



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 07:29 am BST

PDB ID : 2BOZ
Title : Photosynthetic Reaction Center Mutant With Gly M203 Replaced With Leu
Authors : Potter, J.P.; Fyfe, P.K.; Jones, M.R.
Deposited on : 2005-04-15
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

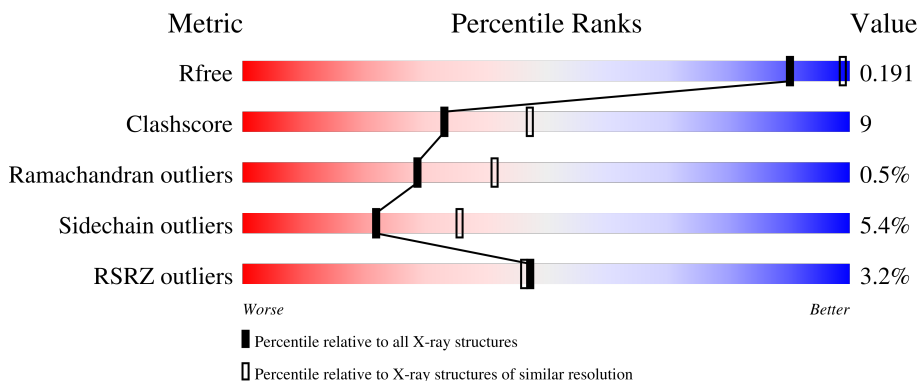
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
2	L	281	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>
3	M	307	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7475 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
			Total	C	N	O	S			
1	H	241	1830	1169	315	337	9	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2232	1507	355	362	8	0	0	0

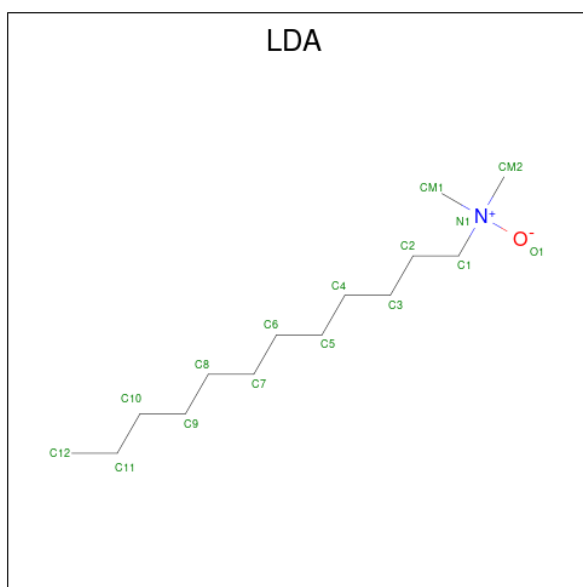
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2413	1611	395	397	10	0	0	1

There is a discrepancy between the modelled and reference sequences:

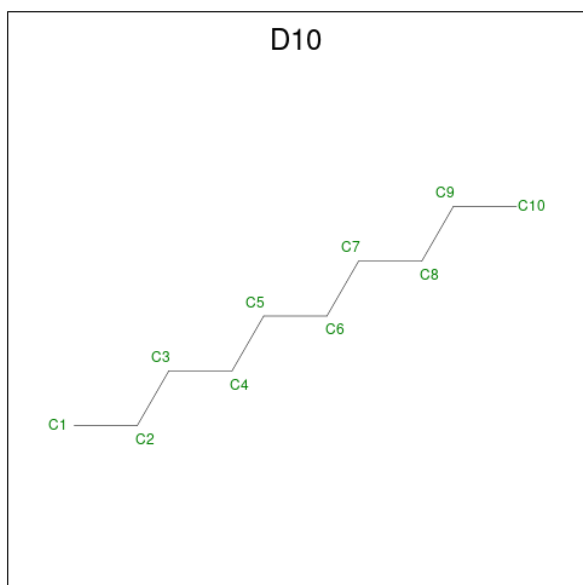
Chain	Residue	Modelled	Actual	Comment	Reference
M	203	LEU	GLY	engineered mutation	UNP P11846

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



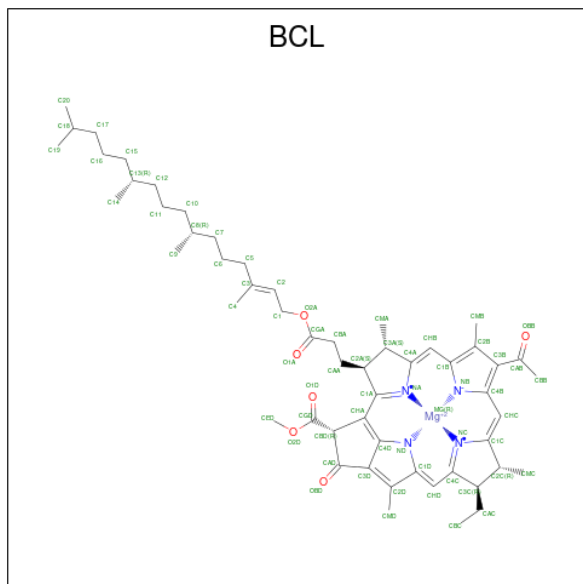
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



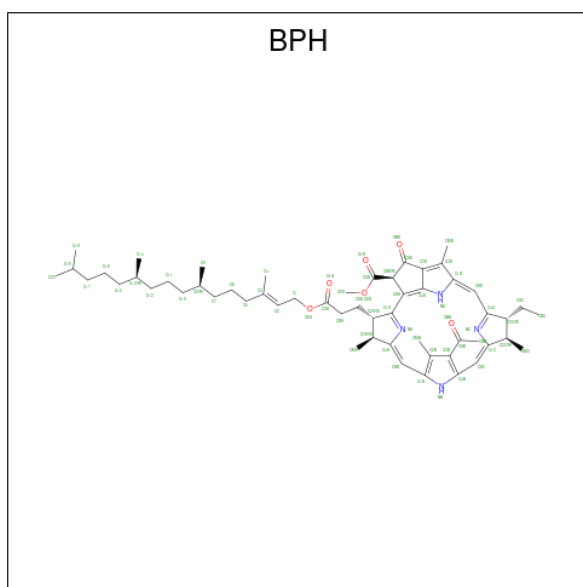
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C 9 9	0	0
5	H	1	Total C 8 8	0	0
5	H	1	Total C 7 7	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



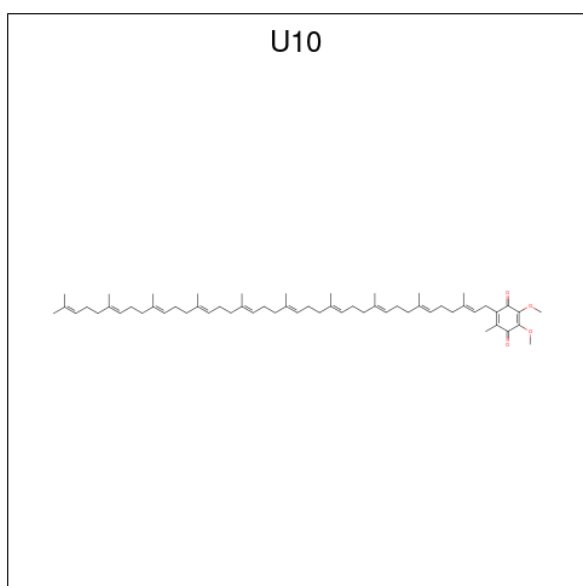
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



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

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

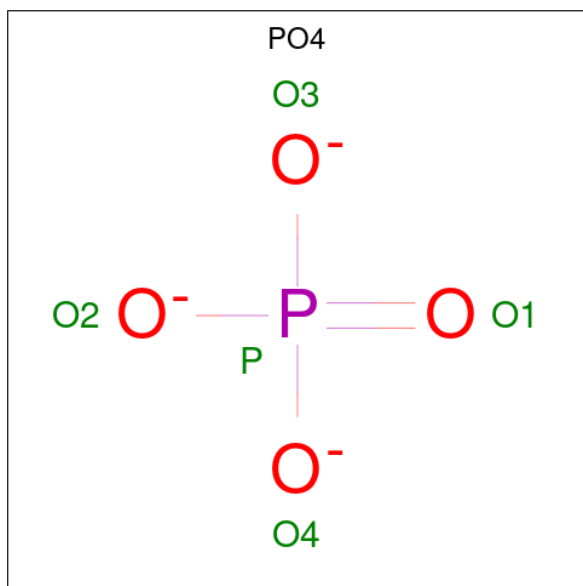


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	48	44	4	14	0
8	M	1	48	44	4	0	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

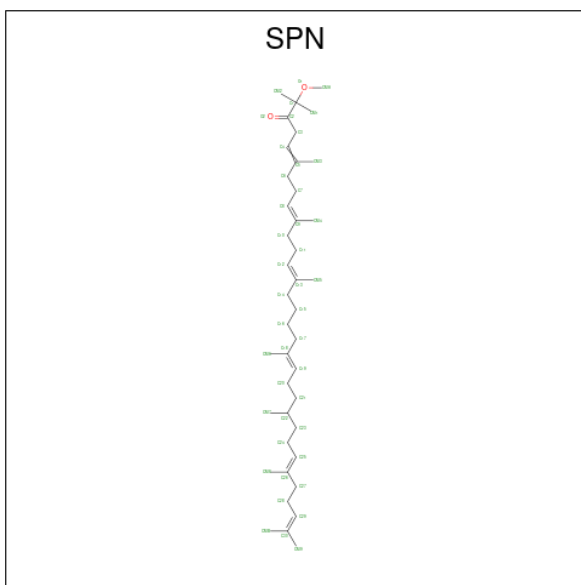
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 11 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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


- Molecule 12 is water.

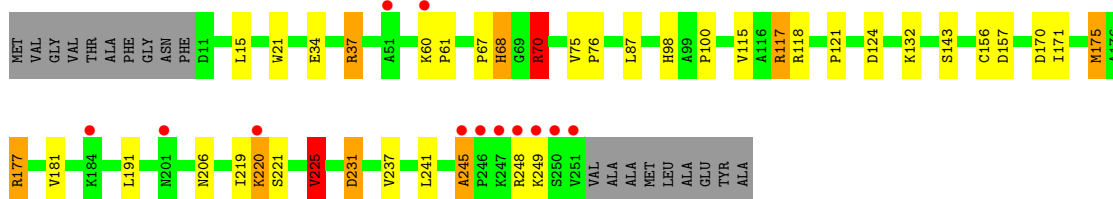
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	174	Total	O	0	0
			174	174		
12	L	95	Total	O	0	0
			95	95		
12	M	99	Total	O	0	0
			99	99		

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.

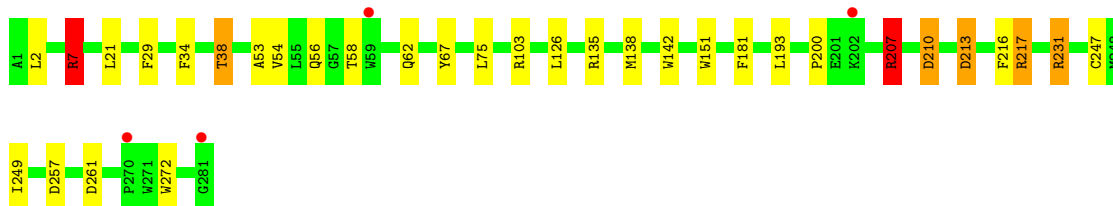
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H: 




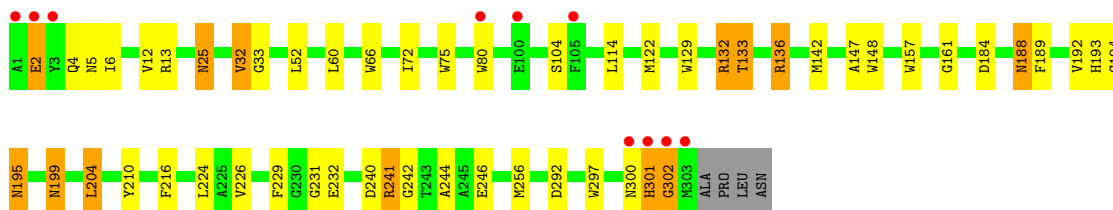
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L: 



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M: 



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.61Å 138.61Å 185.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.96 – 2.40 17.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (17.96-2.40) 99.5 (17.96-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.174 , 0.198 0.167 , 0.191	Depositor DCC
R_{free} test set	3991 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: U10, PO4, BPH, SPN, BCL, D10, FE, LDA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.86	1/1878 (0.1%)	1.06	12/2555 (0.5%)
2	L	0.91	0/2320	0.96	17/3175 (0.5%)
3	M	0.83	0/2505	0.88	8/3421 (0.2%)
All	All	0.87	1/6703 (0.0%)	0.96	37/9151 (0.4%)

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
3	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	68	HIS	N-CA	5.02	1.56	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	37	ARG	NE-CZ-NH2	-14.39	113.10	120.30
3	M	241	ARG	NE-CZ-NH2	-13.27	113.67	120.30
2	L	103	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	L	7	ARG	NE-CZ-NH1	12.07	126.34	120.30
3	M	241	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	L	7	ARG	NE-CZ-NH2	-11.25	114.68	120.30
2	L	135	ARG	NE-CZ-NH2	-10.04	115.28	120.30
2	L	207	ARG	NE-CZ-NH2	-8.87	115.87	120.30
2	L	103	ARG	NE-CZ-NH1	8.65	124.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	231	ARG	NE-CZ-NH1	8.64	124.62	120.30
3	M	136	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	H	37	ARG	NE-CZ-NH1	8.62	124.61	120.30
3	M	132	ARG	NE-CZ-NH1	-8.45	116.08	120.30
2	L	231	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	H	37	ARG	CG-CD-NE	-7.89	95.23	111.80
3	M	136	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	H	67	PRO	C-N-CA	-7.45	103.07	121.70
2	L	135	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	L	210	ASP	CB-CG-OD1	7.34	124.91	118.30
1	H	237	VAL	CG1-CB-CG2	6.70	121.62	110.90
1	H	70	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	H	117	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	H	70	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	H	124	ASP	CB-CG-OD1	6.08	123.77	118.30
1	H	157	ASP	CB-CG-OD2	5.96	123.67	118.30
3	M	240	ASP	CB-CG-OD2	5.96	123.66	118.30
2	L	261	ASP	CB-CG-OD2	5.87	123.58	118.30
2	L	2	LEU	CA-CB-CG	5.62	128.24	115.30
2	L	257	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
1	H	231	ASP	CB-CG-OD2	5.53	123.27	118.30
2	L	207	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	L	213	ASP	CB-CG-OD2	5.49	123.24	118.30
2	L	217	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	L	7	ARG	CD-NE-CZ	5.33	131.06	123.60
3	M	241	ARG	CD-NE-CZ	5.07	130.70	123.60
3	M	292	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

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	1830	0	1836	34	0
2	L	2232	0	2187	24	0
3	M	2413	0	2329	43	0
4	H	16	0	31	3	0
4	M	48	0	93	6	0
5	H	24	0	45	0	0
6	L	132	0	148	5	0
6	M	132	0	148	12	0
7	L	65	0	75	5	0
7	M	65	0	76	10	0
8	L	48	0	60	1	0
8	M	48	0	63	3	0
9	M	1	0	0	0	0
10	M	10	0	0	0	0
11	M	43	0	69	6	0
12	H	174	0	0	4	0
12	L	95	0	0	4	0
12	M	99	0	0	1	0
All	All	7475	0	7160	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (122) 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:220:LYS:HE2	12:H:2104:HOH:O	1.30	1.25
7:M:1311:BPH:H111	7:M:1311:BPH:H171	1.22	1.11
4:H:1251:LDA:H121	4:M:1307:LDA:H91	1.40	0.98
3:M:2:GLU:HG2	3:M:4:GLN:HE22	1.29	0.96
7:M:1311:BPH:HHC	7:M:1311:BPH:HBB3	1.45	0.95
3:M:2:GLU:HG2	3:M:4:GLN:NE2	1.86	0.90
1:H:220:LYS:CE	12:H:2104:HOH:O	1.98	0.90
7:M:1311:BPH:H171	7:M:1311:BPH:C11	2.01	0.90
7:L:1284:BPH:HBB3	7:L:1284:BPH:HHC	1.59	0.84
1:H:68:HIS:ND1	12:H:2050:HOH:O	2.10	0.83
1:H:98:HIS:CD2	2:L:7:ARG:HH11	2.01	0.79
2:L:56:GLN:OE1	12:L:2015:HOH:O	2.04	0.75
2:L:67:TYR:HE1	12:L:2022:HOH:O	1.70	0.73
2:L:34:PHE:O	2:L:38:THR:HG22	1.89	0.72
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.72	0.69
3:M:32:VAL:HG13	3:M:33:GLY:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:301:HIS:CD2	3:M:301:HIS:O	2.47	0.68
1:H:175:MET:HE3	12:L:2084:HOH:O	1.95	0.66
4:H:1251:LDA:C12	4:M:1307:LDA:H91	2.21	0.66
2:L:34:PHE:O	2:L:38:THR:CG2	2.44	0.66
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.79	0.65
2:L:231:ARG:HD3	3:M:5:ASN:O	1.98	0.64
2:L:56:GLN:NE2	12:L:2014:HOH:O	2.30	0.63
6:L:1282:BCL:HMB1	6:L:1282:BCL:CBB	2.29	0.63
3:M:189:PHE:O	3:M:193:HIS:HD2	1.82	0.63
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.34	0.62
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.38	0.62
6:M:1304:BCL:CBB	6:M:1304:BCL:HMB1	2.30	0.61
1:H:117:ARG:HD3	3:M:242:GLY:HA2	1.84	0.59
7:M:1311:BPH:HHC	7:M:1311:BPH:CBB	2.28	0.59
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.27	0.59
6:L:1283:BCL:HMB1	6:L:1283:BCL:HBB2	1.85	0.58
3:M:2:GLU:CG	3:M:4:GLN:HE22	2.10	0.57
1:H:170:ASP:OD2	1:H:177:ARG:NH1	2.31	0.57
1:H:34:GLU:O	1:H:37:ARG:HG3	2.06	0.56
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.88	0.56
6:M:1303:BCL:CBB	6:M:1303:BCL:HMB1	2.36	0.55
1:H:98:HIS:HD2	2:L:7:ARG:HH11	1.52	0.55
2:L:213:ASP:O	2:L:217:ARG:HG3	2.07	0.55
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.37	0.54
2:L:193:LEU:HD23	8:L:1285:U10:C2	2.38	0.54
1:H:245:ALA:HB2	1:H:248:ARG:HH21	1.71	0.54
6:L:1282:BCL:HMB1	6:L:1282:BCL:HBB3	1.88	0.54
1:H:70:ARG:NH2	1:H:121:PRO:O	2.37	0.54
3:M:184:ASP:O	3:M:188:ASN:HB2	2.08	0.54
1:H:156:CYS:HB2	1:H:248:ARG:HG3	1.90	0.53
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.43	0.53
1:H:241:LEU:O	1:H:248:ARG:NH2	2.42	0.53
3:M:199:ASN:HD22	3:M:199:ASN:C	2.11	0.53
1:H:181:VAL:CG2	1:H:191:LEU:HD12	2.39	0.52
2:L:207:ARG:HG2	3:M:142:MET:HG2	1.92	0.52
1:H:132:LYS:HD2	1:H:171:ILE:CD1	2.40	0.52
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.90	0.52
1:H:37:ARG:NH2	1:H:60:LYS:O	2.37	0.52
2:L:56:GLN:HG3	2:L:58:THR:HG22	1.91	0.52
1:H:156:CYS:SG	1:H:248:ARG:HA	2.51	0.51
6:M:1304:BCL:HMB1	6:M:1304:BCL:HBB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:VAL:HG21	1:H:191:LEU:CD1	2.41	0.50
3:M:25:ASN:C	3:M:25:ASN:HD22	2.14	0.49
1:H:21:TRP:HZ2	4:M:1307:LDA:HM11	1.78	0.49
3:M:204:LEU:HD13	4:M:1307:LDA:H12	1.95	0.49
3:M:136:ARG:NE	3:M:136:ARG:HA	2.28	0.48
3:M:133:THR:HG21	3:M:147:ALA:HA	1.96	0.48
6:M:1303:BCL:H71	6:M:1304:BCL:H202	1.96	0.48
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.95	0.48
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.79	0.47
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.45	0.47
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.47
1:H:177:ARG:NH2	3:M:232:GLU:OE2	2.47	0.47
6:M:1303:BCL:HMB1	6:M:1303:BCL:HBB2	1.96	0.47
1:H:156:CYS:SG	1:H:248:ARG:CB	3.03	0.47
4:H:1251:LDA:HM21	4:H:1251:LDA:H21	1.64	0.47
3:M:129:TRP:CH2	3:M:132:ARG:NH1	2.82	0.47
6:L:1283:BCL:HMB1	6:L:1283:BCL:CBB	2.45	0.47
7:M:1311:BPH:HBC2	7:M:1311:BPH:HHB	1.97	0.47
6:M:1303:BCL:H91	6:M:1303:BCL:H111	1.71	0.46
6:M:1303:BCL:C3B	11:M:1312:SPN:H152	2.46	0.46
3:M:256:MET:CE	8:M:1313:U10:H102	2.45	0.46
3:M:133:THR:CG2	3:M:147:ALA:HA	2.46	0.46
3:M:2:GLU:HB2	12:M:2015:HOH:O	2.16	0.46
3:M:161:GLY:HA3	11:M:1312:SPN:H201	1.97	0.45
6:M:1303:BCL:CAB	11:M:1312:SPN:H162	2.46	0.45
2:L:138:MET:SD	2:L:249:ILE:HD11	2.56	0.45
3:M:194:GLY:O	3:M:195:ASN:HB3	2.17	0.45
1:H:132:LYS:HB2	1:H:171:ILE:HD11	1.99	0.45
1:H:21:TRP:CZ2	4:M:1307:LDA:HM11	2.52	0.45
2:L:231:ARG:HD2	3:M:6:ILE:HA	1.99	0.45
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.51	0.45
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.52	0.45
2:L:62:GLN:NE2	2:L:151:TRP:HE1	2.15	0.44
7:L:1284:BPH:HHC	7:L:1284:BPH:CBB	2.37	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.99	0.44
3:M:2:GLU:O	3:M:4:GLN:NE2	2.51	0.44
8:M:1313:U10:H28	8:M:1313:U10:H322	1.74	0.43
2:L:231:ARG:HG2	3:M:224:LEU:HD21	1.98	0.43
6:M:1303:BCL:H141	11:M:1312:SPN:H112	1.99	0.43
3:M:241:ARG:HD3	3:M:246:GLU:HG2	2.01	0.43
6:M:1303:BCL:H141	11:M:1312:SPN:H101	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:133:THR:HG22	3:M:147:ALA:HB2	1.99	0.43
2:L:53:ALA:HB1	2:L:58:THR:O	2.19	0.43
1:H:245:ALA:HB2	1:H:248:ARG:NH2	2.33	0.43
6:L:1282:BCL:NA	6:M:1304:BCL:HBB2	2.34	0.43
3:M:52:LEU:HD12	3:M:52:LEU:HA	1.84	0.43
4:M:1307:LDA:H21	4:M:1307:LDA:HM13	1.42	0.43
1:H:132:LYS:HD2	1:H:171:ILE:HD11	1.99	0.42
6:M:1304:BCL:HAA2	6:M:1304:BCL:HBD	2.02	0.42
2:L:75:LEU:HA	2:L:142:TRP:CD1	2.54	0.42
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.01	0.42
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.01	0.42
1:H:156:CYS:SG	1:H:248:ARG:CA	3.07	0.41
3:M:75:TRP:HB3	3:M:80:TRP:CE3	2.55	0.41
1:H:115:VAL:HG22	1:H:117:ARG:HG2	2.01	0.41
12:H:2119:HOH:O	3:M:13:ARG:HD2	2.20	0.41
3:M:157:TRP:CE2	11:M:1312:SPN:HM73	2.56	0.41
3:M:297:TRP:NE1	3:M:302:GLY:HA2	2.36	0.41
3:M:226:VAL:HG23	3:M:231:GLY:HA3	2.03	0.41
7:L:1284:BPH:NC	7:L:1284:BPH:ND	2.68	0.41
3:M:72:ILE:HD12	3:M:72:ILE:HA	1.96	0.40
3:M:189:PHE:O	3:M:193:HIS:CD2	2.69	0.40
2:L:29:PHE:CE1	8:M:1313:U10:H311	2.56	0.40
7:M:1311:BPH:H6C1	7:M:1311:BPH:H4C1	1.19	0.40
2:L:231:ARG:HD2	3:M:6:ILE:O	2.21	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	239/260 (92%)	234 (98%)	4 (2%)	1 (0%)	34 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	279/281 (99%)	273 (98%)	6 (2%)	0	100	100
3	M	301/307 (98%)	293 (97%)	5 (2%)	3 (1%)	15	23
All	All	819/848 (97%)	800 (98%)	15 (2%)	4 (0%)	29	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	301	HIS
3	M	195	ASN
3	M	302	GLY

5.3.2 Protein sidechains [i](#)

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%)	183 (94%)	12 (6%)	18	29
2	L	220/220 (100%)	210 (96%)	10 (4%)	27	44
3	M	237/241 (98%)	224 (94%)	13 (6%)	21	35
All	All	652/669 (98%)	617 (95%)	35 (5%)	22	36

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

Mol	Chain	Res	Type
1	H	15	LEU
1	H	70	ARG
1	H	118	ARG
1	H	143	SER
1	H	175	MET
1	H	177	ARG
1	H	206	ASN
1	H	220	LYS
1	H	221	SER
1	H	225	VAL

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Mol	Chain	Res	Type
1	H	231	ASP
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	54	VAL
2	L	126	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	247	CYS
2	L	272	TRP
3	M	2	GLU
3	M	12	VAL
3	M	25	ASN
3	M	32	VAL
3	M	60	LEU
3	M	104	SER
3	M	114	LEU
3	M	133	THR
3	M	188	ASN
3	M	192	VAL
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

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

Mol	Chain	Res	Type
1	H	98	HIS
2	L	62	GLN
3	M	4	GLN
3	M	25	ASN
3	M	44	ASN
3	M	193	HIS
3	M	199	ASN
3	M	300	ASN
3	M	301	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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$
10	PO4	M	1309	-	4,4,4	1.43	0	6,6,6	1.04	1 (16%)
4	LDA	M	1305	-	12,15,15	2.24	1 (8%)	14,17,17	3.72	3 (21%)
5	D10	H	1252	-	8,8,9	0.27	0	7,7,8	0.47	0
7	BPH	L	1284	-	51,70,70	0.94	1 (1%)	52,101,101	1.31	9 (17%)
7	BPH	M	1311	-	51,70,70	0.72	1 (1%)	52,101,101	2.11	16 (30%)
6	BCL	M	1304	3	64,74,74	1.53	5 (7%)	78,115,115	1.63	17 (21%)
6	BCL	L	1282	2	64,74,74	1.48	4 (6%)	78,115,115	1.72	19 (24%)
4	LDA	M	1307	-	12,15,15	2.44	1 (8%)	14,17,17	2.66	3 (21%)
6	BCL	L	1283	2	64,74,74	1.19	4 (6%)	78,115,115	1.68	22 (28%)
8	U10	M	1313	-	48,48,63	1.92	4 (8%)	58,61,79	1.46	10 (17%)
10	PO4	M	1310	-	4,4,4	0.69	0	6,6,6	0.53	0
11	SPN	M	1312	-	40,42,42	3.72	16 (40%)	50,52,52	2.15	21 (42%)
6	BCL	M	1303	3	64,74,74	1.03	5 (7%)	78,115,115	1.71	16 (20%)
4	LDA	H	1251	-	12,15,15	2.27	1 (8%)	14,17,17	3.71	3 (21%)
5	D10	H	1253	-	7,7,9	0.25	0	6,6,8	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	D10	H	1254	-	6,6,9	0.73	0	5,5,8	0.55	0
4	LDA	M	1306	-	12,15,15	2.06	1 (8%)	14,17,17	3.57	3 (21%)
8	U10	L	1285	-	48,48,63	2.40	4 (8%)	58,61,79	2.42	17 (29%)

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	1305	-	-	7/13/13/13	-
5	D10	H	1252	-	-	2/6/6/7	-
7	BPH	L	1284	-	-	7/37/105/105	0/5/6/6
7	BPH	M	1311	-	-	17/37/105/105	0/5/6/6
6	BCL	M	1304	3	-	2/37/137/137	-
6	BCL	L	1282	2	-	5/37/137/137	-
4	LDA	M	1307	-	-	5/13/13/13	-
6	BCL	L	1283	2	-	6/37/137/137	-
8	U10	M	1313	-	-	10/45/69/87	0/1/1/1
11	SPN	M	1312	-	-	16/50/51/51	-
6	BCL	M	1303	3	-	15/37/137/137	-
4	LDA	H	1251	-	-	2/13/13/13	-
5	D10	H	1253	-	-	4/5/5/7	-
5	D10	H	1254	-	-	1/4/4/7	-
4	LDA	M	1306	-	-	5/13/13/13	-
8	U10	L	1285	-	-	15/45/69/87	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1285	U10	C27-C28	-11.54	1.12	1.50
11	M	1312	SPN	C3-C4	-10.32	1.35	1.50
6	M	1304	BCL	MG-NA	9.00	2.27	2.06
8	M	1313	U10	C6-C1	8.76	1.51	1.35
4	M	1307	LDA	O1-N1	-8.08	1.23	1.42
6	L	1282	BCL	MG-NA	8.06	2.25	2.06
4	H	1251	LDA	O1-N1	-7.80	1.23	1.42
8	L	1285	U10	C6-C1	7.76	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1305	LDA	O1-N1	-7.70	1.24	1.42
8	M	1313	U10	C36-C34	-7.54	1.35	1.51
11	M	1312	SPN	C17-C18	-7.33	1.36	1.51
4	M	1306	LDA	O1-N1	-7.04	1.25	1.42
11	M	1312	SPN	C14-C13	-7.02	1.36	1.51
11	M	1312	SPN	C8-C9	6.72	1.49	1.33
11	M	1312	SPN	C10-C9	-6.66	1.37	1.51
11	M	1312	SPN	C6-C5	-6.62	1.37	1.51
8	L	1285	U10	C36-C34	-6.13	1.38	1.51
11	M	1312	SPN	C12-C13	5.90	1.47	1.33
11	M	1312	SPN	C19-C18	5.81	1.46	1.33
11	M	1312	SPN	C4-C5	5.60	1.46	1.33
6	L	1282	BCL	C4B-NB	4.92	1.39	1.35
11	M	1312	SPN	C20-C19	-4.58	1.35	1.50
6	L	1283	BCL	C4B-NB	4.41	1.39	1.35
11	M	1312	SPN	C11-C12	-4.28	1.36	1.50
11	M	1312	SPN	C7-C8	-4.27	1.36	1.50
6	M	1304	BCL	C4B-NB	3.83	1.38	1.35
11	M	1312	SPN	C1-C2	-3.53	1.50	1.53
8	L	1285	U10	C4-C3	3.43	1.50	1.36
6	M	1303	BCL	MG-ND	-3.42	1.99	2.05
6	L	1282	BCL	C1B-NB	3.39	1.38	1.35
6	L	1282	BCL	MG-NC	3.35	2.14	2.06
6	M	1303	BCL	C4B-NB	3.32	1.38	1.35
6	L	1283	BCL	MG-NA	3.27	2.14	2.06
8	M	1313	U10	C4-C3	3.14	1.49	1.36
11	M	1312	SPN	C21-C22	-2.99	1.36	1.52
11	M	1312	SPN	C16-C15	-2.91	1.35	1.51
7	L	1284	BPH	C3A-C2A	-2.88	1.52	1.54
6	L	1283	BCL	C1B-NB	2.84	1.37	1.35
6	L	1283	BCL	MG-ND	-2.83	2.00	2.05
6	M	1304	BCL	C1B-NB	2.80	1.37	1.35
6	M	1304	BCL	C4D-ND	-2.27	1.34	1.37
6	M	1303	BCL	C1B-NB	2.26	1.37	1.35
11	M	1312	SPN	C25-C26	2.26	1.38	1.33
8	M	1313	U10	O5-C5	2.21	1.28	1.23
7	M	1311	BPH	C1-C2	2.12	1.55	1.49
6	M	1303	BCL	C1D-ND	2.06	1.40	1.37
6	M	1304	BCL	CHD-C1D	2.03	1.42	1.38
6	M	1303	BCL	C1B-CHB	-2.02	1.35	1.41

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1285	U10	C26-C27-C28	11.34	149.16	111.88
4	M	1305	LDA	CM1-N1-C1	-10.25	88.69	110.23
4	M	1306	LDA	CM2-N1-C1	-9.07	91.19	110.23
4	H	1251	LDA	CM1-N1-C1	-8.73	91.89	110.23
4	H	1251	LDA	CM2-N1-C1	-8.21	92.98	110.23
4	M	1306	LDA	CM1-N1-C1	-7.92	93.59	110.23
7	M	1311	BPH	C1-C2-C3	-6.58	114.66	126.04
4	M	1305	LDA	O1-N1-C1	-6.58	93.13	109.27
4	M	1305	LDA	CM2-N1-C1	-6.40	96.79	110.23
4	H	1251	LDA	O1-N1-C1	-6.31	93.79	109.27
4	M	1307	LDA	CM2-N1-C1	-5.58	98.51	110.23
4	M	1307	LDA	O1-N1-C1	-5.55	95.65	109.27
4	M	1307	LDA	CM1-N1-C1	-5.49	98.71	110.23
4	M	1306	LDA	O1-N1-C1	-5.32	96.23	109.27
6	L	1283	BCL	CMB-C2B-C1B	-5.21	120.45	128.46
7	M	1311	BPH	CAC-C3C-C4C	5.18	125.31	113.73
6	L	1282	BCL	C1C-NC-C4C	5.04	108.97	106.71
6	M	1304	BCL	CAC-C3C-C4C	-4.91	101.70	112.58
8	L	1285	U10	C32-C33-C34	-4.90	115.86	127.66
11	M	1312	SPN	CM3-C5-C6	4.72	123.21	115.27
11	M	1312	SPN	C11-C10-C9	4.44	127.58	112.98
6	M	1303	BCL	CMB-C2B-C1B	-4.41	121.69	128.46
7	M	1311	BPH	C1-O2A-CGA	4.36	127.89	116.44
8	L	1285	U10	C1M-C1-C6	-4.24	117.49	124.40
8	L	1285	U10	C37-C36-C34	4.22	126.86	112.98
7	M	1311	BPH	O2D-CGD-CBD	4.13	116.22	111.00
6	L	1282	BCL	CAA-C2A-C3A	-4.08	101.60	112.78
6	M	1303	BCL	C1-C2-C3	4.06	133.07	126.04
6	M	1304	BCL	C4D-CHA-C1A	4.06	126.19	121.25
6	L	1282	BCL	CHD-C1D-ND	-3.98	120.80	124.45
11	M	1312	SPN	CM4-C9-C10	3.95	121.91	115.27
6	M	1303	BCL	C1-O2A-CGA	3.81	126.45	116.44
11	M	1312	SPN	CM6-C18-C17	3.80	121.67	115.27
8	L	1285	U10	C35-C34-C36	3.70	121.50	115.27
7	M	1311	BPH	CAA-C2A-C3A	-3.68	102.71	112.78
6	M	1304	BCL	CHD-C1D-ND	-3.65	121.10	124.45
6	M	1303	BCL	CAA-C2A-C3A	-3.59	102.94	112.78
6	M	1304	BCL	CHA-C1A-NA	-3.56	118.26	126.40
6	M	1304	BCL	C1C-NC-C4C	3.53	108.30	106.71
6	L	1282	BCL	CAA-C2A-C1A	-3.53	100.40	111.97
6	M	1303	BCL	C5-C3-C2	3.53	128.26	121.12
11	M	1312	SPN	CM5-C13-C14	3.53	121.20	115.27
7	M	1311	BPH	C6-C5-C3	-3.51	104.26	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1303	BCL	CHD-C1D-ND	-3.49	121.25	124.45
6	L	1283	BCL	CAA-C2A-C3A	-3.48	103.25	112.78
8	L	1285	U10	O2-C2-C3	-3.46	113.59	120.93
8	M	1313	U10	C30-C29-C31	3.40	121.00	115.27
6	L	1282	BCL	CMA-C3A-C2A	-3.33	100.38	113.83
6	L	1283	BCL	CAC-C3C-C2C	-3.31	105.99	114.26
6	M	1303	BCL	CMB-C2B-C3B	3.30	130.86	124.68
6	L	1283	BCL	CAC-C3C-C4C	-3.29	105.28	112.58
6	M	1304	BCL	CAC-C3C-C2C	-3.25	106.15	114.26
8	L	1285	U10	C25-C24-C26	3.24	120.73	115.27
8	M	1313	U10	C22-C23-C24	-3.20	119.95	127.66
7	L	1284	BPH	CAC-C3C-C2C	3.18	122.20	114.26
7	M	1311	BPH	CMA-C3A-C4A	-3.17	107.44	114.38
8	M	1313	U10	C32-C33-C34	-3.16	120.04	127.66
7	M	1311	BPH	O2A-C1-C2	-3.16	100.33	108.64
8	L	1285	U10	C27-C28-C29	3.14	135.21	127.66
6	L	1283	BCL	CMC-C2C-C3C	-3.11	101.29	113.83
6	L	1283	BCL	CMB-C2B-C3B	3.11	130.49	124.68
7	L	1284	BPH	C1-C2-C3	-3.10	120.67	126.04
6	M	1303	BCL	C4-C3-C2	-3.10	115.72	123.68
11	M	1312	SPN	C16-C15-C14	3.10	124.34	113.19
11	M	1312	SPN	C7-C6-C5	3.10	123.17	112.98
6	L	1282	BCL	CMB-C2B-C1B	-3.05	123.77	128.46
8	M	1313	U10	C35-C34-C36	3.03	120.37	115.27
11	M	1312	SPN	CM7-C22-C21	3.03	122.26	111.29
6	M	1303	BCL	CMA-C3A-C2A	-3.02	101.66	113.83
6	L	1282	BCL	CHA-C1A-NA	-3.00	119.53	126.40
6	M	1303	BCL	CHA-C1A-NA	-2.92	119.70	126.40
7	M	1311	BPH	CMA-C3A-C2A	-2.92	102.25	113.99
11	M	1312	SPN	CM2-C1-C2	-2.88	103.42	109.43
7	L	1284	BPH	CAA-C2A-C3A	-2.88	104.89	112.78
8	M	1313	U10	C10-C9-C11	2.87	120.10	115.27
6	M	1303	BCL	C4D-CHA-C1A	2.87	124.74	121.25
11	M	1312	SPN	C15-C14-C13	2.83	120.89	113.45
7	L	1284	BPH	CMA-C3A-C2A	-2.80	102.72	113.99
8	L	1285	U10	C35-C34-C33	-2.78	116.56	123.68
7	M	1311	BPH	C5-C3-C2	2.77	126.71	121.12
7	M	1311	BPH	C4C-C3C-C2C	2.76	105.47	102.84
6	M	1304	BCL	CMC-C2C-C3C	-2.73	102.81	113.83
11	M	1312	SPN	C6-C7-C8	2.73	120.84	111.88
8	M	1313	U10	C15-C14-C16	2.73	119.86	115.27
11	M	1312	SPN	CMB-C30-CM9	2.69	120.56	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1285	U10	C15-C14-C16	2.68	119.79	115.27
6	L	1282	BCL	C4D-CHA-C1A	2.67	124.49	121.25
6	M	1303	BCL	C4B-C3B-CAB	-2.64	122.02	127.13
6	L	1283	BCL	C6-C5-C3	-2.64	106.53	113.45
11	M	1312	SPN	C20-C21-C22	2.64	124.90	115.76
7	M	1311	BPH	OBD-CAD-CBD	-2.63	121.96	125.82
11	M	1312	SPN	C16-C17-C18	2.63	120.36	113.45
6	M	1303	BCL	C1B-CHB-C4A	-2.63	124.92	130.12
8	M	1313	U10	C27-C28-C29	-2.60	121.40	127.66
6	L	1282	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
6	M	1304	BCL	C1-C2-C3	-2.60	121.55	126.04
6	L	1283	BCL	O2A-C1-C2	-2.59	101.82	108.64
8	L	1285	U10	C22-C23-C24	-2.55	121.52	127.66
6	L	1283	BCL	C1-O2A-CGA	2.54	123.11	116.44
7	M	1311	BPH	C4B-NB-C1B	2.54	112.30	107.09
6	M	1304	BCL	CMB-C2B-C1B	-2.53	124.57	128.46
6	M	1303	BCL	O2D-CGD-CBD	2.52	115.75	111.27
6	L	1282	BCL	CMB-C2B-C3B	2.51	129.37	124.68
8	L	1285	U10	C3M-O3-C3	2.48	125.25	116.47
11	M	1312	SPN	C17-C18-C19	-2.47	116.11	121.12
7	L	1284	BPH	CAC-C3C-C4C	2.46	119.24	113.73
6	L	1282	BCL	C4B-C3B-CAB	-2.45	122.39	127.13
6	L	1282	BCL	C1D-ND-C4D	2.44	108.07	106.33
6	L	1283	BCL	CHD-C1D-ND	-2.43	122.22	124.45
6	L	1282	BCL	C4-C3-C5	2.42	119.34	115.27
7	L	1284	BPH	CMA-C3A-C4A	-2.40	109.11	114.38
8	L	1285	U10	C31-C32-C33	2.39	119.75	111.88
6	L	1283	BCL	CAA-C2A-C1A	-2.39	104.15	111.97
6	L	1282	BCL	CAC-C3C-C2C	-2.38	108.31	114.26
6	L	1282	BCL	O2A-CGA-O1A	-2.38	117.59	123.59
6	L	1282	BCL	CHD-C1D-C2D	2.36	130.44	125.48
6	L	1283	BCL	CAA-CBA-CGA	2.36	120.14	113.25
11	M	1312	SPN	CM9-C30-C29	-2.36	115.84	122.65
6	L	1283	BCL	O2D-CGD-CBD	2.35	115.45	111.27
8	L	1285	U10	C36-C37-C38	2.35	119.61	111.88
8	M	1313	U10	C37-C38-C39	-2.33	119.78	127.75
11	M	1312	SPN	C3-C4-C5	-2.33	122.91	126.79
6	L	1283	BCL	O2A-CGA-O1A	-2.33	117.71	123.59
6	L	1283	BCL	O2D-CGD-O1D	-2.33	119.29	123.84
8	M	1313	U10	C37-C36-C34	2.29	120.53	112.98
6	L	1283	BCL	C1-C2-C3	-2.29	122.08	126.04
11	M	1312	SPN	CM7-C22-C23	2.28	119.55	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1313	U10	C26-C27-C28	-2.28	104.39	111.88
6	L	1282	BCL	CMC-C2C-C3C	-2.28	104.64	113.83
6	M	1304	BCL	CMD-C2D-C1D	2.26	128.69	124.71
6	L	1283	BCL	CMA-C3A-C2A	-2.25	104.76	113.83
7	L	1284	BPH	O2D-CGD-CBD	2.23	113.83	111.00
6	L	1283	BCL	OBB-CAB-C3B	2.19	123.88	119.99
10	M	1309	PO4	O3-P-O2	2.19	115.00	107.97
7	M	1311	BPH	CMB-C2B-C3B	2.18	128.76	124.68
6	M	1304	BCL	C1D-ND-C4D	2.18	107.88	106.33
7	M	1311	BPH	CAA-CBA-CGA	2.18	119.62	113.25
8	L	1285	U10	C4-C3-C2	-2.17	116.42	120.68
6	M	1304	BCL	C4B-C3B-CAB	-2.17	122.94	127.13
11	M	1312	SPN	C15-C16-C17	2.17	120.98	113.19
6	M	1303	BCL	C4A-NA-C1A	-2.16	105.74	106.71
6	L	1283	BCL	CMA-C3A-C4A	-2.15	106.01	111.77
7	M	1311	BPH	C4-C3-C2	-2.14	118.18	123.68
6	L	1283	BCL	CBA-CAA-C2A	2.14	120.17	113.86
8	L	1285	U10	C30-C29-C31	2.13	118.86	115.27
6	M	1303	BCL	C7-C6-C5	2.13	119.15	113.36
11	M	1312	SPN	C28-C27-C26	-2.13	105.98	112.98
6	L	1283	BCL	CMC-C2C-C1C	-2.12	106.07	111.77
7	L	1284	BPH	CMC-C2C-C3C	2.11	122.47	113.99
6	M	1304	BCL	CHD-C1D-C2D	2.10	129.88	125.48
6	L	1282	BCL	CED-O2D-CGD	2.10	120.68	115.94
7	L	1284	BPH	C7-C6-C5	-2.07	107.73	113.36
6	M	1304	BCL	C2A-C1A-CHA	2.07	127.48	123.86
6	M	1304	BCL	CGD-CBD-CAD	-2.04	104.12	110.73
11	M	1312	SPN	CM3-C5-C4	-2.04	118.45	123.68
6	M	1304	BCL	O2D-CGD-O1D	-2.03	119.87	123.84
8	L	1285	U10	C25-C24-C23	-2.02	118.49	123.68
6	M	1304	BCL	C4B-CHC-C1C	-2.02	126.12	130.12
6	L	1282	BCL	CMA-C3A-C4A	-2.01	106.36	111.77
6	L	1283	BCL	OBB-CAB-CBB	-2.01	115.65	120.17

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1306	LDA	C2-C1-N1-O1
4	M	1306	LDA	C2-C1-N1-CM1
4	M	1306	LDA	C2-C1-N1-CM2
4	M	1307	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
4	M	1307	LDA	C2-C1-N1-CM2
7	M	1311	BPH	C4C-C3C-CAC-CBC
7	M	1311	BPH	C2C-C3C-CAC-CBC
8	L	1285	U10	C27-C28-C29-C30
8	L	1285	U10	C27-C28-C29-C31
8	L	1285	U10	C32-C33-C34-C35
8	L	1285	U10	C32-C33-C34-C36
8	M	1313	U10	C27-C28-C29-C30
8	M	1313	U10	C27-C28-C29-C31
11	M	1312	SPN	C20-C21-C22-CM7
11	M	1312	SPN	C14-C15-C16-C17
7	M	1311	BPH	C4-C3-C5-C6
11	M	1312	SPN	CM3-C5-C6-C7
11	M	1312	SPN	C11-C10-C9-CM4
11	M	1312	SPN	CM5-C13-C14-C15
11	M	1312	SPN	C16-C17-C18-CM6
7	M	1311	BPH	C2-C3-C5-C6
11	M	1312	SPN	C4-C5-C6-C7
11	M	1312	SPN	C11-C10-C9-C8
11	M	1312	SPN	C12-C13-C14-C15
11	M	1312	SPN	C16-C17-C18-C19
6	L	1282	BCL	C14-C13-C15-C16
7	M	1311	BPH	C6-C7-C8-C9
6	L	1282	BCL	C13-C15-C16-C17
8	M	1313	U10	C37-C38-C39-C41
8	L	1285	U10	C17-C18-C19-C20
6	M	1303	BCL	C6-C7-C8-C10
7	M	1311	BPH	C12-C13-C15-C16
8	M	1313	U10	C24-C26-C27-C28
8	M	1313	U10	C29-C31-C32-C33
7	M	1311	BPH	C15-C16-C17-C18
8	L	1285	U10	C37-C38-C39-C40
6	L	1283	BCL	C16-C17-C18-C19
4	M	1307	LDA	C3-C4-C5-C6
7	L	1284	BPH	C4-C3-C5-C6
11	M	1312	SPN	C3-C4-C5-CM3
6	L	1283	BCL	C14-C13-C15-C16
4	M	1305	LDA	C4-C5-C6-C7
4	H	1251	LDA	C11-C10-C9-C8
5	H	1252	D10	C5-C6-C7-C8
7	M	1311	BPH	C16-C17-C18-C19
7	M	1311	BPH	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
4	M	1305	LDA	C2-C3-C4-C5
7	L	1284	BPH	C2-C3-C5-C6
4	M	1305	LDA	C3-C4-C5-C6
4	M	1307	LDA	C11-C10-C9-C8
6	M	1303	BCL	C2-C1-O2A-CGA
4	M	1305	LDA	C5-C6-C7-C8
8	L	1285	U10	C37-C38-C39-C41
8	M	1313	U10	C37-C38-C39-C40
8	L	1285	U10	C35-C34-C36-C37
6	L	1283	BCL	C12-C13-C15-C16
6	M	1304	BCL	C16-C17-C18-C20
8	L	1285	U10	C29-C31-C32-C33
4	M	1306	LDA	C4-C5-C6-C7
8	M	1313	U10	C28-C29-C31-C32
6	M	1303	BCL	C5-C6-C7-C8
6	L	1283	BCL	C16-C17-C18-C20
5	H	1253	D10	C2-C3-C4-C5
4	M	1307	LDA	C1-C2-C3-C4
8	M	1313	U10	C30-C29-C31-C32
5	H	1252	D10	C2-C3-C4-C5
6	M	1303	BCL	C12-C13-C15-C16
7	M	1311	BPH	C11-C10-C8-C7
8	L	1285	U10	C33-C34-C36-C37
11	M	1312	SPN	C21-C22-C23-C24
6	M	1303	BCL	C6-C7-C8-C9
7	M	1311	BPH	C11-C10-C8-C9
7	M	1311	BPH	C14-C13-C15-C16
4	H	1251	LDA	C6-C7-C8-C9
4	M	1305	LDA	C6-C7-C8-C9
8	L	1285	U10	C15-C14-C16-C17
4	M	1306	LDA	C1-C2-C3-C4
5	H	1253	D10	C1-C2-C3-C4
7	M	1311	BPH	C3-C5-C6-C7
8	L	1285	U10	C13-C14-C16-C17
6	M	1303	BCL	C11-C12-C13-C14
6	M	1303	BCL	C15-C16-C17-C18
6	M	1304	BCL	C16-C17-C18-C19
6	M	1303	BCL	C11-C12-C13-C15
6	L	1282	BCL	CAD-CBD-CGD-O2D
6	M	1303	BCL	CAD-CBD-CGD-O2D
7	L	1284	BPH	CAD-CBD-CGD-O2D
4	M	1305	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	L	1282	BCL	C12-C13-C15-C16
6	M	1303	BCL	C14-C13-C15-C16
6	M	1303	BCL	C8-C10-C11-C12
5	H	1254	D10	C3-C4-C5-C6
4	M	1305	LDA	C1-C2-C3-C4
6	M	1303	BCL	C16-C17-C18-C20
7	L	1284	BPH	O2A-C1-C2-C3
7	M	1311	BPH	C6-C7-C8-C10
5	H	1253	D10	C5-C6-C7-C8
8	M	1313	U10	C5-C4-O4-C4M
8	L	1285	U10	C14-C16-C17-C18
6	L	1283	BCL	C3-C5-C6-C7
8	L	1285	U10	C30-C29-C31-C32
6	M	1303	BCL	C4C-C3C-CAC-CBC
7	M	1311	BPH	C8-C10-C11-C12
6	M	1303	BCL	C16-C17-C18-C19
6	M	1303	BCL	C13-C15-C16-C17
8	L	1285	U10	C20-C19-C21-C22
5	H	1253	D10	C3-C4-C5-C6
6	L	1283	BCL	CAD-CBD-CGD-O2D
7	M	1311	BPH	CAD-CBD-CGD-O2D
8	M	1313	U10	C25-C24-C26-C27
7	L	1284	BPH	C11-C10-C8-C9
11	M	1312	SPN	C10-C11-C12-C13
11	M	1312	SPN	C18-C19-C20-C21
7	M	1311	BPH	C5-C6-C7-C8
11	M	1312	SPN	C6-C7-C8-C9
11	M	1312	SPN	C3-C4-C5-C6
6	L	1282	BCL	C11-C12-C13-C15
7	L	1284	BPH	C11-C10-C8-C7
7	L	1284	BPH	C8-C10-C11-C12

There are no ring outliers.

11 monomers are involved in 44 short contacts:

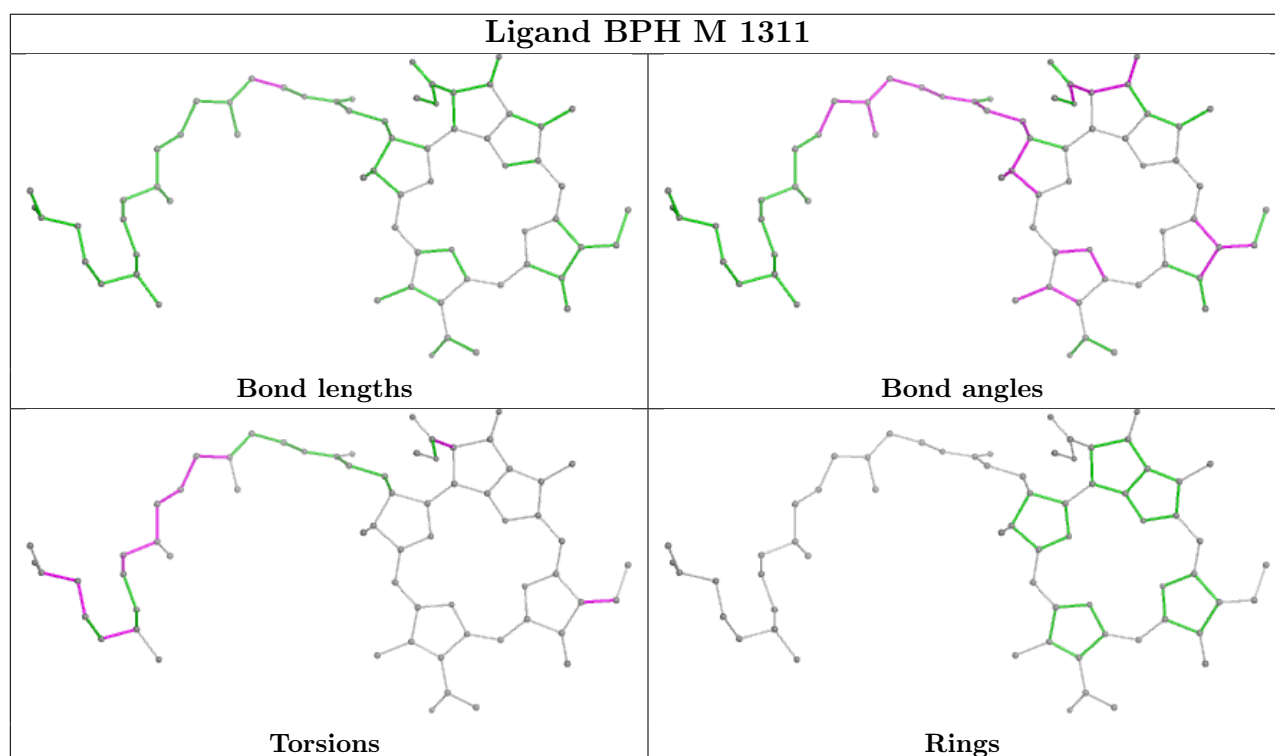
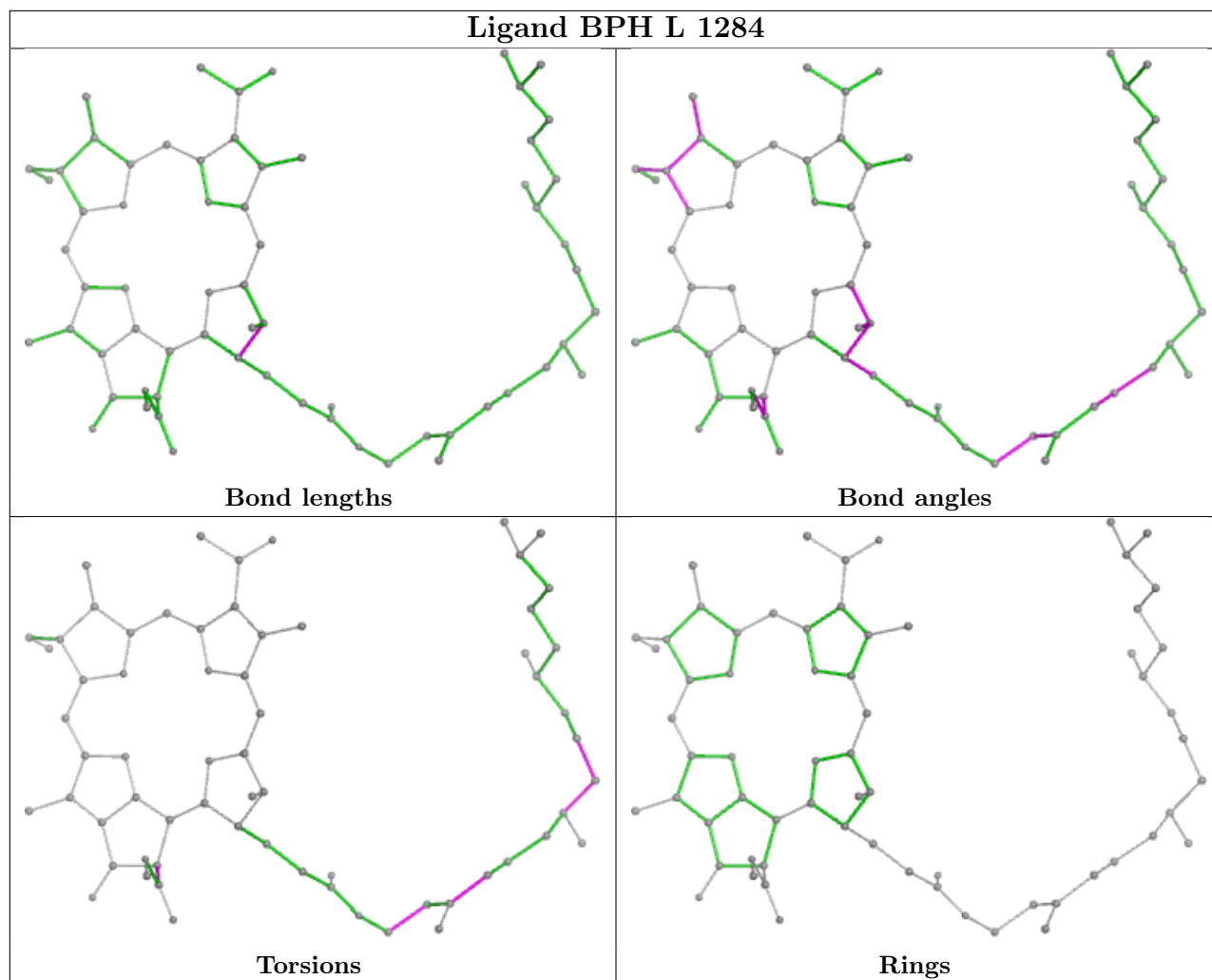
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1284	BPH	5	0
7	M	1311	BPH	10	0
6	M	1304	BCL	5	0
6	L	1282	BCL	3	0
4	M	1307	LDA	6	0
6	L	1283	BCL	2	0

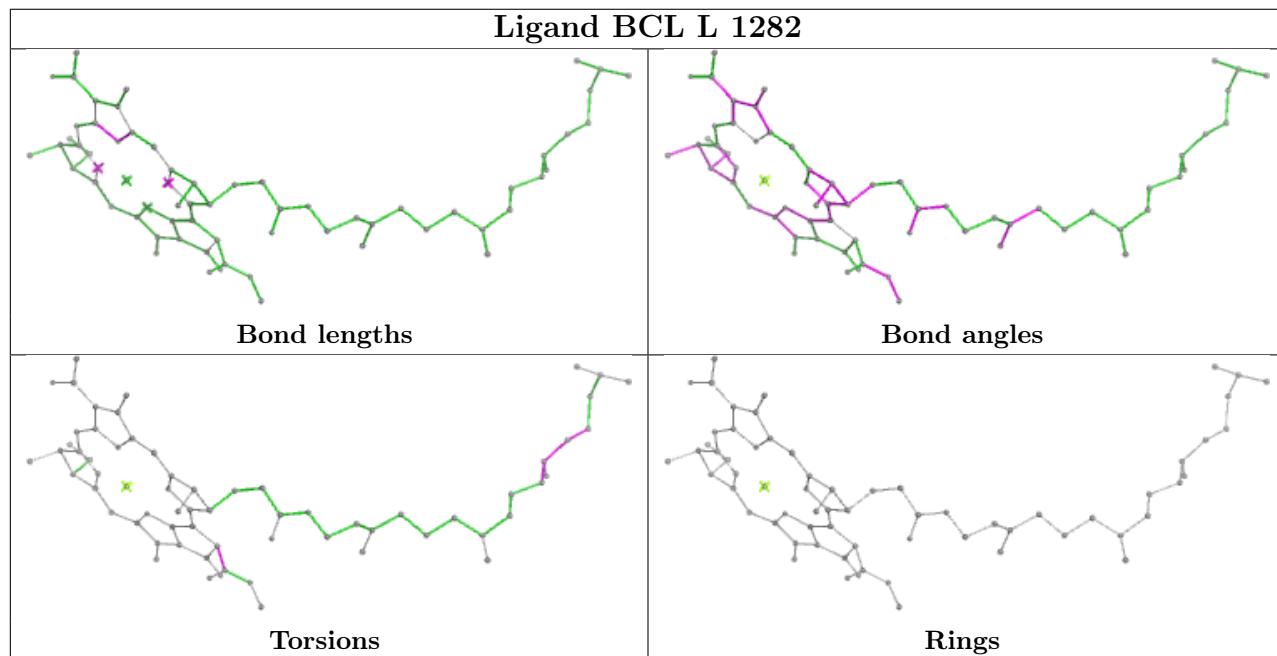
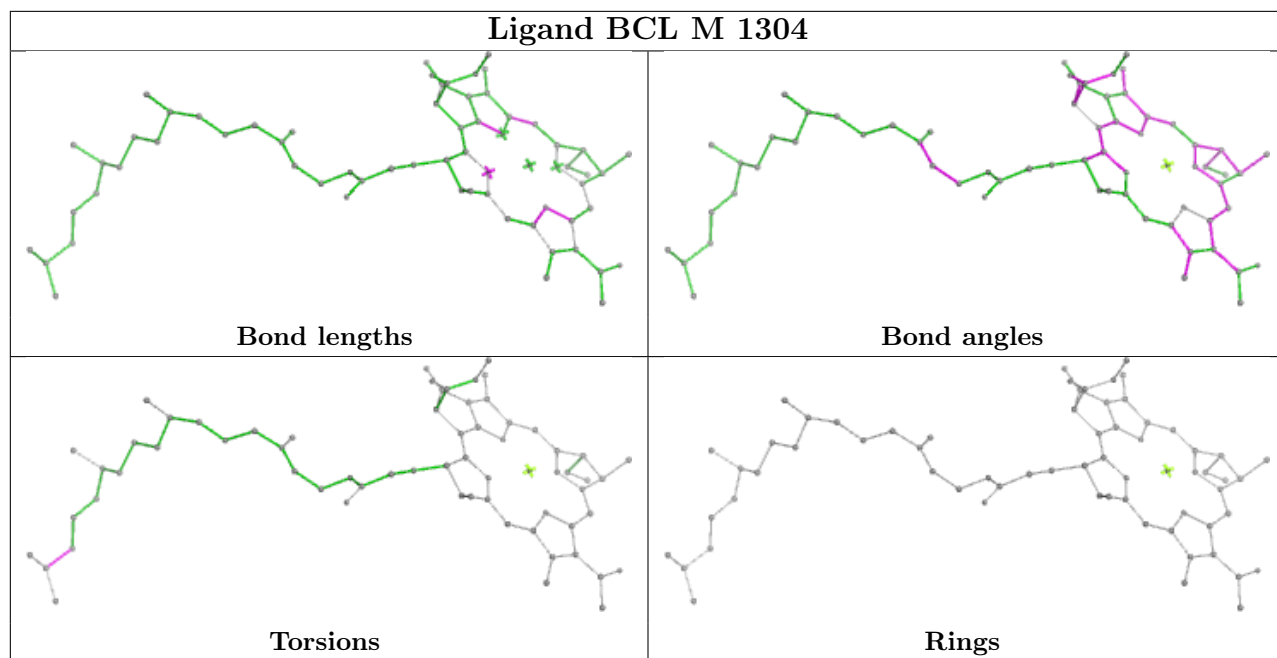
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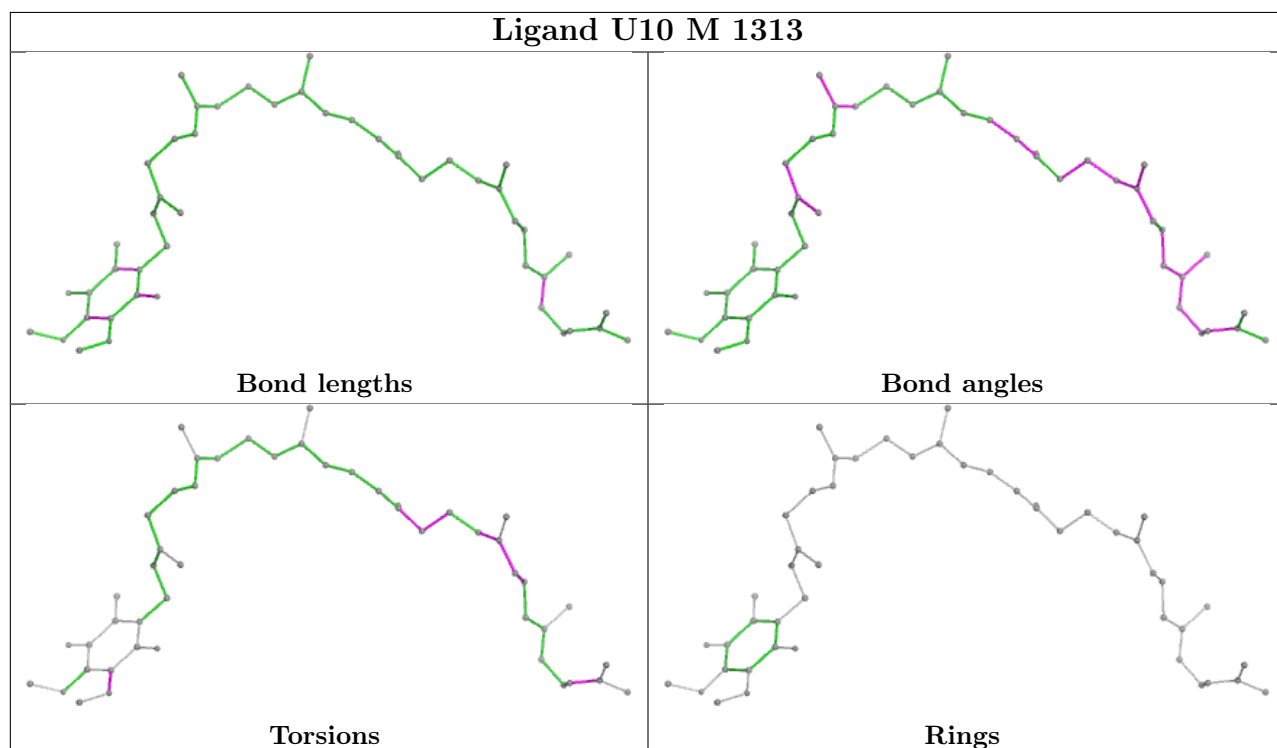
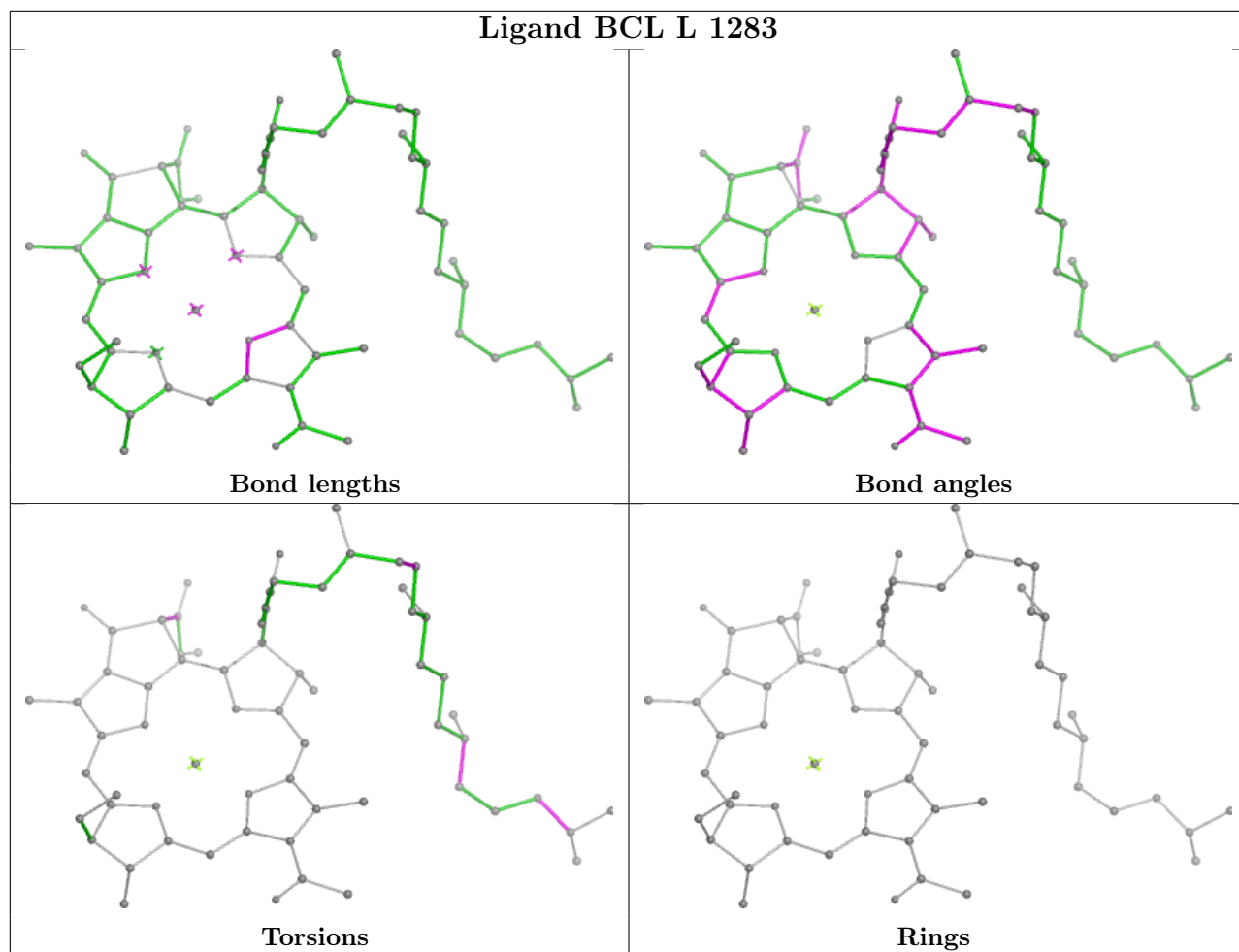
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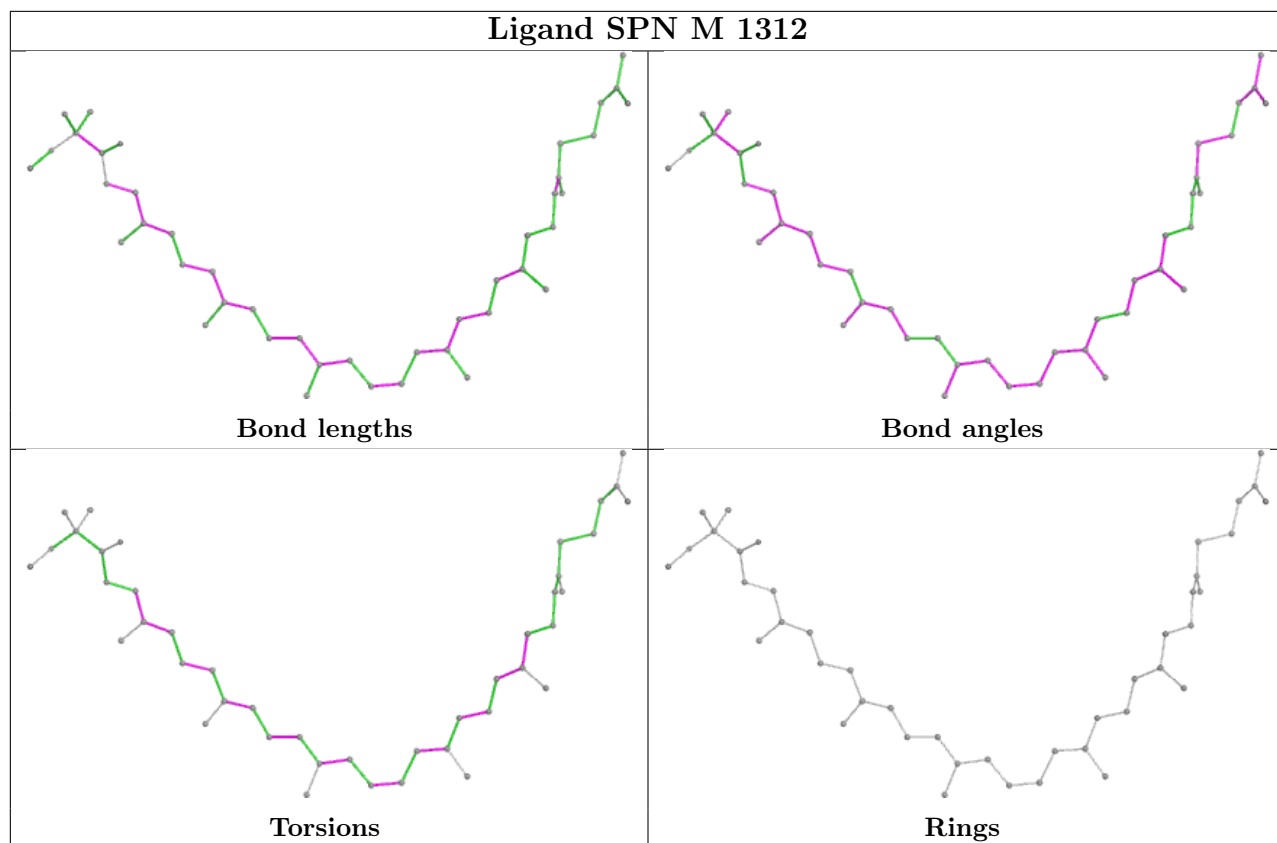
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1313	U10	3	0
11	M	1312	SPN	6	0
6	M	1303	BCL	8	0
4	H	1251	LDA	3	0
8	L	1285	U10	1	0

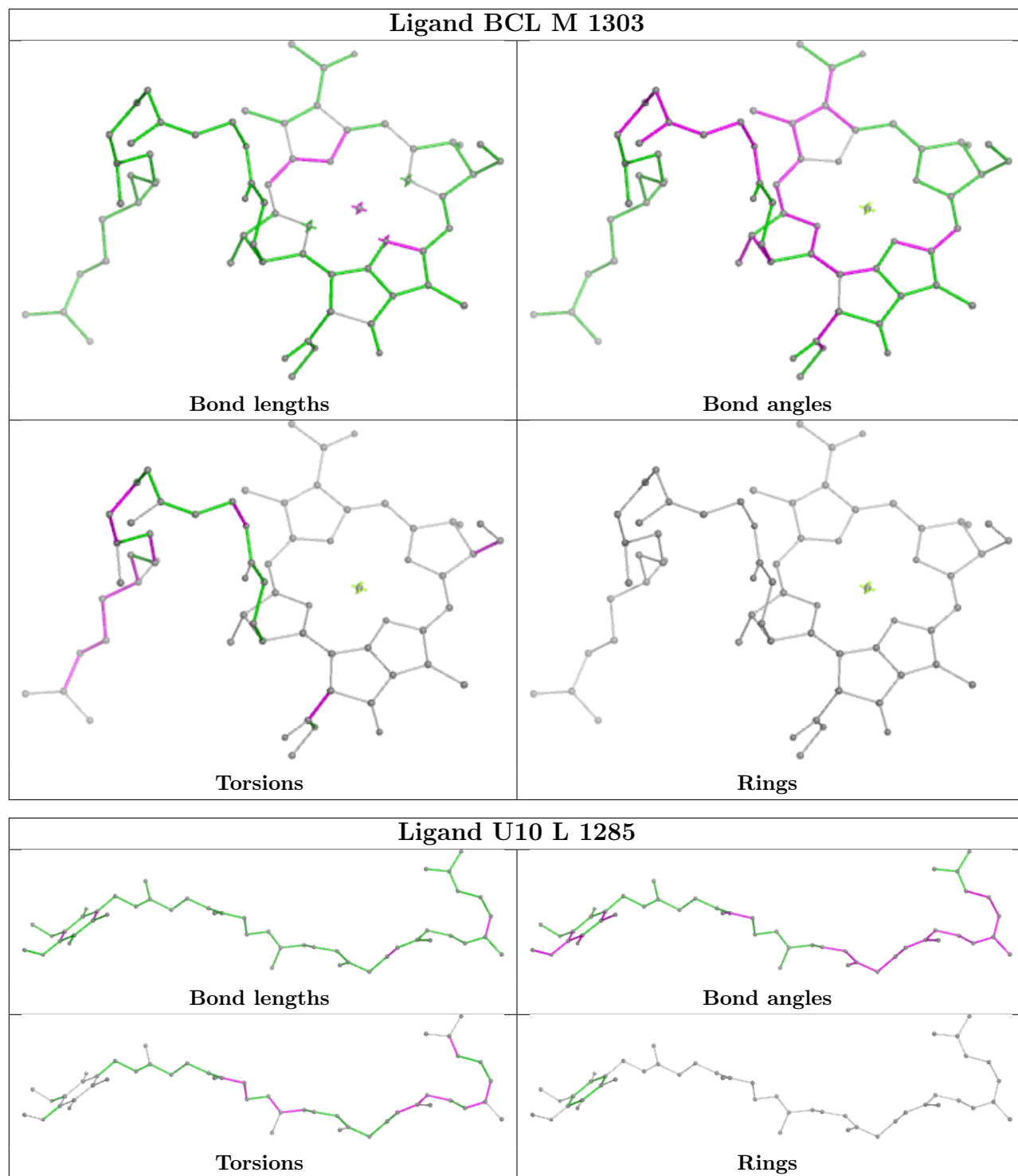
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	241/260 (92%)	-0.18	12 (4%) 28 27	24, 31, 42, 100	0
2	L	281/281 (100%)	-0.48	4 (1%) 75 73	27, 35, 49, 55	0
3	M	303/307 (98%)	-0.23	10 (3%) 46 45	29, 36, 48, 77	0
All	All	825/848 (97%)	-0.30	26 (3%) 47 46	24, 35, 48, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	13.0
3	M	303	MET	12.6
3	M	1	ALA	10.4
1	H	250	SER	9.4
3	M	302	GLY	8.5
1	H	249	LYS	7.6
1	H	245	ALA	7.2
1	H	246	PRO	6.0
1	H	247	LYS	5.7
3	M	301	HIS	5.1
3	M	2	GLU	4.6
1	H	248	ARG	3.3
2	L	270	PRO	3.1
2	L	59	TRP	2.9
3	M	3	TYR	2.9
2	L	281	GLY	2.6
1	H	60	LYS	2.6
1	H	220	LYS	2.3
1	H	201	ASN	2.3
3	M	100	GLU	2.2
1	H	184	LYS	2.2
1	H	51	ALA	2.1
2	L	202	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	80	TRP	2.1
3	M	105	PHE	2.1
3	M	300	ASN	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](#)

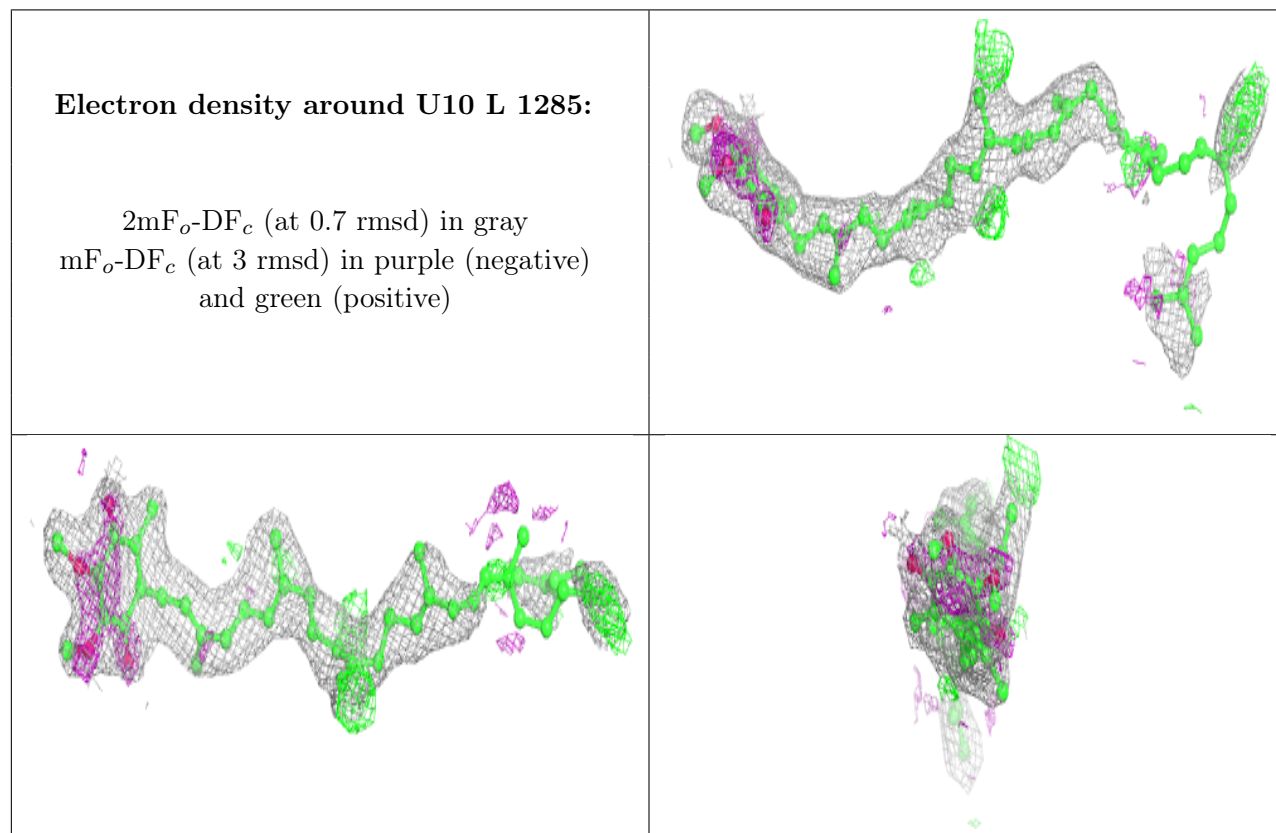
There are no monosaccharides in this entry.

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.

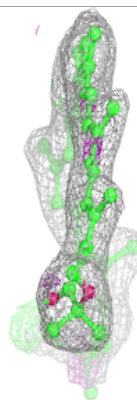
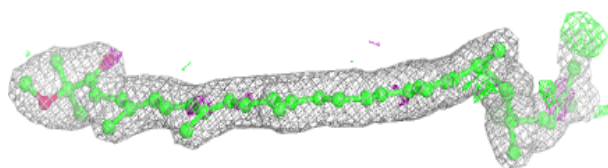
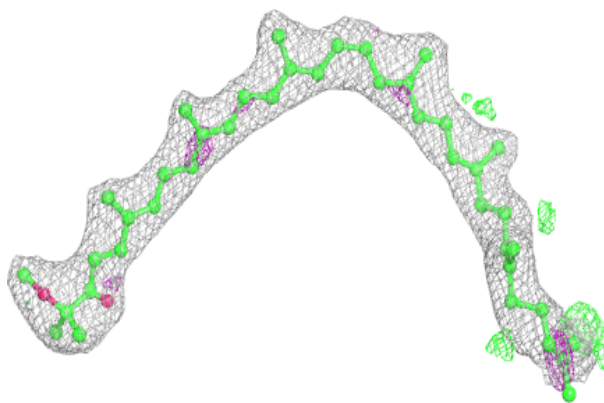
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LDA	M	1306	16/16	0.60	0.31	66,71,91,92	0
4	LDA	M	1307	16/16	0.66	0.28	31,59,69,70	0
5	D10	H	1254	7/10	0.79	0.23	77,77,77,78	0
5	D10	H	1253	8/10	0.84	0.27	66,67,71,72	0
4	LDA	M	1305	16/16	0.89	0.24	78,80,85,87	0
5	D10	H	1252	9/10	0.89	0.20	74,74,76,76	0
10	PO4	M	1310	5/5	0.89	0.35	74,75,76,77	0
4	LDA	H	1251	16/16	0.90	0.14	57,60,65,66	0
8	U10	L	1285	48/63	0.91	0.21	37,51,81,82	14
11	SPN	M	1312	43/43	0.91	0.13	22,37,59,63	0
7	BPH	M	1311	65/65	0.92	0.12	22,28,81,82	0
8	U10	M	1313	48/63	0.94	0.12	12,27,53,55	0
6	BCL	M	1303	66/66	0.95	0.11	19,23,65,67	0
6	BCL	M	1304	66/66	0.97	0.08	17,24,38,51	0
6	BCL	L	1283	66/66	0.97	0.11	12,17,38,41	0
7	BPH	L	1284	65/65	0.98	0.08	12,19,25,28	0
6	BCL	L	1282	66/66	0.98	0.08	15,21,33,41	0
10	PO4	M	1309	5/5	0.99	0.22	39,42,44,46	0
9	FE	M	1308	1/1	1.00	0.07	20,20,20,20	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.

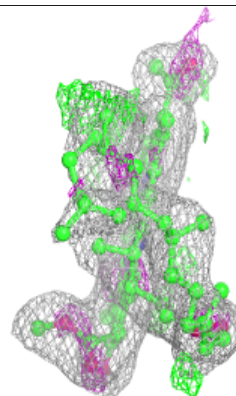
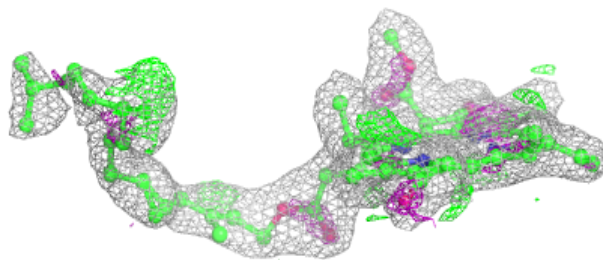
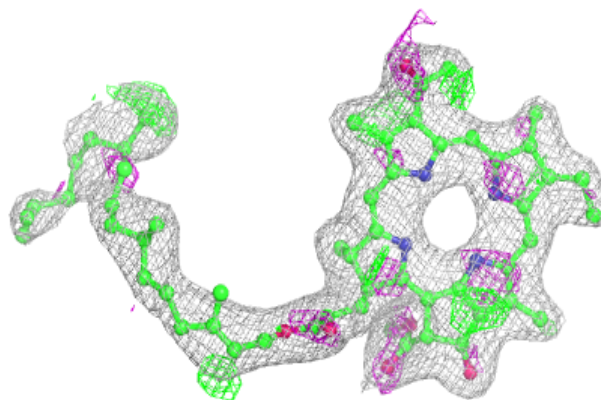


Electron density around SPN M 1312:

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

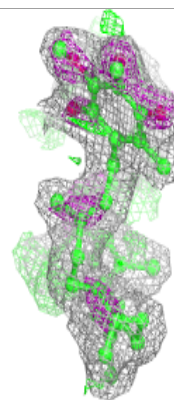
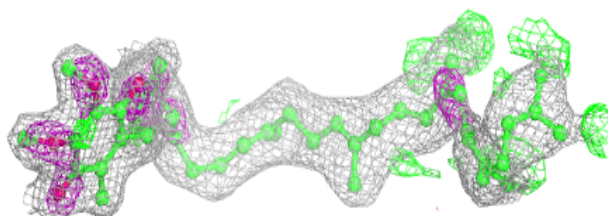
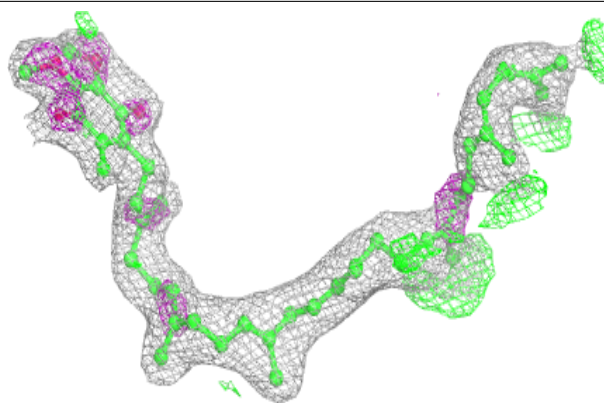
**Electron density around BPH M 1311:**

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

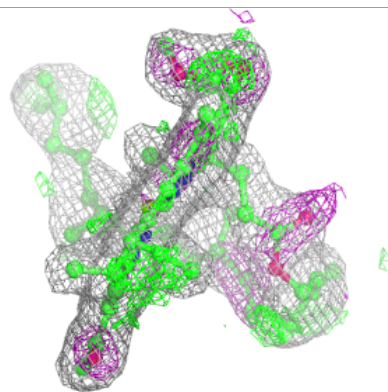
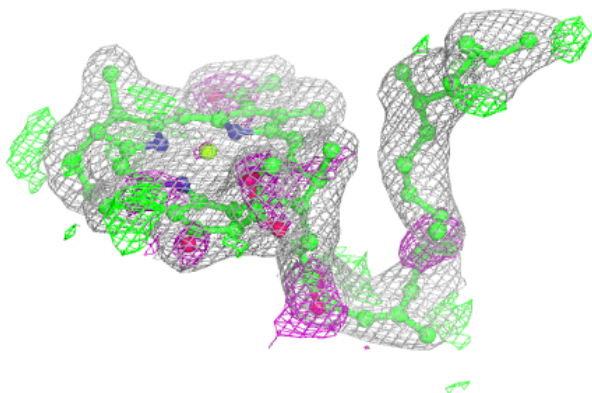
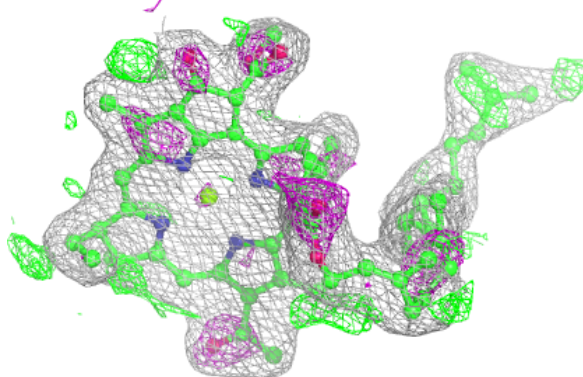


Electron density around U10 M 1313:

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

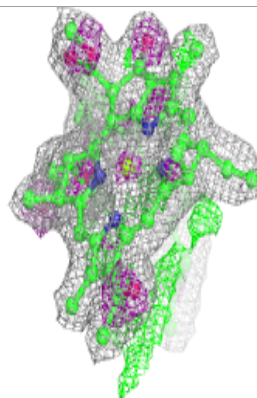
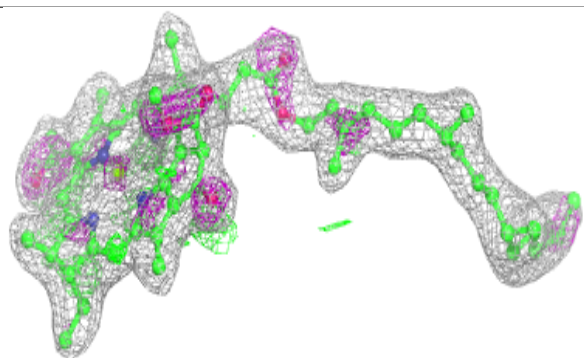
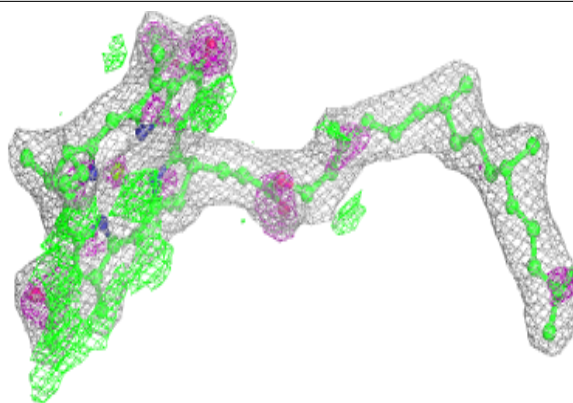
**Electron density around BCL M 1303:**

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

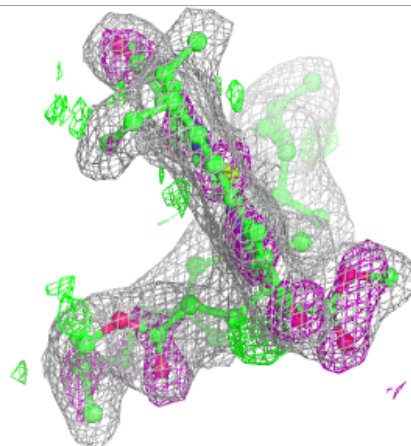
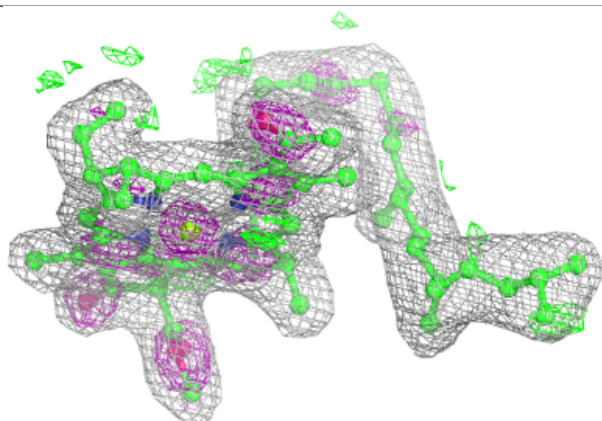
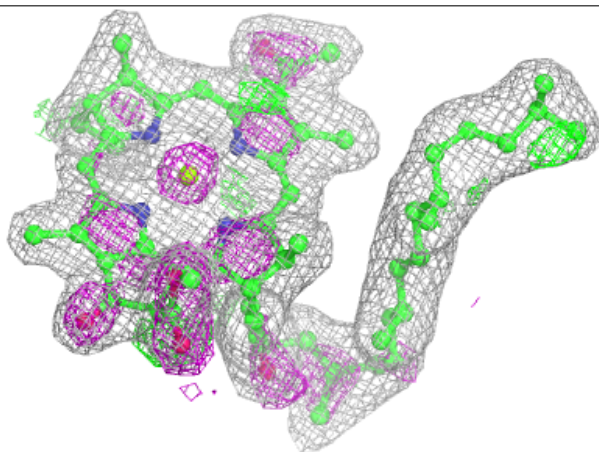


Electron density around BCL M 1304:

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

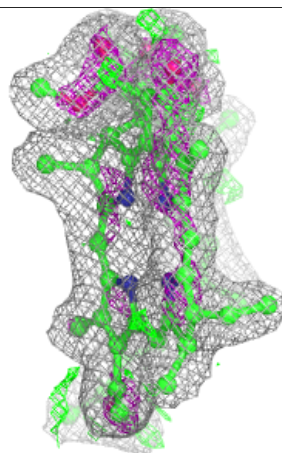
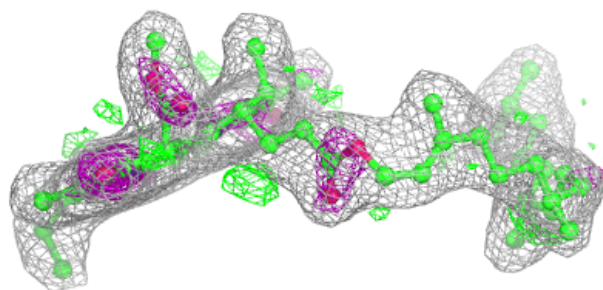
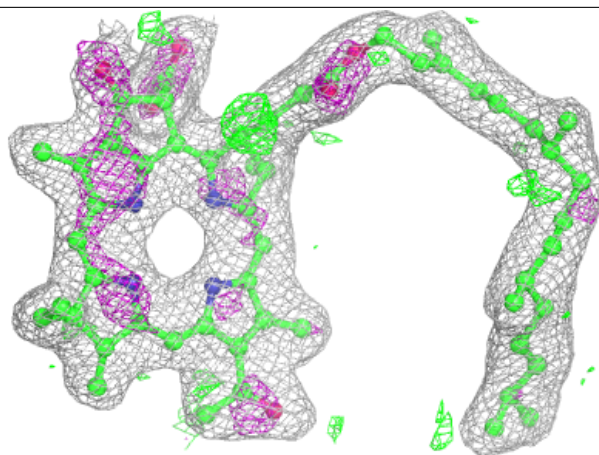
**Electron density around BCL L 1283:**

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

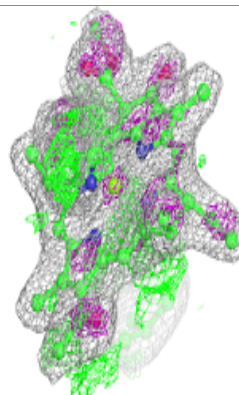
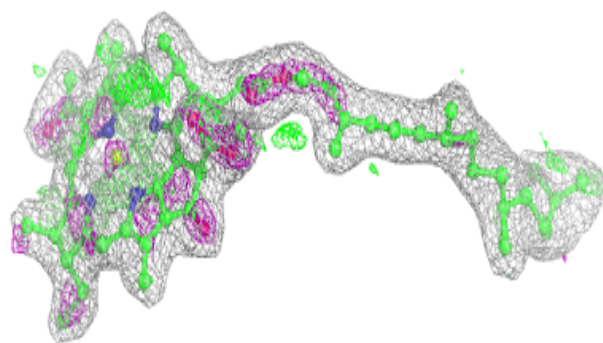
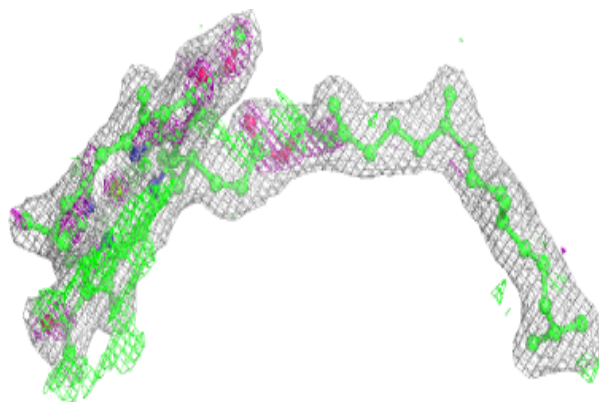


Electron density around BPH L 1284:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.