:SER:OG	2.32	0.48
1:H:190:LEU:N	1:H:190:LEU:HD23	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:207:ARG:HG2	2:L:211:HIS:CD2	2.49	0.47
2:L:133:LEU:HD23	2:L:134:PHE:CE1	2.49	0.47
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.49	0.47
2:L:207:ARG:CG	2:L:211:HIS:CG	2.98	0.47
3:M:31:GLY:O	3:M:32:VAL:C	2.58	0.47
3:M:36:SER:O	3:M:37:THR:C	2.58	0.47
3:M:189:PHE:O	3:M:193:HIS:HD2	1.98	0.46
2:L:97:PHE:CE1	6:L:1283:BCL:H121	2.51	0.46
2:L:266:TRP:NE1	8:M:1313:HTO:H62	2.30	0.46
3:M:195:ASN:OD1	3:M:195:ASN:C	2.58	0.46
2:L:266:TRP:CE2	8:M:1313:HTO:H3	2.51	0.46
9:L:1288:BPH:H7C1	6:M:1304:BCL:H202	1.97	0.46
4:M:1306:LDA:H91	4:M:1307:LDA:C12	2.28	0.46
1:H:193:MET:C	1:H:195:MET:H	2.24	0.46
3:M:144:LYS:HA	3:M:144:LYS:HD3	1.87	0.46
1:H:67:PRO:HA	2:L:205:GLU:OE2	2.16	0.46
3:M:110:LYS:HE3	3:M:110:LYS:HB2	1.69	0.46
4:M:1309:LDA:HM21	4:M:1309:LDA:H22	1.74	0.46
3:M:271:TRP:HH2	10:M:1305:CDL:H731	1.80	0.45
2:L:266:TRP:CD1	8:M:1313:HTO:H62	2.52	0.45
6:L:1282:BCL:CBB	12:M:1315:SPN:HM63	2.47	0.45
2:L:201:GLU:HG2	3:M:144:LYS:HZ1	1.81	0.45
2:L:62:GLN:HG3	14:L:2033:HOH:O	2.17	0.45
3:M:119:SER:OG	3:M:177:TYR:OH	2.27	0.45
3:M:16:ALA:CB	3:M:32:VAL:HG11	2.47	0.45
3:M:270:ILE:O	3:M:274:VAL:HG13	2.16	0.44
6:L:1282:BCL:HED1	3:M:179:ILE:HG23	1.98	0.44
14:L:2022:HOH:O	13:M:1316:U10:H322	2.17	0.44
9:L:1288:BPH:HHC	9:L:1288:BPH:CBB	2.43	0.44
2:L:207:ARG:CG	2:L:211:HIS:CD2	3.01	0.44
2:L:230:HIS:NE2	3:M:223:ILE:HG13	2.33	0.44
3:M:123:PHE:O	3:M:124:VAL:C	2.60	0.44
6:L:1283:BCL:H41	6:M:1304:BCL:HBB3	1.99	0.44
3:M:260:ALA:C	13:M:1316:U10:H4M3	2.43	0.44
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.18	0.44
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.52	0.43
1:H:23:PHE:CD2	1:H:23:PHE:C	2.96	0.43
2:L:7:ARG:O	2:L:7:ARG:HG3	2.15	0.43
3:M:259:ASN:C	3:M:259:ASN:HD22	2.26	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.42	0.43
3:M:134:TYR:C	3:M:134:TYR:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.00	0.43
3:M:90:PHE:HB2	8:M:1313:HTO:H73	2.01	0.42
1:H:173:GLU:O	1:H:174:GLN:C	2.60	0.42
2:L:185:LEU:CD1	9:M:1314:BPH:C1D	2.98	0.42
3:M:138:GLN:O	3:M:139:ALA:C	2.61	0.42
3:M:271:TRP:HD1	14:M:2075:HOH:O	1.85	0.42
1:H:113:SER:HB2	2:L:9:TYR:CE1	2.54	0.42
2:L:266:TRP:CD2	8:M:1313:HTO:H3	2.54	0.42
3:M:20:MET:HE3	3:M:20:MET:HB3	1.57	0.42
3:M:97:PRO:O	3:M:172:SER:HB3	2.19	0.42
2:L:8:LYS:HG2	14:L:2005:HOH:O	2.19	0.42
2:L:85:LEU:O	2:L:89:ILE:HG13	2.19	0.42
3:M:136:ARG:HA	3:M:136:ARG:NH1	2.34	0.42
2:L:185:LEU:CD1	9:M:1314:BPH:ND	2.82	0.42
6:L:1283:BCL:H2C	6:M:1303:BCL:HBC2	2.02	0.42
3:M:70:ILE:HD13	12:M:1315:SPN:H102	2.02	0.42
9:L:1288:BPH:H192	6:M:1304:BCL:C2B	2.49	0.42
3:M:89:LEU:HA	3:M:92:PHE:CD2	2.55	0.42
3:M:197:PHE:HZ	6:M:1303:BCL:CBB	2.22	0.42
3:M:202:HIS:CE1	3:M:206:ILE:CD1	3.01	0.42
9:M:1314:BPH:HHC	9:M:1314:BPH:CBB	2.43	0.42
3:M:278:LEU:HD11	10:M:1305:CDL:H382	2.02	0.42
1:H:167:ILE:HG22	1:H:169:VAL:CG1	2.49	0.42
1:H:201:ASN:O	1:H:202:ARG:HB3	2.20	0.42
3:M:13:ARG:NH2	3:M:35:PHE:HB3	2.35	0.42
3:M:52:LEU:CG	3:M:53:GLY:H	2.32	0.42
3:M:269:ALA:O	3:M:270:ILE:C	2.58	0.42
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.01	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.01	0.41
2:L:44:LEU:HD23	2:L:92:CYS:SG	2.60	0.41
6:L:1282:BCL:CAB	12:M:1315:SPN:H162	2.51	0.41
3:M:24:VAL:HG22	3:M:139:ALA:HB1	2.02	0.41
2:L:28:PRO:O	3:M:254:TRP:HA	2.20	0.41
2:L:66:VAL:HG12	2:L:86:TRP:HB2	2.02	0.41
3:M:29:ARG:C	3:M:30:SER:O	2.62	0.41
3:M:90:PHE:CD2	8:M:1313:HTO:H51	2.56	0.41
3:M:98:ALA:O	3:M:99:PRO:C	2.62	0.41
3:M:156:LEU:HD23	6:M:1303:BCL:H43	2.02	0.41
3:M:157:TRP:CD1	12:M:1315:SPN:H202	2.56	0.41
2:L:100:TRP:CZ2	13:M:1316:U10:H251	2.56	0.41
2:L:79:PRO:O	2:L:80:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:ALA:HB1	14:L:2040:HOH:O	2.21	0.40
6:L:1282:BCL:H111	6:M:1303:BCL:H192	2.03	0.40
2:L:69:PRO:HD3	2:L:83:GLY:O	2.21	0.40
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.91	0.40
1:H:22:ILE:O	1:H:23:PHE:C	2.61	0.40
1:H:132:LYS:HB2	1:H:171:ILE:HD11	2.03	0.40
3:M:260:ALA:O	13:M:1316:U10:H4M3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	198/260 (76%)	186 (94%)	11 (6%)	1 (0%)	24	36
2	L	103/281 (37%)	90 (87%)	13 (13%)	0	100	100
3	M	300/307 (98%)	273 (91%)	21 (7%)	6 (2%)	6	8
All	All	601/848 (71%)	549 (91%)	45 (8%)	7 (1%)	10	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	48	GLY
3	M	124	VAL
3	M	22	GLU
3	M	30	SER
1	H	45	GLU
3	M	195	ASN
3	M	107	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	185 (95%)	10 (5%)	21	35
2	L	220/220 (100%)	205 (93%)	15 (7%)	14	23
3	M	236/240 (98%)	219 (93%)	17 (7%)	13	21
All	All	651/668 (98%)	609 (94%)	42 (6%)	15	26

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	ILE
1	H	75	VAL
1	H	83	ARG
1	H	106	LYS
1	H	135	LYS
1	H	197	LYS
1	H	200	SER
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	49	ILE
2	L	52	SER
2	L	59	TRP
2	L	85	LEU
2	L	113	ILE
2	L	158	SER
2	L	181	ARG
2	L	207	ARG
2	L	210	ASP
2	L	217	ARG
2	L	235	LEU
2	L	251	THR
3	M	26	LEU

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Mol	Chain	Res	Type
3	M	32	VAL
3	M	52	LEU
3	M	54	SER
3	M	55	LEU
3	M	59	SER
3	M	62	SER
3	M	72	ILE
3	M	109	LEU
3	M	136	ARG
3	M	144	LYS
3	M	182	HIS
3	M	192	VAL
3	M	205	SER
3	M	259	ASN
3	M	265	ILE
3	M	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	199	GLN
1	H	206	ASN
2	L	60	ASN
2	L	62	GLN
2	L	183	ASN
2	L	199	ASN
2	L	258	GLN
2	L	280	ASN
3	M	193	HIS
3	M	300	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	LDA	M	1307	-	13,15,15	2.15	2 (15%)	14,17,17	0.70	0
8	HTO	M	1313	-	9,9,9	1.08	1 (11%)	10,10,10	1.24	1 (10%)
6	BCL	M	1303	3	69,74,74	1.20	5 (7%)	79,115,115	1.95	13 (16%)
8	HTO	L	1286	-	9,9,9	1.25	1 (11%)	10,10,10	2.18	4 (40%)
9	BPH	L	1288	-	59,70,70	1.50	5 (8%)	59,101,101	2.00	13 (22%)
7	GOL	L	1285	-	5,5,5	0.46	0	5,5,5	0.49	0
4	LDA	H	1251	-	13,15,15	2.28	2 (15%)	14,17,17	0.44	0
7	GOL	L	1284	-	5,5,5	0.41	0	5,5,5	0.29	0
8	HTO	L	1287	-	9,9,9	0.77	0	10,10,10	1.47	3 (30%)
9	BPH	M	1314	-	59,70,70	1.71	7 (11%)	59,101,101	2.42	17 (28%)
4	LDA	M	1310	-	13,15,15	2.04	2 (15%)	14,17,17	0.77	0
13	U10	M	1316	-	48,48,63	2.80	15 (31%)	60,61,79	1.93	16 (26%)
6	BCL	L	1282	3,14	69,74,74	1.31	6 (8%)	79,115,115	1.89	15 (18%)
6	BCL	L	1283	2	69,74,74	1.32	6 (8%)	79,115,115	1.82	16 (20%)
12	SPN	M	1315	-	42,42,42	0.65	0	50,52,52	1.66	12 (24%)
4	LDA	M	1306	-	13,15,15	1.98	1 (7%)	14,17,17	1.00	1 (7%)
10	CDL	M	1305	-	80,80,99	1.28	4 (5%)	86,92,111	1.31	11 (12%)
4	LDA	M	1309	-	13,15,15	2.17	2 (15%)	14,17,17	0.57	0
4	LDA	M	1308	-	13,15,15	2.05	2 (15%)	14,17,17	0.68	0
6	BCL	M	1304	2	69,74,74	1.44	8 (11%)	79,115,115	2.48	25 (31%)

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	LDA	M	1307	-	-	3/13/13/13	-
8	HTO	M	1313	-	1/1/2/2	4/10/10/10	-
6	BCL	M	1303	3	-	3/41/137/137	-
8	HTO	L	1286	-	1/1/2/2	2/10/10/10	-
9	BPH	L	1288	-	2/2/18/22	12/37/105/105	0/5/6/6
7	GOL	L	1285	-	-	0/4/4/4	-
8	HTO	L	1287	-	1/1/2/2	2/10/10/10	-
9	BPH	M	1314	-	2/2/18/22	13/37/105/105	0/5/6/6
4	LDA	H	1251	-	-	7/13/13/13	-
7	GOL	L	1284	-	-	2/4/4/4	-
4	LDA	M	1310	-	-	6/13/13/13	-
13	U10	M	1316	-	-	8/45/69/87	0/1/1/1
6	BCL	L	1282	3,14	-	9/41/137/137	-
6	BCL	L	1283	2	-	4/41/137/137	-
12	SPN	M	1315	-	-	18/50/51/51	-
4	LDA	M	1306	-	-	7/13/13/13	-
10	CDL	M	1305	-	-	40/91/91/110	-
4	LDA	M	1309	-	-	11/13/13/13	-
4	LDA	M	1308	-	-	4/13/13/13	-
6	BCL	M	1304	2	-	10/41/137/137	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1314	BPH	C1D-C2D	8.76	1.49	1.39
9	L	1288	BPH	C1D-C2D	8.55	1.48	1.39
4	H	1251	LDA	O1-N1	-6.91	1.25	1.42
13	M	1316	U10	C33-C34	6.86	1.48	1.33
13	M	1316	U10	C13-C14	6.79	1.48	1.33
13	M	1316	U10	C18-C19	6.78	1.48	1.33
4	M	1309	LDA	O1-N1	-6.71	1.25	1.42
4	M	1307	LDA	O1-N1	-6.68	1.25	1.42
4	M	1306	LDA	O1-N1	-6.66	1.25	1.42
4	M	1310	LDA	O1-N1	-6.62	1.25	1.42
4	M	1308	LDA	O1-N1	-6.44	1.26	1.42
13	M	1316	U10	C23-C24	6.44	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1316	U10	C28-C29	6.33	1.47	1.33
6	L	1283	BCL	MG-ND	-5.85	1.94	2.05
6	M	1304	BCL	MG-NB	-5.69	1.94	2.05
13	M	1316	U10	C8-C9	5.62	1.46	1.33
10	M	1305	CDL	OA6-CA5	5.42	1.49	1.34
13	M	1316	U10	C38-C39	5.40	1.48	1.32
6	L	1282	BCL	MG-NB	-5.37	1.95	2.05
10	M	1305	CDL	OA8-CA7	5.32	1.48	1.33
6	M	1303	BCL	MG-NB	-4.86	1.96	2.05
10	M	1305	CDL	OB8-CB7	4.76	1.47	1.33
13	M	1316	U10	O4-C4	-4.76	1.25	1.36
6	M	1304	BCL	MG-ND	-4.67	1.96	2.05
10	M	1305	CDL	OB6-CB5	4.55	1.47	1.34
13	M	1316	U10	O3-C3	-4.39	1.26	1.36
4	H	1251	LDA	C1-N1	-4.13	1.47	1.51
6	L	1283	BCL	C1D-C2D	-4.06	1.37	1.45
6	M	1304	BCL	C4B-NB	3.98	1.43	1.37
6	M	1303	BCL	MG-ND	-3.80	1.98	2.05
6	M	1304	BCL	C1B-NB	3.78	1.42	1.37
4	M	1307	LDA	C1-N1	-3.75	1.47	1.51
6	L	1283	BCL	MG-NB	-3.68	1.98	2.05
4	M	1309	LDA	C1-N1	-3.66	1.47	1.51
6	L	1282	BCL	MG-ND	-3.65	1.98	2.05
9	M	1314	BPH	OBD-CAD	-3.36	1.17	1.22
9	M	1314	BPH	C4D-CHA	-3.31	1.34	1.39
4	M	1308	LDA	C1-N1	-3.31	1.48	1.51
9	L	1288	BPH	C4D-CHA	-3.30	1.34	1.39
6	L	1282	BCL	C1B-NB	3.17	1.42	1.37
6	L	1282	BCL	C4B-NB	3.07	1.41	1.37
6	L	1282	BCL	C1D-C2D	-3.00	1.39	1.45
9	L	1288	BPH	C3D-C2D	-2.99	1.34	1.39
6	M	1304	BCL	MG-NC	-2.98	1.99	2.06
6	M	1303	BCL	C4B-NB	2.98	1.41	1.37
6	M	1303	BCL	C1D-C2D	-2.91	1.39	1.45
9	M	1314	BPH	C4D-ND	-2.83	1.34	1.38
9	M	1314	BPH	C3D-C2D	-2.80	1.34	1.39
9	M	1314	BPH	C2C-C3C	-2.80	1.52	1.54
6	M	1304	BCL	C1D-ND	2.79	1.41	1.37
13	M	1316	U10	C6-C5	-2.75	1.38	1.46
6	L	1283	BCL	C4B-NB	2.71	1.41	1.37
13	M	1316	U10	C4-C5	-2.65	1.41	1.48
4	M	1310	LDA	C1-N1	-2.62	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1303	BCL	C1B-C2B	-2.40	1.37	1.43
6	L	1283	BCL	C1B-NB	2.39	1.41	1.37
13	M	1316	U10	C3-C2	-2.36	1.42	1.48
6	L	1282	BCL	C1B-C2B	-2.35	1.37	1.43
9	L	1288	BPH	C3D-C4D	2.35	1.44	1.41
8	M	1313	HTO	C4-C3	2.35	1.56	1.52
6	L	1283	BCL	C1B-C2B	-2.33	1.37	1.43
13	M	1316	U10	C6-C1	2.33	1.39	1.35
6	M	1304	BCL	C1D-C2D	-2.33	1.40	1.45
6	M	1304	BCL	MG-NA	-2.30	2.00	2.06
8	L	1286	HTO	O3-C3	2.30	1.48	1.43
13	M	1316	U10	C1-C2	-2.22	1.39	1.47
9	M	1314	BPH	C1B-C2B	-2.15	1.37	1.39
9	L	1288	BPH	CMD-C2D	-2.05	1.47	1.51
13	M	1316	U10	O4-C4M	-2.02	1.40	1.45

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1304	BCL	C1D-ND-C4D	-12.59	97.47	106.31
6	L	1282	BCL	C1D-ND-C4D	-8.53	100.33	106.31
6	M	1303	BCL	C1D-ND-C4D	-8.24	100.53	106.31
9	M	1314	BPH	C4D-CHA-CBD	7.67	112.14	108.45
9	M	1314	BPH	C2D-C1D-ND	-7.59	103.95	109.43
6	L	1283	BCL	C1D-ND-C4D	-7.49	101.06	106.31
6	M	1303	BCL	C1C-NC-C4C	7.31	110.01	106.68
9	M	1314	BPH	O2D-CGD-CBD	7.10	118.75	110.95
9	L	1288	BPH	C4D-CHA-CBD	6.59	111.61	108.45
6	M	1304	BCL	O2D-CGD-CBD	6.26	122.17	111.23
6	M	1304	BCL	C2D-C1D-ND	6.16	116.22	110.13
9	L	1288	BPH	C2D-C1D-ND	-6.15	104.99	109.43
10	M	1305	CDL	OA6-CA5-C11	5.02	122.34	111.48
13	M	1316	U10	C30-C29-C31	4.98	123.87	115.23
10	M	1305	CDL	OB6-CB5-C51	4.78	121.81	111.48
6	L	1282	BCL	C1C-NC-C4C	4.62	108.79	106.68
9	L	1288	BPH	C2B-C1B-NB	-4.42	106.23	109.43
9	L	1288	BPH	C4C-C3C-C2C	-4.42	98.64	102.84
6	L	1283	BCL	C1-O2A-CGA	4.42	127.34	116.65
6	M	1304	BCL	C1C-NC-C4C	4.37	108.67	106.68
6	L	1282	BCL	CHD-C1D-ND	-4.34	118.70	124.80
6	M	1303	BCL	CHD-C1D-ND	-4.31	118.74	124.80
13	M	1316	U10	C15-C14-C16	4.30	122.68	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1315	SPN	CM4-C9-C10	4.15	122.43	115.23
9	M	1314	BPH	C6-C5-C3	4.06	123.36	113.47
6	L	1283	BCL	O2A-CGA-CBA	4.03	124.13	111.83
12	M	1315	SPN	CM5-C13-C14	4.01	122.19	115.23
6	M	1304	BCL	C16-C15-C13	-3.98	102.72	115.97
9	M	1314	BPH	C2B-C1B-NB	-3.96	106.56	109.43
6	M	1303	BCL	O2A-CGA-CBA	3.93	123.82	111.83
6	M	1304	BCL	C4A-NA-C1A	3.88	108.45	106.68
6	L	1283	BCL	O2D-CGD-CBD	3.81	117.89	111.23
6	M	1304	BCL	C1D-CHD-C4C	-3.78	117.50	126.62
9	M	1314	BPH	C4D-ND-C1D	3.78	113.41	108.87
6	M	1304	BCL	CHB-C4A-NA	3.75	129.81	124.40
9	M	1314	BPH	O1D-CGD-CBD	-3.72	119.09	124.72
13	M	1316	U10	C17-C18-C19	-3.72	119.12	127.62
6	L	1282	BCL	O2A-CGA-CBA	3.71	123.15	111.83
13	M	1316	U10	C22-C23-C24	-3.68	119.20	127.62
6	M	1304	BCL	C3C-C4C-CHD	-3.65	115.69	123.39
6	L	1283	BCL	C11-C12-C13	-3.64	103.86	115.97
9	M	1314	BPH	C1-C2-C3	3.59	132.08	126.20
8	L	1286	HTO	O3-C3-C2	3.56	117.06	109.57
13	M	1316	U10	C6-C1-C2	3.49	121.92	119.17
10	M	1305	CDL	OB6-CB5-OB7	-3.49	115.55	123.70
6	L	1283	BCL	C2D-C1D-ND	3.47	113.56	110.13
13	M	1316	U10	C32-C33-C34	-3.45	119.72	127.62
6	M	1303	BCL	O2D-CGD-CBD	3.43	117.23	111.23
6	L	1283	BCL	C1C-NC-C4C	3.43	108.24	106.68
8	L	1286	HTO	C1-C2-C3	3.42	119.96	113.00
6	L	1282	BCL	O1D-CGD-CBD	-3.41	117.79	124.52
6	M	1304	BCL	C3D-C4D-ND	3.41	115.53	109.99
13	M	1316	U10	C10-C9-C11	3.39	121.12	115.23
9	M	1314	BPH	C1A-C2A-C3A	-3.38	99.63	102.84
13	M	1316	U10	C7-C8-C9	-3.33	121.10	126.83
6	M	1304	BCL	O1D-CGD-CBD	-3.30	118.01	124.52
9	L	1288	BPH	CAA-CBA-CGA	-3.28	103.91	113.21
9	L	1288	BPH	CBC-CAC-C3C	3.27	120.21	113.78
6	L	1283	BCL	CED-O2D-CGD	3.26	123.30	115.92
8	L	1286	HTO	C5-C4-C3	-3.23	108.82	114.11
6	M	1304	BCL	C5-C3-C2	-3.21	113.96	121.17
13	M	1316	U10	C27-C28-C29	-3.21	120.28	127.62
6	L	1282	BCL	C2D-C1D-ND	3.18	113.28	110.13
6	M	1303	BCL	C3D-C4D-ND	3.17	115.13	109.99
12	M	1315	SPN	CM6-C18-C17	3.16	120.72	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	1305	CDL	OA8-CA7-C31	3.13	121.39	111.83
9	L	1288	BPH	OBB-CAB-C3B	3.10	125.17	119.99
6	L	1282	BCL	C1-C2-C3	3.09	131.25	126.20
6	M	1303	BCL	C2D-C1D-ND	3.03	113.13	110.13
6	L	1283	BCL	C1-C2-C3	3.02	131.14	126.20
6	L	1282	BCL	O2D-CGD-CBD	3.02	116.50	111.23
6	L	1282	BCL	C2C-C3C-C4C	3.01	105.85	101.34
12	M	1315	SPN	CM3-C5-C6	3.00	120.43	115.23
10	M	1305	CDL	OB8-CB7-C71	2.98	120.93	111.83
6	M	1304	BCL	C6-C5-C3	-2.98	106.22	113.47
8	M	1313	HTO	O3-C3-C4	2.97	115.88	109.14
12	M	1315	SPN	C7-C8-C9	-2.94	120.89	127.62
13	M	1316	U10	C1M-C1-C6	-2.93	119.63	124.45
6	M	1304	BCL	CHD-C1D-ND	-2.92	120.69	124.80
6	M	1304	BCL	OBD-CAD-C3D	-2.88	121.68	128.42
6	L	1282	BCL	C3D-C4D-ND	2.88	114.67	109.99
13	M	1316	U10	C35-C34-C36	2.87	120.22	115.23
9	L	1288	BPH	CMA-C3A-C4A	-2.86	108.44	114.61
9	L	1288	BPH	OBB-CAB-CBB	-2.86	114.09	120.19
9	M	1314	BPH	C3D-CAD-CBD	2.85	111.36	107.61
9	M	1314	BPH	CBA-CAA-C2A	-2.79	105.57	113.78
6	M	1303	BCL	CHB-C4A-NA	2.77	128.40	124.40
6	L	1282	BCL	O2A-C1-C2	2.75	118.70	108.11
6	L	1282	BCL	CMC-C2C-C3C	-2.73	103.41	113.98
9	L	1288	BPH	O2D-CGD-CBD	2.73	113.95	110.95
6	M	1304	BCL	C4-C3-C5	2.73	119.97	115.23
4	M	1306	LDA	O1-N1-C1	2.73	115.96	109.27
9	M	1314	BPH	CMA-C3A-C4A	-2.70	108.79	114.61
6	L	1283	BCL	CHD-C1D-ND	-2.69	121.02	124.80
9	M	1314	BPH	OBB-CAB-CBB	-2.68	114.47	120.19
6	L	1282	BCL	C1-O2A-CGA	2.68	123.13	116.65
10	M	1305	CDL	CB4-OB6-CB5	-2.67	111.41	117.80
9	M	1314	BPH	OBB-CAB-C3B	2.66	124.43	119.99
6	L	1282	BCL	CHB-C4A-NA	2.63	128.20	124.40
6	M	1303	BCL	O2D-CGD-O1D	-2.59	118.80	123.85
10	M	1305	CDL	OA8-CA6-CA4	2.58	115.82	108.40
12	M	1315	SPN	C23-C24-C25	-2.56	105.44	112.16
6	L	1283	BCL	CAC-C3C-C4C	-2.54	106.94	112.58
6	M	1304	BCL	CAA-CBA-CGA	2.54	120.43	113.21
6	M	1303	BCL	CED-O2D-CGD	2.53	121.65	115.92
12	M	1315	SPN	C21-C20-C19	-2.52	105.53	112.16
6	M	1304	BCL	C16-C17-C18	-2.51	104.73	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1316	U10	C41-C39-C40	2.50	120.33	114.59
12	M	1315	SPN	CMB-C30-CM9	2.48	120.31	114.59
9	L	1288	BPH	C4D-ND-C1D	2.45	111.81	108.87
9	L	1288	BPH	C1A-C2A-C3A	-2.44	100.52	102.84
12	M	1315	SPN	C16-C17-C18	-2.44	107.53	113.47
10	M	1305	CDL	CB6-CB4-CB3	-2.44	106.11	111.78
13	M	1316	U10	C20-C19-C21	2.43	119.44	115.23
6	M	1303	BCL	O2A-CGA-O1A	-2.39	117.65	123.63
6	L	1283	BCL	O1D-CGD-CBD	-2.37	119.83	124.52
8	L	1287	HTO	O1-C1-C2	2.36	116.11	111.16
6	M	1303	BCL	CMA-C3A-C2A	-2.34	104.93	113.98
6	L	1283	BCL	C3C-C4C-CHD	-2.33	118.48	123.39
8	L	1287	HTO	C1-C2-C3	-2.32	108.28	113.00
9	M	1314	BPH	OBD-CAD-CBD	-2.32	122.42	125.82
13	M	1316	U10	C12-C13-C14	-2.32	122.32	127.62
6	M	1304	BCL	CHC-C4B-NB	-2.31	120.58	124.05
6	L	1283	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
6	M	1304	BCL	C1-O2A-CGA	2.31	122.24	116.65
6	L	1283	BCL	CHC-C4B-NB	-2.27	120.65	124.05
6	L	1282	BCL	CMD-C2D-C1D	2.23	128.66	124.73
10	M	1305	CDL	OB8-CB7-OB9	-2.21	118.10	123.63
10	M	1305	CDL	OA8-CA7-OA9	-2.20	118.12	123.63
8	L	1287	HTO	O2-C2-C1	2.17	113.97	109.03
6	M	1304	BCL	CHC-C1C-NC	2.15	127.51	124.40
13	M	1316	U10	C7-C6-C1	-2.15	121.20	124.89
12	M	1315	SPN	CMA-O1-C1	2.13	124.98	114.23
9	M	1314	BPH	C4C-C3C-C2C	-2.12	100.82	102.84
12	M	1315	SPN	CM5-C13-C12	-2.09	118.25	123.63
6	M	1303	BCL	CMD-C2D-C1D	2.09	128.41	124.73
6	L	1283	BCL	C4A-NA-C1A	-2.09	105.73	106.68
6	M	1304	BCL	CMD-C2D-C1D	2.08	128.40	124.73
13	M	1316	U10	C40-C39-C38	-2.07	116.44	122.66
6	M	1304	BCL	O2D-CGD-O1D	-2.07	119.82	123.85
9	M	1314	BPH	CMD-C2D-C3D	2.06	128.80	124.68
8	L	1286	HTO	O2-C2-C1	-2.06	104.34	109.03
9	L	1288	BPH	C4-C3-C2	2.03	128.85	123.63
6	M	1304	BCL	OBB-CAB-CBB	-2.03	115.22	119.77
12	M	1315	SPN	O1-C1-C2	2.02	113.03	108.90
10	M	1305	CDL	CA6-OA8-CA7	2.01	124.47	117.12
6	M	1304	BCL	CBA-CAA-C2A	-2.01	107.81	113.79

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	1286	HTO	C2
8	L	1287	HTO	C2
8	M	1313	HTO	C2
9	L	1288	BPH	C8
9	L	1288	BPH	C13
9	M	1314	BPH	C8
9	M	1314	BPH	C13

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1306	LDA	C2-C1-N1-CM1
4	M	1309	LDA	C2-C1-N1-O1
4	M	1309	LDA	C2-C1-N1-CM1
4	M	1309	LDA	C2-C1-N1-CM2
4	M	1309	LDA	N1-C1-C2-C3
4	M	1310	LDA	N1-C1-C2-C3
6	L	1282	BCL	C4C-C3C-CAC-CBC
6	M	1304	BCL	CHA-CBD-CGD-O1D
6	M	1304	BCL	CHA-CBD-CGD-O2D
8	L	1287	HTO	C1-C2-C3-O3
8	M	1313	HTO	O2-C2-C3-C4
8	M	1313	HTO	C2-C3-C4-C5
8	M	1313	HTO	O3-C3-C4-C5
9	M	1314	BPH	C2C-C3C-CAC-CBC
9	M	1314	BPH	C11-C10-C8-C9
10	M	1305	CDL	CA2-OA2-PA1-OA3
10	M	1305	CDL	CA2-OA2-PA1-OA4
10	M	1305	CDL	CA2-OA2-PA1-OA5
10	M	1305	CDL	CA3-OA5-PA1-OA4
10	M	1305	CDL	CB2-OB2-PB2-OB3
10	M	1305	CDL	CB2-OB2-PB2-OB4
10	M	1305	CDL	CB2-OB2-PB2-OB5
13	M	1316	U10	C27-C28-C29-C30
13	M	1316	U10	C27-C28-C29-C31
12	M	1315	SPN	C11-C10-C9-CM4
13	M	1316	U10	C37-C38-C39-C40
9	M	1314	BPH	C3-C5-C6-C7
10	M	1305	CDL	O1-C1-CA2-OA2
12	M	1315	SPN	C16-C17-C18-CM6
12	M	1315	SPN	C16-C17-C18-C19
8	L	1286	HTO	O1-C1-C2-C3
12	M	1315	SPN	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
13	M	1316	U10	C37-C38-C39-C41
12	M	1315	SPN	CM7-C22-C23-C24
9	M	1314	BPH	C12-C13-C15-C16
12	M	1315	SPN	C26-C27-C28-C29
13	M	1316	U10	C29-C31-C32-C33
12	M	1315	SPN	C14-C15-C16-C17
6	L	1282	BCL	C10-C11-C12-C13
6	L	1282	BCL	C15-C16-C17-C18
9	M	1314	BPH	C13-C15-C16-C17
9	L	1288	BPH	CBD-CGD-O2D-CED
6	M	1303	BCL	C5-C6-C7-C8
6	L	1283	BCL	C16-C17-C18-C19
7	L	1284	GOL	O1-C1-C2-C3
6	L	1282	BCL	O2A-C1-C2-C3
4	M	1308	LDA	C2-C3-C4-C5
10	M	1305	CDL	C73-C74-C75-C76
10	M	1305	CDL	C39-C40-C41-C42
6	L	1282	BCL	C6-C7-C8-C10
9	L	1288	BPH	C11-C10-C8-C7
10	M	1305	CDL	C51-C52-C53-C54
10	M	1305	CDL	CB2-C1-CA2-OA2
6	L	1283	BCL	C16-C17-C18-C20
9	L	1288	BPH	C14-C13-C15-C16
4	M	1309	LDA	C1-C2-C3-C4
10	M	1305	CDL	C76-C77-C78-C79
10	M	1305	CDL	C54-C55-C56-C57
6	M	1304	BCL	C16-C17-C18-C19
10	M	1305	CDL	C79-C80-C81-C82
10	M	1305	CDL	CB5-C51-C52-C53
10	M	1305	CDL	C56-C57-C58-C59
9	M	1314	BPH	C10-C11-C12-C13
4	M	1309	LDA	C4-C5-C6-C7
10	M	1305	CDL	C71-C72-C73-C74
10	M	1305	CDL	OB5-CB3-CB4-CB6
12	M	1315	SPN	C21-C22-C23-C24
6	M	1304	BCL	C16-C17-C18-C20
6	M	1304	BCL	C13-C15-C16-C17
4	M	1309	LDA	C7-C8-C9-C10
6	L	1282	BCL	C6-C7-C8-C9
6	M	1304	BCL	C14-C13-C15-C16
12	M	1315	SPN	C20-C21-C22-CM7
10	M	1305	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	M	1310	LDA	C3-C4-C5-C6
9	L	1288	BPH	O1D-CGD-O2D-CED
9	L	1288	BPH	C2-C3-C5-C6
4	M	1307	LDA	C5-C6-C7-C8
4	M	1306	LDA	C1-C2-C3-C4
9	L	1288	BPH	O2A-C1-C2-C3
6	M	1303	BCL	C15-C16-C17-C18
10	M	1305	CDL	C51-CB5-OB6-CB4
9	L	1288	BPH	C4-C3-C5-C6
8	M	1313	HTO	C4-C5-C6-C7
4	M	1310	LDA	C1-C2-C3-C4
9	M	1314	BPH	C8-C10-C11-C12
4	M	1309	LDA	C3-C4-C5-C6
7	L	1284	GOL	O1-C1-C2-O2
6	L	1283	BCL	C11-C12-C13-C14
9	M	1314	BPH	C14-C13-C15-C16
10	M	1305	CDL	C53-C54-C55-C56
4	M	1307	LDA	C9-C10-C11-C12
4	H	1251	LDA	C11-C10-C9-C8
6	L	1283	BCL	C11-C12-C13-C15
6	M	1304	BCL	C12-C13-C15-C16
10	M	1305	CDL	C61-C62-C63-C64
10	M	1305	CDL	C74-C75-C76-C77
10	M	1305	CDL	C35-C36-C37-C38
12	M	1315	SPN	CM1-C1-C2-O2
12	M	1315	SPN	CM1-C1-C2-C3
10	M	1305	CDL	C80-C81-C82-C83
13	M	1316	U10	C14-C16-C17-C18
9	L	1288	BPH	C10-C11-C12-C13
4	M	1308	LDA	C4-C5-C6-C7
4	M	1309	LDA	C6-C7-C8-C9
10	M	1305	CDL	OB5-CB3-CB4-OB6
10	M	1305	CDL	C36-C37-C38-C39
10	M	1305	CDL	C41-C42-C43-C44
8	L	1286	HTO	O1-C1-C2-O2
12	M	1315	SPN	O1-C1-C2-O2
10	M	1305	CDL	C59-C60-C61-C62
9	M	1314	BPH	C5-C6-C7-C8
10	M	1305	CDL	OB7-CB5-OB6-CB4
12	M	1315	SPN	CM8-C26-C27-C28
6	M	1304	BCL	C3-C5-C6-C7
4	H	1251	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	M	1305	CDL	OA6-CA4-CA6-OA8
4	H	1251	LDA	C3-C4-C5-C6
4	M	1310	LDA	C5-C6-C7-C8
4	M	1306	LDA	C2-C1-N1-CM2
4	H	1251	LDA	C2-C3-C4-C5
12	M	1315	SPN	C25-C26-C27-C28
9	L	1288	BPH	C3-C5-C6-C7
9	M	1314	BPH	C6-C7-C8-C10
6	L	1282	BCL	C8-C10-C11-C12
10	M	1305	CDL	CB3-CB4-CB6-OB8
4	M	1309	LDA	C9-C10-C11-C12
6	L	1282	BCL	CHA-CBD-CGD-O1D
6	L	1282	BCL	CHA-CBD-CGD-O2D
8	L	1287	HTO	O2-C2-C3-O3
10	M	1305	CDL	CA3-OA5-PA1-OA2
10	M	1305	CDL	CA3-OA5-PA1-OA3
12	M	1315	SPN	CM3-C5-C6-C7
4	M	1307	LDA	C7-C8-C9-C10
12	M	1315	SPN	C4-C5-C6-C7
4	M	1310	LDA	C11-C10-C9-C8
10	M	1305	CDL	C13-C14-C15-C16
4	H	1251	LDA	C1-C2-C3-C4
9	L	1288	BPH	C11-C10-C8-C9
12	M	1315	SPN	C19-C20-C21-C22
4	M	1309	LDA	C2-C3-C4-C5
10	M	1305	CDL	C1-CB2-OB2-PB2
13	M	1316	U10	C5-C4-O4-C4M
4	M	1310	LDA	C6-C7-C8-C9
4	M	1306	LDA	C3-C4-C5-C6
4	M	1306	LDA	C9-C10-C11-C12
4	M	1308	LDA	C9-C10-C11-C12
9	M	1314	BPH	C11-C10-C8-C7
4	M	1308	LDA	C1-C2-C3-C4
9	L	1288	BPH	C8-C10-C11-C12
9	M	1314	BPH	C6-C7-C8-C9
10	M	1305	CDL	C31-C32-C33-C34
4	H	1251	LDA	N1-C1-C2-C3
4	M	1306	LDA	C11-C10-C9-C8
9	L	1288	BPH	C11-C12-C13-C15
4	H	1251	LDA	C2-C1-N1-CM2
10	M	1305	CDL	C72-C71-CB7-OB8
12	M	1315	SPN	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
6	M	1304	BCL	C2B-C3B-CAB-CBB
6	M	1304	BCL	C4B-C3B-CAB-CBB
10	M	1305	CDL	C72-C71-CB7-OB9
4	M	1306	LDA	C2-C1-N1-O1
13	M	1316	U10	C1-C6-C7-C8
6	M	1303	BCL	CAA-CBA-CGA-O2A
9	M	1314	BPH	C4C-C3C-CAC-CBC

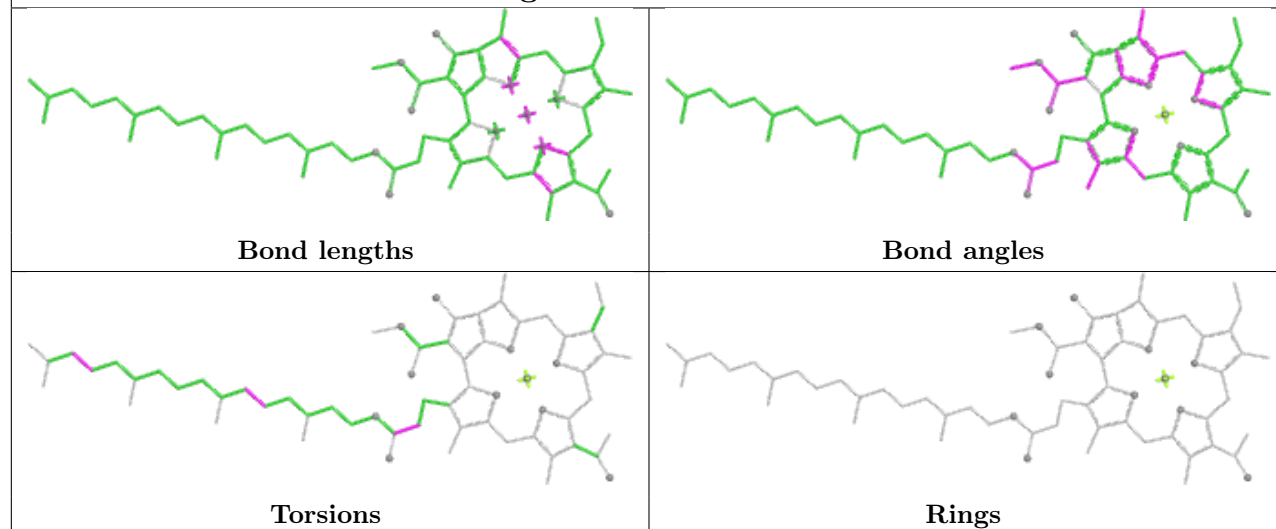
There are no ring outliers.

17 monomers are involved in 76 short contacts:

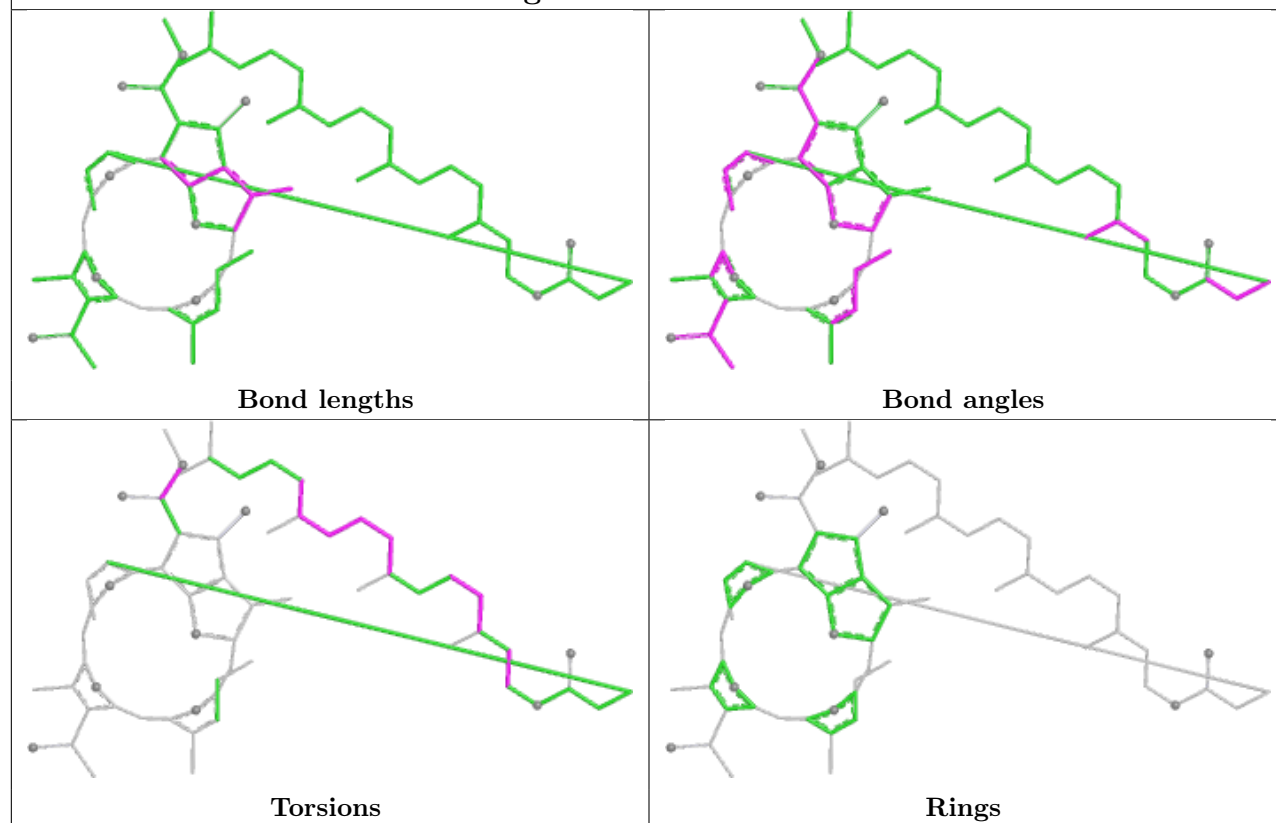
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1307	LDA	4	0
8	M	1313	HTO	7	0
6	M	1303	BCL	12	0
8	L	1286	HTO	1	0
9	L	1288	BPH	8	0
4	H	1251	LDA	2	0
8	L	1287	HTO	3	0
9	M	1314	BPH	7	0
4	M	1310	LDA	2	0
13	M	1316	U10	5	0
6	L	1282	BCL	12	0
6	L	1283	BCL	6	0
12	M	1315	SPN	10	0
4	M	1306	LDA	3	0
10	M	1305	CDL	3	0
4	M	1309	LDA	2	0
6	M	1304	BCL	6	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.

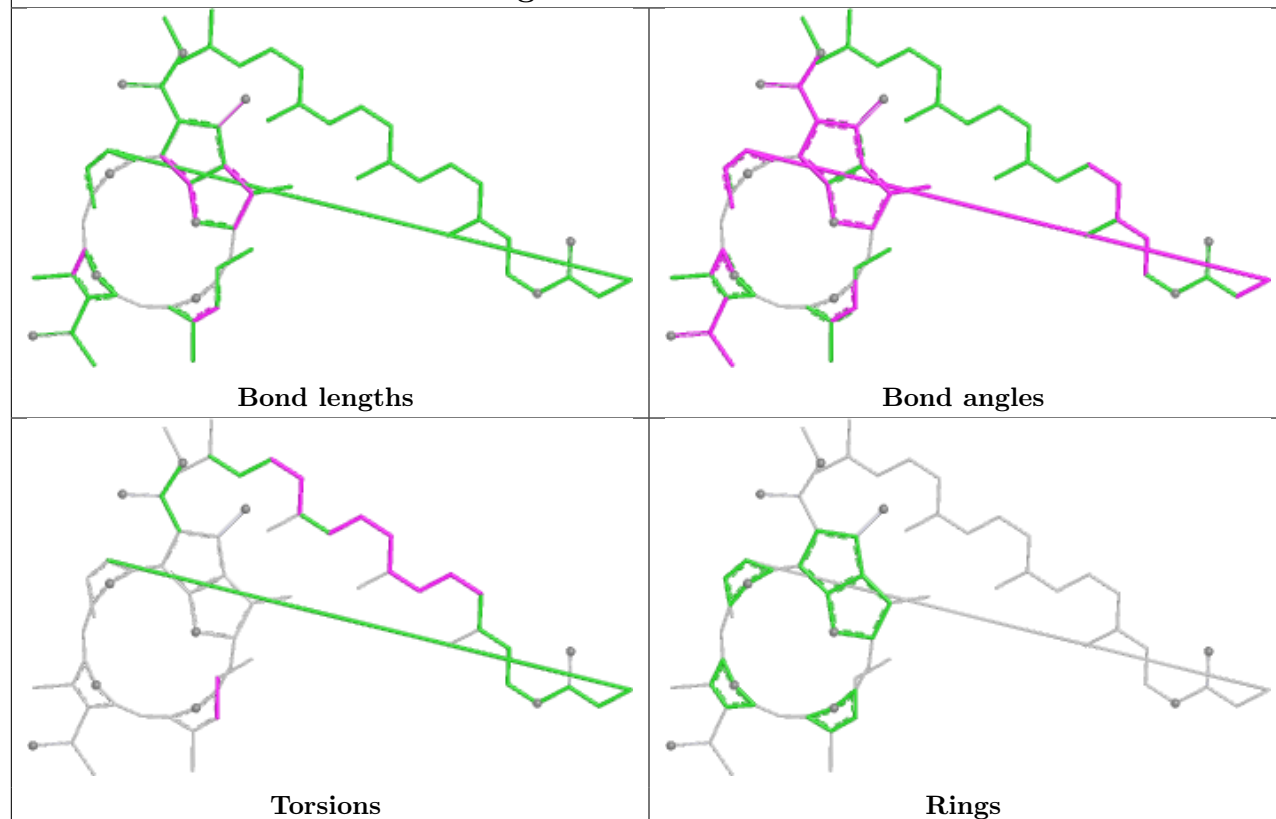
Ligand BCL M 1303



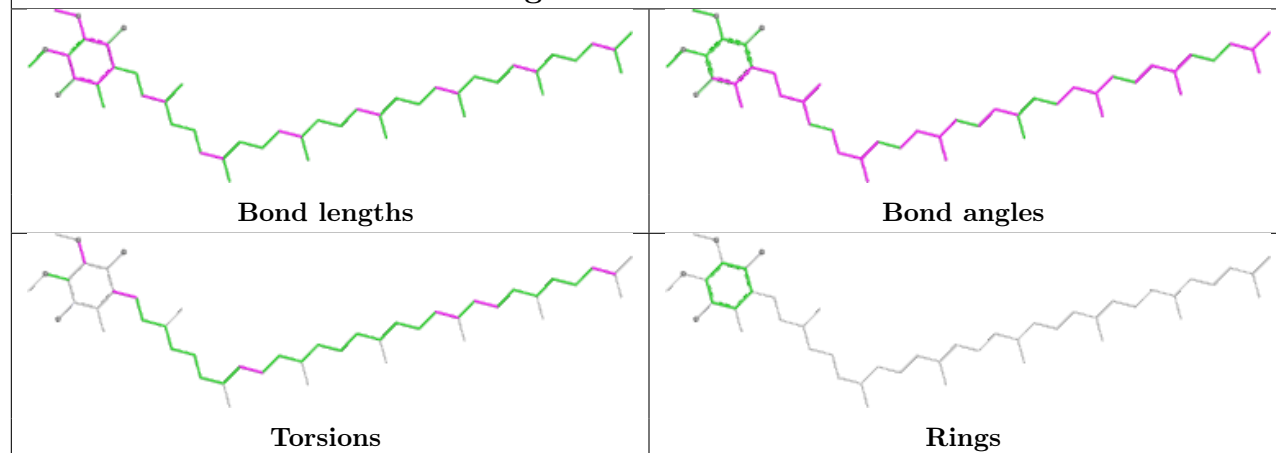
Ligand BPH L 1288

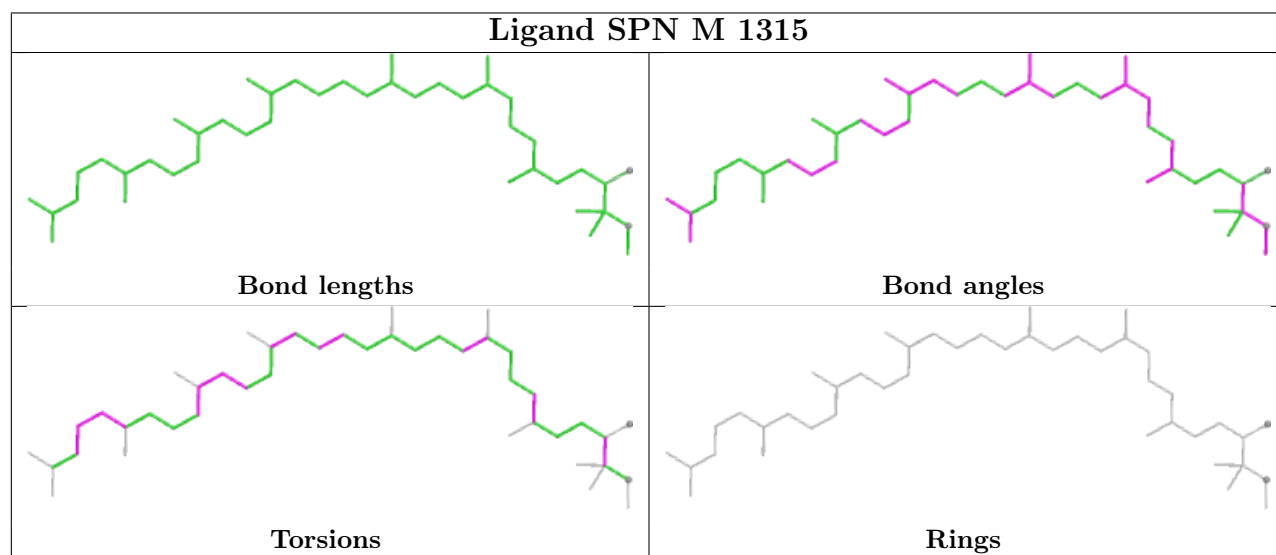
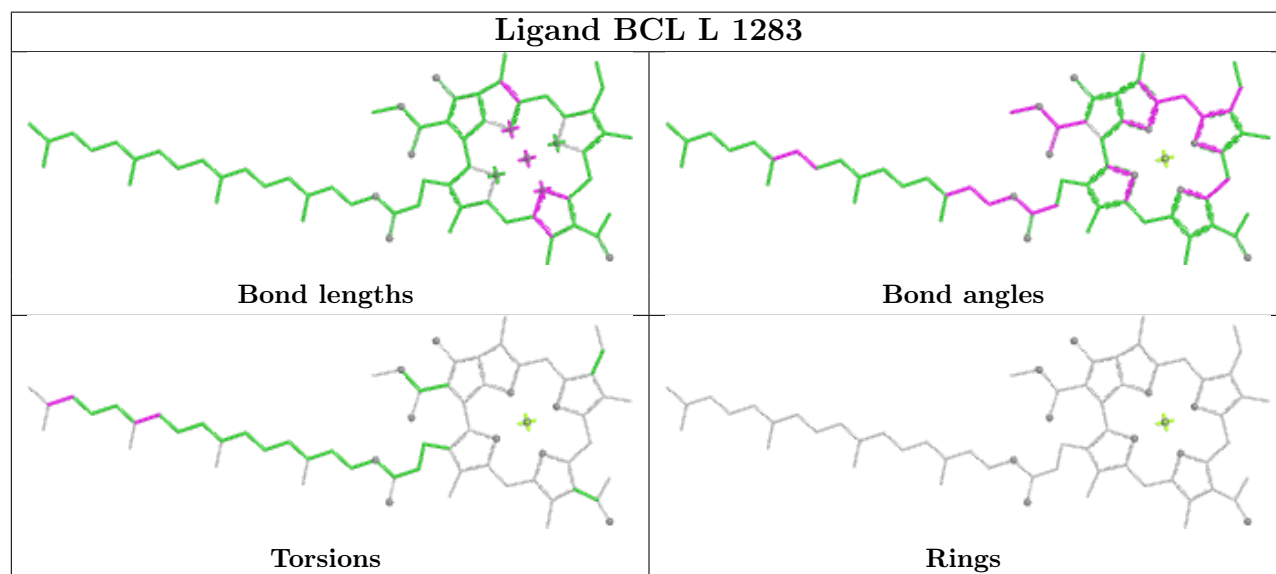
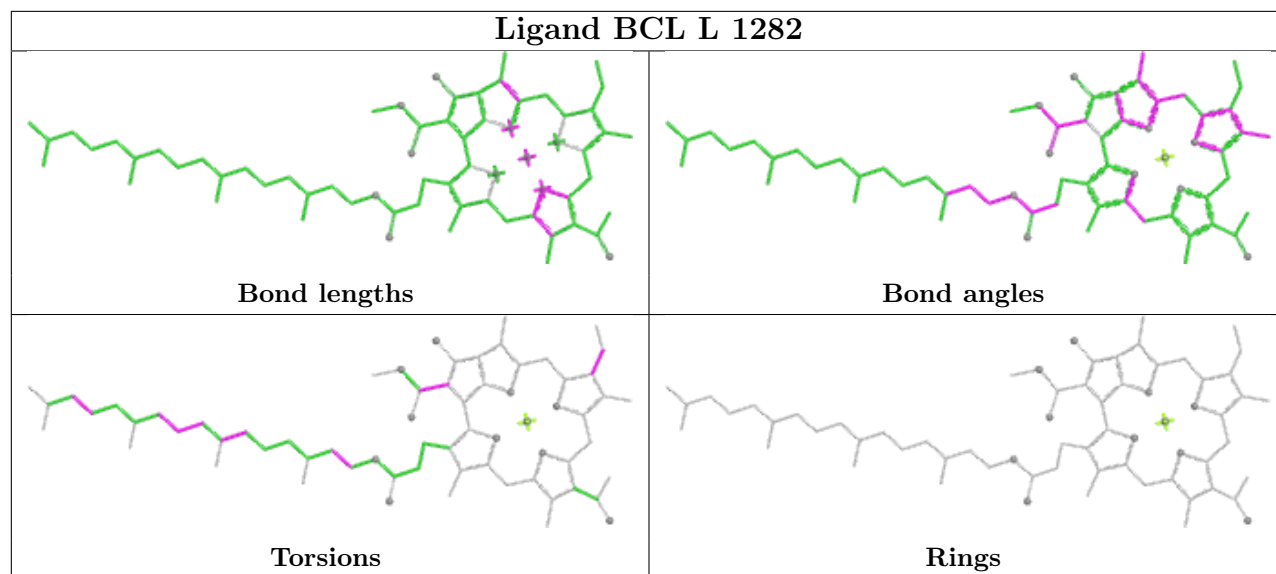


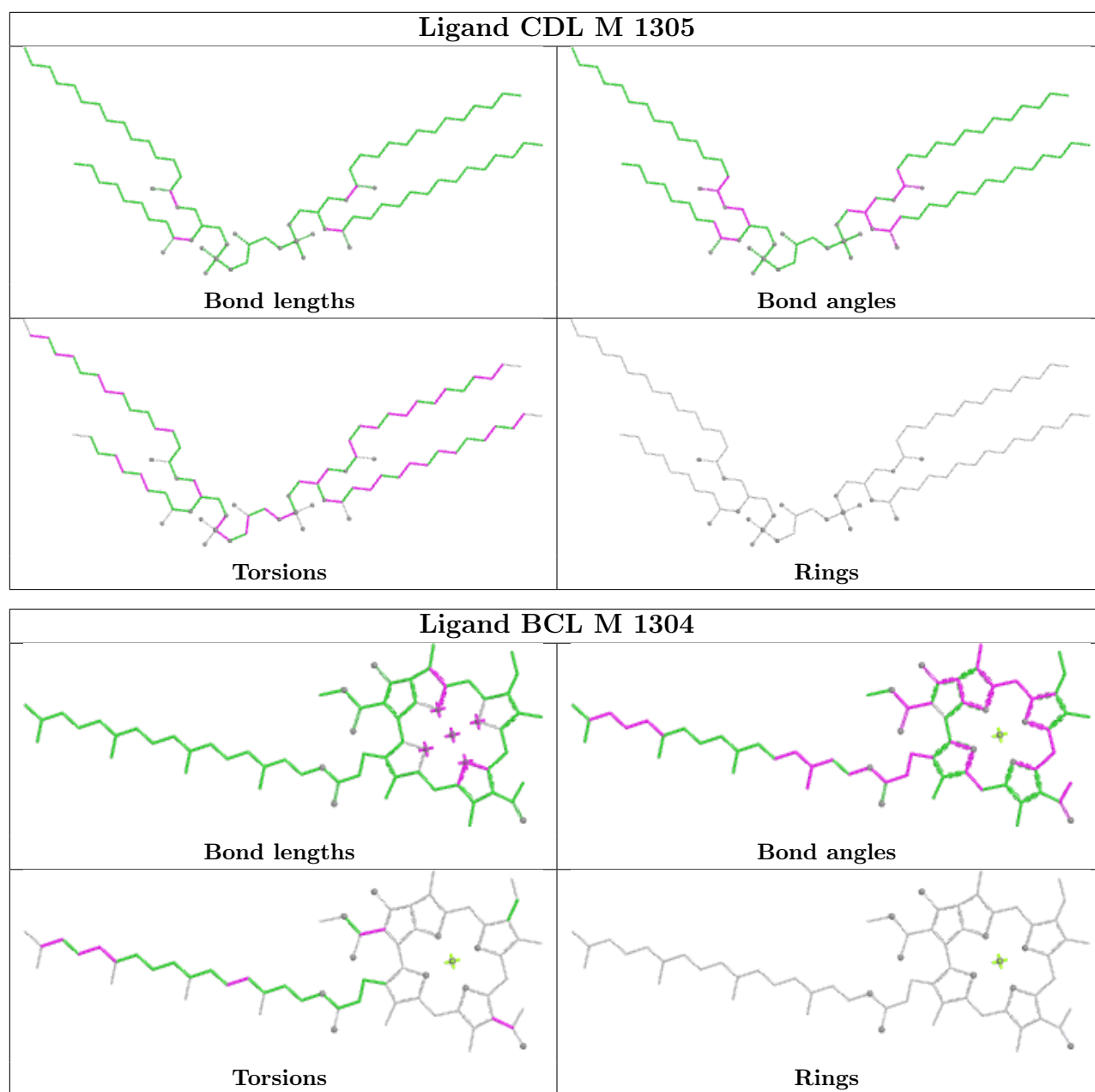
Ligand BPH M 1314



Ligand U10 M 1316







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	H	240/260 (92%)	0.79	17 (7%)	22 18	48, 63, 84, 171	0
2	L	281/281 (100%)	0.99	42 (14%)	5 4	42, 62, 103, 129	0
3	M	302/307 (98%)	0.89	31 (10%)	12 9	42, 64, 101, 118	0
All	All	823/848 (97%)	0.90	90 (10%)	10 8	42, 63, 99, 171	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	245	ALA	6.6
2	L	83	GLY	6.2
1	H	248	ARG	6.1
1	H	246	PRO	5.4
1	H	250	SER	5.4
2	L	59	TRP	4.8
3	M	52	LEU	4.8
1	H	247	LYS	4.5
2	L	51	TRP	4.2
3	M	1	ALA	4.1
2	L	82	LYS	3.8
2	L	1	ALA	3.8
2	L	46	ILE	3.7
3	M	83	ALA	3.6
2	L	87	GLN	3.6
3	M	169	GLY	3.6
3	M	105	PHE	3.6
3	M	109	LEU	3.5
1	H	249	LYS	3.5
2	L	58	THR	3.4
2	L	273	ALA	3.4
2	L	73	TYR	3.4
2	L	80	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	M	84	VAL	3.4
2	L	55	LEU	3.2
2	L	269	LEU	3.2
3	M	283	GLY	3.0
2	L	268	LYS	3.0
2	L	90	THR	2.9
3	M	76	TYR	2.9
2	L	81	ALA	2.9
3	M	78	ALA	2.8
1	H	79	GLU	2.8
2	L	54	VAL	2.8
2	L	72	GLU	2.8
3	M	302	GLY	2.7
2	L	84	GLY	2.7
2	L	155	ASP	2.7
2	L	40	PHE	2.6
3	M	97	PRO	2.6
1	H	127	GLY	2.5
2	L	67	TYR	2.5
3	M	2	GLU	2.5
3	M	7	PHE	2.5
2	L	14	GLY	2.5
3	M	28	ASN	2.4
1	H	221	SER	2.4
3	M	101	TYR	2.4
2	L	275	ILE	2.4
2	L	43	ALA	2.4
2	L	222	TYR	2.4
1	H	124	ASP	2.4
2	L	277	GLY	2.4
3	M	236	GLU	2.3
2	L	50	ALA	2.3
2	L	71	LEU	2.3
2	L	134	PHE	2.3
2	L	192	ALA	2.3
2	L	270	PRO	2.3
3	M	294	TRP	2.3
2	L	133	LEU	2.3
3	M	45	ALA	2.2
3	M	112	GLY	2.2
1	H	156	CYS	2.2
2	L	74	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	143	GLY	2.2
3	M	111	GLU	2.2
3	M	82	PRO	2.2
2	L	62	GLN	2.2
2	L	235	LEU	2.2
3	M	298	GLY	2.2
3	M	59	SER	2.2
1	H	128	HIS	2.2
3	M	27	ALA	2.2
3	M	205	SER	2.2
1	H	80	SER	2.1
3	M	72	ILE	2.1
2	L	47	ILE	2.1
1	H	207	ALA	2.1
2	L	271	TRP	2.1
3	M	168	MET	2.1
3	M	114	LEU	2.1
2	L	144	TYR	2.1
2	L	137	VAL	2.1
2	L	141	ALA	2.0
3	M	98	ALA	2.0
1	H	52	ASN	2.0
1	H	155	GLY	2.0
3	M	170	SER	2.0
1	H	206	ASN	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 ⓘ

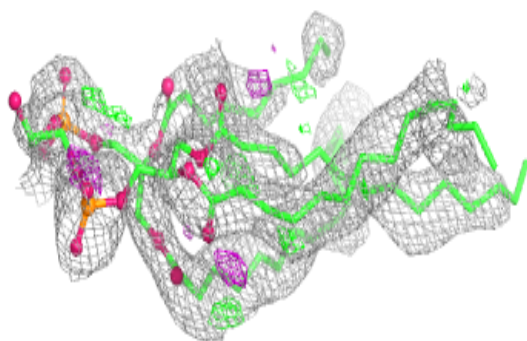
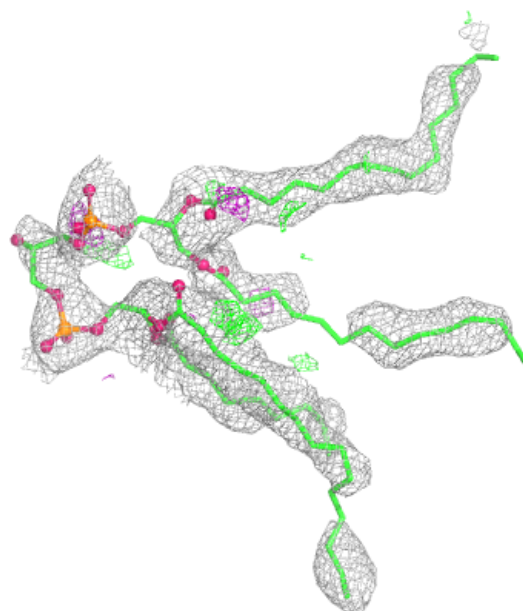
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	HTO	L	1287	10/10	0.56	0.20	92,97,101,102	0
4	LDA	M	1309	16/16	0.59	0.38	115,132,147,148	0
4	LDA	H	1251	16/16	0.67	0.30	98,130,149,151	0
7	GOL	L	1284	6/6	0.72	0.22	84,90,95,95	0
4	LDA	M	1308	16/16	0.76	0.27	74,113,155,156	0
4	LDA	M	1310	16/16	0.77	0.24	74,88,126,127	0
8	HTO	L	1286	10/10	0.79	0.24	71,75,90,97	0
7	GOL	L	1285	6/6	0.79	0.15	86,106,108,109	0
10	CDL	M	1305	81/100	0.80	0.22	52,98,114,118	0
8	HTO	M	1313	10/10	0.81	0.18	77,89,95,97	0
4	LDA	M	1306	16/16	0.84	0.18	52,89,101,102	0
4	LDA	M	1307	16/16	0.87	0.20	88,98,122,123	0
6	BCL	L	1282	66/66	0.87	0.17	42,57,125,132	0
9	BPH	M	1314	65/65	0.88	0.15	44,71,128,133	0
5	NA	M	1311	1/1	0.89	0.17	71,71,71,71	0
12	SPN	M	1315	43/43	0.89	0.17	47,77,114,118	0
13	U10	M	1316	48/63	0.90	0.14	40,68,98,105	0
6	BCL	M	1303	66/66	0.92	0.11	39,56,78,103	0
6	BCL	L	1283	66/66	0.93	0.12	39,56,67,83	0
9	BPH	L	1288	65/65	0.94	0.10	30,52,77,81	0
6	BCL	M	1304	66/66	0.95	0.10	14,45,78,88	0
5	NA	H	1252	1/1	0.98	0.04	45,45,45,45	0
11	FE	M	1312	1/1	1.00	0.01	49,49,49,49	0

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

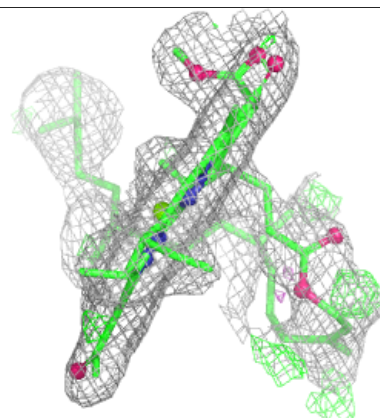
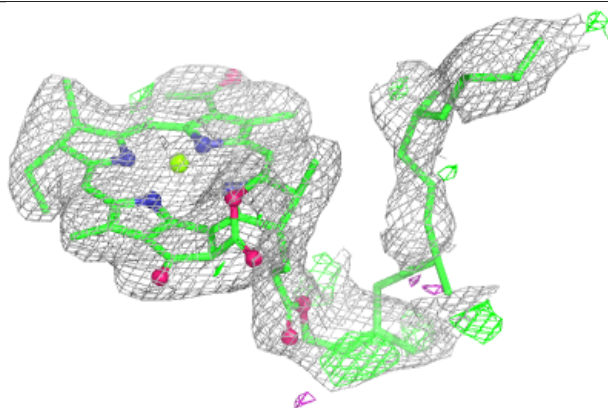
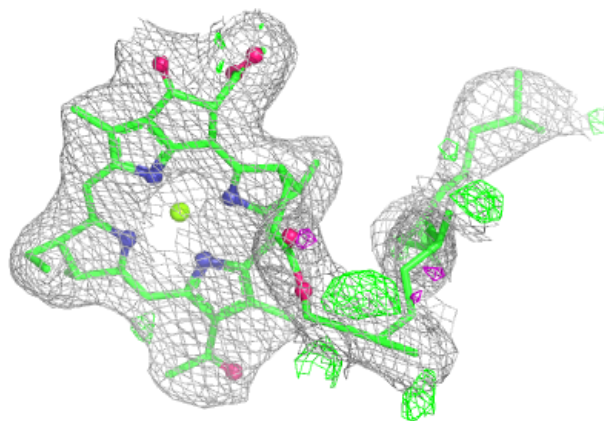
Electron density around CDL M 1305:

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

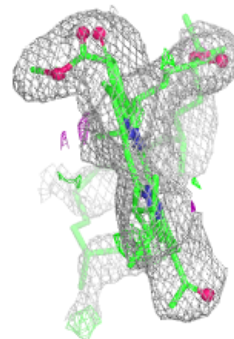
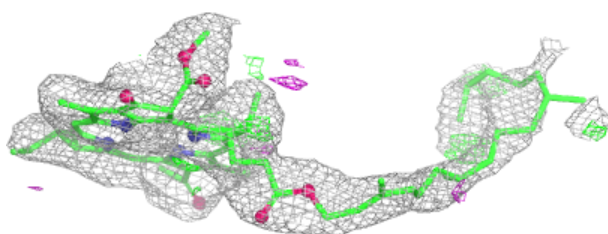
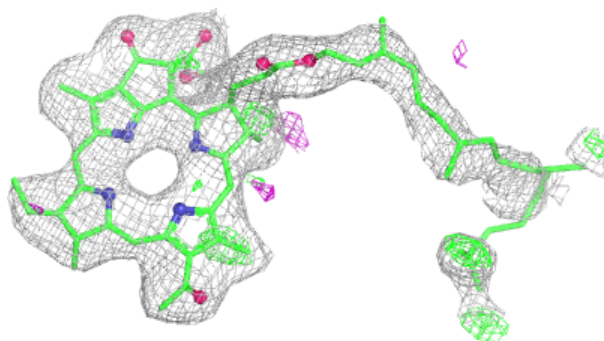


Electron density around BCL L 1282:

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

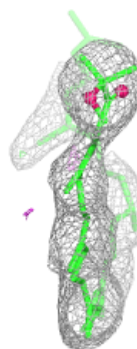
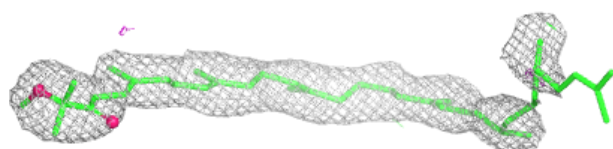
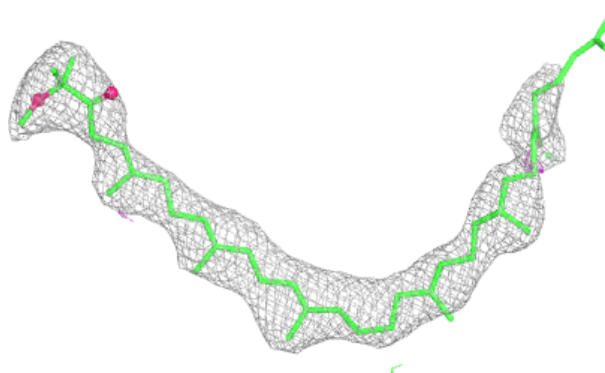
**Electron density around BPH M 1314:**

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

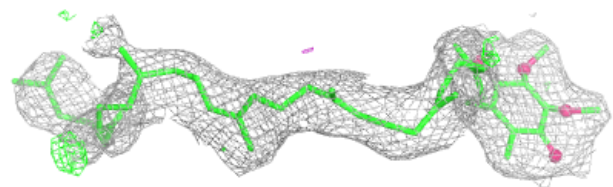
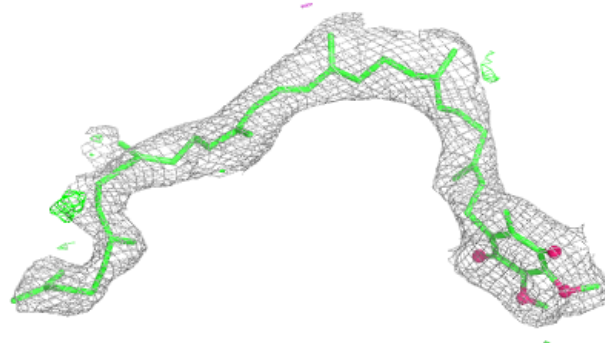


Electron density around SPN M 1315:

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

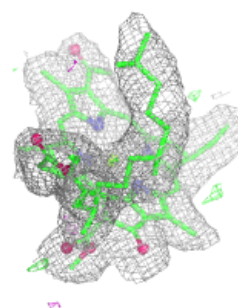
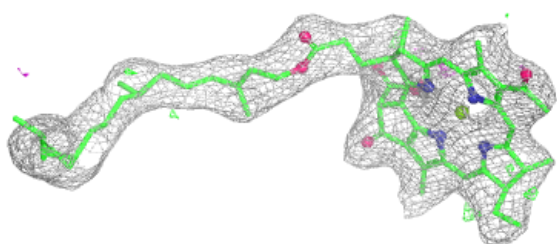
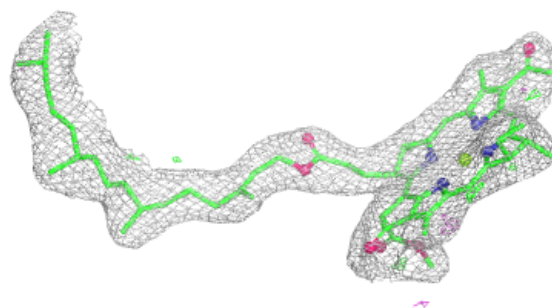
**Electron density around U10 M 1316:**

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

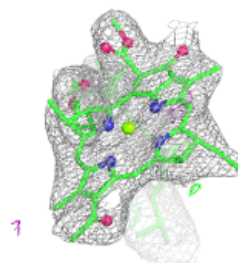
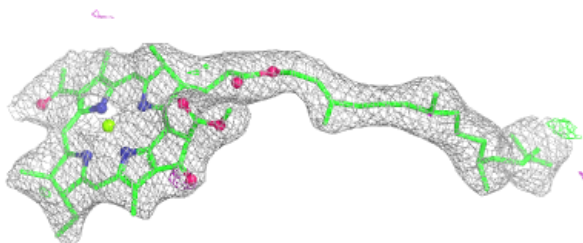
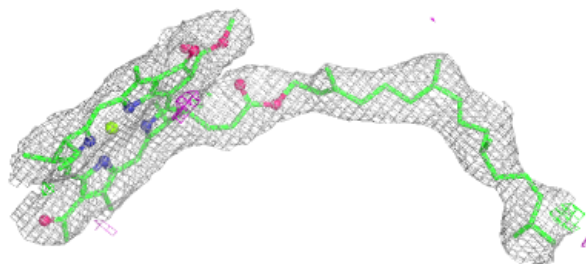


Electron density around BCL M 1303:

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

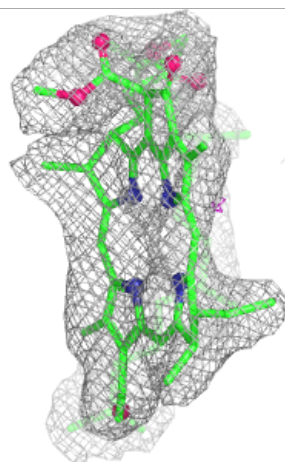
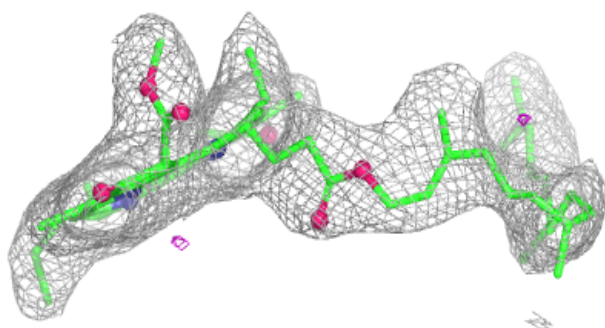
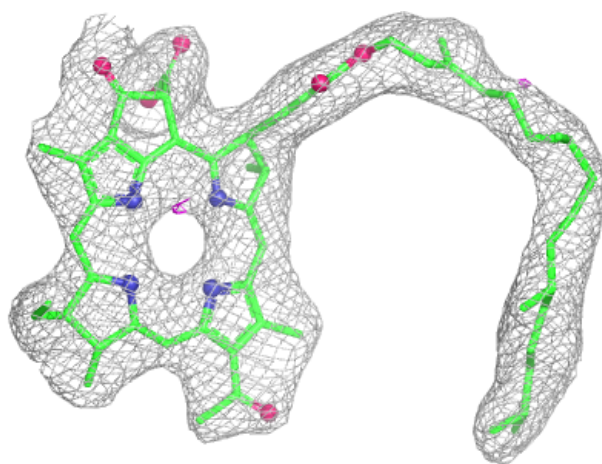
**Electron density around BCL L 1283:**

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



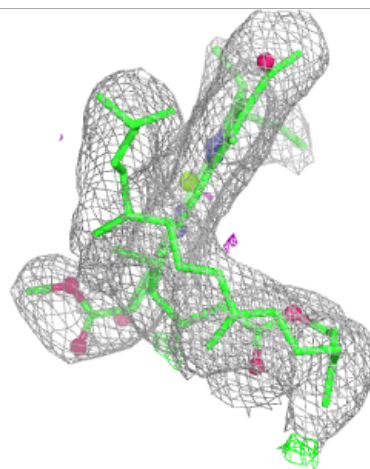
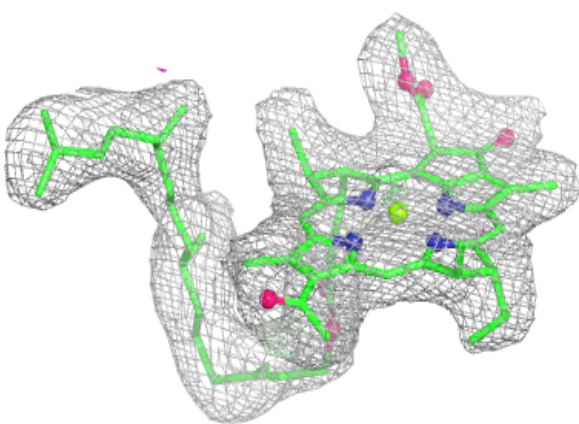
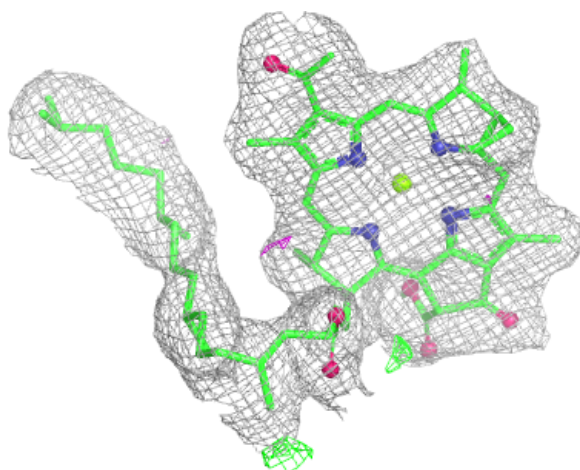
Electron density around BPH L 1288:

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



Electron density around BCL M 1304:

$2mF_o-DF_c$ (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.