



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 AM UTC

PDB ID : 3ZUW / pdb_00003zuw
Title : Photosynthetic Reaction Centre Mutant with TYR L128 replaced with HIS
Authors : Gibasiewicz, K.; Pajzderska, M.; Potter, J.A.; Fyfe, P.K.; Dobek, A.; Brettel, K.; Jones, M.R.
Deposited on : 2011-07-20
Resolution : 2.31 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

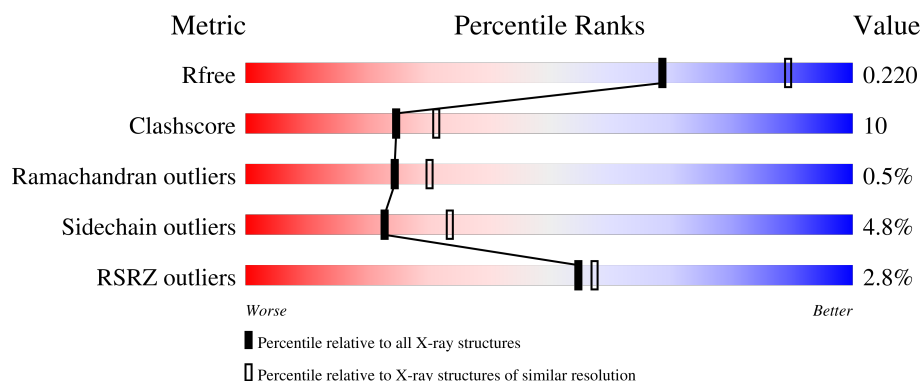
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	3% 77% 13% • 7%
2	L	281	4% 84% 14% ••
3	M	307	2% 83% 13% ••

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
4	LDA	L	1284	-	-	X	-
6	BPH	L	1285	X	-	-	-
6	BPH	M	1311	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7456 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	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2230	1504	357	361	8			

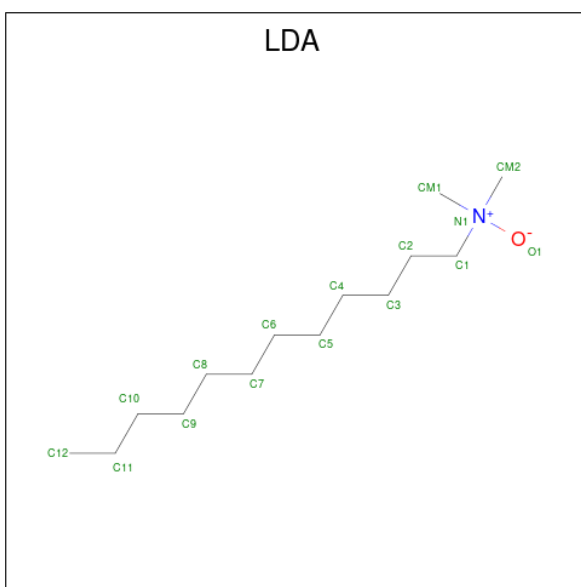
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	128	HIS	TYR	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2414	1610	397	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 16 14 1 1	0	0
4	H	1	Total C 12 12	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	L	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



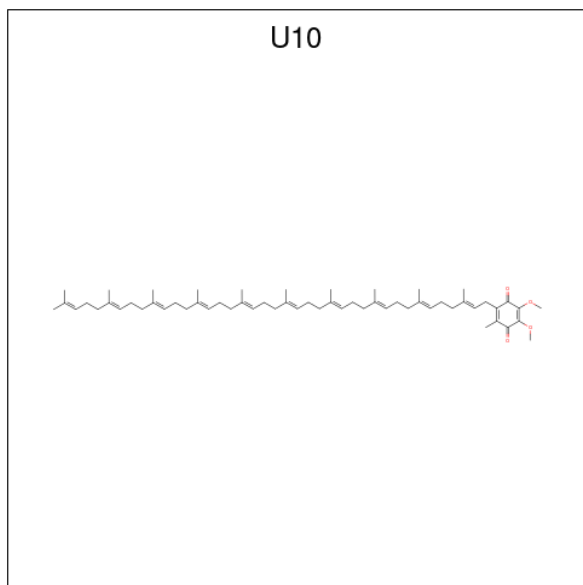
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

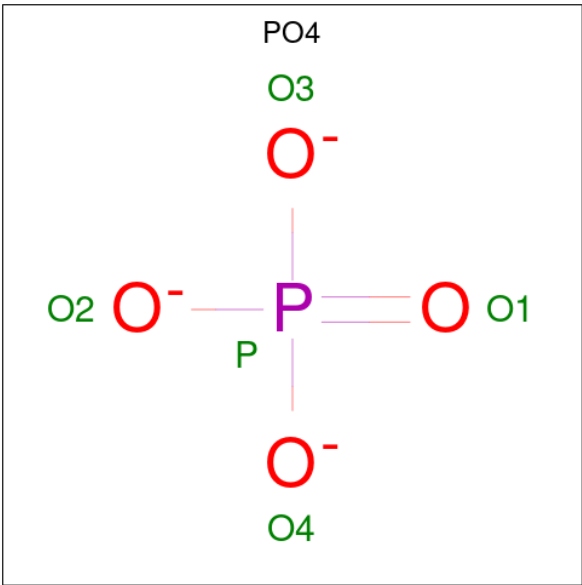


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	1	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

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

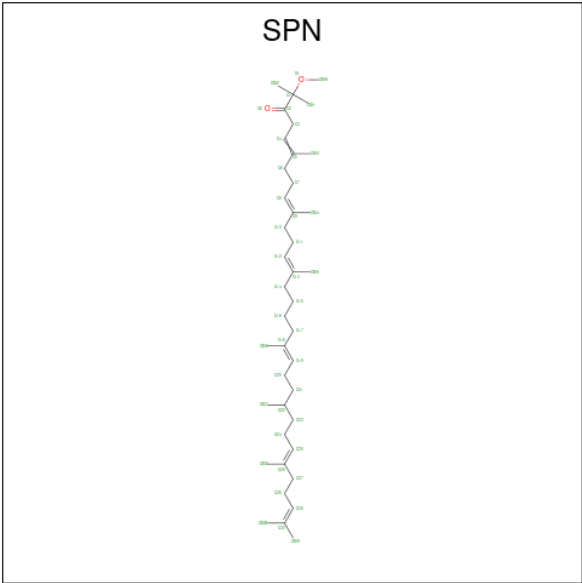
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 10 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂).



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

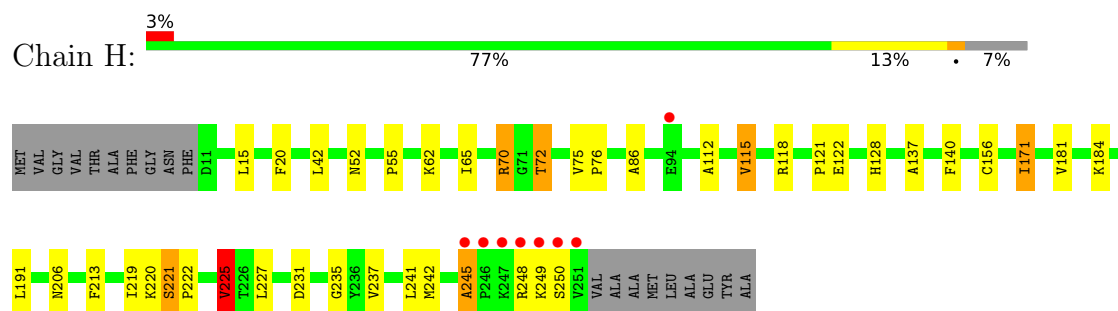
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	152	Total 152	O 152	0	0
11	L	81	Total 81	O 81	0	0
11	M	65	Total 65	O 65	0	0

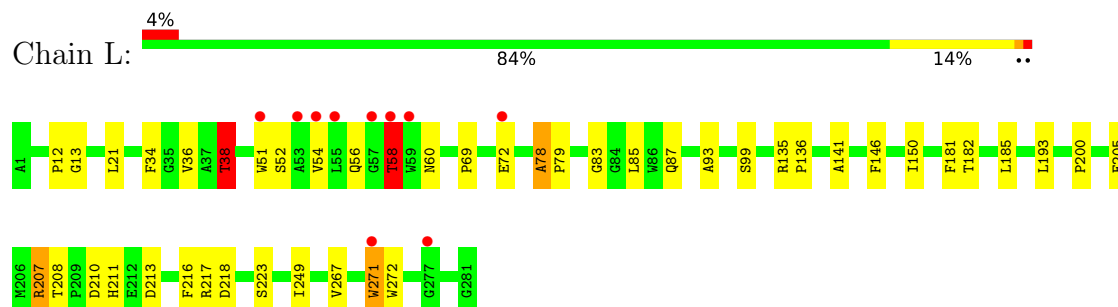
3 Residue-property plots [i](#)

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

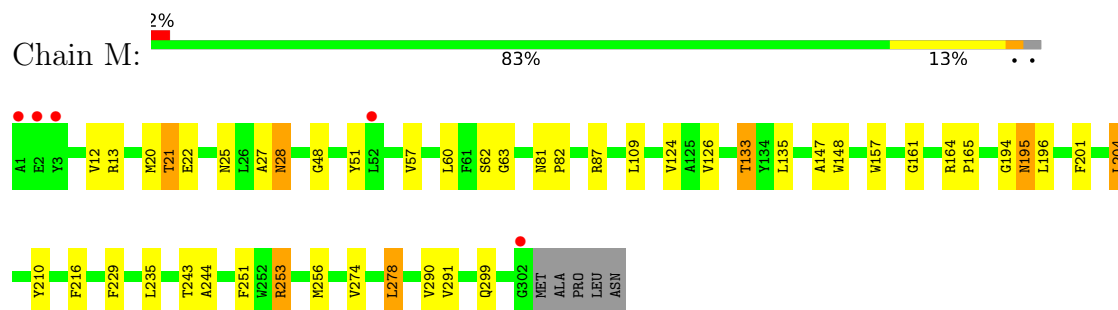
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER 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	139.87Å 139.87Å 184.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.87 – 2.31 17.87 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.87-2.31) 94.8 (17.87-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.192 , 0.224 0.189 , 0.220	Depositor DCC
R_{free} test set	4341 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BPH, FE, U10, SPN, BCL, 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	1.23	3/1878 (0.2%)	1.16	5/2555 (0.2%)
2	L	1.19	2/2318 (0.1%)	1.13	9/3172 (0.3%)
3	M	1.12	2/2511 (0.1%)	1.07	8/3427 (0.2%)
All	All	1.18	7/6707 (0.1%)	1.12	22/9154 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	250	SER	C-N	-6.23	1.24	1.33
3	M	57	VAL	CA-CB	6.01	1.61	1.54
1	H	137	ALA	C-O	5.49	1.30	1.23
2	L	36	VAL	CA-CB	5.22	1.60	1.54
3	M	126	VAL	CA-CB	5.20	1.60	1.54
2	L	249	ILE	CA-CB	5.14	1.61	1.54
1	H	86	ALA	CA-CB	5.11	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	78	ALA	CA-C-N	-8.75	110.96	119.89
2	L	78	ALA	C-N-CA	-8.75	110.96	119.89
1	H	225	VAL	CB-CA-C	-6.87	99.93	110.50
2	L	58	THR	N-CA-C	6.48	120.19	110.14
1	H	245	ALA	N-CA-C	6.13	123.35	109.81
3	M	135	LEU	N-CA-C	6.09	118.42	111.11
2	L	146	PHE	CA-C-N	-5.94	114.43	120.85
2	L	146	PHE	C-N-CA	-5.94	114.43	120.85
3	M	21	THR	N-CA-C	-5.90	105.17	112.72
2	L	141	ALA	N-CA-C	5.81	117.23	108.46
3	M	201	PHE	N-CA-C	5.54	118.08	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	208	THR	CA-C-N	-5.31	114.14	119.56
2	L	208	THR	C-N-CA	-5.31	114.14	119.56
3	M	299	GLN	N-CA-C	-5.28	105.58	112.23
3	M	27	ALA	N-CA-C	-5.27	106.11	112.54
2	L	38	THR	N-CA-CB	5.21	117.87	110.16
1	H	62	LYS	N-CA-C	-5.17	101.51	109.52
1	H	171	ILE	CA-C-N	-5.07	114.39	119.56
1	H	171	ILE	C-N-CA	-5.07	114.39	119.56
3	M	253[A]	ARG	N-CA-C	-5.03	105.71	111.14
3	M	253[B]	ARG	N-CA-C	-5.03	105.71	111.14
3	M	28	ASN	N-CA-C	5.02	119.28	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1830	0	1836	33	0
2	L	2230	0	2185	33	0
3	M	2414	0	2330	33	0
4	H	76	0	147	9	0
4	L	16	0	31	9	0
4	M	48	0	93	9	0
5	L	132	0	148	4	0
5	M	132	0	148	17	0
6	L	65	0	76	7	0
6	M	65	0	76	10	0
7	L	48	0	58	15	0
7	M	48	0	63	2	0
8	M	1	0	0	0	0
9	M	10	0	0	1	0
10	M	43	0	70	7	0
11	H	152	0	0	10	0
11	L	81	0	0	2	0
11	M	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7456	0	7261	141	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 10.

All (141) 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:52:ASN:HB3	11:H:2041:HOH:O	1.48	1.10
7:L:1286:U10:H351	7:L:1286:U10:C46	1.84	1.08
1:H:220:LYS:HE3	11:H:2095:HOH:O	1.62	0.99
6:L:1285:BPH:HHC	6:L:1285:BPH:HBB3	1.46	0.96
3:M:253[B]:ARG:HH22	4:M:1309:LDA:HM23	1.37	0.90
1:H:184:LYS:O	1:H:184:LYS:HD3	1.72	0.89
1:H:242:MET:HE1	2:L:12:PRO:O	1.80	0.81
7:L:1286:U10:C46	7:L:1286:U10:C35	2.61	0.79
6:M:1311:BPH:HHC	6:M:1311:BPH:HBB3	1.65	0.76
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.66	0.76
4:H:1253:LDA:H121	4:L:1284:LDA:H121	1.66	0.75
3:M:253[B]:ARG:NH2	4:M:1309:LDA:HM23	2.01	0.74
6:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.68	0.74
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.23	0.73
5:M:1303:BCL:HMB3	5:M:1303:BCL:HBB2	1.70	0.73
2:L:271:TRP:H	2:L:271:TRP:CD1	2.04	0.72
7:L:1286:U10:C45	5:M:1303:BCL:C20	2.67	0.72
4:H:1253:LDA:H121	4:L:1284:LDA:C12	2.19	0.71
2:L:181:PHE:HB3	6:M:1311:BPH:HBB2	1.71	0.71
6:L:1285:BPH:HHC	6:L:1285:BPH:CBB	2.23	0.68
5:L:1283:BCL:HMB3	5:L:1283:BCL:HBB2	1.74	0.68
4:M:1308:LDA:H91	4:M:1309:LDA:H121	1.75	0.67
2:L:34:PHE:O	2:L:38:THR:HG23	1.94	0.67
2:L:181:PHE:CD2	6:M:1311:BPH:HBB1	2.30	0.67
9:M:1307:PO4:O4	4:M:1310:LDA:HM11	1.95	0.67
3:M:161:GLY:HA3	10:M:1312:SPN:H201	1.76	0.66
5:M:1303:BCL:HMB3	5:M:1303:BCL:CBB	2.26	0.66
2:L:51:TRP:O	2:L:54:VAL:HG22	1.96	0.66
1:H:72:THR:HG23	11:H:2058:HOH:O	1.95	0.65
1:H:242:MET:HE2	11:H:2151:HOH:O	1.97	0.65
3:M:278:LEU:HD11	4:M:1310:LDA:H122	1.79	0.64
1:H:242:MET:CE	11:H:2151:HOH:O	2.45	0.64
2:L:93:ALA:HA	6:L:1285:BPH:H9C2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.16	0.61
7:L:1286:U10:C33	7:L:1286:U10:C26	2.79	0.61
1:H:72:THR:CG2	11:H:2058:HOH:O	2.48	0.60
3:M:157:TRP:CZ2	10:M:1312:SPN:H22	2.36	0.60
2:L:38:THR:HG22	2:L:99:SER:HB3	1.85	0.59
3:M:21:THR:O	3:M:22:GLU:C	2.45	0.59
1:H:220:LYS:NZ	11:H:2094:HOH:O	2.35	0.59
6:M:1311:BPH:HBC3	6:M:1311:BPH:HHD	1.85	0.58
4:H:1253:LDA:H112	4:L:1284:LDA:H123	1.86	0.58
7:L:1286:U10:C45	5:M:1303:BCL:H202	2.33	0.58
6:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.39	0.57
2:L:181:PHE:HB3	6:M:1311:BPH:CBB	2.35	0.57
6:M:1311:BPH:H111	6:M:1311:BPH:H161	1.85	0.57
4:H:1253:LDA:C12	4:L:1284:LDA:C12	2.83	0.56
2:L:34:PHE:O	2:L:38:THR:CG2	2.53	0.56
7:L:1286:U10:H422	7:L:1286:U10:H361	1.88	0.56
7:L:1286:U10:H361	7:L:1286:U10:C43	2.35	0.56
7:L:1286:U10:C45	5:M:1303:BCL:H203	2.36	0.55
5:M:1304:BCL:HMB3	5:M:1304:BCL:HBB2	1.89	0.55
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.89	0.55
1:H:42:LEU:HD11	4:M:1309:LDA:HM12	1.87	0.55
1:H:242:MET:CE	2:L:13:GLY:HA3	2.37	0.54
5:M:1303:BCL:H172	10:M:1312:SPN:H72	1.89	0.54
5:M:1303:BCL:CBB	5:M:1303:BCL:CMB	2.85	0.54
1:H:220:LYS:CE	11:H:2095:HOH:O	2.36	0.54
4:H:1252:LDA:H62	4:H:1254:LDA:H62	1.88	0.54
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.88	0.54
2:L:223:SER:HA	7:L:1286:U10:H103	1.89	0.54
7:L:1286:U10:H361	7:L:1286:U10:C42	2.38	0.53
1:H:75:VAL:HA	1:H:76:PRO:C	2.33	0.53
7:L:1286:U10:H451	5:M:1303:BCL:H202	1.89	0.53
1:H:241:LEU:O	1:H:248:ARG:NH2	2.42	0.53
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.52
4:L:1284:LDA:HM12	11:L:2081:HOH:O	2.10	0.51
1:H:115:VAL:HG13	3:M:243:THR:N	2.27	0.50
2:L:271:TRP:CD1	2:L:271:TRP:N	2.79	0.50
5:L:1283:BCL:HMB3	5:L:1283:BCL:CBB	2.41	0.49
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.95	0.49
3:M:157:TRP:CE2	10:M:1312:SPN:H22	2.48	0.49
4:H:1253:LDA:C12	4:L:1284:LDA:H121	2.37	0.49
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1304:BCL:HMB3	5:M:1304:BCL:CBB	2.42	0.49
3:M:133:THR:CG2	3:M:147:ALA:HA	2.42	0.49
1:H:242:MET:HE1	2:L:13:GLY:HA3	1.93	0.48
7:L:1286:U10:H451	5:M:1303:BCL:C20	2.41	0.48
6:M:1311:BPH:HBC3	6:M:1311:BPH:CHD	2.43	0.47
2:L:216:PHE:CD1	7:L:1286:U10:H102	2.49	0.47
5:M:1304:BCL:OBB	5:M:1304:BCL:HHC	2.14	0.47
1:H:181:VAL:CG2	1:H:191:LEU:HD12	2.39	0.47
1:H:70:ARG:NH2	1:H:121:PRO:O	2.47	0.47
3:M:133:THR:HG21	3:M:147:ALA:HA	1.97	0.47
2:L:83:GLY:O	2:L:87:GLN:HG3	2.15	0.47
2:L:38:THR:HG22	2:L:99:SER:CB	2.44	0.46
1:H:112:ALA:HA	1:H:235:GLY:O	2.16	0.46
4:H:1253:LDA:C12	4:L:1284:LDA:H123	2.45	0.46
1:H:20:PHE:CD1	1:H:20:PHE:C	2.93	0.45
2:L:193:LEU:HD23	7:L:1286:U10:C2	2.47	0.45
5:L:1282:BCL:HMB3	5:L:1282:BCL:CBB	2.47	0.45
3:M:161:GLY:HA3	10:M:1312:SPN:HM72	1.98	0.45
5:M:1303:BCL:CAB	10:M:1312:SPN:H162	2.47	0.45
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.99	0.45
6:L:1285:BPH:CBB	6:L:1285:BPH:CHC	2.89	0.45
5:L:1283:BCL:H13	5:L:1283:BCL:H172	1.74	0.44
7:M:1313:U10:H8	7:M:1313:U10:H1M3	1.99	0.44
4:H:1253:LDA:C11	4:L:1284:LDA:H123	2.47	0.44
7:L:1286:U10:H452	5:M:1303:BCL:C20	2.48	0.44
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.53	0.44
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.85	0.44
1:H:55:PRO:HB2	4:H:1254:LDA:H52	2.00	0.43
3:M:133:THR:CG2	3:M:147:ALA:HB2	2.48	0.43
2:L:78:ALA:O	2:L:79:PRO:C	2.60	0.43
3:M:63:GLY:HA3	6:M:1311:BPH:H5C1	2.01	0.43
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.01	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.18	0.43
6:L:1285:BPH:H112	6:L:1285:BPH:H7C2	1.89	0.43
2:L:207:ARG:HD2	2:L:207:ARG:N	2.32	0.42
1:H:118:ARG:NH2	11:H:2093:HOH:O	2.52	0.42
1:H:221:SER:HA	1:H:222:PRO:HD3	1.83	0.42
2:L:182:THR:OG1	5:M:1303:BCL:H2	2.20	0.42
6:M:1311:BPH:HHC	6:M:1311:BPH:CBB	2.43	0.42
10:M:1312:SPN:H111	10:M:1312:SPN:HM41	1.85	0.42
3:M:148:TRP:HB3	4:M:1310:LDA:H62	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1308:LDA:H91	4:M:1309:LDA:C12	2.48	0.42
1:H:65:ILE:HG22	2:L:205:GLU:HG2	2.01	0.42
1:H:128:HIS:HD2	11:H:2102:HOH:O	2.02	0.42
2:L:85:LEU:HD23	2:L:85:LEU:HA	1.92	0.42
6:M:1311:BPH:HHD	6:M:1311:BPH:CBC	2.50	0.42
3:M:256:MET:CE	7:M:1313:U10:H102	2.49	0.42
2:L:200:PRO:HB3	2:L:207:ARG:HD3	2.02	0.41
3:M:194:GLY:O	3:M:195:ASN:HB3	2.21	0.41
3:M:251:PHE:CD1	3:M:251:PHE:C	2.98	0.41
2:L:69:PRO:HB2	11:L:2019:HOH:O	2.19	0.41
5:M:1303:BCL:C4	5:M:1303:BCL:C7	2.99	0.41
2:L:217:ARG:O	2:L:218:ASP:C	2.63	0.41
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.84	0.41
1:H:184:LYS:HD3	1:H:184:LYS:C	2.39	0.41
3:M:25:ASN:OD1	3:M:25:ASN:C	2.64	0.41
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.55	0.41
2:L:58:THR:HB	2:L:60:ASN:H	1.86	0.41
2:L:213:ASP:O	2:L:217:ARG:HG3	2.20	0.41
3:M:133:THR:HG23	3:M:147:ALA:HB2	2.02	0.41
1:H:70:ARG:HH11	1:H:70:ARG:HD2	1.69	0.40
1:H:156:CYS:HB3	1:H:206:ASN:O	2.22	0.40
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.85	0.40
4:L:1284:LDA:HM13	4:L:1284:LDA:H21	1.90	0.40
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.56	0.40
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.03	0.40
3:M:204:LEU:HD13	4:M:1308:LDA:H12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	37
2	L	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
3	M	301/307 (98%)	285 (95%)	13 (4%)	3 (1%)	12	14
All	All	819/848 (97%)	784 (96%)	31 (4%)	4 (0%)	24	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	48	GLY
3	M	195	ASN
3	M	109	LEU

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	31
2	L	220/220 (100%)	209 (95%)	11 (5%)	22	32
3	M	237/240 (99%)	227 (96%)	10 (4%)	26	39
All	All	652/668 (98%)	621 (95%)	31 (5%)	23	33

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	70	ARG
1	H	72	THR
1	H	115	VAL
1	H	171	ILE
1	H	221	SER
1	H	225	VAL
1	H	231	ASP
1	H	237	VAL

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Mol	Chain	Res	Type
1	H	249	LYS
2	L	21	LEU
2	L	38	THR
2	L	56	GLN
2	L	58	THR
2	L	72	GLU
2	L	150	ILE
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	267	VAL
2	L	271	TRP
3	M	12	VAL
3	M	60	LEU
3	M	62	SER
3	M	124	VAL
3	M	133	THR
3	M	196	LEU
3	M	204	LEU
3	M	216	PHE
3	M	274	VAL
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	68	HIS
2	L	280	ASN
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 21 ligands modelled in this entry, 1 is 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	1308	-	13,15,15	2.17	2 (15%)	14,17,17	1.31	1 (7%)
7	U10	M	1313	-	48,48,63	2.75	12 (25%)	60,61,79	1.84	14 (23%)
9	PO4	M	1307	-	4,4,4	2.14	2 (50%)	6,6,6	0.67	0
5	BCL	L	1283	2	69,74,74	1.57	8 (11%)	79,115,115	1.86	18 (22%)
4	LDA	L	1284	-	13,15,15	2.01	2 (15%)	14,17,17	0.38	0
4	LDA	M	1310	-	13,15,15	1.81	1 (7%)	14,17,17	0.71	0
6	BPH	L	1285	-	59,70,70	1.78	9 (15%)	59,101,101	2.19	11 (18%)
6	BPH	M	1311	-	59,70,70	1.60	4 (6%)	59,101,101	2.41	13 (22%)
10	SPN	M	1312	-	42,42,42	0.77	0	50,52,52	1.78	11 (22%)
4	LDA	M	1309	-	13,15,15	2.34	2 (15%)	14,17,17	1.53	3 (21%)
9	PO4	M	1306	-	4,4,4	0.98	0	6,6,6	0.50	0
5	BCL	L	1282	2	69,74,74	1.26	6 (8%)	79,115,115	1.81	14 (17%)
4	LDA	H	1254	-	13,15,15	2.11	2 (15%)	14,17,17	0.38	0
5	BCL	M	1303	3	69,74,74	1.38	6 (8%)	79,115,115	1.87	14 (17%)
4	LDA	H	1256	-	13,15,15	1.96	2 (15%)	14,17,17	0.53	0
4	LDA	H	1253	-	11,11,15	0.29	0	10,10,17	0.62	0
4	LDA	H	1252	-	13,15,15	1.93	2 (15%)	14,17,17	0.59	0
5	BCL	M	1304	3	69,74,74	1.36	7 (10%)	79,115,115	1.91	18 (22%)
7	U10	L	1286	-	47,47,63	3.13	14 (29%)	57,59,79	1.95	16 (28%)
4	LDA	H	1255	-	13,15,15	2.22	2 (15%)	14,17,17	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BPH	L	1285	-	2/2/18/22	12/37/105/105	0/5/6/6
4	LDA	M	1308	-	-	3/13/13/13	-
7	U10	M	1313	-	-	13/45/69/87	0/1/1/1
6	BPH	M	1311	-	2/2/18/22	7/37/105/105	0/5/6/6
5	BCL	L	1283	2	-	5/41/137/137	-
5	BCL	M	1303	3	-	7/41/137/137	-
4	LDA	L	1284	-	-	3/13/13/13	-
5	BCL	M	1304	3	-	1/41/137/137	-
7	U10	L	1286	-	-	22/41/65/87	0/1/1/1
4	LDA	H	1256	-	-	5/13/13/13	-
10	SPN	M	1312	-	-	16/50/51/51	-
4	LDA	H	1253	-	-	4/9/9/13	-
4	LDA	M	1309	-	-	4/13/13/13	-
4	LDA	M	1310	-	-	9/13/13/13	-
4	LDA	H	1252	-	-	5/13/13/13	-
5	BCL	L	1282	2	-	6/41/137/137	-
4	LDA	H	1255	-	-	5/13/13/13	-
4	LDA	H	1254	-	-	4/13/13/13	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1286	U10	C27-C26	-10.37	1.07	1.51
6	L	1285	BPH	C1D-C2D	10.24	1.50	1.39
6	M	1311	BPH	C1D-C2D	9.81	1.50	1.39
7	L	1286	U10	C38-C39	7.37	1.50	1.33
7	M	1313	U10	C33-C34	7.33	1.49	1.33
7	L	1286	U10	C18-C19	7.22	1.49	1.33
4	M	1309	LDA	O1-N1	-7.06	1.24	1.42
4	M	1308	LDA	O1-N1	-7.05	1.24	1.42
7	L	1286	U10	C13-C14	6.96	1.49	1.33
7	M	1313	U10	C13-C14	6.84	1.48	1.33
4	H	1255	LDA	O1-N1	-6.59	1.26	1.42
7	M	1313	U10	C28-C29	6.44	1.47	1.33
4	H	1254	LDA	O1-N1	-6.39	1.26	1.42
4	H	1252	LDA	O1-N1	-6.35	1.26	1.42
4	H	1256	LDA	O1-N1	-6.34	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1284	LDA	O1-N1	-6.31	1.26	1.42
7	M	1313	U10	C18-C19	6.22	1.47	1.33
5	L	1283	BCL	MG-ND	-6.15	1.93	2.05
4	M	1310	LDA	O1-N1	-6.10	1.27	1.42
7	L	1286	U10	C23-C24	6.09	1.47	1.33
7	M	1313	U10	C8-C9	6.06	1.47	1.33
5	L	1283	BCL	MG-NB	-6.01	1.93	2.05
7	M	1313	U10	C23-C24	5.98	1.46	1.33
7	L	1286	U10	C8-C9	5.85	1.46	1.33
7	M	1313	U10	C38-C39	5.52	1.49	1.32
7	L	1286	U10	C43-C44	5.34	1.48	1.32
5	M	1303	BCL	MG-ND	-5.30	1.95	2.05
5	M	1303	BCL	MG-NB	-5.28	1.95	2.05
7	L	1286	U10	C33-C34	5.25	1.48	1.33
5	L	1282	BCL	MG-ND	-4.63	1.96	2.05
4	M	1309	LDA	C1-N1	-4.58	1.46	1.51
5	L	1283	BCL	C4B-NB	4.39	1.43	1.37
4	H	1255	LDA	C1-N1	-4.27	1.47	1.51
5	M	1304	BCL	MG-ND	-4.25	1.97	2.05
7	L	1286	U10	O4-C4	-4.16	1.26	1.36
5	M	1303	BCL	C1B-NB	4.16	1.43	1.37
4	H	1254	LDA	C1-N1	-3.94	1.47	1.51
5	M	1304	BCL	C4B-NB	3.86	1.42	1.37
7	M	1313	U10	O3-C3	-3.82	1.27	1.36
5	L	1282	BCL	C4B-NB	3.76	1.42	1.37
7	M	1313	U10	O4-C4	-3.72	1.27	1.36
5	L	1282	BCL	C1D-C2D	-3.70	1.38	1.45
5	M	1304	BCL	MG-NB	-3.63	1.98	2.05
5	L	1282	BCL	C1B-NB	3.55	1.42	1.37
5	M	1304	BCL	C1B-NB	3.54	1.42	1.37
5	L	1283	BCL	C1B-NB	3.47	1.42	1.37
5	M	1304	BCL	C1D-C2D	-3.46	1.38	1.45
6	L	1285	BPH	C3D-C4D	3.44	1.45	1.41
5	M	1303	BCL	C1D-C2D	-3.44	1.38	1.45
6	L	1285	BPH	C4D-CHA	-3.39	1.34	1.39
4	L	1284	LDA	C1-N1	-3.31	1.48	1.51
9	M	1307	PO4	P-O3	-3.28	1.45	1.54
7	L	1286	U10	O3-C3	-3.27	1.28	1.36
6	L	1285	BPH	C3B-C4B	-3.07	1.36	1.41
5	M	1304	BCL	C3D-C4D	-3.06	1.37	1.44
5	L	1283	BCL	C1D-C2D	-2.94	1.39	1.45
6	M	1311	BPH	C4D-CHA	-2.86	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1311	BPH	C3D-C2D	-2.81	1.34	1.39
5	L	1283	BCL	MG-NA	-2.78	1.99	2.06
7	M	1313	U10	C4-C5	-2.71	1.41	1.48
7	L	1286	U10	C3-C2	-2.70	1.41	1.48
7	M	1313	U10	C6-C1	2.69	1.40	1.35
4	H	1256	LDA	C1-N1	-2.69	1.48	1.51
5	L	1282	BCL	MG-NB	-2.67	2.00	2.05
7	L	1286	U10	C6-C1	2.61	1.39	1.35
9	M	1307	PO4	P-O1	2.59	1.56	1.50
7	L	1286	U10	C6-C5	-2.56	1.39	1.46
5	L	1282	BCL	C1B-C2B	-2.48	1.37	1.43
5	M	1304	BCL	C1B-C2B	-2.46	1.37	1.43
5	M	1303	BCL	C1D-ND	2.45	1.41	1.37
4	H	1252	LDA	C1-N1	-2.44	1.49	1.51
5	M	1303	BCL	C1B-C2B	-2.36	1.37	1.43
6	L	1285	BPH	C3D-C2D	-2.29	1.35	1.39
6	L	1285	BPH	CMD-C2D	-2.24	1.47	1.51
7	L	1286	U10	C4-C5	-2.10	1.42	1.48
6	M	1311	BPH	CBD-CGD	-2.09	1.49	1.52
6	L	1285	BPH	C3B-CAB	-2.08	1.43	1.49
7	M	1313	U10	C3-C2	-2.06	1.42	1.48
5	L	1283	BCL	CAA-C2A	2.05	1.57	1.54
4	M	1308	LDA	C1-N1	-2.04	1.49	1.51
6	L	1285	BPH	C2-C3	2.03	1.37	1.33
6	L	1285	BPH	CHA-CBD	2.02	1.54	1.51
5	L	1283	BCL	CMA-C3A	2.00	1.57	1.53

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1311	BPH	C4D-CHA-CBD	11.06	113.76	108.45
5	M	1303	BCL	C1D-ND-C4D	-9.55	99.61	106.31
6	M	1311	BPH	C2D-C1D-ND	-8.78	103.08	109.43
5	L	1283	BCL	C1D-ND-C4D	-8.35	100.45	106.31
6	L	1285	BPH	C4D-CHA-CBD	8.35	112.46	108.45
5	L	1282	BCL	C1D-ND-C4D	-8.12	100.61	106.31
6	L	1285	BPH	C2D-C1D-ND	-7.48	104.02	109.43
5	M	1304	BCL	C1D-ND-C4D	-7.27	101.21	106.31
5	M	1304	BCL	C1C-NC-C4C	6.69	109.73	106.68
5	L	1282	BCL	C1C-NC-C4C	6.61	109.69	106.68
7	L	1286	U10	C1M-C1-C6	-5.37	115.61	124.45
5	M	1304	BCL	O2D-CGD-CBD	5.37	120.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1311	BPH	C2B-C1B-NB	-5.18	105.68	109.43
6	L	1285	BPH	C2B-C1B-NB	-5.16	105.70	109.43
10	M	1312	SPN	CM5-C13-C14	4.92	123.77	115.23
5	M	1303	BCL	C1-O2A-CGA	4.84	128.38	116.65
5	L	1283	BCL	O2D-CGD-CBD	4.75	119.54	111.23
7	L	1286	U10	C7-C8-C9	-4.72	118.70	126.83
7	M	1313	U10	C17-C18-C19	-4.67	116.93	127.62
6	L	1285	BPH	C4C-C3C-C2C	-4.41	98.64	102.84
7	M	1313	U10	C30-C29-C31	4.34	122.77	115.23
7	L	1286	U10	C25-C24-C26	4.32	121.22	116.13
7	M	1313	U10	C10-C9-C11	4.32	122.72	115.23
5	M	1303	BCL	C2D-C1D-ND	4.26	114.35	110.13
7	L	1286	U10	C3M-O3-C3	4.13	130.98	116.47
4	M	1309	LDA	CM1-N1-C1	-4.09	101.64	110.23
5	M	1303	BCL	C1C-NC-C4C	4.09	108.54	106.68
10	M	1312	SPN	CM6-C18-C17	3.97	122.11	115.23
5	L	1283	BCL	C1C-NC-C4C	3.93	108.47	106.68
10	M	1312	SPN	C21-C20-C19	-3.90	101.92	112.16
4	M	1308	LDA	CM1-N1-C1	3.79	118.20	110.23
6	L	1285	BPH	OBB-CAB-C3B	3.74	126.25	119.99
7	M	1313	U10	C22-C23-C24	-3.63	119.32	127.62
7	M	1313	U10	C32-C33-C34	-3.56	119.47	127.62
6	L	1285	BPH	C4D-ND-C1D	3.55	113.13	108.87
5	M	1303	BCL	C3D-C4D-ND	3.51	115.69	109.99
7	M	1313	U10	C27-C28-C29	-3.46	119.71	127.62
7	L	1286	U10	C15-C14-C16	3.44	121.20	115.23
5	M	1304	BCL	O2D-CGD-O1D	-3.39	117.25	123.85
5	M	1304	BCL	CHD-C1D-ND	-3.39	120.03	124.80
6	M	1311	BPH	C4D-ND-C1D	3.39	112.93	108.87
10	M	1312	SPN	CM4-C9-C10	3.38	121.09	115.23
6	M	1311	BPH	OBB-CAB-C3B	3.37	125.63	119.99
6	L	1285	BPH	C1A-C2A-C3A	-3.35	99.66	102.84
5	M	1303	BCL	O2D-CGD-CBD	3.32	117.03	111.23
7	L	1286	U10	C22-C23-C24	-3.29	120.10	127.62
5	L	1283	BCL	C2D-C1D-ND	3.26	113.35	110.13
5	L	1283	BCL	C3D-C4D-ND	3.24	115.25	109.99
7	M	1313	U10	C35-C34-C36	3.24	120.85	115.23
7	L	1286	U10	C27-C26-C24	3.22	129.00	113.70
5	L	1282	BCL	C2D-C1D-ND	3.21	113.31	110.13
5	L	1283	BCL	O2A-CGA-CBA	3.18	121.55	111.83
5	L	1282	BCL	C4-C3-C5	3.13	120.67	115.23
7	L	1286	U10	C25-C24-C23	-3.13	115.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1313	U10	C25-C24-C26	3.12	120.64	115.23
5	L	1283	BCL	CHB-C4A-NA	3.08	128.85	124.40
7	L	1286	U10	C10-C9-C11	3.08	120.57	115.23
5	L	1282	BCL	CHD-C1D-ND	-3.07	120.48	124.80
5	L	1282	BCL	C11-C12-C13	-3.04	105.86	115.97
5	M	1303	BCL	C4-C3-C2	-3.00	115.91	123.63
5	L	1283	BCL	O2D-CGD-O1D	-2.99	118.02	123.85
10	M	1312	SPN	CM3-C5-C6	2.96	120.36	115.23
5	L	1283	BCL	C1D-CHD-C4C	-2.95	119.50	126.62
5	M	1303	BCL	C3C-C4C-CHD	-2.90	117.28	123.39
7	M	1313	U10	C15-C14-C16	2.85	120.18	115.23
6	M	1311	BPH	O2D-CGD-CBD	2.81	114.03	110.95
7	L	1286	U10	C40-C39-C41	2.80	120.08	115.23
6	L	1285	BPH	C4-C3-C5	-2.79	110.38	115.23
6	M	1311	BPH	CBA-CAA-C2A	-2.79	105.55	113.78
5	L	1283	BCL	O2A-CGA-O1A	-2.76	116.72	123.63
10	M	1312	SPN	CM2-C1-C2	-2.73	103.74	109.43
5	L	1282	BCL	C1-O2A-CGA	2.73	123.25	116.65
10	M	1312	SPN	C3-C4-C5	-2.71	122.17	126.83
10	M	1312	SPN	CM8-C26-C27	2.69	119.90	115.23
4	M	1309	LDA	CM2-N1-C1	2.66	115.83	110.23
5	L	1282	BCL	O2D-CGD-CBD	2.65	115.87	111.23
7	M	1313	U10	C4M-O4-C4	2.64	125.73	116.47
5	L	1283	BCL	CMA-C3A-C4A	2.63	118.85	111.77
5	M	1304	BCL	C11-C12-C13	-2.63	107.22	115.97
6	L	1285	BPH	CMA-C3A-C4A	-2.63	108.95	114.61
5	M	1304	BCL	O2A-CGA-CBA	2.62	119.82	111.83
5	M	1304	BCL	C3D-C4D-ND	2.60	114.22	109.99
5	L	1282	BCL	C4A-NA-C1A	-2.59	105.50	106.68
5	L	1283	BCL	C3C-C4C-CHD	-2.59	117.94	123.39
5	L	1282	BCL	C1D-CHD-C4C	-2.55	120.47	126.62
6	M	1311	BPH	C4C-C3C-C2C	-2.55	100.41	102.84
7	L	1286	U10	O5-C5-C6	-2.55	116.86	121.79
5	M	1304	BCL	CMD-C2D-C1D	2.52	129.16	124.73
5	M	1304	BCL	CHB-C4A-NA	2.46	127.94	124.40
6	L	1285	BPH	C7-C6-C5	-2.43	106.79	113.26
5	M	1303	BCL	CHD-C1D-ND	-2.42	121.40	124.80
5	L	1282	BCL	O2A-CGA-CBA	2.40	119.16	111.83
7	M	1313	U10	C41-C39-C40	2.39	120.09	114.59
5	M	1303	BCL	O2A-CGA-CBA	2.37	119.06	111.83
6	M	1311	BPH	C5-C3-C2	2.36	126.47	121.17
6	L	1285	BPH	C1-O2A-CGA	-2.35	110.95	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1283	BCL	CHD-C1D-ND	-2.35	121.49	124.80
6	M	1311	BPH	OBB-CAB-CBB	-2.35	115.18	120.19
5	L	1283	BCL	C1-O2A-CGA	2.32	122.27	116.65
6	M	1311	BPH	CMD-C2D-C3D	2.31	129.31	124.68
7	L	1286	U10	C15-C14-C13	-2.31	117.69	123.63
10	M	1312	SPN	C14-C13-C12	-2.29	116.03	121.17
5	M	1304	BCL	CED-O2D-CGD	2.29	121.11	115.92
7	L	1286	U10	C7-C6-C1	-2.29	120.97	124.89
5	L	1283	BCL	C4D-CHA-C1A	-2.26	118.54	121.24
5	L	1283	BCL	OBD-CAD-C3D	-2.26	123.13	128.42
10	M	1312	SPN	C20-C19-C18	-2.26	122.45	127.62
5	M	1304	BCL	CAA-C2A-C3A	-2.26	106.90	113.00
6	M	1311	BPH	C6-C5-C3	2.24	118.93	113.47
5	M	1304	BCL	C1-C2-C3	-2.23	122.54	126.20
5	M	1303	BCL	CBC-CAC-C3C	-2.22	108.71	113.41
10	M	1312	SPN	CMB-C30-CM9	2.22	119.69	114.59
7	L	1286	U10	O2-C2-C3	-2.21	116.34	121.03
5	L	1282	BCL	CHC-C4B-NB	-2.21	120.74	124.05
5	L	1282	BCL	C3D-C4D-ND	2.16	113.49	109.99
5	M	1303	BCL	C5-C3-C2	2.13	125.95	121.17
5	M	1304	BCL	C4-C3-C5	2.13	118.93	115.23
5	M	1304	BCL	C16-C15-C13	-2.13	108.89	115.97
7	M	1313	U10	C11-C9-C8	-2.12	116.42	121.17
5	M	1303	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
5	L	1283	BCL	C2A-C1A-CHA	-2.11	120.21	123.87
5	M	1304	BCL	CMD-C2D-C3D	-2.11	122.85	127.69
7	M	1313	U10	C25-C24-C23	-2.11	118.22	123.63
5	M	1303	BCL	O2A-CGA-O1A	-2.08	118.43	123.63
6	M	1311	BPH	C1A-C2A-C3A	-2.07	100.87	102.84
7	L	1286	U10	C1M-C1-C2	2.04	123.92	116.93
5	M	1304	BCL	C4-C3-C2	-2.04	118.38	123.63
7	M	1313	U10	C7-C6-C1	-2.04	121.39	124.89
5	L	1282	BCL	O2A-CGA-O1A	-2.03	118.54	123.63
5	L	1283	BCL	C17-C16-C15	-2.03	104.19	113.28
7	L	1286	U10	C37-C38-C39	-2.01	123.02	127.62
5	M	1304	BCL	C2A-C1A-CHA	-2.01	120.38	123.87
4	M	1309	LDA	C8-C7-C6	-2.01	104.23	114.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1285	BPH	C8

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Mol	Chain	Res	Type	Atom
6	L	1285	BPH	C13
6	M	1311	BPH	C8
6	M	1311	BPH	C13

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	LDA	C2-C1-N1-CM2
4	H	1254	LDA	C2-C1-N1-CM1
4	H	1254	LDA	C2-C1-N1-CM2
4	H	1256	LDA	N1-C1-C2-C3
4	M	1310	LDA	C2-C1-N1-O1
4	M	1310	LDA	C2-C1-N1-CM1
6	L	1285	BPH	C6-C7-C8-C9
7	L	1286	U10	C22-C23-C24-C25
7	L	1286	U10	C23-C24-C26-C27
7	L	1286	U10	C25-C24-C26-C27
7	L	1286	U10	C33-C34-C36-C37
7	L	1286	U10	C35-C34-C36-C37
7	L	1286	U10	C37-C38-C39-C40
7	L	1286	U10	C37-C38-C39-C41
7	L	1286	U10	C39-C41-C42-C43
7	M	1313	U10	C27-C28-C29-C31
7	M	1313	U10	C32-C33-C34-C35
7	M	1313	U10	C32-C33-C34-C36
10	M	1312	SPN	CM3-C5-C6-C7
7	L	1286	U10	C42-C43-C44-C45
7	L	1286	U10	C42-C43-C44-C46
10	M	1312	SPN	C11-C10-C9-CM4
10	M	1312	SPN	C4-C5-C6-C7
10	M	1312	SPN	C11-C10-C9-C8
7	M	1313	U10	C27-C28-C29-C30
10	M	1312	SPN	C16-C17-C18-CM6
10	M	1312	SPN	C16-C17-C18-C19
7	L	1286	U10	C34-C36-C37-C38
7	L	1286	U10	C17-C18-C19-C20
10	M	1312	SPN	C14-C15-C16-C17
10	M	1312	SPN	CM5-C13-C14-C15
10	M	1312	SPN	C12-C13-C14-C15
10	M	1312	SPN	C20-C21-C22-CM7
10	M	1312	SPN	CM7-C22-C23-C24
5	M	1303	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
6	L	1285	BPH	C11-C10-C8-C7
6	L	1285	BPH	C11-C12-C13-C15
7	M	1313	U10	C24-C26-C27-C28
5	M	1303	BCL	C13-C15-C16-C17
6	M	1311	BPH	C15-C16-C17-C18
5	M	1303	BCL	C3-C5-C6-C7
6	M	1311	BPH	C8-C10-C11-C12
5	L	1283	BCL	C15-C16-C17-C18
7	M	1313	U10	C37-C38-C39-C41
7	M	1313	U10	C34-C36-C37-C38
4	M	1310	LDA	C1-C2-C3-C4
5	M	1303	BCL	C15-C16-C17-C18
6	M	1311	BPH	C16-C17-C18-C19
4	L	1284	LDA	C11-C10-C9-C8
4	M	1310	LDA	C3-C4-C5-C6
4	H	1255	LDA	C4-C5-C6-C7
6	M	1311	BPH	C16-C17-C18-C20
4	H	1253	LDA	C6-C7-C8-C9
6	L	1285	BPH	C8-C10-C11-C12
4	H	1256	LDA	C11-C10-C9-C8
4	M	1308	LDA	C3-C4-C5-C6
7	L	1286	U10	C22-C23-C24-C26
4	H	1253	LDA	C3-C4-C5-C6
5	L	1283	BCL	C16-C17-C18-C20
4	H	1252	LDA	C4-C5-C6-C7
5	L	1282	BCL	C16-C17-C18-C19
4	H	1254	LDA	C5-C6-C7-C8
4	M	1309	LDA	C6-C7-C8-C9
10	M	1312	SPN	C21-C22-C23-C24
6	L	1285	BPH	C2-C3-C5-C6
5	L	1282	BCL	C16-C17-C18-C20
7	L	1286	U10	C20-C19-C21-C22
5	M	1303	BCL	C8-C10-C11-C12
6	L	1285	BPH	O2A-C1-C2-C3
4	H	1252	LDA	C2-C3-C4-C5
4	M	1310	LDA	C6-C7-C8-C9
5	M	1303	BCL	C11-C10-C8-C9
6	L	1285	BPH	C11-C10-C8-C9
6	L	1285	BPH	C14-C13-C15-C16
4	M	1308	LDA	C1-C2-C3-C4
7	L	1286	U10	C18-C19-C21-C22
10	M	1312	SPN	CM1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	M	1312	SPN	CM1-C1-C2-C3
5	L	1283	BCL	C16-C17-C18-C19
4	L	1284	LDA	C6-C7-C8-C9
4	H	1255	LDA	C7-C8-C9-C10
6	L	1285	BPH	C4-C3-C5-C6
7	M	1313	U10	C37-C38-C39-C40
10	M	1312	SPN	O1-C1-C2-O2
6	M	1311	BPH	C3-C5-C6-C7
5	L	1282	BCL	C11-C12-C13-C15
4	M	1309	LDA	C1-C2-C3-C4
4	H	1252	LDA	C2-C1-N1-CM1
4	H	1255	LDA	C2-C1-N1-CM1
4	M	1310	LDA	C2-C1-N1-CM2
7	M	1313	U10	C25-C24-C26-C27
4	H	1253	LDA	C2-C3-C4-C5
6	L	1285	BPH	C6-C7-C8-C10
4	H	1254	LDA	C2-C1-N1-O1
5	L	1283	BCL	CHA-CBD-CGD-O1D
7	M	1313	U10	C23-C24-C26-C27
4	H	1253	LDA	C4-C5-C6-C7
4	H	1256	LDA	C4-C5-C6-C7
4	H	1256	LDA	C2-C3-C4-C5
4	M	1310	LDA	C9-C10-C11-C12
5	L	1282	BCL	C11-C12-C13-C14
10	M	1312	SPN	C19-C20-C21-C22
5	M	1303	BCL	C5-C6-C7-C8
5	L	1283	BCL	C13-C15-C16-C17
4	H	1255	LDA	C6-C7-C8-C9
7	L	1286	U10	C12-C11-C9-C10
7	M	1313	U10	C5-C4-O4-C4M
5	L	1282	BCL	C14-C13-C15-C16
7	L	1286	U10	C15-C14-C16-C17
4	M	1310	LDA	C5-C6-C7-C8
7	L	1286	U10	C12-C11-C9-C8
4	L	1284	LDA	C1-C2-C3-C4
4	M	1309	LDA	C9-C10-C11-C12
6	L	1285	BPH	C10-C11-C12-C13
7	M	1313	U10	C35-C34-C36-C37
7	L	1286	U10	C17-C18-C19-C21
4	M	1310	LDA	C2-C3-C4-C5
6	L	1285	BPH	C16-C17-C18-C20
5	M	1304	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	M	1311	BPH	C2-C3-C5-C6
7	L	1286	U10	C13-C14-C16-C17
7	M	1313	U10	C33-C34-C36-C37
6	M	1311	BPH	C11-C10-C8-C7
5	L	1282	BCL	C2-C1-O2A-CGA
4	H	1256	LDA	C3-C4-C5-C6
7	L	1286	U10	C3-C4-O4-C4M
4	M	1309	LDA	C5-C6-C7-C8
7	L	1286	U10	C5-C4-O4-C4M
4	H	1252	LDA	C2-C1-N1-O1
4	H	1255	LDA	C2-C1-N1-O1
4	M	1308	LDA	C9-C10-C11-C12

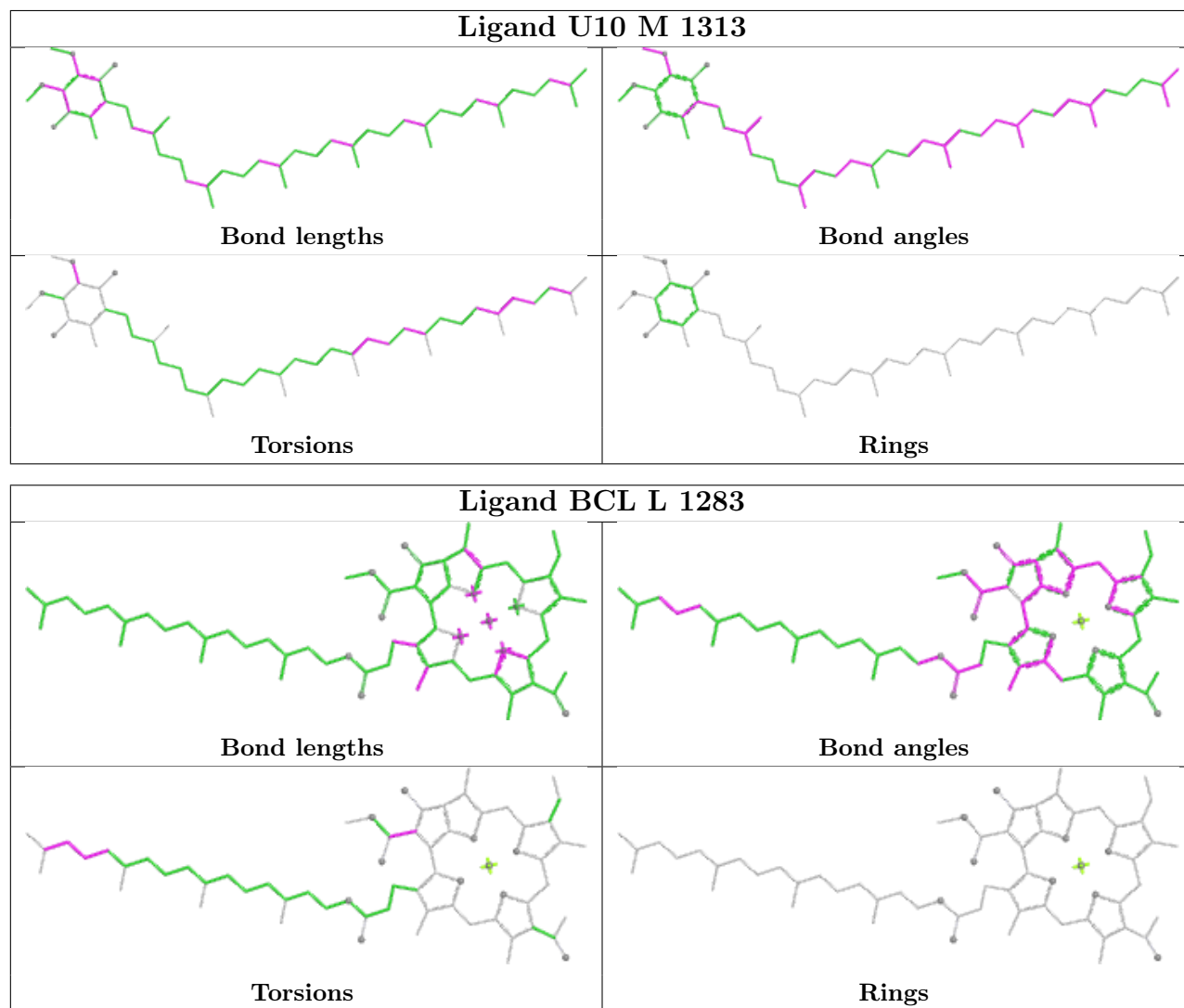
There are no ring outliers.

17 monomers are involved in 74 short contacts:

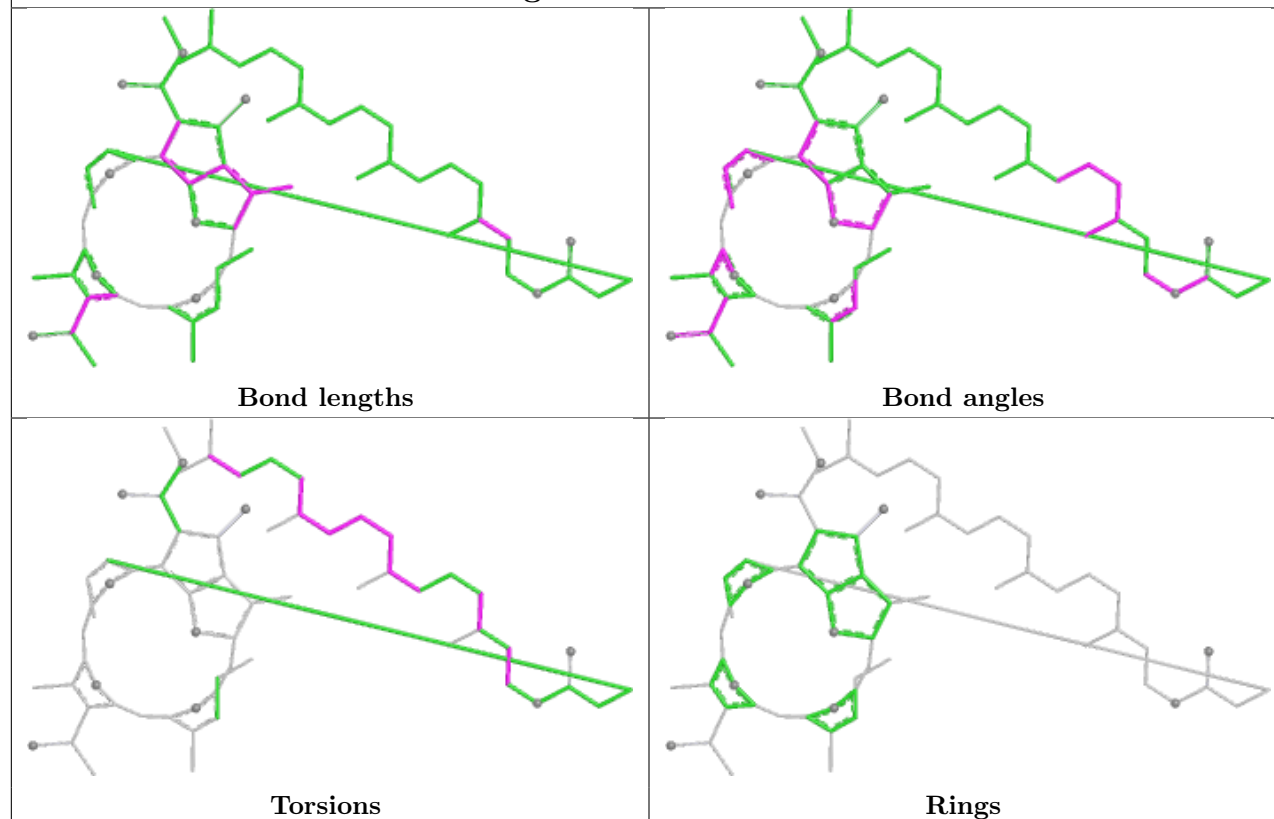
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1308	LDA	3	0
7	M	1313	U10	2	0
9	M	1307	PO4	1	0
5	L	1283	BCL	3	0
4	L	1284	LDA	9	0
4	M	1310	LDA	3	0
6	L	1285	BPH	7	0
6	M	1311	BPH	10	0
10	M	1312	SPN	7	0
4	M	1309	LDA	5	0
5	L	1282	BCL	1	0
4	H	1254	LDA	2	0
5	M	1303	BCL	13	0
4	H	1253	LDA	7	0
4	H	1252	LDA	1	0
5	M	1304	BCL	4	0
7	L	1286	U10	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

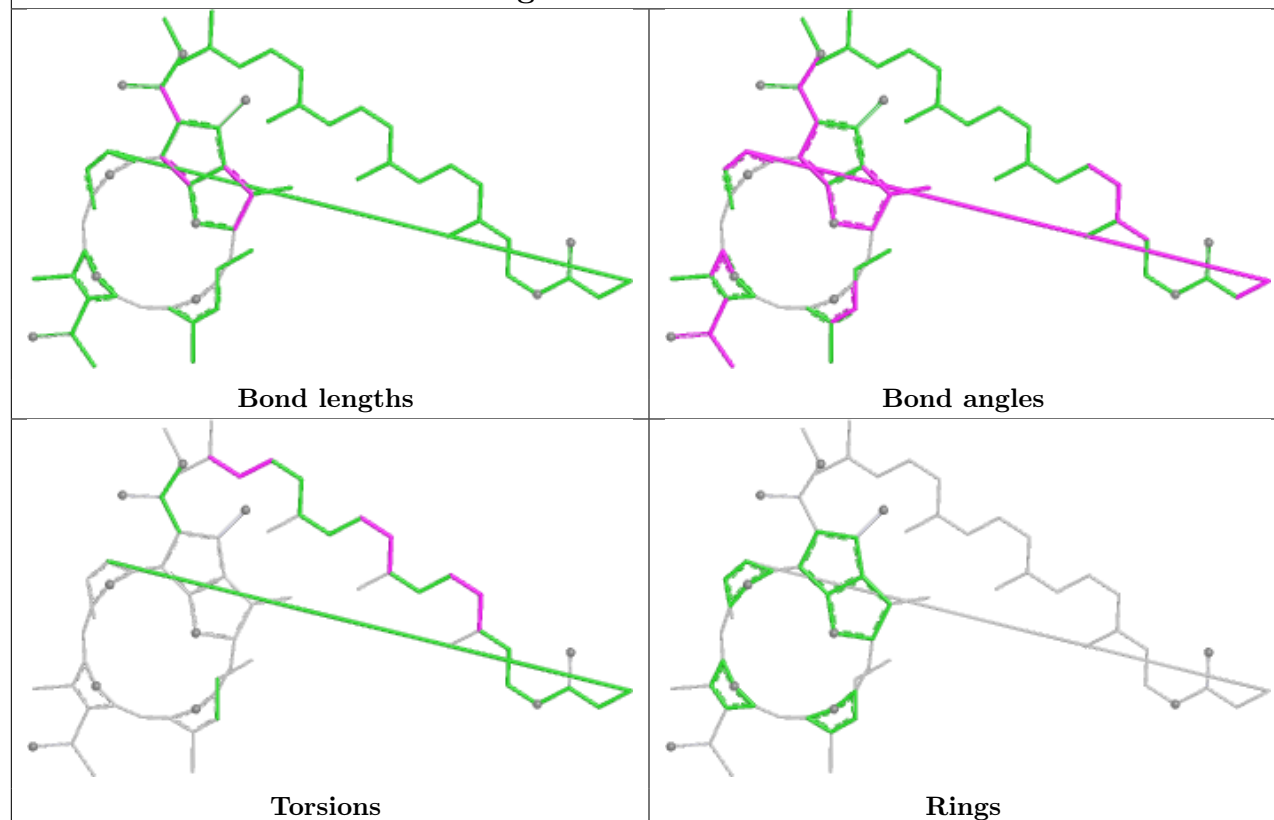
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

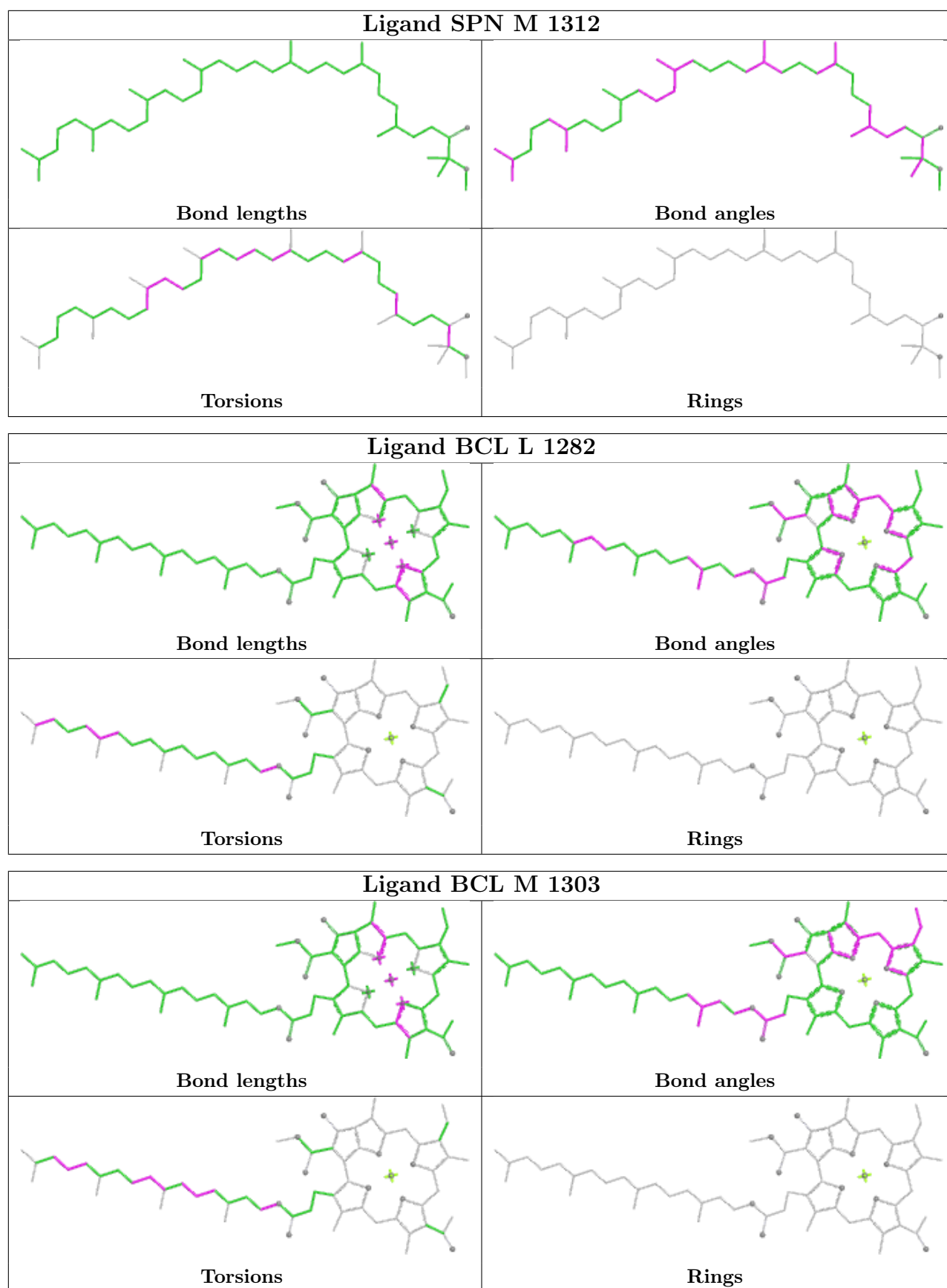


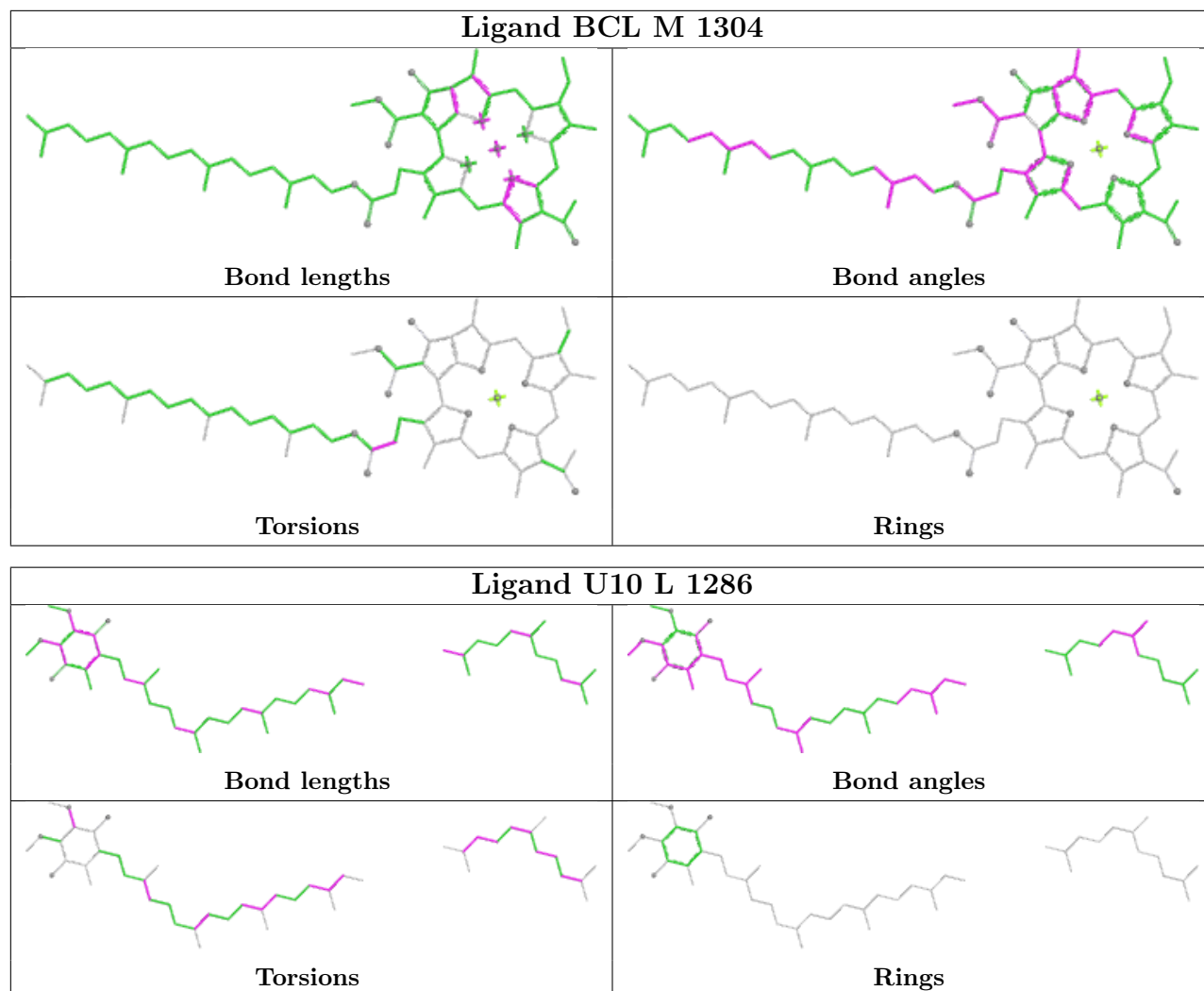
Ligand BPH L 1285



Ligand BPH M 1311







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	241/260 (92%)	-0.42	8 (3%)	49	52	26, 35, 52, 113	0
2	L	281/281 (100%)	-0.25	10 (3%)	46	49	24, 34, 64, 86	0
3	M	302/307 (98%)	-0.34	5 (1%)	69	71	15, 37, 61, 84	1 (0%)
All	All	824/848 (97%)	-0.33	23 (2%)	55	57	15, 35, 61, 113	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	3	TYR	5.2
1	H	245	ALA	4.8
1	H	249	LYS	4.8
3	M	2	GLU	4.3
1	H	247	LYS	4.1
3	M	1	ALA	4.0
1	H	248	ARG	3.9
1	H	251	VAL	3.8
2	L	57	GLY	3.5
1	H	250	SER	3.3
2	L	53	ALA	3.3
1	H	246	PRO	3.3
2	L	58	THR	3.2
2	L	271	TRP	2.4
2	L	51	TRP	2.3
2	L	54	VAL	2.2
2	L	277	GLY	2.2
2	L	72	GLU	2.1
3	M	302	GLY	2.1
1	H	94	GLU	2.0
3	M	52	LEU	2.0
2	L	59	TRP	2.0
2	L	55	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

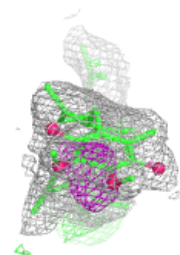
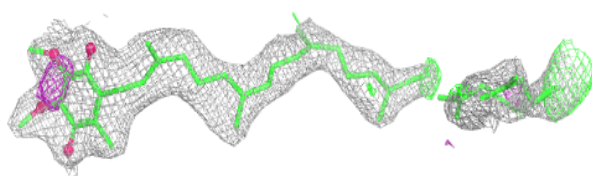
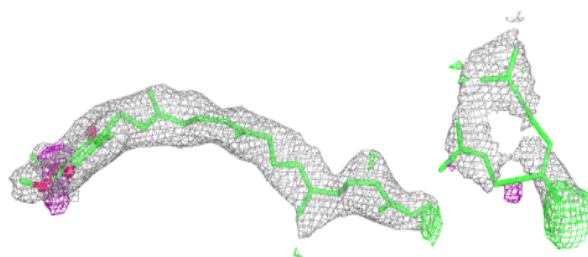
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	L	1284	16/16	0.75	0.18	65,80,102,102	0
4	LDA	H	1254	16/16	0.77	0.20	68,81,117,117	0
4	LDA	M	1310	16/16	0.77	0.20	59,64,92,93	0
4	LDA	H	1255	16/16	0.78	0.16	74,81,92,93	0
4	LDA	H	1256	16/16	0.79	0.26	70,79,106,107	0
7	U10	L	1286	48/63	0.79	0.19	38,67,112,114	1
4	LDA	H	1253	12/16	0.84	0.14	64,67,73,74	0
4	LDA	H	1252	16/16	0.86	0.16	61,72,107,107	0
4	LDA	M	1308	16/16	0.89	0.09	35,47,53,54	0
4	LDA	M	1309	16/16	0.92	0.09	42,53,65,65	0
7	U10	M	1313	48/63	0.93	0.09	16,38,66,68	0
9	PO4	M	1306	5/5	0.93	0.09	66,68,71,72	0
10	SPN	M	1312	43/43	0.93	0.09	26,42,72,80	0
9	PO4	M	1307	5/5	0.94	0.16	36,50,55,58	0
6	BPH	M	1311	65/65	0.94	0.09	22,38,103,105	0
5	BCL	L	1283	66/66	0.96	0.06	13,25,44,55	0
5	BCL	M	1303	66/66	0.96	0.08	18,31,73,75	0
5	BCL	L	1282	66/66	0.97	0.05	20,29,41,44	0
5	BCL	M	1304	66/66	0.97	0.06	19,29,50,64	0
6	BPH	L	1285	65/65	0.97	0.05	17,27,41,48	0
8	FE	M	1305	1/1	0.99	0.03	26,26,26,26	0

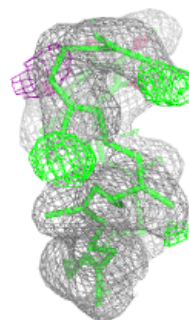
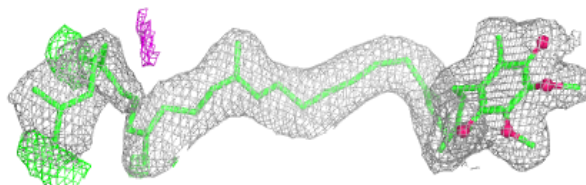
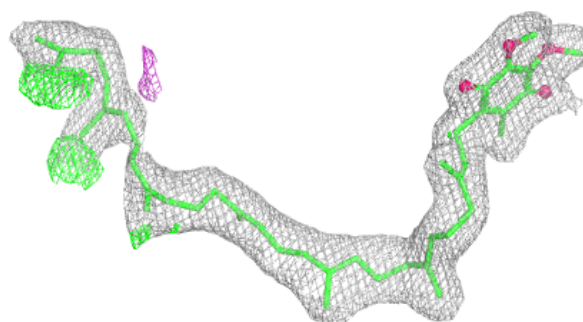
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 L 1286:

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

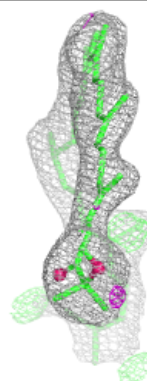
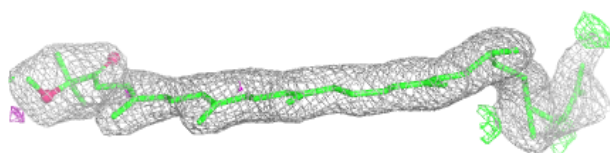
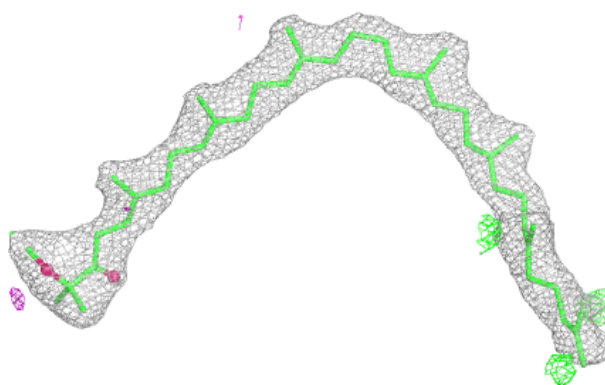
**Electron density around U10 M 1313:**

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

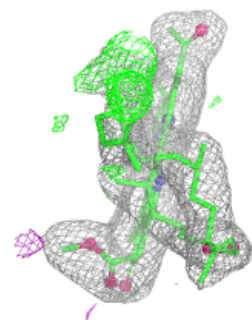
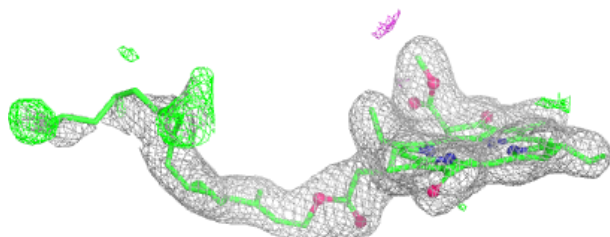
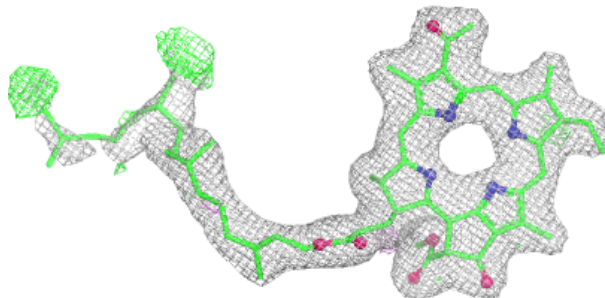


Electron density around SPN M 1312:

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

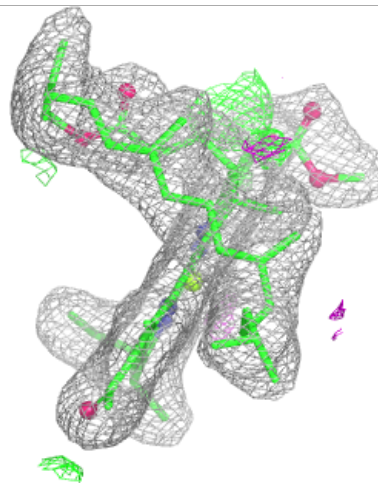
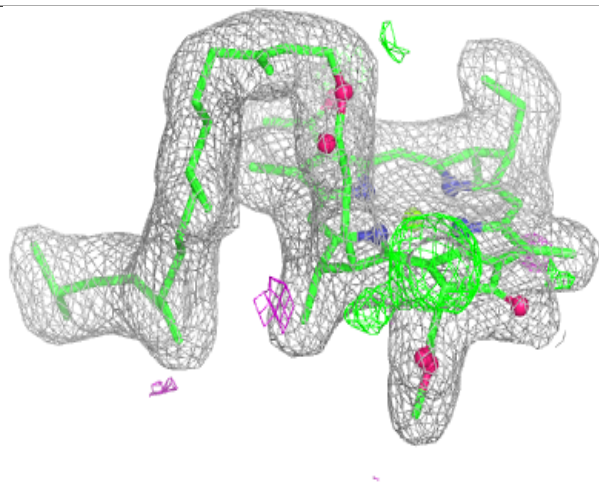
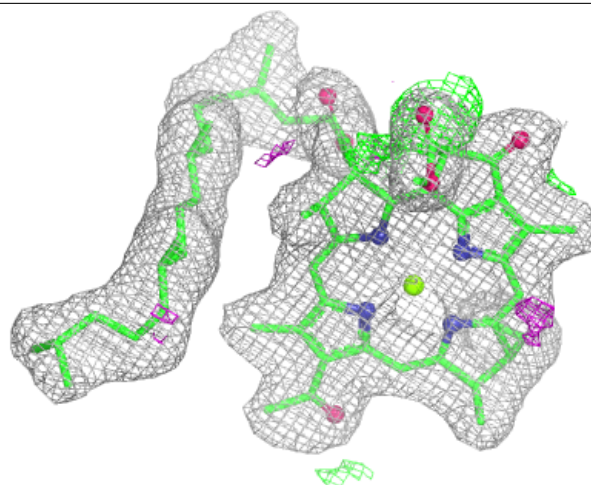
**Electron density around BPH M 1311:**

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



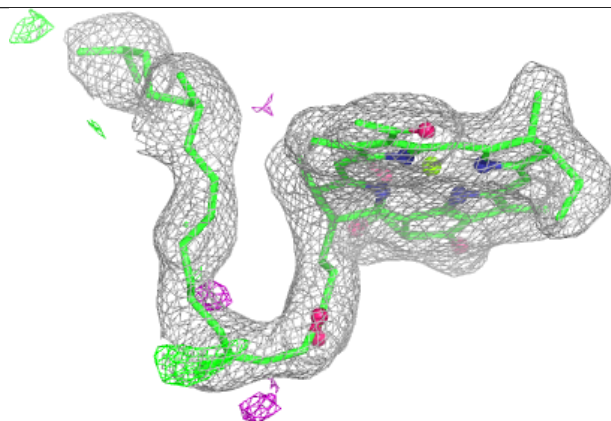
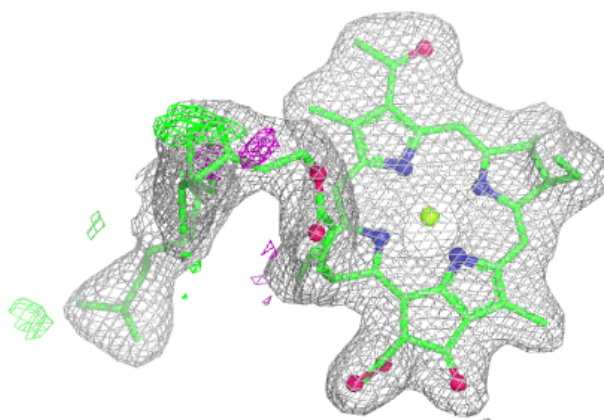
Electron density around BCL L 1283:

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

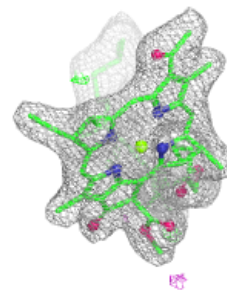
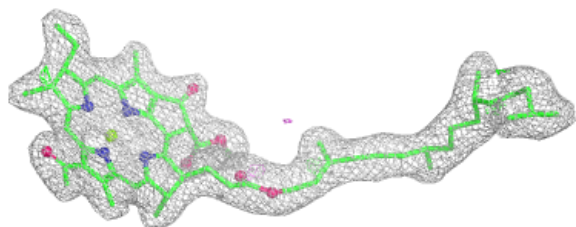
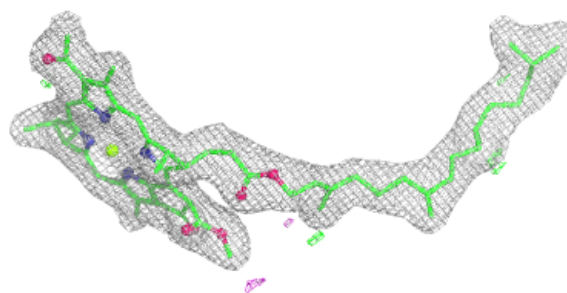


Electron density around BCL M 1303:

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and green (positive)

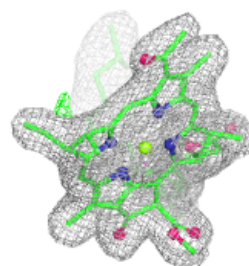
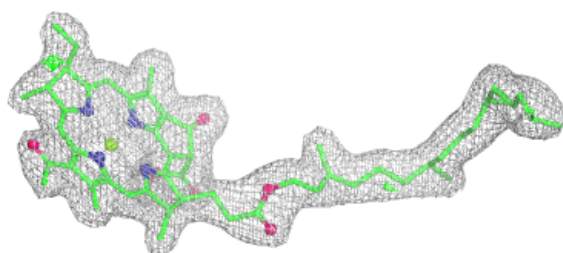
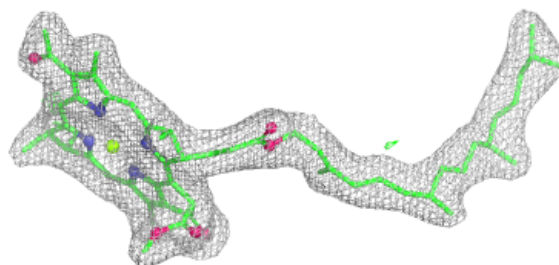
**Electron density around BCL L 1282:**

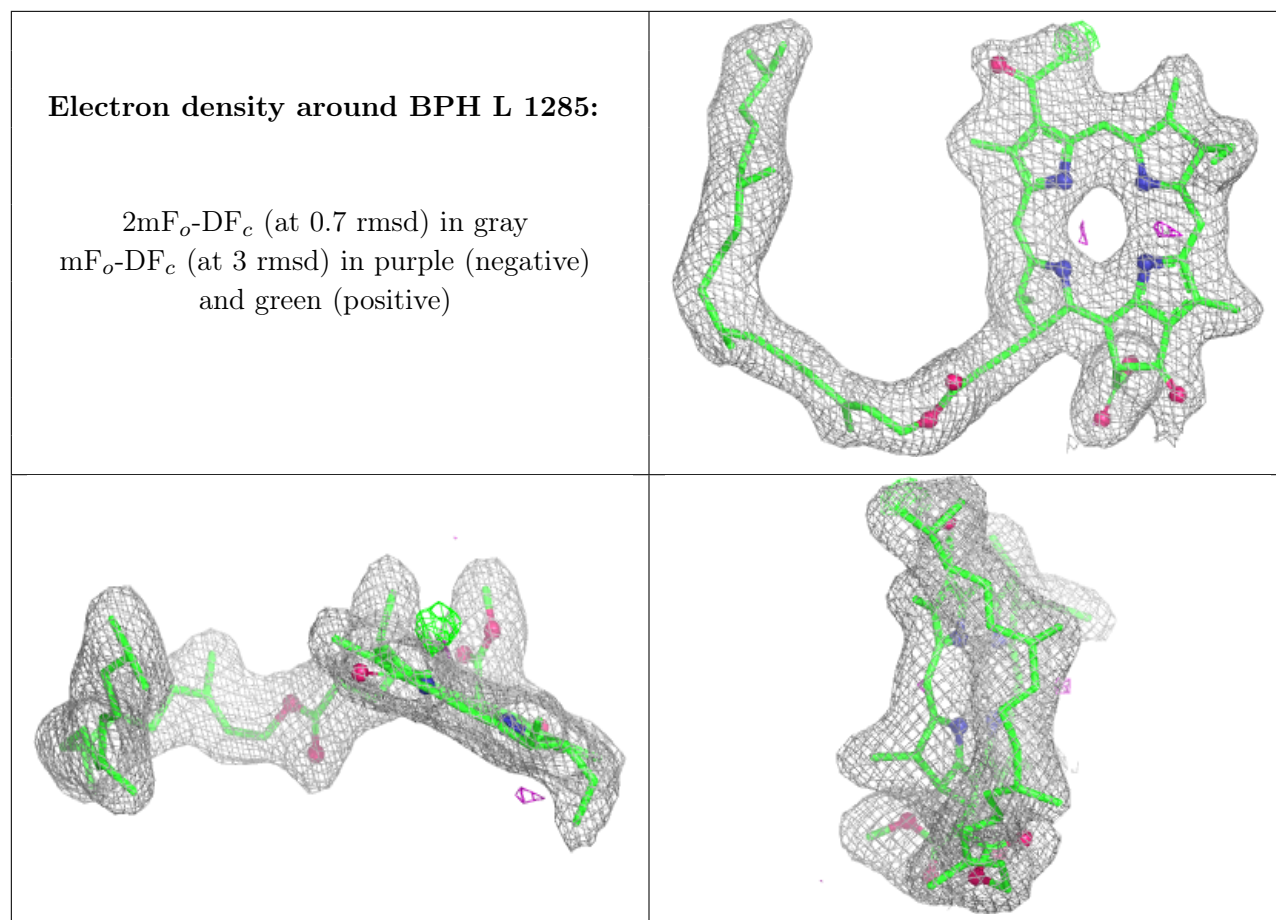
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.