Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:42 PM EDT

PDB ID	:	1AIG / pdb_00001aig
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE D+QB-CHARGE SEPARATED STATE
Authors	:	Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Feher, G.
Deposited on	:	1997-04-17
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

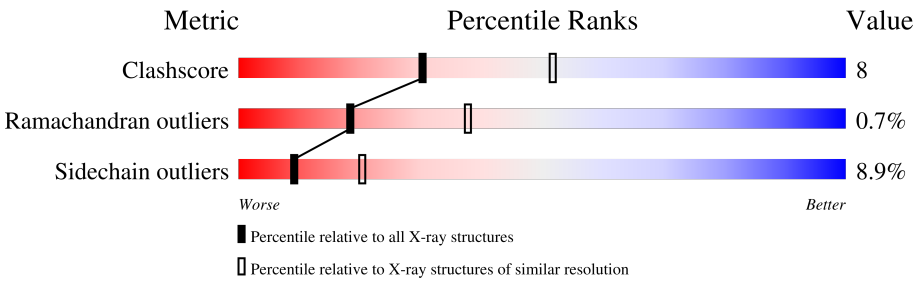
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	66% 27% 7%
1	N	281	67% 27% 6% •
2	M	307	67% 26% • • •
2	O	307	66% 25% 6% •
3	H	260	63% 28% • • 5%
3	P	260	63% 28% • • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	309	X	-	-	-
4	BCL	M	310	X	-	-	-
4	BCL	N	282	X	-	-	-
4	BCL	O	309	X	-	-	-
5	BPH	L	284	X	-	-	-
5	BPH	L	285	X	-	-	-
5	BPH	N	285	X	-	-	-
5	BPH	O	310	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14138 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 PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT).

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	299	2390	1597	391	392	10	0	0	0
2	O	299	2390	1597	391	392	10	0	0	0

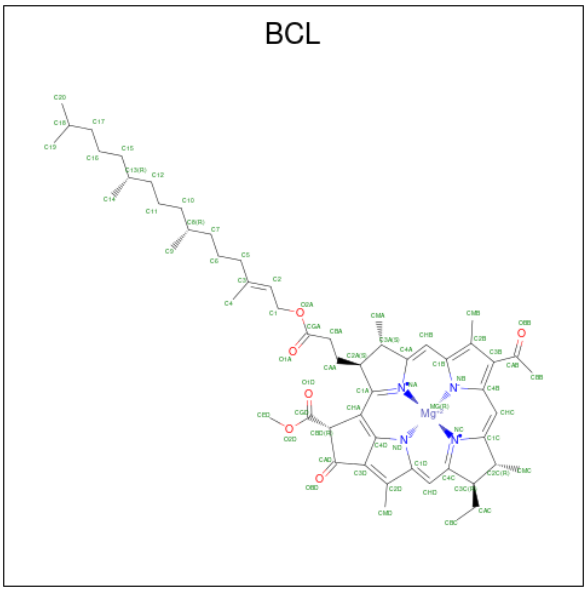
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	248	1883	1204	322	347	10	0	0	0
3	P	248	1883	1204	322	347	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
P	8	GLN	GLY	conflict	UNP P11846

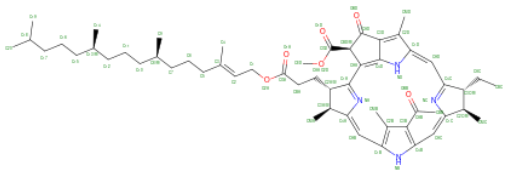
- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	N	1	66	55	1	4	6	12	0
			Total	C	Mg	N	O		
4	N	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	N	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	O	1	66	55	1	4	6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

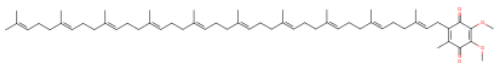
BPH



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	14	0
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
			Total	C	N	O		
5	N	1	65	55	4	6	0	0
			Total	C	N	O		
5	O	1	65	55	4	6	0	0

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

U10



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	63	59	4	0	0
6	M	1	63	59	4	0	0
6	N	1	63	59	4	19	0
6	O	1	63	59	4	0	0

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	19	19	19	0	0
8	M	21	21	21	0	0
8	H	13	13	13	0	0
8	N	13	13	13	0	0
8	O	15	15	15	0	0
8	P	5	5	5	0	0

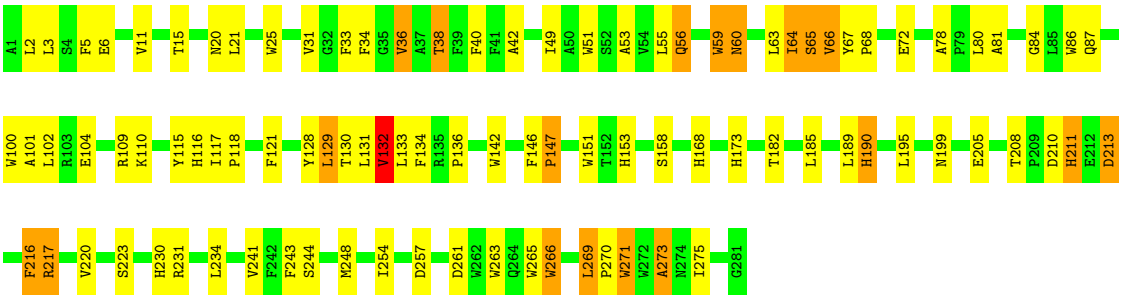
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

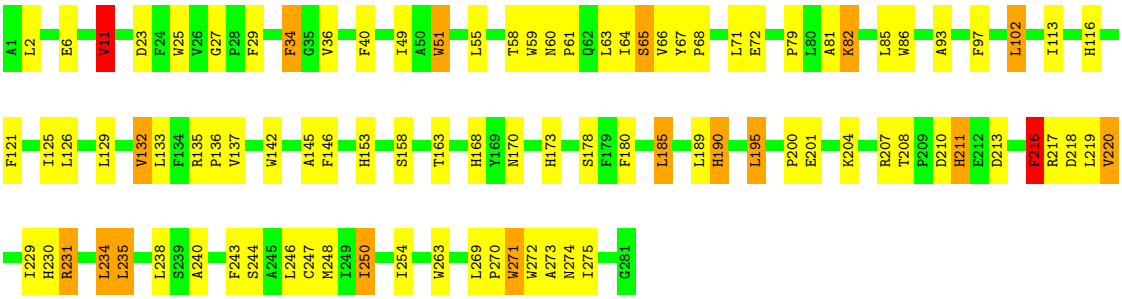
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

Chain L: 66% 27% 7%



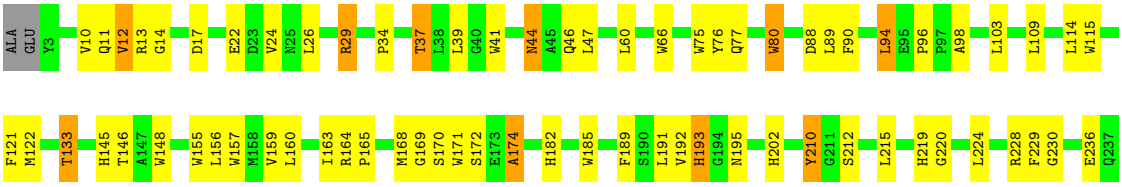
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

Chain N: 67% 27% 6%



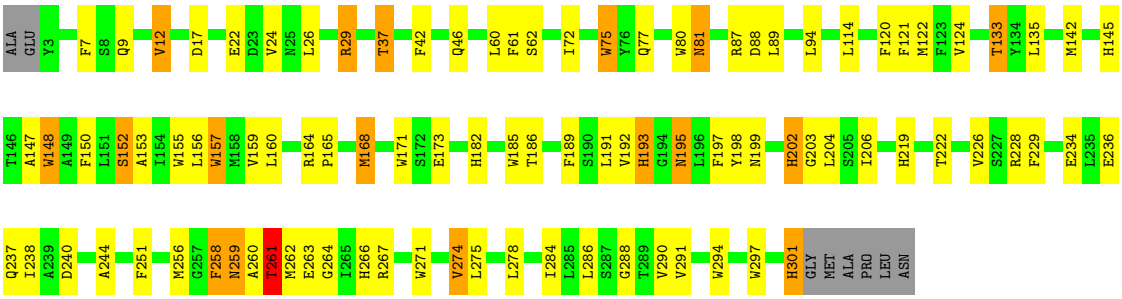
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain M: 67% 26%



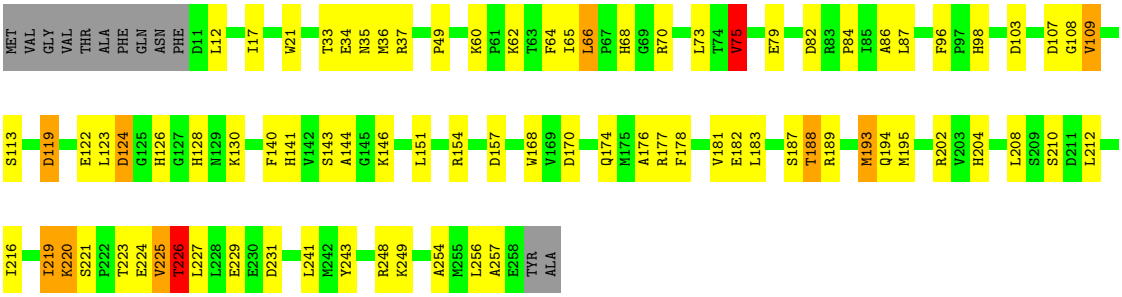
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain O:



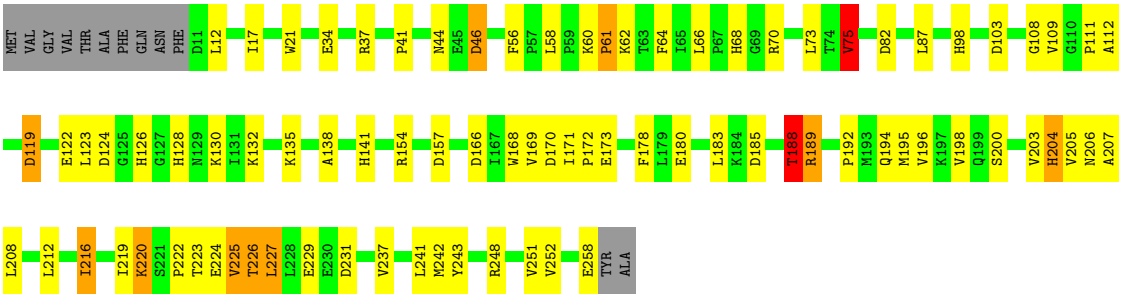
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain P:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.10Å 140.10Å 271.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.89	Depositor
R, R_{free}	0.215 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

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: BCL, BPH, U10, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	L	1.07	12/2320 (0.5%)	1.80	60/3175 (1.9%)
1	N	1.01	9/2320 (0.4%)	1.77	51/3175 (1.6%)
2	M	1.05	9/2482 (0.4%)	1.77	49/3389 (1.4%)
2	O	1.05	12/2482 (0.5%)	1.71	45/3389 (1.3%)
3	H	0.98	6/1931 (0.3%)	1.76	33/2627 (1.3%)
3	P	0.96	6/1931 (0.3%)	1.75	38/2627 (1.4%)
All	All	1.02	54/13466 (0.4%)	1.76	276/18382 (1.5%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	211	HIS	CD2-NE2	-7.82	1.29	1.37
2	O	145	HIS	CD2-NE2	-7.20	1.29	1.37
2	M	145	HIS	CD2-NE2	-7.07	1.30	1.37
3	H	128	HIS	CD2-NE2	-7.06	1.30	1.37
1	L	211	HIS	CD2-NE2	-6.98	1.30	1.37
1	L	66	VAL	CA-CB	6.97	1.64	1.54
2	O	193	HIS	CD2-NE2	-6.92	1.30	1.37
1	N	116	HIS	CD2-NE2	-6.92	1.30	1.37
1	L	36	VAL	CA-CB	6.86	1.63	1.54
3	P	204	HIS	CD2-NE2	-6.79	1.30	1.37
3	H	98	HIS	CD2-NE2	-6.78	1.30	1.37
3	P	126	HIS	CD2-NE2	-6.71	1.30	1.37
2	M	193	HIS	CD2-NE2	-6.62	1.30	1.37
3	P	98	HIS	CD2-NE2	-6.61	1.30	1.37
2	O	182	HIS	CD2-NE2	-6.59	1.30	1.37
1	N	168	HIS	CD2-NE2	-6.54	1.30	1.37
1	L	116	HIS	CD2-NE2	-6.52	1.30	1.37
2	O	301	HIS	CD2-NE2	-6.45	1.30	1.37
2	O	266	HIS	CD2-NE2	-6.33	1.30	1.37
3	P	128	HIS	CD2-NE2	-6.30	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	266	HIS	CD2-NE2	-6.24	1.30	1.37
3	P	141	HIS	CD2-NE2	-6.22	1.31	1.37
3	P	68	HIS	CD2-NE2	-6.17	1.31	1.37
1	L	153	HIS	CD2-NE2	-6.15	1.31	1.37
2	M	301	HIS	CD2-NE2	-6.11	1.31	1.37
3	H	126	HIS	CD2-NE2	-6.08	1.31	1.37
2	M	182	HIS	CD2-NE2	-6.04	1.31	1.37
1	N	153	HIS	CD2-NE2	-6.04	1.31	1.37
1	L	168	HIS	CD2-NE2	-6.03	1.31	1.37
3	H	204	HIS	CD2-NE2	-6.02	1.31	1.37
2	O	192	VAL	CA-CB	6.02	1.61	1.54
2	M	219	HIS	CD2-NE2	-5.96	1.31	1.37
2	M	202	HIS	CD2-NE2	-5.96	1.31	1.37
2	O	219	HIS	CD2-NE2	-5.84	1.31	1.37
1	L	230	HIS	CG-ND1	-5.82	1.31	1.38
1	L	190	HIS	CD2-NE2	-5.80	1.31	1.37
3	H	141	HIS	CD2-NE2	-5.78	1.31	1.37
1	N	190	HIS	CD2-NE2	-5.77	1.31	1.37
1	N	173	HIS	CD2-NE2	-5.71	1.31	1.37
1	L	153	HIS	CG-ND1	-5.65	1.32	1.38
2	M	219	HIS	CG-ND1	-5.57	1.32	1.38
3	H	68	HIS	CD2-NE2	-5.51	1.31	1.37
1	L	147	PRO	CA-CB	-5.50	1.47	1.54
1	N	36	VAL	CA-CB	5.48	1.61	1.54
2	O	202	HIS	CD2-NE2	-5.46	1.31	1.37
1	N	211	HIS	CG-ND1	-5.37	1.32	1.38
2	O	145	HIS	CG-ND1	-5.37	1.32	1.38
2	O	182	HIS	CG-ND1	-5.36	1.32	1.38
1	L	230	HIS	CD2-NE2	-5.28	1.32	1.37
2	O	266	HIS	CG-ND1	-5.27	1.32	1.38
1	N	230	HIS	CD2-NE2	-5.26	1.32	1.37
1	L	49	ILE	CA-CB	5.19	1.61	1.54
2	O	219	HIS	CG-ND1	-5.17	1.32	1.38
2	M	182	HIS	CG-ND1	-5.02	1.32	1.38

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	75	VAL	N-CA-CB	-11.56	100.11	112.37
1	N	220	VAL	N-CA-CB	-9.88	100.58	112.33
3	H	124	ASP	CA-CB-CG	9.65	122.25	112.60
3	H	75	VAL	CB-CA-C	9.51	119.35	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	124	ASP	CA-CB-CG	8.91	121.51	112.60
1	N	216	PHE	CA-CB-CG	-8.16	105.64	113.80
1	N	65	SER	N-CA-C	8.14	124.01	113.18
1	L	261	ASP	CA-CB-CG	8.14	120.74	112.60
2	O	258	PHE	N-CA-C	8.10	124.96	114.75
1	N	210	ASP	CA-CB-CG	7.97	120.57	112.60
2	O	258	PHE	CA-CB-CG	7.89	121.69	113.80
2	O	259	ASN	N-CA-C	7.86	127.54	110.80
2	M	90	PHE	N-CA-C	7.84	120.73	111.71
3	H	225	VAL	CB-CA-C	-7.82	98.97	110.62
2	M	259	ASN	N-CA-C	7.81	127.44	110.80
2	M	258	PHE	N-CA-C	7.80	125.71	114.16
2	O	12	VAL	N-CA-CB	-7.68	101.66	111.64
2	M	44	ASN	CA-CB-CG	7.66	120.26	112.60
1	L	173	HIS	CA-CB-CG	7.63	121.43	113.80
1	L	273	ALA	N-CA-C	7.63	120.48	111.71
1	L	5	PHE	CA-CB-CG	7.54	121.34	113.80
1	L	67	TYR	N-CA-C	7.49	119.50	110.07
1	L	2	LEU	N-CA-C	7.47	121.03	110.50
3	H	157	ASP	CA-CB-CG	7.46	120.06	112.60
2	O	46	GLN	N-CA-C	7.46	120.55	109.59
1	L	132	VAL	N-CA-CB	-7.36	102.19	112.35
2	M	261	THR	CA-CB-OG1	-7.32	98.63	109.60
2	O	17	ASP	CA-CB-CG	7.21	119.81	112.60
1	N	271	TRP	CA-CB-CG	7.21	127.29	113.60
3	H	256	LEU	N-CA-C	-7.14	103.50	111.71
1	N	11	VAL	N-CA-CB	-7.13	101.23	111.21
1	L	220	VAL	N-CA-CB	-7.09	102.55	112.12
1	N	132	VAL	N-CA-CB	-7.06	99.77	111.98
3	P	12	LEU	N-CA-C	6.97	118.88	111.28
2	M	88	ASP	CA-CB-CG	6.89	119.49	112.60
1	L	213	ASP	CA-CB-CG	6.89	119.49	112.60
2	O	135	LEU	N-CA-C	6.88	118.78	111.28
3	P	157	ASP	CA-CB-CG	6.88	119.48	112.60
2	O	182	HIS	CB-CG-CD2	-6.87	122.27	131.20
2	O	182	HIS	CA-CB-CG	6.87	120.67	113.80
2	O	7	PHE	CA-CB-CG	-6.82	106.98	113.80
3	P	75	VAL	N-CA-CB	-6.81	101.67	111.21
2	M	109	LEU	N-CA-C	6.80	118.69	111.28
1	L	11	VAL	N-CA-CB	-6.78	101.72	111.21
1	N	27	GLY	CA-C-N	6.75	126.21	118.85
1	N	27	GLY	C-N-CA	6.75	126.21	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	146	PHE	CA-CB-CG	6.75	120.55	113.80
2	O	290	VAL	N-CA-C	-6.72	105.16	111.48
1	L	216	PHE	CA-CB-CG	-6.65	107.15	113.80
3	P	243	TYR	N-CA-C	6.64	120.64	112.54
3	P	61	PRO	N-CA-C	6.64	121.25	111.03
3	H	243	TYR	N-CA-C	6.60	120.54	112.23
1	N	173	HIS	CA-CB-CG	6.59	120.39	113.80
1	L	20	ASN	CA-CB-CG	6.59	119.19	112.60
1	L	153	HIS	CA-CB-CG	6.58	120.38	113.80
1	N	153	HIS	CA-CB-CG	6.56	120.36	113.80
1	N	153	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	N	68	PRO	N-CA-C	6.50	118.63	110.70
2	M	210	TYR	O-C-N	6.49	128.76	122.07
2	M	148	TRP	CG-CD2-CE3	6.49	140.39	133.90
3	P	200	SER	N-CA-C	6.48	120.28	112.38
1	N	116	HIS	N-CA-C	6.43	119.11	111.71
2	O	301	HIS	CA-CB-CG	-6.40	107.40	113.80
2	M	182	HIS	CA-CB-CG	6.35	120.15	113.80
3	H	226	THR	N-CA-CB	-6.34	100.32	110.46
1	N	163	THR	CA-CB-OG1	-6.34	100.09	109.60
1	N	34	PHE	CA-CB-CG	-6.33	107.47	113.80
1	N	58	THR	N-CA-C	6.33	119.78	109.59
1	L	243	PHE	CA-CB-CG	-6.33	107.47	113.80
2	O	148	TRP	CG-CD2-CE3	6.32	140.22	133.90
1	L	134	PHE	N-CA-C	6.31	118.68	111.11
3	H	220	LYS	CA-CB-CG	6.30	126.70	114.10
2	M	261	THR	CA-CB-CG2	6.28	121.17	110.50
2	M	259	ASN	CA-C-O	6.28	129.49	120.51
1	N	6	GLU	N-CA-C	6.27	119.09	111.82
2	M	170	SER	N-CA-C	6.24	119.57	109.40
1	N	211	HIS	CB-CG-CD2	-6.22	123.11	131.20
3	H	170	ASP	CA-CB-CG	6.19	118.79	112.60
1	L	65	SER	N-CA-C	6.17	123.94	110.80
3	P	166	ASP	CA-CB-CG	6.17	118.77	112.60
3	P	56	PHE	N-CA-C	6.16	117.80	109.24
2	O	193	HIS	CB-CG-CD2	-6.14	123.22	131.20
2	M	14	GLY	CA-C-N	6.13	126.16	119.90
2	M	14	GLY	C-N-CA	6.13	126.16	119.90
3	H	193	MET	N-CA-C	6.11	118.73	111.71
1	N	273	ALA	N-CA-C	6.09	118.70	111.33
3	H	225	VAL	N-CA-CB	6.08	121.96	111.39
3	H	109	VAL	N-CA-CB	-6.07	102.27	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	269	LEU	CA-C-O	-6.06	114.32	119.59
2	M	171	TRP	CG-CD2-CE3	6.06	139.96	133.90
2	M	17	ASP	CA-CB-CG	6.05	118.65	112.60
1	L	56	GLN	N-CA-C	-6.04	106.45	113.88
3	H	126	HIS	CA-CB-CG	-6.04	107.76	113.80
3	H	248	ARG	N-CA-C	6.04	118.14	108.41
2	O	259	ASN	CA-CB-CG	6.01	118.61	112.60
1	L	271	TRP	CA-CB-CG	5.99	124.99	113.60
3	H	96	PHE	CA-CB-CG	-5.96	107.84	113.80
2	M	261	THR	N-CA-CB	-5.96	101.55	111.20
2	O	261	THR	CA-CB-OG1	-5.96	100.67	109.60
1	L	132	VAL	CB-CA-C	5.95	117.37	110.88
3	P	252	VAL	CB-CA-C	-5.95	104.20	111.87
1	L	210	ASP	CA-CB-CG	5.94	118.54	112.60
3	P	119	ASP	CA-CB-CG	5.91	118.51	112.60
1	L	153	HIS	CB-CG-CD2	-5.89	123.54	131.20
2	M	182	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	N	190	HIS	CB-CG-CD2	-5.87	123.57	131.20
2	M	174	ALA	N-CA-C	5.86	117.62	110.41
1	N	71	LEU	N-CA-C	5.84	119.23	111.75
1	N	116	HIS	CB-CG-CD2	-5.82	123.63	131.20
3	H	188	THR	CA-CB-OG1	-5.82	100.87	109.60
2	M	193	HIS	CA-CB-CG	-5.81	107.99	113.80
2	M	98	ALA	CA-C-N	5.81	125.94	119.32
2	M	98	ALA	C-N-CA	5.81	125.94	119.32
1	L	151	TRP	CG-CD2-CE3	5.80	139.70	133.90
1	N	220	VAL	CB-CA-C	5.79	116.88	110.62
2	O	160	LEU	N-CA-C	5.79	117.26	111.07
2	O	301	HIS	CB-CG-CD2	-5.77	123.70	131.20
3	H	103	ASP	CA-CB-CG	5.77	118.37	112.60
1	L	86	TRP	CG-CD2-CE3	5.76	139.66	133.90
1	N	219	LEU	N-CA-C	5.76	117.36	111.14
2	M	46	GLN	N-CA-C	5.75	118.05	109.59
1	N	269	LEU	CA-C-O	-5.75	114.34	119.75
3	H	119	ASP	CA-CB-CG	5.75	118.35	112.60
2	O	291	VAL	N-CA-C	5.75	116.07	107.51
3	P	204	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	L	265	TRP	CG-CD2-CE3	5.73	139.63	133.90
1	N	25	TRP	CG-CD2-CE3	5.72	139.62	133.90
1	L	130	THR	CA-CB-OG1	-5.72	101.03	109.60
2	O	185	TRP	CG-CD2-CE3	5.70	139.60	133.90
2	M	171	TRP	CB-CG-CD1	-5.69	118.36	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	271	TRP	CG-CD2-CE3	5.68	139.58	133.90
1	L	244	SER	N-CA-CB	-5.67	101.85	110.07
2	M	37	THR	CA-CB-OG1	-5.66	101.11	109.60
3	H	86	ALA	N-CA-C	5.65	118.39	108.56
3	H	226	THR	CB-CA-C	5.65	119.71	109.83
3	H	181	VAL	N-CA-C	5.59	116.17	107.28
2	O	240	ASP	CA-CB-CG	5.59	118.19	112.60
2	O	81	ASN	CA-CB-CG	5.58	118.18	112.60
1	L	40	PHE	CA-CB-CG	5.56	119.36	113.80
3	H	107	ASP	N-CA-C	5.56	119.68	113.01
1	L	211	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	O	148	TRP	CB-CG-CD1	-5.56	118.56	126.90
1	N	213	ASP	CA-CB-CG	5.55	118.15	112.60
1	L	72	GLU	CB-CA-C	-5.55	100.01	110.67
1	L	142	TRP	CG-CD2-CE3	5.55	139.45	133.90
2	M	258	PHE	CA-C-O	-5.55	112.42	118.52
3	P	46	ASP	CA-CB-CG	5.55	118.15	112.60
1	L	59	TRP	CG-CD2-CE3	5.54	139.44	133.90
3	P	171	ILE	CA-C-O	-5.54	112.53	119.95
2	M	148	TRP	CB-CG-CD1	-5.54	118.60	126.90
3	P	225	VAL	N-CA-CB	5.53	118.77	111.25
3	H	249	LYS	CA-CB-CG	-5.53	103.05	114.10
1	N	40	PHE	CA-CB-CG	5.53	119.33	113.80
2	O	260	ALA	N-CA-C	5.53	115.58	108.34
3	H	210	SER	N-CA-C	5.52	117.73	111.11
2	O	199	ASN	CA-C-N	5.51	125.16	119.05
2	O	199	ASN	C-N-CA	5.51	125.16	119.05
1	L	25	TRP	CG-CD2-CE3	5.50	139.41	133.90
1	L	72	GLU	CA-CB-CG	5.50	125.09	114.10
3	P	189	ARG	CA-CB-CG	-5.49	103.13	114.10
2	O	261	THR	CA-CB-CG2	5.45	119.76	110.50
2	O	145	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	N	25	TRP	CE2-CD2-CG	-5.43	100.68	107.20
3	P	258	GLU	CB-CG-CD	5.42	121.81	112.60
3	H	12	LEU	N-CA-C	5.41	117.18	111.28
1	N	86	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	N	218	ASP	CA-CB-CG	5.41	118.01	112.60
2	O	77	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	L	116	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	M	171	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	L	142	TRP	CE2-CD2-CG	-5.38	100.75	107.20
1	N	263	TRP	CG-CD2-CE3	5.38	139.28	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	265	TRP	CB-CG-CD1	-5.38	118.84	126.90
3	P	135	LYS	CB-CG-CD	-5.38	98.93	111.30
3	H	174	GLN	N-CA-C	5.37	117.74	111.02
2	O	204	LEU	N-CA-CB	-5.37	102.21	110.16
1	N	29	PHE	N-CA-C	5.37	117.49	109.59
2	M	145	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	L	100	TRP	CG-CD2-CE3	5.36	139.26	133.90
3	H	21	TRP	CG-CD2-CE3	5.36	139.26	133.90
1	N	59	TRP	CG-CD2-CE3	5.36	139.26	133.90
2	M	121	PHE	CA-CB-CG	-5.34	108.46	113.80
1	N	59	TRP	CE2-CD2-CG	-5.34	100.79	107.20
2	M	12	VAL	N-CA-CB	-5.34	103.73	111.52
2	O	148	TRP	CE2-CD2-CG	-5.33	100.80	107.20
2	M	77	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	N	170	ASN	CA-C-N	5.32	124.50	118.97
1	N	170	ASN	C-N-CA	5.32	124.50	118.97
1	L	266	TRP	CG-CD2-CE3	5.32	139.22	133.90
2	M	41	TRP	CG-CD2-CE3	5.30	139.20	133.90
3	P	132	LYS	CA-CB-CG	5.30	124.70	114.10
2	M	148	TRP	CE2-CD2-CG	-5.30	100.84	107.20
3	P	103	ASP	CA-C-N	5.30	125.36	119.32
3	P	103	ASP	C-N-CA	5.30	125.36	119.32
2	O	81	ASN	CA-C-N	5.30	124.93	119.05
2	O	81	ASN	C-N-CA	5.30	124.93	119.05
2	O	150	PHE	CA-CB-CG	5.30	119.10	113.80
3	P	222	PRO	N-CA-C	5.30	120.97	114.35
1	L	271	TRP	CB-CG-CD1	-5.29	118.96	126.90
2	M	41	TRP	CE2-CD2-CG	-5.29	100.85	107.20
2	M	296	VAL	N-CA-CB	-5.29	104.36	110.55
1	L	257	ASP	CA-CB-CG	5.28	117.88	112.60
1	L	168	HIS	CA-CB-CG	5.28	119.08	113.80
3	H	128	HIS	CB-CG-CD2	-5.27	124.34	131.20
3	P	169	VAL	N-CA-CB	-5.27	102.43	110.86
3	P	220	LYS	CA-CB-CG	5.26	124.62	114.10
2	M	26	LEU	N-CA-C	5.25	118.79	112.38
1	L	59	TRP	CE2-CD2-CG	-5.24	100.91	107.20
3	P	170	ASP	CA-CB-CG	5.23	117.83	112.60
1	L	142	TRP	CB-CG-CD1	-5.23	119.06	126.90
1	N	63	LEU	N-CA-C	5.22	119.70	112.45
1	N	146	PHE	CA-C-N	5.20	125.65	120.14
1	N	146	PHE	C-N-CA	5.20	125.65	120.14
3	P	56	PHE	CA-C-N	5.20	125.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	56	PHE	C-N-CA	5.20	125.20	119.90
3	P	126	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	L	51	TRP	CE2-CD2-CG	-5.20	100.97	107.20
3	P	188	THR	CA-CB-OG1	-5.19	101.81	109.60
1	L	151	TRP	CB-CG-CD1	-5.19	119.12	126.90
2	M	193	HIS	CB-CG-CD2	-5.19	124.45	131.20
2	M	212	SER	N-CA-C	-5.18	105.32	111.69
3	P	141	HIS	CB-CG-CD2	-5.18	124.47	131.20
2	M	80	TRP	CE2-CD2-CG	-5.17	100.99	107.20
2	M	254	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	N	243	PHE	CA-CB-CG	-5.17	108.63	113.80
1	N	2	LEU	N-CA-C	5.17	118.49	110.17
2	O	297	TRP	CE2-CD2-CG	-5.17	101.00	107.20
2	M	160	LEU	N-CA-C	5.16	116.91	111.28
2	M	251	PHE	N-CA-C	-5.15	105.36	110.97
2	O	37	THR	CA-CB-OG1	-5.14	101.89	109.60
1	L	146	PHE	CA-CB-CG	5.14	118.94	113.80
1	L	72	GLU	N-CA-CB	5.14	118.24	110.28
2	M	155	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	N	142	TRP	CE2-CD2-CG	-5.13	101.05	107.20
2	O	294	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	L	266	TRP	CB-CG-CD1	-5.12	119.23	126.90
2	O	294	TRP	CE2-CD2-CG	-5.11	101.07	107.20
3	P	216	ILE	CA-C-N	5.10	125.10	119.90
3	P	216	ILE	C-N-CA	5.10	125.10	119.90
1	N	23	ASP	CA-CB-CG	5.09	117.69	112.60
3	P	103	ASP	CA-CB-CG	5.09	117.69	112.60
1	N	51	TRP	CE2-CD2-CG	-5.09	101.09	107.20
3	P	21	TRP	CE2-CD2-CG	-5.09	101.09	107.20
2	M	76	TYR	N-CA-C	-5.09	105.81	111.36
2	O	185	TRP	CB-CG-CD1	-5.09	119.27	126.90
3	P	185	ASP	N-CA-C	5.09	119.58	113.17
3	P	252	VAL	N-CA-C	-5.08	105.64	110.42
2	O	88	ASP	CA-CB-CG	5.08	117.68	112.60
1	L	263	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	N	274	ASN	CA-CB-CG	-5.08	107.52	112.60
1	L	275	ILE	N-CA-C	-5.06	104.28	108.63
1	L	25	TRP	CB-CG-CD1	-5.06	119.31	126.90
2	O	157	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	L	68	PRO	N-CA-C	5.05	116.87	110.70
2	M	10	VAL	CA-C-O	5.05	125.72	120.36
1	N	82	LYS	CA-C-O	5.05	124.84	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	61	PHE	CA-CB-CG	-5.05	108.75	113.80
1	L	60	ASN	CA-C-N	5.05	125.07	119.32
1	L	60	ASN	C-N-CA	5.05	125.07	119.32
1	L	151	TRP	CE2-CD2-CG	-5.04	101.15	107.20
3	H	225	VAL	N-CA-C	-5.04	101.22	108.48
1	L	230	HIS	CA-CB-CG	-5.04	108.76	113.80
2	M	185	TRP	CE2-CD2-CG	-5.04	101.15	107.20
2	M	297	TRP	CE2-CD2-CG	-5.04	101.16	107.20
3	H	219	ILE	CB-CA-C	-5.04	104.31	111.21
3	P	225	VAL	CB-CA-C	-5.03	103.33	110.83
1	L	190	HIS	CB-CG-CD2	-5.03	124.67	131.20
2	O	271	TRP	CE2-CD2-CG	-5.02	101.17	107.20
2	O	75	TRP	CE2-CD2-CG	-5.02	101.18	107.20
2	O	171	TRP	CE2-CD2-CG	-5.02	101.18	107.20
3	P	44	ASN	N-CA-C	-5.02	104.06	110.53
3	H	66	LEU	CA-C-N	5.01	124.91	119.85
3	H	66	LEU	C-N-CA	5.01	124.91	119.85
1	L	21	LEU	O-C-N	5.00	127.22	122.07
1	N	25	TRP	CB-CG-CD1	-5.00	119.40	126.90
1	N	132	VAL	CB-CA-C	5.00	118.35	110.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	38	0
1	N	2232	0	2187	39	0
2	M	2390	0	2304	37	0
2	O	2390	0	2304	47	0
3	H	1883	0	1895	31	0
3	P	1883	0	1895	33	0
4	L	132	0	148	7	0
4	M	132	0	148	11	0
4	N	198	0	222	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	66	0	74	7	0
5	L	130	0	152	11	0
5	N	65	0	76	7	0
5	O	65	0	76	4	0
6	L	63	0	90	4	0
6	M	63	0	90	1	0
6	N	63	0	90	6	0
6	O	63	0	90	3	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
8	H	13	0	0	3	0
8	L	19	0	0	4	0
8	M	21	0	0	0	0
8	N	13	0	0	0	0
8	O	15	0	0	1	0
8	P	5	0	0	0	0
All	All	14138	0	14028	235	0

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

All (235) 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)
2:O:122:MET:HE3	2:O:157:TRP:HE1	1.37	0.89
2:M:275:LEU:O	2:M:279:THR:HB	1.86	0.75
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.52	0.75
4:N:282:BCL:HBB3	4:O:309:BCL:H41	1.71	0.72
4:N:284:BCL:HED2	2:O:203:GLY:HA3	1.72	0.70
2:M:261:THR:HG22	2:M:264:GLY:H	1.55	0.70
3:H:226:THR:HG22	3:H:229:GLU:H	1.55	0.70
1:L:241:VAL:HG21	5:L:285:BPH:HAC2	1.74	0.70
5:L:285:BPH:HHC	5:L:285:BPH:HBB3	1.74	0.68
2:O:197:PHE:HZ	4:O:309:BCL:HBB2	1.60	0.67
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.76	0.67
5:L:285:BPH:H142	5:L:285:BPH:H102	1.78	0.65
1:N:229:ILE:HD13	6:N:286:U10:H102	1.79	0.64
5:N:285:BPH:CBB	5:N:285:BPH:HHC	2.28	0.64
1:L:60:ASN:O	1:L:64:ILE:HG22	1.98	0.63
2:M:133:THR:HG23	2:M:146:THR:HG22	1.81	0.62
1:N:93:ALA:HA	5:N:285:BPH:H9C2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:ARG:HD2	1:N:248:MET:O	1.99	0.62
1:L:53:ALA:HB2	1:L:64:ILE:HG13	1.83	0.61
4:O:309:BCL:H42	5:O:310:BPH:HBB2	1.83	0.60
3:P:154:ARG:HE	3:P:204:HIS:HD2	1.48	0.60
2:O:275:LEU:HD23	2:O:278:LEU:HD23	1.84	0.59
1:L:65:SER:HB2	8:L:289:HOH:O	2.02	0.59
1:L:208:THR:H	1:L:211:HIS:HD2	1.51	0.59
2:O:197:PHE:CZ	4:O:309:BCL:HBB2	2.38	0.59
3:P:168:TRP:HB2	3:P:178:PHE:HB2	1.85	0.58
2:M:157:TRP:HB2	4:M:310:BCL:H71	1.85	0.58
3:P:70:ARG:NH2	3:P:123:LEU:HD13	2.19	0.58
3:H:183:LEU:HD11	3:H:189:ARG:HD2	1.86	0.57
1:N:195:LEU:HD11	2:O:267:ARG:HG2	1.86	0.57
3:H:119:ASP:OD1	3:H:226:THR:HG21	2.04	0.57
5:N:285:BPH:HHC	5:N:285:BPH:HBB2	1.87	0.57
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.57
2:O:155:TRP:O	2:O:159:VAL:HG23	2.05	0.57
3:H:189:ARG:HD3	3:H:216:ILE:HB	1.86	0.57
2:M:103:LEU:HG	2:M:169:GLY:O	2.03	0.57
1:N:185:LEU:HD13	5:O:310:BPH:ND	2.20	0.56
4:O:309:BCL:HBB3	4:O:309:BCL:HHC	1.88	0.56
1:N:11:VAL:HG23	3:P:87:LEU:HD11	1.87	0.55
2:O:153:ALA:HB2	5:O:310:BPH:HAC1	1.88	0.55
2:M:39:LEU:HD12	2:M:47:LEU:HD11	1.88	0.55
1:L:42:ALA:HB2	5:L:285:BPH:H4C1	1.89	0.55
2:O:9:GLN:NE2	3:P:198:VAL:H	2.04	0.54
1:N:97:PHE:HB3	1:N:125:ILE:HG12	1.89	0.54
6:N:286:U10:H322	2:O:42:PHE:CD1	2.43	0.54
2:O:228:ARG:HA	3:P:194:GLN:CG	2.37	0.53
2:M:230:GLY:HA2	8:H:267:HOH:O	2.07	0.53
4:N:282:BCL:HHC	4:N:282:BCL:HBB2	1.88	0.53
4:N:282:BCL:HBB1	2:O:157:TRP:HD1	1.73	0.53
3:H:34:GLU:O	3:H:37:ARG:HG3	2.08	0.53
3:H:37:ARG:HB3	3:H:75:VAL:HG13	1.90	0.53
2:O:228:ARG:HA	3:P:194:GLN:HG3	1.91	0.53
2:O:237:GLN:HB2	2:O:262:MET:HG2	1.90	0.53
4:M:310:BCL:OBB	4:M:310:BCL:HHC	2.09	0.53
1:L:131:LEU:HD21	1:L:248:MET:HG3	1.90	0.53
1:N:178:SER:HA	4:N:282:BCL:HBA2	1.89	0.53
3:P:226:THR:HG22	3:P:229:GLU:H	1.72	0.53
2:O:261:THR:HG22	2:O:263:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:GLN:HE22	1:L:64:ILE:HA	1.73	0.52
1:N:201:GLU:HB2	1:N:204:LYS:HD2	1.90	0.52
1:L:208:THR:H	1:L:211:HIS:CD2	2.27	0.52
3:H:176:ALA:HB1	3:H:193:MET:HG3	1.90	0.52
3:P:183:LEU:HD11	3:P:189:ARG:HD2	1.90	0.52
2:O:168:MET:HE1	2:O:288:GLY:HA3	1.92	0.52
3:H:219:ILE:HG23	3:H:229:GLU:OE1	2.10	0.51
2:O:24:VAL:HG11	2:O:29:ARG:NH1	2.26	0.51
4:L:282:BCL:H151	5:L:285:BPH:H2	1.92	0.51
1:N:246:LEU:O	1:N:250:ILE:HB	2.11	0.51
2:O:9:GLN:HE22	3:P:198:VAL:H	1.59	0.51
4:N:282:BCL:HHC	4:N:282:BCL:CBB	2.41	0.51
3:H:119:ASP:HA	3:H:226:THR:HG23	1.93	0.50
2:M:189:PHE:O	2:M:193:HIS:HD2	1.95	0.50
2:O:234:GLU:O	2:O:238:ILE:HG13	2.10	0.50
1:N:208:THR:H	1:N:211:HIS:CD2	2.28	0.50
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.76	0.50
1:L:269:LEU:O	1:L:273:ALA:HB2	2.12	0.50
5:L:285:BPH:HHC	5:L:285:BPH:CBB	2.41	0.50
2:M:260:ALA:HA	3:H:35:ASN:HB3	1.94	0.50
2:M:236:GLU:HG3	3:H:122:GLU:CD	2.37	0.49
4:O:309:BCL:HHC	4:O:309:BCL:CBB	2.42	0.49
2:M:13:ARG:O	3:H:140:PHE:HA	2.12	0.49
3:H:108:GLY:O	3:H:113:SER:HA	2.12	0.49
1:N:185:LEU:CD2	4:N:282:BCL:H43	2.42	0.49
5:L:285:BPH:HBB2	2:M:210:TYR:HB3	1.94	0.49
3:P:119:ASP:HA	3:P:226:THR:HG23	1.94	0.49
3:P:130:LYS:NZ	3:P:173:GLU:HG3	2.27	0.49
3:P:62:LYS:HE2	3:P:64:PHE:CZ	2.47	0.49
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.28	0.49
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.12	0.49
1:N:81:ALA:H	1:N:85:LEU:HB2	1.78	0.49
3:P:41:PRO:HG3	3:P:58:LEU:HD11	1.95	0.49
4:M:309:BCL:H41	4:M:309:BCL:H61	1.61	0.48
3:P:154:ARG:HH21	3:P:204:HIS:CD2	2.31	0.48
6:L:286:U10:H162	4:M:309:BCL:H92	1.96	0.48
3:H:62:LYS:HE2	3:H:64:PHE:CZ	2.48	0.48
1:L:213:ASP:O	1:L:217:ARG:HB2	2.13	0.48
2:O:261:THR:HG22	2:O:264:GLY:H	1.77	0.48
3:P:37:ARG:O	3:P:75:VAL:HG22	2.13	0.48
3:P:207:ALA:HB1	3:P:237:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:LEU:HD13	5:L:284:BPH:ND	2.29	0.47
1:N:208:THR:OG1	1:N:211:HIS:HD2	1.97	0.47
1:L:182:THR:OG1	4:M:309:BCL:H11	2.14	0.47
6:L:286:U10:H252	6:L:286:U10:H201	1.97	0.47
3:P:195:MET:HE3	3:P:195:MET:HA	1.96	0.47
1:L:33:PHE:O	1:L:36:VAL:HG22	2.14	0.47
1:L:190:HIS:HA	6:L:286:U10:O2	2.14	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
1:N:136:PRO:HG2	1:N:145:ALA:HB2	1.96	0.47
2:M:96:PRO:HB2	2:M:172:SER:HA	1.96	0.47
3:P:196:VAL:HG12	3:P:205:VAL:HG22	1.97	0.47
2:M:157:TRP:HD1	4:M:309:BCL:HBB1	1.79	0.47
5:L:284:BPH:HMA1	4:M:310:BCL:H192	1.97	0.46
3:H:177:ARG:NH1	8:H:267:HOH:O	2.46	0.46
1:N:231:ARG:O	1:N:235:LEU:HB2	2.15	0.46
3:P:37:ARG:NH2	3:P:62:LYS:HB2	2.30	0.46
1:L:110:LYS:HD2	2:M:254:TRP:CZ3	2.51	0.46
1:N:79:PRO:HG2	1:N:82:LYS:HB3	1.96	0.46
2:O:202:HIS:HD2	4:O:309:BCL:HED2	1.80	0.46
3:P:130:LYS:NZ	3:P:172:PRO:HG2	2.30	0.46
2:M:94:LEU:HD13	2:M:115:TRP:HA	1.96	0.46
1:N:180:PHE:CE2	1:N:240:ALA:HB1	2.51	0.46
6:L:286:U10:H563	6:L:286:U10:H501	1.96	0.46
8:L:295:HOH:O	3:H:130:LYS:HE2	2.15	0.46
1:N:121:PHE:CZ	5:N:285:BPH:HBA2	2.50	0.46
1:N:190:HIS:HA	6:N:286:U10:O2	2.16	0.46
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.51	0.46
4:N:283:BCL:CGA	4:N:284:BCL:HBC1	2.46	0.46
4:N:284:BCL:HMD1	2:O:197:PHE:CE1	2.51	0.46
2:M:168:MET:HE1	2:M:288:GLY:HA3	1.98	0.46
3:H:66:LEU:HB3	3:H:70:ARG:HB2	1.97	0.46
3:P:189:ARG:HD3	3:P:216:ILE:HB	1.98	0.46
2:O:168:MET:HG2	2:O:173:GLU:HG3	1.99	0.46
3:H:154:ARG:NH2	8:H:270:HOH:O	2.48	0.45
1:L:3:LEU:HB2	1:L:6:GLU:HB2	1.97	0.45
3:H:195:MET:HE1	3:H:241:LEU:HD11	1.97	0.45
2:O:222:THR:O	2:O:226:VAL:HG22	2.17	0.45
1:N:272:TRP:CE2	2:O:87:ARG:HB3	2.51	0.45
4:N:282:BCL:H3C	2:O:186:THR:OG1	2.16	0.45
4:N:282:BCL:O1A	5:O:310:BPH:HMB1	2.17	0.45
2:O:256:MET:HE1	6:O:311:U10:H13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:GLU:HG2	3:H:65:ILE:HG22	1.98	0.45
3:P:119:ASP:HA	3:P:226:THR:CG2	2.47	0.45
4:M:309:BCL:HBB2	4:M:309:BCL:HMB3	1.99	0.45
3:H:182:GLU:HA	3:H:187:SER:O	2.16	0.45
1:N:34:PHE:CE1	1:N:102:LEU:HD23	2.51	0.45
1:L:185:LEU:CD2	4:M:309:BCL:H52	2.47	0.45
2:M:238:ILE:HG23	2:M:263:GLU:HB2	1.99	0.45
3:H:219:ILE:HG21	3:H:224:GLU:O	2.16	0.45
6:N:286:U10:H322	2:O:42:PHE:CG	2.51	0.45
2:M:75:TRP:HB3	2:M:80:TRP:CE3	2.51	0.45
6:N:286:U10:H1M1	6:N:286:U10:H71	1.77	0.44
1:L:129:LEU:HG	1:L:133:LEU:HD23	1.99	0.44
1:L:199:ASN:HD21	2:M:267:ARG:HH12	1.64	0.44
1:L:60:ASN:HB3	1:L:63:LEU:HD12	2.00	0.44
8:L:300:HOH:O	3:H:79:GLU:HB2	2.17	0.44
4:N:283:BCL:H11	4:N:284:BCL:HBC3	2.00	0.44
2:O:164:ARG:HB3	2:O:165:PRO:HD3	2.00	0.43
2:O:237:GLN:CB	2:O:262:MET:HG2	2.48	0.43
3:P:111:PRO:HG3	3:P:242:MET:HE3	1.99	0.43
3:P:122:GLU:HB2	3:P:227:LEU:HD11	2.00	0.43
1:N:244:SER:OG	4:N:283:BCL:HBA2	2.18	0.43
1:N:275:ILE:HG21	2:O:81:ASN:ND2	2.33	0.43
4:L:282:BCL:H2C	4:M:310:BCL:H2C	2.00	0.43
1:N:234:LEU:HD22	1:N:238:LEU:HD22	2.00	0.43
4:N:283:BCL:H122	5:N:285:BPH:H3A	2.01	0.43
4:N:283:BCL:HHC	4:N:283:BCL:OBB	2.19	0.43
2:O:237:GLN:HG3	2:O:262:MET:HE3	1.99	0.43
4:L:282:BCL:HBD	4:L:283:BCL:HAC1	2.00	0.43
2:O:236:GLU:HG3	3:P:122:GLU:CD	2.43	0.43
3:P:108:GLY:HA2	3:P:112:ALA:O	2.19	0.43
1:L:147:PRO:HB2	8:L:289:HOH:O	2.18	0.43
2:O:62:SER:HB3	2:O:121:PHE:O	2.19	0.43
1:N:93:ALA:HA	5:N:285:BPH:C9	2.48	0.42
2:O:164:ARG:HD2	2:O:284:ILE:HG22	2.01	0.42
2:M:165:PRO:HG2	2:M:174:ALA:HB2	2.00	0.42
1:L:34:PHE:O	1:L:38:THR:HB	2.19	0.42
1:L:78:ALA:H	1:L:87:GLN:HE22	1.66	0.42
6:O:311:U10:H421	6:O:311:U10:H401	1.85	0.42
1:L:121:PHE:CZ	5:L:285:BPH:HBA2	2.54	0.42
4:L:283:BCL:H172	5:L:285:BPH:H142	2.01	0.42
2:M:228:ARG:HA	3:H:194:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:241:LEU:HA	3:P:248:ARG:NH2	2.34	0.42
1:N:200:PRO:HB3	1:N:207:ARG:HD3	2.02	0.42
1:L:266:TRP:O	1:L:269:LEU:HB2	2.19	0.42
4:L:282:BCL:HAA2	4:L:283:BCL:HBC1	2.01	0.42
2:M:11:GLN:HB2	3:H:144:ALA:HB3	2.02	0.42
1:L:158:SER:HA	4:L:282:BCL:HBC1	2.01	0.42
2:M:13:ARG:HB2	3:H:143:SER:HB3	2.02	0.42
2:M:159:VAL:HA	2:M:163:ILE:HB	2.02	0.42
2:M:215:LEU:HD13	6:M:311:U10:H153	2.01	0.42
2:O:152:SER:OG	2:O:274:VAL:HG13	2.19	0.42
1:N:60:ASN:HA	1:N:61:PRO:HD3	1.75	0.42
1:N:180:PHE:CD2	1:N:240:ALA:HB1	2.55	0.42
2:O:229:PHE:HB2	2:O:244:ALA:HB2	2.02	0.42
3:P:192:PRO:HB2	3:P:195:MET:HB2	2.02	0.41
1:L:115:TYR:O	1:L:118:PRO:HG2	2.20	0.41
1:L:128:TYR:O	1:L:132:VAL:HB	2.20	0.41
2:M:220:GLY:O	2:M:224:LEU:HG	2.20	0.41
8:O:322:HOH:O	3:P:34:GLU:HG3	2.19	0.41
3:P:130:LYS:HZ1	3:P:173:GLU:HG3	1.84	0.41
1:N:135:ARG:HB3	1:N:136:PRO:HD3	2.02	0.41
2:O:261:THR:HG22	2:O:263:GLU:N	2.35	0.41
3:H:254:ALA:O	3:H:257:ALA:HB3	2.20	0.41
1:L:109:ARG:HG3	1:L:115:TYR:HE1	1.86	0.41
1:L:117:ILE:H	1:L:117:ILE:HD12	1.86	0.41
2:M:34:PRO:O	2:M:47:LEU:HB2	2.20	0.41
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.02	0.41
3:H:33:THR:O	3:H:36:MET:HB2	2.19	0.41
1:N:207:ARG:HG2	2:O:142:MET:HG2	2.02	0.41
2:O:120:PHE:O	2:O:124:VAL:HG23	2.20	0.41
1:N:55:LEU:HD13	1:N:81:ALA:HB2	2.02	0.41
1:N:65:SER:HG	1:N:67:TYR:HE1	1.66	0.41
3:P:180:GLU:OE2	3:P:188:THR:HG21	2.21	0.41
2:M:75:TRP:HB3	2:M:80:TRP:CZ3	2.56	0.41
2:O:75:TRP:HB3	2:O:80:TRP:CE3	2.56	0.41
2:O:189:PHE:O	2:O:193:HIS:HD2	2.04	0.41
3:P:206:ASN:O	3:P:248:ARG:NH1	2.54	0.41
2:M:243:THR:O	2:M:247:ARG:HG3	2.20	0.41
1:N:133:LEU:O	1:N:137:VAL:HG23	2.20	0.41
3:H:146:LYS:NZ	3:H:151:LEU:HD21	2.36	0.41
1:N:113:ILE:HD11	2:O:251:PHE:CD2	2.56	0.41
1:N:216:PHE:CG	6:N:286:U10:H72	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:CYS:O	1:N:250:ILE:HG22	2.21	0.41
1:L:15:THR:N	1:L:109:ARG:HH12	2.19	0.40
1:L:185:LEU:HD23	4:M:309:BCL:H52	2.03	0.40
1:N:51:TRP:CE3	1:N:51:TRP:HA	2.57	0.40
2:O:133:THR:CG2	2:O:147:ALA:HA	2.52	0.40
2:O:202:HIS:CE1	2:O:206:ILE:HD11	2.57	0.40
2:O:258:PHE:HE1	6:O:311:U10:H211	1.86	0.40
1:N:238:LEU:HD12	5:N:285:BPH:CBC	2.51	0.40
2:O:195:ASN:HB3	2:O:198:TYR:HD2	1.86	0.40
4:N:284:BCL:H18	4:N:284:BCL:H141	2.03	0.40
1:L:101:ALA:O	1:L:104:GLU:HB2	2.20	0.40
1:L:223:SER:O	2:M:44:ASN:HB2	2.22	0.40
4:L:282:BCL:CGA	4:L:283:BCL:HBC1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	261 (94%)	14 (5%)	4 (1%)	9	19
1	N	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	11	25
2	M	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	18	38
2	O	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	18	38
3	H	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
3	P	246/260 (95%)	238 (97%)	7 (3%)	1 (0%)	30	51
All	All	1644/1696 (97%)	1566 (95%)	66 (4%)	12 (1%)	18	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	270	PRO
2	M	259	ASN
2	O	259	ASN
1	L	271	TRP
2	M	195	ASN
1	N	271	TRP
2	O	195	ASN
1	N	270	PRO
1	L	66	VAL
3	P	138	ALA
1	N	66	VAL
1	L	31	VAL

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	L	220/220 (100%)	205 (93%)	15 (7%)	14	32
1	N	220/220 (100%)	200 (91%)	20 (9%)	9	19
2	M	235/240 (98%)	217 (92%)	18 (8%)	12	27
2	O	235/240 (98%)	215 (92%)	20 (8%)	10	22
3	H	200/209 (96%)	178 (89%)	22 (11%)	6	13
3	P	200/209 (96%)	178 (89%)	22 (11%)	6	13
All	All	1310/1338 (98%)	1193 (91%)	117 (9%)	9	20

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	THR
1	L	59	TRP
1	L	64	ILE
1	L	80	LEU
1	L	102	LEU
1	L	129	LEU
1	L	132	VAL

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Mol	Chain	Res	Type
1	L	136	PRO
1	L	189	LEU
1	L	195	LEU
1	L	216	PHE
1	L	217	ARG
1	L	231	ARG
1	L	234	LEU
1	L	254	ILE
2	M	12	VAL
2	M	22	GLU
2	M	29	ARG
2	M	37	THR
2	M	60	LEU
2	M	89	LEU
2	M	94	LEU
2	M	114	LEU
2	M	133	THR
2	M	156	LEU
2	M	191	LEU
2	M	192	VAL
2	M	259	ASN
2	M	261	THR
2	M	279	THR
2	M	286	LEU
2	M	292	ASP
2	M	300	ASN
3	H	17	ILE
3	H	49	PRO
3	H	60	LYS
3	H	73	LEU
3	H	75	VAL
3	H	82	ASP
3	H	84	PRO
3	H	87	LEU
3	H	109	VAL
3	H	123	LEU
3	H	124	ASP
3	H	188	THR
3	H	202	ARG
3	H	208	LEU
3	H	212	LEU
3	H	220	LYS

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Mol	Chain	Res	Type
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	226	THR
3	H	227	LEU
3	H	231	ASP
1	N	11	VAL
1	N	49	ILE
1	N	64	ILE
1	N	72	GLU
1	N	102	LEU
1	N	126	LEU
1	N	129	LEU
1	N	132	VAL
1	N	158	SER
1	N	185	LEU
1	N	189	LEU
1	N	195	LEU
1	N	216	PHE
1	N	217	ARG
1	N	220	VAL
1	N	231	ARG
1	N	234	LEU
1	N	235	LEU
1	N	250	ILE
1	N	254	ILE
2	O	12	VAL
2	O	22	GLU
2	O	26	LEU
2	O	29	ARG
2	O	37	THR
2	O	60	LEU
2	O	72	ILE
2	O	89	LEU
2	O	94	LEU
2	O	114	LEU
2	O	133	THR
2	O	148	TRP
2	O	152	SER
2	O	156	LEU
2	O	168	MET
2	O	191	LEU

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Mol	Chain	Res	Type
2	O	261	THR
2	O	274	VAL
2	O	286	LEU
2	O	301	HIS
3	P	17	ILE
3	P	46	ASP
3	P	60	LYS
3	P	61	PRO
3	P	66	LEU
3	P	73	LEU
3	P	75	VAL
3	P	82	ASP
3	P	109	VAL
3	P	188	THR
3	P	203	VAL
3	P	208	LEU
3	P	212	LEU
3	P	219	ILE
3	P	220	LYS
3	P	223	THR
3	P	224	GLU
3	P	225	VAL
3	P	226	THR
3	P	227	LEU
3	P	231	ASP
3	P	251	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
1	L	87	GLN
1	L	159	ASN
1	L	199	ASN
1	L	211	HIS
2	M	9	GLN
2	M	81	ASN
2	M	138	GLN
2	M	145	HIS
2	M	187	ASN
2	M	193	HIS
2	M	300	ASN

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Mol	Chain	Res	Type
2	M	301	HIS
3	H	199	GLN
3	H	204	HIS
1	N	87	GLN
1	N	159	ASN
1	N	199	ASN
1	N	211	HIS
2	O	9	GLN
2	O	11	GLN
2	O	138	GLN
2	O	145	HIS
2	O	193	HIS
3	P	52	ASN
3	P	199	GLN
3	P	204	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	L	282	1	69,74,74	1.19	7 (10%)	79,115,115	1.71	20 (25%)
4	BCL	N	283	1	69,74,74	1.14	5 (7%)	79,115,115	1.98	22 (27%)
6	U10	M	311	-	63,63,63	1.74	14 (22%)	78,79,79	1.29	7 (8%)
6	U10	N	286	-	63,63,63	1.73	16 (25%)	78,79,79	1.59	9 (11%)
6	U10	O	311	-	63,63,63	1.61	14 (22%)	78,79,79	1.19	11 (14%)
4	BCL	M	310	2	69,74,74	1.10	5 (7%)	79,115,115	1.97	20 (25%)
4	BCL	N	284	1	69,74,74	1.20	9 (13%)	79,115,115	2.12	24 (30%)
4	BCL	L	283	1	69,74,74	1.15	6 (8%)	79,115,115	1.99	25 (31%)
5	BPH	L	285	-	59,70,70	1.61	7 (11%)	59,101,101	2.39	21 (35%)
4	BCL	O	309	2	69,74,74	1.10	7 (10%)	79,115,115	1.76	17 (21%)
5	BPH	N	285	-	59,70,70	1.44	6 (10%)	59,101,101	2.82	19 (32%)
4	BCL	M	309	2	69,74,74	1.22	8 (11%)	79,115,115	2.18	24 (30%)
5	BPH	O	310	-	59,70,70	1.39	7 (11%)	59,101,101	2.86	20 (33%)
4	BCL	N	282	2	69,74,74	1.28	8 (11%)	79,115,115	1.85	19 (24%)
5	BPH	L	284	-	59,70,70	1.72	9 (15%)	59,101,101	2.45	20 (33%)
6	U10	L	286	-	63,63,63	1.74	16 (25%)	78,79,79	1.32	8 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	282	1	-	3/41/137/137	-
4	BCL	N	283	1	-	11/41/137/137	-
6	U10	M	311	-	-	15/63/87/87	0/1/1/1
6	U10	N	286	-	-	19/63/87/87	0/1/1/1
6	U10	O	311	-	-	13/63/87/87	0/1/1/1
4	BCL	M	310	2	2/2/21/25	3/41/137/137	-
4	BCL	N	284	1	-	5/41/137/137	-
5	BPH	L	285	-	1/1/18/22	10/37/105/105	0/5/6/6
5	BPH	N	285	-	1/1/18/22	9/37/105/105	0/5/6/6
4	BCL	O	309	2	1/1/21/25	4/41/137/137	-
4	BCL	L	283	1	-	6/41/137/137	-
4	BCL	M	309	2	2/2/21/25	11/41/137/137	-
5	BPH	O	310	-	1/1/18/22	10/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	N	282	2	2/2/21/25	6/41/137/137	-
5	BPH	L	284	-	2/2/18/22	9/37/105/105	0/5/6/6
6	U10	L	286	-	-	13/63/87/87	0/1/1/1

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	285	BPH	C3A-C2A	-7.85	1.47	1.54
5	L	284	BPH	C2C-C3C	-6.89	1.48	1.54
5	L	284	BPH	C3A-C2A	-5.74	1.49	1.54
5	N	285	BPH	C3D-CAD	-5.04	1.38	1.47
5	O	310	BPH	C3D-CAD	-5.00	1.38	1.47
5	L	284	BPH	C3D-CAD	-4.93	1.38	1.47
6	L	286	U10	C7-C8	-4.57	1.43	1.50
5	N	285	BPH	C3A-C2A	-4.55	1.50	1.54
6	M	311	U10	C7-C8	-4.42	1.43	1.50
5	L	285	BPH	C3D-CAD	-4.36	1.39	1.47
4	L	282	BCL	O2D-CGD	-4.33	1.22	1.33
5	O	310	BPH	C2C-C3C	-4.11	1.51	1.54
6	N	286	U10	C7-C8	-4.02	1.44	1.50
5	L	285	BPH	C2C-C3C	-4.01	1.51	1.54
4	O	309	BCL	O2D-CGD	-3.98	1.23	1.33
6	O	311	U10	C6-C1	3.98	1.42	1.35
4	L	283	BCL	O2D-CGD	-3.88	1.23	1.33
4	L	282	BCL	C1D-C2D	-3.80	1.37	1.45
6	N	286	U10	C32-C33	-3.79	1.39	1.50
6	N	286	U10	C6-C1	3.76	1.41	1.35
5	N	285	BPH	C2C-C3C	-3.71	1.51	1.54
4	N	282	BCL	C1D-C2D	-3.66	1.38	1.45
4	N	282	BCL	O2D-CGD	-3.66	1.24	1.33
6	L	286	U10	C23-C24	3.55	1.41	1.33
5	L	284	BPH	O2D-CGD	-3.55	1.24	1.33
4	N	283	BCL	O2D-CGD	-3.53	1.24	1.33
5	N	285	BPH	C3B-CAB	-3.52	1.39	1.49
6	O	311	U10	C28-C29	3.48	1.41	1.33
6	L	286	U10	C28-C29	3.47	1.41	1.33
4	M	309	BCL	C1D-C2D	-3.46	1.38	1.45
6	M	311	U10	C38-C39	3.46	1.41	1.33
4	N	284	BCL	O2D-CGD	-3.43	1.24	1.33
6	M	311	U10	C43-C44	3.43	1.41	1.33
5	L	284	BPH	O2A-CGA	-3.40	1.23	1.33
4	N	282	BCL	C2-C3	3.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	286	U10	C48-C49	3.37	1.40	1.33
4	M	309	BCL	O2D-CGD	-3.36	1.25	1.33
4	N	282	BCL	CAA-C2A	3.36	1.60	1.54
6	M	311	U10	C6-C1	3.32	1.41	1.35
4	N	283	BCL	CAA-C2A	-3.31	1.48	1.54
4	M	309	BCL	C1D-ND	-3.31	1.33	1.37
5	N	285	BPH	O2D-CGD	-3.31	1.25	1.33
5	O	310	BPH	C3A-C2A	-3.30	1.51	1.54
5	O	310	BPH	O2A-CGA	-3.29	1.23	1.33
6	M	311	U10	C48-C49	3.28	1.40	1.33
6	L	286	U10	C3-C2	-3.27	1.39	1.48
6	N	286	U10	C28-C29	3.27	1.40	1.33
4	N	283	BCL	O2A-CGA	-3.23	1.23	1.33
4	N	284	BCL	C1D-C2D	-3.23	1.38	1.45
4	M	310	BCL	C1D-C2D	-3.19	1.39	1.45
4	M	310	BCL	O2D-CGD	-3.19	1.25	1.33
5	L	285	BPH	O2D-CGD	-3.19	1.25	1.33
6	N	286	U10	C18-C19	3.16	1.40	1.33
5	L	285	BPH	O2A-CGA	-3.13	1.24	1.33
4	L	283	BCL	C1D-C2D	-3.12	1.39	1.45
5	O	310	BPH	O2D-CGD	-3.07	1.25	1.33
4	M	309	BCL	O2A-CGA	-3.07	1.24	1.33
6	L	286	U10	C38-C39	3.05	1.40	1.33
6	M	311	U10	C33-C34	3.04	1.40	1.33
6	N	286	U10	C4-C5	-3.02	1.40	1.48
4	N	282	BCL	O2A-CGA	-3.02	1.24	1.33
6	O	311	U10	C3-C2	-3.00	1.40	1.48
5	N	285	BPH	O2A-CGA	-2.99	1.24	1.33
6	L	286	U10	C33-C34	2.99	1.40	1.33
4	O	309	BCL	O2A-CGA	-2.98	1.24	1.33
6	O	311	U10	C8-C9	2.94	1.39	1.33
6	M	311	U10	C18-C19	2.94	1.39	1.33
4	O	309	BCL	C1D-C2D	-2.93	1.39	1.45
4	L	282	BCL	O2A-CGA	-2.93	1.24	1.33
6	N	286	U10	C38-C39	2.91	1.39	1.33
6	N	286	U10	C23-C24	2.91	1.39	1.33
6	O	311	U10	C4-C5	-2.89	1.40	1.48
4	M	310	BCL	O2A-CGA	-2.89	1.25	1.33
6	O	311	U10	C23-C24	2.85	1.39	1.33
6	N	286	U10	C13-C14	2.84	1.39	1.33
6	O	311	U10	C43-C44	2.82	1.39	1.33
6	M	311	U10	C3-C2	-2.82	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	286	U10	C6-C1	2.81	1.40	1.35
4	N	283	BCL	C1D-C2D	-2.80	1.39	1.45
6	M	311	U10	C13-C14	2.79	1.39	1.33
6	N	286	U10	C3-C2	-2.79	1.40	1.48
6	N	286	U10	C43-C44	2.79	1.39	1.33
6	L	286	U10	C18-C19	2.75	1.39	1.33
6	L	286	U10	C43-C44	2.75	1.39	1.33
6	L	286	U10	C4-C5	-2.75	1.40	1.48
6	O	311	U10	C38-C39	2.72	1.39	1.33
4	L	283	BCL	O2A-CGA	-2.72	1.25	1.33
6	O	311	U10	C18-C19	2.68	1.39	1.33
6	M	311	U10	C4-C5	-2.68	1.41	1.48
6	N	286	U10	C48-C49	2.64	1.39	1.33
4	N	284	BCL	CAA-CBA	2.64	1.60	1.52
6	M	311	U10	C23-C24	2.63	1.39	1.33
6	O	311	U10	C33-C34	2.62	1.39	1.33
4	O	309	BCL	C2-C3	2.62	1.39	1.33
4	L	282	BCL	C2-C3	2.61	1.39	1.33
6	O	311	U10	C48-C49	2.59	1.39	1.33
4	N	283	BCL	C2-C3	2.57	1.39	1.33
5	L	285	BPH	C3B-CAB	-2.56	1.42	1.49
4	M	310	BCL	C2-C3	2.54	1.38	1.33
6	M	311	U10	C53-C54	2.54	1.40	1.32
4	M	309	BCL	C3D-CAD	-2.53	1.36	1.45
6	M	311	U10	C28-C29	2.50	1.38	1.33
5	O	310	BPH	C2-C3	2.50	1.38	1.33
4	N	284	BCL	C2-C3	2.48	1.38	1.33
5	O	310	BPH	C3B-CAB	-2.48	1.42	1.49
5	L	284	BPH	C2-C3	2.47	1.38	1.33
4	N	284	BCL	O2A-CGA	-2.47	1.26	1.33
5	L	284	BPH	C3B-CAB	-2.47	1.42	1.49
4	L	283	BCL	C2-C3	2.46	1.38	1.33
4	L	282	BCL	C1D-ND	-2.45	1.34	1.37
6	O	311	U10	C7-C6	2.42	1.55	1.51
4	O	309	BCL	C1B-C2B	-2.40	1.37	1.43
4	M	309	BCL	C2-C3	2.38	1.38	1.33
4	L	283	BCL	C3D-CAD	-2.36	1.37	1.45
5	L	285	BPH	CBD-CGD	2.35	1.55	1.52
6	O	311	U10	C13-C14	2.34	1.38	1.33
4	N	282	BCL	C3A-C2A	-2.30	1.48	1.54
6	L	286	U10	C6-C5	-2.29	1.40	1.46
4	N	284	BCL	C1D-ND	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	282	BCL	CAA-CBA	2.26	1.59	1.52
6	O	311	U10	C53-C54	2.25	1.39	1.32
4	L	282	BCL	C2C-C3C	-2.22	1.48	1.54
4	O	309	BCL	C3B-CAB	-2.21	1.40	1.46
6	L	286	U10	C13-C14	2.20	1.38	1.33
4	L	282	BCL	CAA-C2A	-2.20	1.50	1.54
6	N	286	U10	C53-C54	2.19	1.39	1.32
4	M	309	BCL	C3D-C4D	-2.18	1.39	1.44
4	M	310	BCL	C3D-CAD	-2.18	1.38	1.45
4	M	309	BCL	C1B-C2B	-2.18	1.38	1.43
6	L	286	U10	C53-C54	2.17	1.39	1.32
4	N	284	BCL	MG-NC	-2.14	2.01	2.06
4	N	282	BCL	C2C-C3C	-2.14	1.48	1.54
4	N	284	BCL	CMC-C2C	-2.14	1.48	1.53
6	L	286	U10	C12-C13	-2.13	1.44	1.50
4	L	283	BCL	C1D-ND	-2.13	1.35	1.37
5	L	284	BPH	CMC-C2C	-2.11	1.49	1.53
5	L	284	BPH	C1D-C2D	-2.07	1.37	1.39
6	M	311	U10	C8-C9	2.06	1.37	1.33
6	N	286	U10	C33-C34	2.06	1.37	1.33
6	N	286	U10	C1-C2	-2.05	1.40	1.47
6	N	286	U10	C35-C34	2.04	1.55	1.50
4	N	284	BCL	C1B-NB	-2.04	1.35	1.37
6	L	286	U10	C8-C9	2.03	1.37	1.33
4	O	309	BCL	C1D-ND	-2.01	1.35	1.37

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	285	BPH	O2D-CGD-CBD	9.79	121.70	110.95
5	O	310	BPH	O2D-CGD-CBD	9.55	121.44	110.95
5	O	310	BPH	C4D-CHA-CBD	-9.44	103.93	108.45
4	M	309	BCL	C1C-NC-C4C	8.00	110.33	106.68
5	N	285	BPH	C4D-CHA-CBD	-7.92	104.66	108.45
5	L	284	BPH	O2D-CGD-CBD	7.37	119.04	110.95
4	N	284	BCL	C1C-NC-C4C	7.33	110.02	106.68
5	O	310	BPH	O1D-CGD-CBD	-6.96	114.17	124.72
5	L	284	BPH	C4D-CHA-CBD	-6.94	105.13	108.45
5	L	285	BPH	C4D-CHA-CBD	-6.72	105.23	108.45
4	L	283	BCL	C1C-NC-C4C	6.70	109.73	106.68
5	L	285	BPH	C3D-C4D-ND	6.48	116.02	107.71
5	N	285	BPH	C4D-ND-C1D	-6.32	101.30	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	285	BPH	C3D-C4D-ND	6.17	115.62	107.71
5	L	285	BPH	O2D-CGD-CBD	6.16	117.72	110.95
4	M	310	BCL	C1C-NC-C4C	6.07	109.45	106.68
5	L	284	BPH	C3D-C4D-ND	5.91	115.28	107.71
4	N	283	BCL	C1C-NC-C4C	5.88	109.36	106.68
5	N	285	BPH	O1D-CGD-CBD	-5.81	115.92	124.72
5	O	310	BPH	C4D-ND-C1D	-5.67	102.08	108.87
4	M	310	BCL	C4A-NA-C1A	5.65	109.26	106.68
4	N	282	BCL	CBA-CAA-C2A	5.64	130.57	113.79
5	O	310	BPH	C3D-C4D-ND	5.56	114.83	107.71
5	L	285	BPH	C4D-ND-C1D	-5.39	102.41	108.87
4	N	284	BCL	C4A-NA-C1A	5.30	109.10	106.68
4	M	309	BCL	C1-C2-C3	-5.20	117.68	126.20
4	N	284	BCL	C1D-ND-C4D	-5.18	102.68	106.31
5	L	284	BPH	C4D-ND-C1D	-5.15	102.70	108.87
4	L	283	BCL	C4D-C3D-CAD	-5.10	102.56	108.11
6	N	286	U10	C7-C6-C1	-5.09	116.16	124.89
4	L	283	BCL	C1D-ND-C4D	-5.06	102.76	106.31
5	L	285	BPH	C3D-CAD-CBD	5.06	114.26	107.61
4	O	309	BCL	C1C-NC-C4C	4.98	108.95	106.68
6	N	286	U10	C7-C6-C5	4.88	124.18	118.52
6	N	286	U10	C35-C34-C36	4.83	123.61	115.23
4	N	283	BCL	C1D-ND-C4D	-4.82	102.93	106.31
4	M	310	BCL	C4D-CHA-C1A	4.61	126.74	121.24
5	O	310	BPH	C2B-C1B-NB	4.54	112.71	109.43
4	M	309	BCL	C4D-CHA-C1A	4.53	126.65	121.24
5	L	284	BPH	O1D-CGD-CBD	-4.49	117.92	124.72
5	N	285	BPH	C7-C6-C5	-4.47	101.34	113.26
5	L	284	BPH	C3D-CAD-CBD	4.47	113.49	107.61
4	M	309	BCL	C1D-ND-C4D	-4.42	103.21	106.31
4	O	309	BCL	C4D-CHA-C1A	4.39	126.48	121.24
4	M	309	BCL	C4A-NA-C1A	4.38	108.68	106.68
4	M	309	BCL	O2D-CGD-CBD	4.36	118.86	111.23
4	N	282	BCL	C4D-CHA-C1A	4.35	126.43	121.24
4	N	282	BCL	C4D-C3D-CAD	-4.34	103.39	108.11
5	N	285	BPH	C2D-C1D-ND	4.34	112.57	109.43
6	N	286	U10	C7-C8-C9	-4.27	119.48	126.83
4	L	283	BCL	C3D-C4D-ND	4.25	116.90	109.99
4	N	284	BCL	C4D-CHA-C1A	4.24	126.31	121.24
4	L	283	BCL	C4D-CHA-C1A	4.22	126.28	121.24
4	N	283	BCL	C4A-NA-C1A	4.22	108.60	106.68
4	N	282	BCL	O2D-CGD-CBD	4.17	118.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	282	BCL	C1D-ND-C4D	-4.15	103.40	106.31
4	M	310	BCL	C4D-C3D-CAD	-4.15	103.60	108.11
4	O	309	BCL	C4D-C3D-CAD	-4.14	103.61	108.11
4	M	309	BCL	C3D-C4D-ND	4.10	116.66	109.99
5	N	285	BPH	OBD-CAD-C3D	-4.08	121.53	127.89
4	M	310	BCL	C1D-ND-C4D	-4.08	103.45	106.31
4	N	282	BCL	C3D-C2D-C1D	4.06	111.37	105.83
4	N	282	BCL	C4A-NA-C1A	4.06	108.53	106.68
4	M	309	BCL	C4D-C3D-CAD	-4.06	103.70	108.11
4	N	283	BCL	C4D-C3D-CAD	-4.05	103.70	108.11
4	L	282	BCL	C4D-C3D-CAD	-4.03	103.72	108.11
5	L	285	BPH	O1D-CGD-CBD	-3.99	118.67	124.72
6	N	286	U10	C8-C7-C6	3.98	121.89	112.08
4	N	283	BCL	C3D-C4D-ND	3.97	116.44	109.99
4	L	282	BCL	C4D-CHA-C1A	3.97	125.98	121.24
4	N	284	BCL	C3D-C4D-ND	3.96	116.43	109.99
4	N	283	BCL	C4D-CHA-C1A	3.94	125.95	121.24
5	N	285	BPH	C3D-CAD-CBD	3.94	112.79	107.61
4	N	284	BCL	C4D-C3D-CAD	-3.93	103.84	108.11
5	O	310	BPH	OBD-CAD-C3D	-3.92	121.78	127.89
4	O	309	BCL	O2D-CGD-CBD	3.92	118.08	111.23
5	L	284	BPH	C2B-C1B-NB	3.89	112.24	109.43
4	N	282	BCL	C3D-C4D-ND	3.87	116.28	109.99
4	M	310	BCL	O2D-CGD-CBD	3.84	117.95	111.23
4	M	309	BCL	O1D-CGD-CBD	-3.81	117.00	124.52
5	O	310	BPH	C3D-CAD-CBD	3.80	112.61	107.61
4	M	310	BCL	C1-O2A-CGA	3.79	125.83	116.65
4	N	282	BCL	C1C-NC-C4C	3.78	108.40	106.68
5	O	310	BPH	C2D-C1D-ND	3.78	112.16	109.43
4	L	282	BCL	C1C-NC-C4C	3.76	108.39	106.68
4	M	310	BCL	C3D-C4D-ND	3.72	116.03	109.99
4	L	282	BCL	C3D-C4D-ND	3.71	116.02	109.99
5	L	284	BPH	C4-C3-C5	3.67	121.61	115.23
5	O	310	BPH	C1B-NB-C4B	-3.67	103.46	108.82
5	L	284	BPH	C1-O2A-CGA	3.66	125.52	116.65
4	O	309	BCL	C1-O2A-CGA	3.62	125.40	116.65
4	N	284	BCL	CAA-CBA-CGA	3.58	123.37	113.21
5	L	284	BPH	CMB-C2B-C3B	3.57	131.81	124.68
5	O	310	BPH	CMA-C3A-C4A	-3.55	106.95	114.61
4	N	284	BCL	CED-O2D-CGD	3.50	123.84	115.92
4	L	283	BCL	CAA-CBA-CGA	3.46	123.03	113.21
5	L	285	BPH	OBD-CAD-C3D	-3.43	122.55	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	310	BPH	C1-O2A-CGA	3.42	124.94	116.65
6	L	286	U10	C7-C8-C9	-3.39	121.00	126.83
5	N	285	BPH	C2B-C1B-NB	3.38	111.88	109.43
4	N	283	BCL	C4-C3-C5	3.38	121.10	115.23
4	O	309	BCL	C3D-C4D-ND	3.37	115.47	109.99
5	O	310	BPH	C3B-C4B-NB	3.36	112.94	108.05
5	N	285	BPH	CMA-C3A-C4A	-3.35	107.39	114.61
4	L	282	BCL	C3D-C2D-C1D	3.35	110.40	105.83
5	L	284	BPH	OBD-CAD-C3D	-3.31	122.72	127.89
4	M	309	BCL	C11-C12-C13	3.29	126.90	115.97
4	L	283	BCL	C4A-NA-C1A	3.26	108.17	106.68
5	L	285	BPH	CED-O2D-CGD	3.26	123.30	115.92
5	N	285	BPH	C17-C16-C15	-3.25	98.73	113.28
5	L	285	BPH	C4-C3-C5	3.24	120.86	115.23
4	M	309	BCL	CBA-CAA-C2A	3.22	123.38	113.79
4	N	283	BCL	C1-C2-C3	-3.21	120.93	126.20
4	O	309	BCL	C1D-ND-C4D	-3.18	104.08	106.31
5	N	285	BPH	C4-C3-C5	3.18	120.74	115.23
6	L	286	U10	C50-C49-C51	3.14	120.68	115.23
5	L	285	BPH	C6-C5-C3	-3.13	105.85	113.47
6	M	311	U10	C30-C29-C31	3.11	120.62	115.23
4	O	309	BCL	C4A-NA-C1A	3.10	108.09	106.68
4	L	283	BCL	CHA-C4D-ND	-3.04	126.27	132.55
4	L	283	BCL	C6-C5-C3	-3.04	106.06	113.47
4	N	283	BCL	O2D-CGD-CBD	3.04	116.54	111.23
4	N	284	BCL	C3D-C2D-C1D	3.04	109.97	105.83
4	N	283	BCL	CBC-CAC-C3C	3.02	119.83	113.41
4	N	284	BCL	CAA-C2A-C3A	-3.02	104.84	113.00
5	N	285	BPH	CMC-C2C-C1C	-2.99	108.16	114.61
5	L	284	BPH	C4A-C3A-C2A	2.99	105.68	102.84
4	M	309	BCL	C3D-C2D-C1D	2.98	109.89	105.83
6	M	311	U10	C1M-C1-C6	-2.95	119.61	124.45
6	N	286	U10	C36-C34-C33	-2.94	114.57	121.17
4	L	283	BCL	CMB-C2B-C1B	-2.94	120.95	125.42
4	N	282	BCL	O1D-CGD-CBD	-2.93	118.73	124.52
5	L	285	BPH	OBB-CAB-C3B	2.93	124.89	119.99
4	L	282	BCL	CAC-C3C-C4C	-2.93	106.08	112.58
4	M	310	BCL	CMB-C2B-C1B	-2.91	120.99	125.42
4	M	309	BCL	CHA-C4D-ND	-2.90	126.57	132.55
6	O	311	U10	C40-C39-C41	2.89	120.25	115.23
4	N	284	BCL	CHA-C4D-ND	-2.89	126.58	132.55
5	O	310	BPH	C4-C3-C5	2.89	120.24	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	283	BCL	CBA-CAA-C2A	-2.87	105.26	113.79
6	L	286	U10	C20-C19-C21	2.85	120.18	115.23
4	M	310	BCL	O1D-CGD-CBD	-2.85	118.90	124.52
5	L	285	BPH	C1-C2-C3	-2.85	121.53	126.20
4	O	309	BCL	CAB-C3B-C2B	-2.84	121.85	127.74
5	L	284	BPH	CMC-C2C-C1C	-2.83	108.51	114.61
4	N	283	BCL	CHA-C4D-ND	-2.82	126.73	132.55
4	N	284	BCL	OBD-CAD-C3D	-2.82	121.83	128.42
5	L	284	BPH	C1B-NB-C4B	-2.81	104.72	108.82
6	M	311	U10	C10-C9-C11	2.80	120.09	115.23
5	N	285	BPH	CMB-C2B-C3B	2.80	130.27	124.68
4	L	283	BCL	C3D-C2D-C1D	2.79	109.64	105.83
5	L	284	BPH	C1C-C2C-C3C	2.78	105.49	102.84
4	N	282	BCL	O2A-CGA-CBA	2.78	120.32	111.83
4	N	282	BCL	CAA-CBA-CGA	2.76	121.05	113.21
4	N	282	BCL	CHA-C4D-ND	-2.75	126.87	132.55
4	M	310	BCL	CED-O2D-CGD	2.75	122.16	115.92
4	N	284	BCL	C1-C2-C3	-2.70	121.77	126.20
4	N	284	BCL	C2B-C1B-NB	2.70	113.13	110.33
4	N	282	BCL	C1D-ND-C4D	-2.70	104.42	106.31
6	M	311	U10	C50-C49-C51	2.70	119.91	115.23
4	O	309	BCL	CED-O2D-CGD	2.69	122.01	115.92
4	L	283	BCL	C4-C3-C5	2.68	119.88	115.23
4	M	310	BCL	CAC-C3C-C4C	-2.68	106.64	112.58
5	N	285	BPH	C1B-NB-C4B	-2.67	104.92	108.82
4	M	310	BCL	CHA-C4D-ND	-2.66	127.06	132.55
6	L	286	U10	C40-C39-C41	2.66	119.84	115.23
4	N	283	BCL	C3D-C2D-C1D	2.65	109.45	105.83
4	L	282	BCL	CED-O2D-CGD	2.65	121.92	115.92
6	O	311	U10	C35-C34-C36	2.64	119.82	115.23
6	L	286	U10	C45-C44-C46	2.64	119.81	115.23
5	O	310	BPH	CMB-C2B-C3B	2.62	129.92	124.68
5	O	310	BPH	CMC-C2C-C1C	-2.62	108.96	114.61
4	N	283	BCL	O2A-CGA-CBA	2.61	119.80	111.83
4	O	309	BCL	C3D-C2D-C1D	2.60	109.38	105.83
4	L	283	BCL	C2B-C1B-NB	2.60	113.02	110.33
4	N	284	BCL	C16-C17-C18	2.60	127.52	115.94
4	M	309	BCL	O2A-CGA-CBA	2.60	119.75	111.83
5	L	285	BPH	C2B-C1B-NB	2.59	111.30	109.43
4	M	309	BCL	CAC-C3C-C4C	-2.57	106.88	112.58
4	M	309	BCL	CMB-C2B-C1B	-2.57	121.51	125.42
4	N	283	BCL	C3A-C2A-C1A	2.51	105.10	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	311	U10	C4M-O4-C4	2.51	125.29	116.47
4	L	282	BCL	CBC-CAC-C3C	2.50	118.72	113.41
5	O	310	BPH	C11-C10-C8	2.48	124.22	115.97
4	N	284	BCL	CHB-C4A-NA	2.45	127.94	124.40
5	N	285	BPH	C1-O2A-CGA	2.45	122.59	116.65
4	L	282	BCL	CHA-C4D-ND	-2.45	127.50	132.55
6	L	286	U10	C56-C54-C55	2.44	120.21	114.59
4	N	282	BCL	CHC-C4B-NB	-2.44	120.39	124.05
5	L	284	BPH	O2A-C1-C2	-2.44	98.72	108.11
4	L	283	BCL	CMB-C2B-C3B	2.43	133.34	125.67
4	L	282	BCL	CHA-C1A-NA	-2.43	120.90	126.39
4	N	284	BCL	CHD-C1D-ND	-2.43	121.39	124.80
4	M	310	BCL	C3D-C2D-C1D	2.41	109.11	105.83
6	M	311	U10	C35-C34-C36	2.40	119.40	115.23
5	L	285	BPH	C17-C16-C15	2.40	124.02	113.28
4	L	282	BCL	C7-C6-C5	-2.39	106.89	113.26
4	M	310	BCL	CMB-C2B-C3B	2.35	133.09	125.67
5	L	284	BPH	C3B-C4B-NB	2.35	111.47	108.05
4	L	283	BCL	O2D-CGD-CBD	2.34	115.31	111.23
4	N	284	BCL	C3B-C4B-NB	2.33	112.84	109.76
5	L	284	BPH	CMA-C3A-C2A	-2.33	105.13	114.13
4	L	282	BCL	C4-C3-C5	2.32	119.25	115.23
4	N	283	BCL	O1D-CGD-CBD	-2.32	119.94	124.52
4	M	309	BCL	CAA-CBA-CGA	2.31	119.77	113.21
4	L	283	BCL	CAA-C2A-C3A	-2.31	106.76	113.00
5	L	285	BPH	C12-C11-C10	2.30	123.59	113.28
6	N	286	U10	C40-C39-C41	2.29	119.20	115.23
4	L	283	BCL	CMC-C2C-C3C	-2.29	105.13	113.98
5	O	310	BPH	CED-O2D-CGD	2.29	121.11	115.92
4	N	284	BCL	C4-C3-C5	2.28	119.19	115.23
4	M	310	BCL	CMC-C2C-C1C	-2.28	105.64	111.77
4	N	283	BCL	C2A-C1A-CHA	2.28	127.82	123.87
4	O	309	BCL	CHA-C1A-NA	-2.28	121.23	126.39
4	O	309	BCL	CHA-C4D-ND	-2.27	127.86	132.55
4	N	283	BCL	O2A-C1-C2	2.27	116.83	108.11
5	O	310	BPH	C11-C12-C13	2.26	123.49	115.97
4	N	284	BCL	C2A-C3A-C4A	2.25	105.51	101.87
4	L	282	BCL	CMB-C2B-C1B	-2.25	121.99	125.42
4	N	283	BCL	CAA-C2A-C3A	-2.25	106.92	113.00
4	L	283	BCL	C1-C2-C3	-2.24	122.52	126.20
4	N	284	BCL	CHC-C4B-NB	-2.23	120.71	124.05
4	L	282	BCL	CHC-C4B-NB	-2.23	120.71	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	309	BCL	O2A-C1-C2	2.22	116.65	108.11
4	L	282	BCL	CAA-C2A-C3A	-2.21	107.03	113.00
4	L	282	BCL	C3C-C2C-C1C	2.21	105.43	101.87
4	M	310	BCL	C7-C6-C5	-2.20	107.40	113.26
4	L	282	BCL	C1-C2-C3	-2.20	122.59	126.20
6	N	286	U10	C17-C16-C14	2.20	120.46	113.19
6	L	286	U10	C15-C14-C16	2.19	119.04	115.23
4	O	309	BCL	CMD-C2D-C3D	-2.19	122.66	127.69
4	L	283	BCL	OBD-CAD-C3D	-2.19	123.30	128.42
4	L	283	BCL	C12-C11-C10	-2.19	103.49	113.28
4	M	310	BCL	CHA-C1A-NA	-2.18	121.46	126.39
4	L	282	BCL	CMC-C2C-C3C	-2.17	105.60	113.98
4	N	284	BCL	CHA-C1A-NA	-2.17	121.48	126.39
5	L	284	BPH	CAA-C2A-C3A	-2.16	107.15	113.00
4	N	283	BCL	CMA-C3A-C4A	-2.16	105.97	111.77
6	O	311	U10	C3M-O3-C3	2.16	124.06	116.47
4	M	310	BCL	C2A-C1A-CHA	2.16	127.61	123.87
6	L	286	U10	C1M-C1-C6	-2.14	120.93	124.45
5	N	285	BPH	CBA-CAA-C2A	2.14	120.07	113.78
5	L	285	BPH	CBA-CAA-C2A	2.14	120.07	113.78
4	N	283	BCL	CHD-C1D-ND	-2.13	121.80	124.80
5	L	285	BPH	CMB-C2B-C3B	2.13	128.93	124.68
5	L	285	BPH	CMA-C3A-C4A	-2.13	110.03	114.61
6	O	311	U10	C50-C49-C51	2.12	118.91	115.23
4	M	309	BCL	CED-O2D-CGD	2.12	120.73	115.92
4	N	283	BCL	OBB-CAB-CBB	-2.12	115.03	119.77
5	L	285	BPH	C2D-C1D-ND	2.11	110.95	109.43
4	N	284	BCL	CMC-C2C-C1C	-2.11	106.11	111.77
5	O	310	BPH	C14-C13-C12	2.10	118.77	111.27
4	M	309	BCL	C2A-C1A-CHA	2.10	127.51	123.87
4	M	309	BCL	CMB-C2B-C3B	2.10	132.29	125.67
6	M	311	U10	C7-C6-C1	-2.09	121.30	124.89
4	N	284	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
4	L	283	BCL	C16-C15-C13	-2.09	109.03	115.97
5	L	285	BPH	C1C-C2C-C3C	2.08	104.82	102.84
6	O	311	U10	C56-C54-C55	2.07	119.35	114.59
6	O	311	U10	C20-C19-C21	2.07	118.82	115.23
6	O	311	U10	C1-C6-C5	-2.07	117.61	119.62
4	M	310	BCL	C2A-C3A-C4A	2.07	105.21	101.87
5	L	285	BPH	CMC-C2C-C1C	-2.07	110.16	114.61
6	O	311	U10	C15-C14-C16	2.06	118.81	115.23
4	L	283	BCL	CHD-C1D-ND	-2.06	121.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	309	BCL	CMA-C3A-C4A	-2.06	106.24	111.77
6	O	311	U10	C37-C38-C39	-2.06	122.91	127.62
4	N	282	BCL	C2C-C3C-C4C	2.06	104.42	101.34
4	O	309	BCL	C2B-C1B-NB	2.05	112.46	110.33
5	N	285	BPH	C11-C12-C13	2.05	122.78	115.97
6	N	286	U10	C3M-O3-C3	2.05	123.68	116.47
4	N	282	BCL	C2A-C3A-C4A	2.05	105.18	101.87
4	N	282	BCL	OBB-CAB-CBB	-2.05	115.19	119.77
4	M	309	BCL	CHA-C1A-NA	-2.04	121.76	126.39
4	O	309	BCL	CAC-C3C-C4C	-2.04	108.05	112.58
6	O	311	U10	C45-C44-C46	2.04	118.76	115.23
5	L	284	BPH	CED-O2D-CGD	2.04	120.53	115.92
4	N	282	BCL	C3A-C2A-C1A	2.03	104.38	101.34
6	O	311	U10	C4M-O4-C4	2.03	123.60	116.47
4	L	282	BCL	C16-C15-C13	-2.02	109.24	115.97
4	L	283	BCL	CAC-C3C-C4C	-2.02	108.10	112.58
4	O	309	BCL	C4-C3-C5	2.02	118.74	115.23
4	M	309	BCL	C3A-C2A-C1A	2.01	104.35	101.34
4	L	283	BCL	CHC-C4B-NB	-2.01	121.03	124.05
4	N	282	BCL	CHA-C1A-NA	-2.00	121.86	126.39
4	L	283	BCL	CHA-C1A-NA	-2.00	121.86	126.39

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	309	BCL	C13
4	M	309	BCL	C8
4	M	310	BCL	C13
4	M	310	BCL	C8
4	N	282	BCL	C13
4	N	282	BCL	C8
4	O	309	BCL	C8
5	L	284	BPH	C13
5	L	284	BPH	C8
5	L	285	BPH	C8
5	N	285	BPH	C8
5	O	310	BPH	C13

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	283	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	N	283	BCL	CBD-CGD-O2D-CED
4	N	284	BCL	CBD-CGD-O2D-CED
5	N	285	BPH	C4C-C3C-CAC-CBC
5	O	310	BPH	C4C-C3C-CAC-CBC
5	O	310	BPH	C2C-C3C-CAC-CBC
6	N	286	U10	C24-C26-C27-C28
6	N	286	U10	C29-C31-C32-C33
4	N	283	BCL	O1D-CGD-O2D-CED
4	O	309	BCL	O1D-CGD-O2D-CED
4	N	282	BCL	CBD-CGD-O2D-CED
4	O	309	BCL	CBD-CGD-O2D-CED
4	L	283	BCL	O1D-CGD-O2D-CED
4	N	284	BCL	O1D-CGD-O2D-CED
5	L	284	BPH	CBD-CGD-O2D-CED
4	M	309	BCL	C3-C5-C6-C7
4	N	282	BCL	C3-C5-C6-C7
4	M	310	BCL	CBD-CGD-O2D-CED
5	N	285	BPH	CBD-CGD-O2D-CED
4	N	282	BCL	O1D-CGD-O2D-CED
4	M	309	BCL	C4-C3-C5-C6
5	L	284	BPH	C4-C3-C5-C6
6	O	311	U10	C40-C39-C41-C42
4	M	309	BCL	C2-C3-C5-C6
5	L	284	BPH	C2-C3-C5-C6
6	O	311	U10	C38-C39-C41-C42
4	N	283	BCL	CBA-CGA-O2A-C1
4	N	283	BCL	O1A-CGA-O2A-C1
5	L	284	BPH	O1D-CGD-O2D-CED
4	N	283	BCL	C4-C3-C5-C6
4	N	283	BCL	C2-C3-C5-C6
6	L	286	U10	C14-C16-C17-C18
6	M	311	U10	C24-C26-C27-C28
6	M	311	U10	C34-C36-C37-C38
6	M	311	U10	C39-C41-C42-C43
6	M	311	U10	C49-C51-C52-C53
6	N	286	U10	C19-C21-C22-C23
6	N	286	U10	C39-C41-C42-C43
6	N	286	U10	C44-C46-C47-C48
6	N	286	U10	C49-C51-C52-C53
6	O	311	U10	C14-C16-C17-C18
6	O	311	U10	C39-C41-C42-C43
5	L	285	BPH	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	M	309	BCL	O1A-CGA-O2A-C1
4	M	309	BCL	CBA-CGA-O2A-C1
4	M	310	BCL	O1D-CGD-O2D-CED
5	L	285	BPH	C14-C13-C15-C16
5	O	310	BPH	CBD-CGD-O2D-CED
5	N	285	BPH	O1D-CGD-O2D-CED
4	N	283	BCL	C15-C16-C17-C18
5	L	285	BPH	C8-C10-C11-C12
6	L	286	U10	C19-C21-C22-C23
6	O	311	U10	C24-C26-C27-C28
4	L	283	BCL	C13-C15-C16-C17
4	L	282	BCL	C13-C15-C16-C17
5	O	310	BPH	O1A-CGA-O2A-C1
5	O	310	BPH	CBA-CGA-O2A-C1
4	M	309	BCL	C15-C16-C17-C18
5	L	285	BPH	C5-C6-C7-C8
6	N	286	U10	C40-C39-C41-C42
6	L	286	U10	C39-C41-C42-C43
6	M	311	U10	C14-C16-C17-C18
5	N	285	BPH	C3-C5-C6-C7
4	N	284	BCL	C3-C5-C6-C7
5	L	284	BPH	O1A-CGA-O2A-C1
4	N	283	BCL	C5-C6-C7-C8
5	L	285	BPH	O1D-CGD-O2D-CED
4	N	283	BCL	C3A-C2A-CAA-CBA
5	L	284	BPH	CBA-CGA-O2A-C1
6	N	286	U10	C9-C11-C12-C13
4	L	283	BCL	C3-C5-C6-C7
6	N	286	U10	C38-C39-C41-C42
6	N	286	U10	C20-C19-C21-C22
6	L	286	U10	C49-C51-C52-C53
6	M	311	U10	C44-C46-C47-C48
5	N	285	BPH	C2C-C3C-CAC-CBC
6	N	286	U10	C18-C19-C21-C22
5	O	310	BPH	O1D-CGD-O2D-CED
4	N	283	BCL	C1A-C2A-CAA-CBA
5	O	310	BPH	C3-C5-C6-C7
4	M	309	BCL	C12-C13-C15-C16
6	N	286	U10	C30-C29-C31-C32
6	M	311	U10	C33-C34-C36-C37
6	N	286	U10	C28-C29-C31-C32
4	L	283	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	L	282	BCL	C2A-CAA-CBA-CGA
4	N	284	BCL	C15-C16-C17-C18
5	N	285	BPH	C11-C10-C8-C7
6	M	311	U10	C35-C34-C36-C37
6	M	311	U10	C48-C49-C51-C52
5	N	285	BPH	C4-C3-C5-C6
6	M	311	U10	C50-C49-C51-C52
5	O	310	BPH	C8-C10-C11-C12
6	L	286	U10	C9-C11-C12-C13
6	N	286	U10	C1-C6-C7-C8
5	N	285	BPH	C2-C3-C5-C6
6	N	286	U10	C5-C6-C7-C8
5	L	285	BPH	C2C-C3C-CAC-CBC
4	M	309	BCL	C8-C10-C11-C12
4	N	282	BCL	C1A-C2A-CAA-CBA
6	L	286	U10	C45-C44-C46-C47
5	L	285	BPH	C12-C13-C15-C16
5	O	310	BPH	C10-C11-C12-C13
6	N	286	U10	C25-C24-C26-C27
6	O	311	U10	C25-C24-C26-C27
4	O	309	BCL	CAD-CBD-CGD-O2D
4	O	309	BCL	CAD-CBD-CGD-O1D
4	N	284	BCL	C13-C15-C16-C17
6	M	311	U10	C5-C4-O4-C4M
6	O	311	U10	C29-C31-C32-C33
6	L	286	U10	C50-C49-C51-C52
6	N	286	U10	C45-C44-C46-C47
4	M	309	BCL	C14-C13-C15-C16
6	M	311	U10	C30-C29-C31-C32
6	O	311	U10	C23-C24-C26-C27
6	L	286	U10	C12-C11-C9-C10
6	O	311	U10	C20-C19-C21-C22
5	L	284	BPH	C2C-C3C-CAC-CBC
6	N	286	U10	C43-C44-C46-C47
6	L	286	U10	C26-C27-C28-C29
6	L	286	U10	C12-C11-C9-C8
6	M	311	U10	C28-C29-C31-C32
6	M	311	U10	C25-C24-C26-C27
6	L	286	U10	C48-C49-C51-C52
6	O	311	U10	C18-C19-C21-C22
6	L	286	U10	C43-C44-C46-C47
6	N	286	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
6	O	311	U10	C5-C4-O4-C4M
4	M	310	BCL	C14-C13-C15-C16
4	L	283	BCL	C2A-CAA-CBA-CGA
5	O	310	BPH	C11-C12-C13-C14
4	L	282	BCL	C2-C1-O2A-CGA
4	M	309	BCL	C2A-CAA-CBA-CGA
4	M	309	BCL	C13-C15-C16-C17
5	L	284	BPH	C3-C5-C6-C7
6	M	311	U10	C45-C44-C46-C47
5	L	285	BPH	C11-C10-C8-C9
6	O	311	U10	C45-C44-C46-C47
4	N	282	BCL	C2A-CAA-CBA-CGA
6	L	286	U10	C40-C39-C41-C42
4	N	282	BCL	C11-C10-C8-C9
5	N	285	BPH	C11-C10-C8-C9
5	L	284	BPH	C4C-C3C-CAC-CBC
5	L	285	BPH	C4C-C3C-CAC-CBC
4	N	283	BCL	C2-C1-O2A-CGA
6	O	311	U10	C16-C17-C18-C19
5	L	285	BPH	CAA-CBA-CGA-O2A

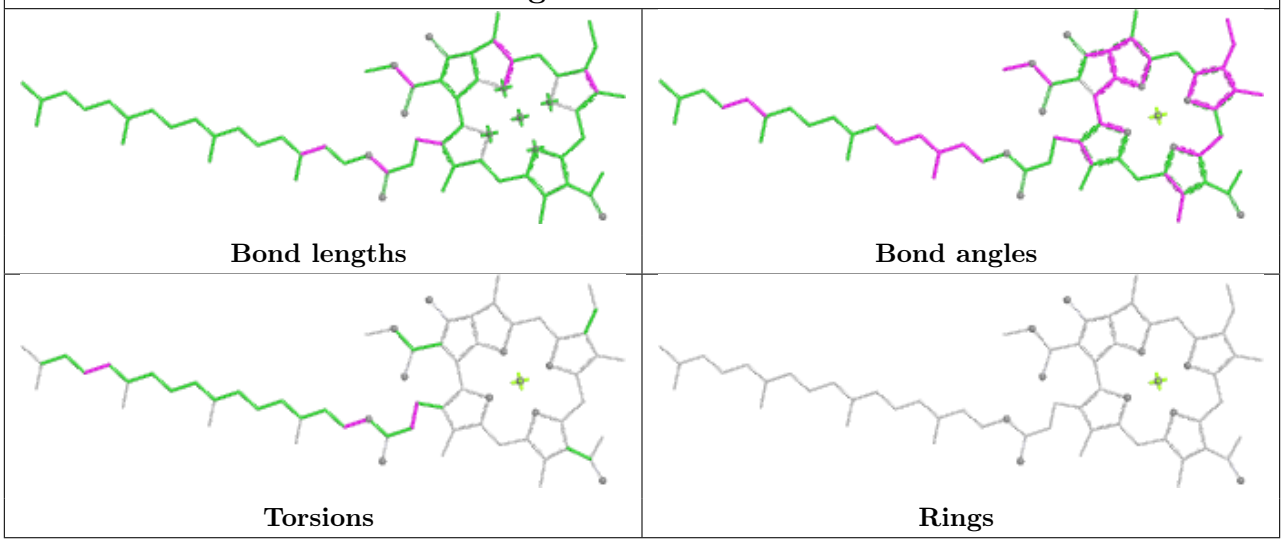
There are no ring outliers.

16 monomers are involved in 68 short contacts:

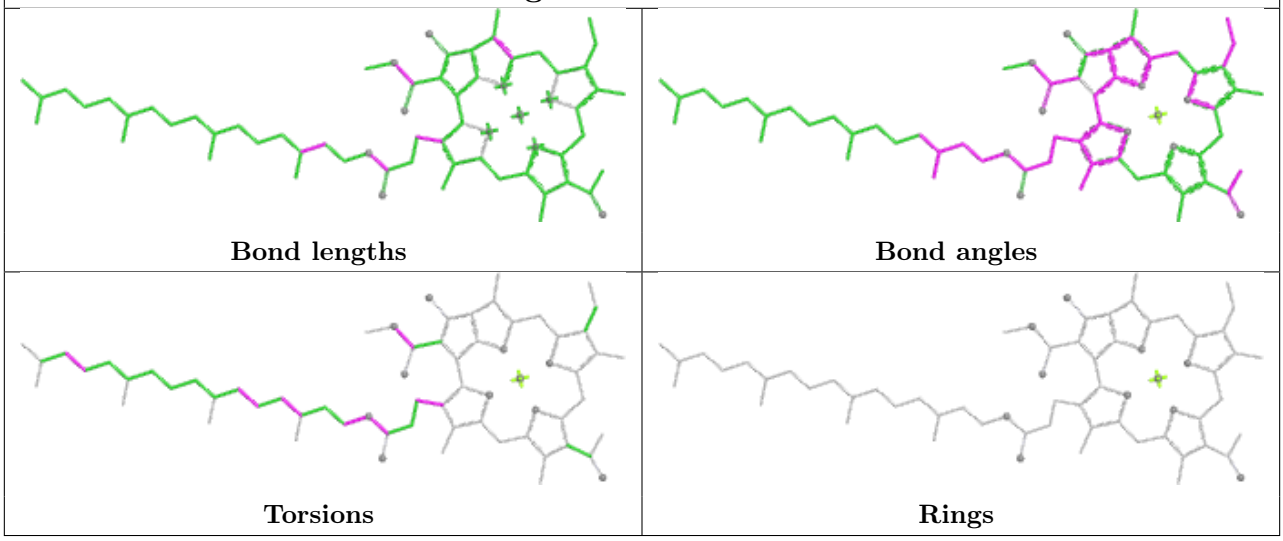
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	282	BCL	6	0
4	N	283	BCL	5	0
6	M	311	U10	1	0
6	N	286	U10	6	0
6	O	311	U10	3	0
4	M	310	BCL	4	0
4	N	284	BCL	5	0
4	L	283	BCL	4	0
5	L	285	BPH	9	0
4	O	309	BCL	7	0
5	N	285	BPH	7	0
4	M	309	BCL	7	0
5	O	310	BPH	4	0
4	N	282	BCL	8	0
5	L	284	BPH	2	0
6	L	286	U10	4	0

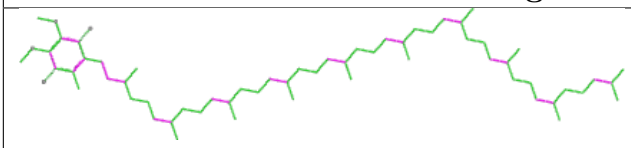
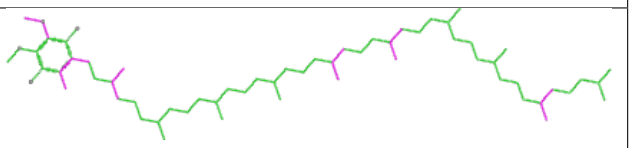
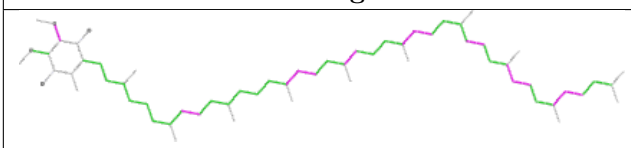
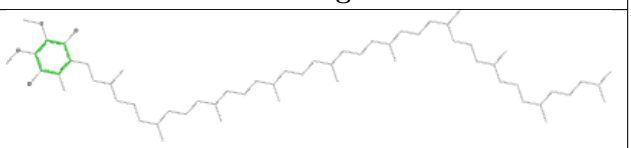
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

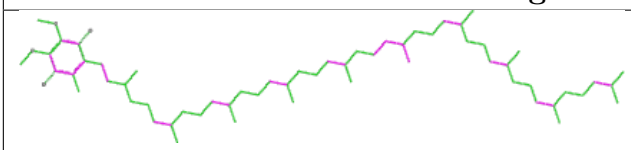
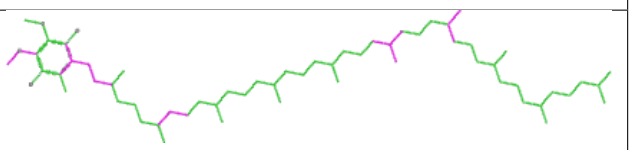
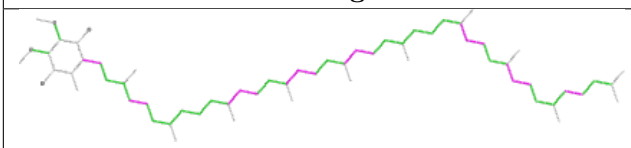
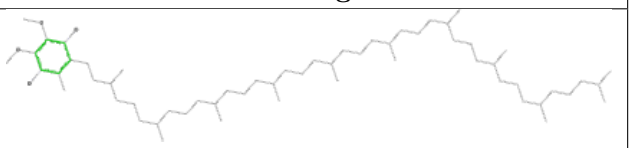
Ligand BCL L 282

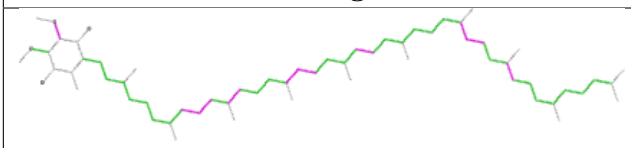
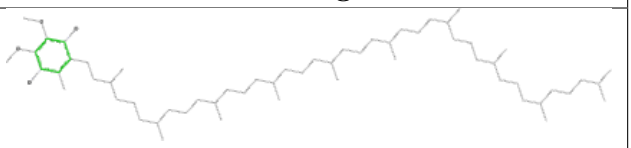


Ligand BCL N 283

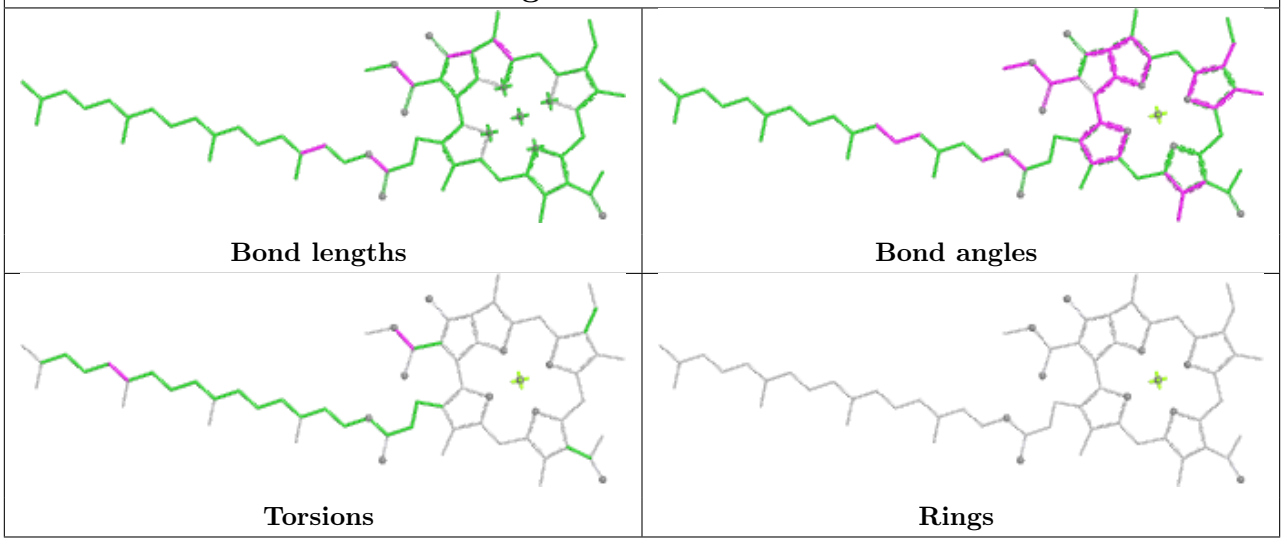


Ligand U10 M 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

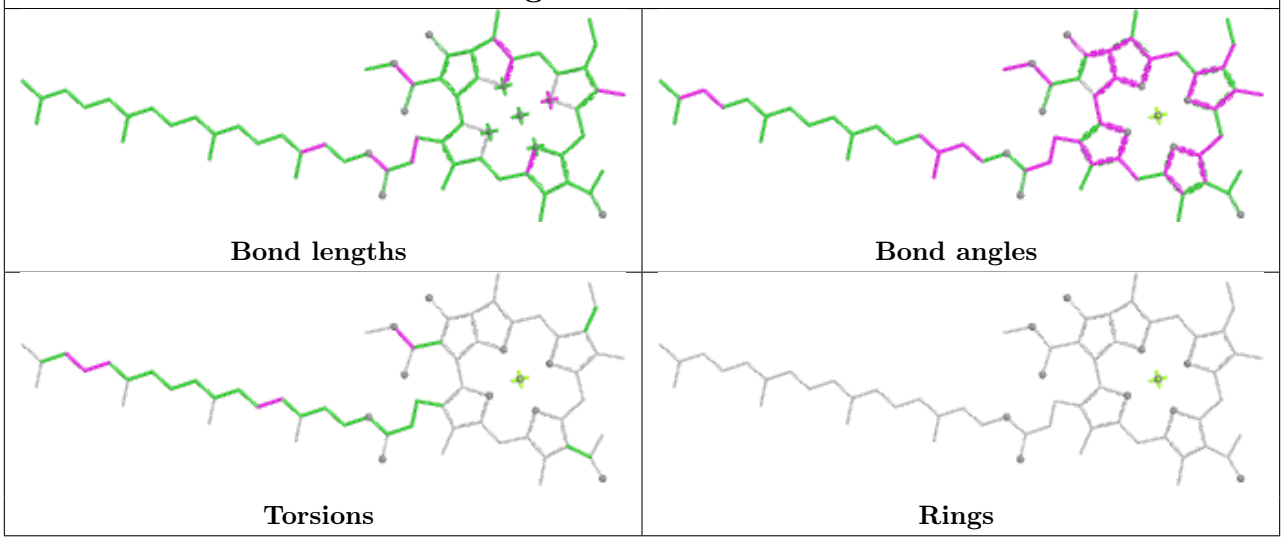
Ligand U10 N 286	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U10 O 311	
Bond lengths	Bond angles
 Torsions	 Rings

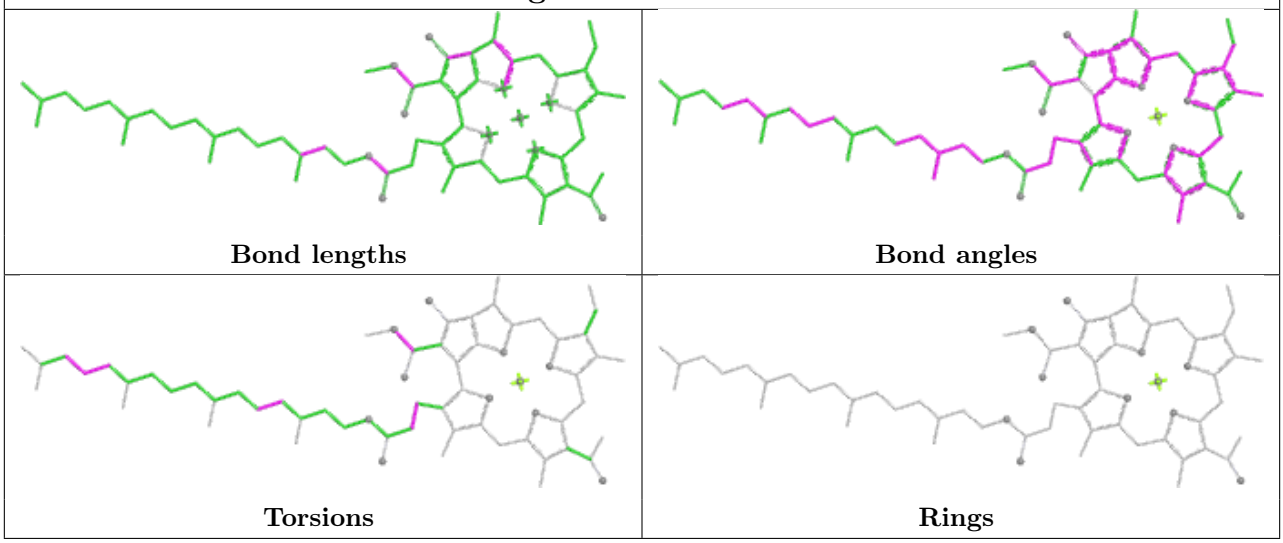
Ligand BCL M 310



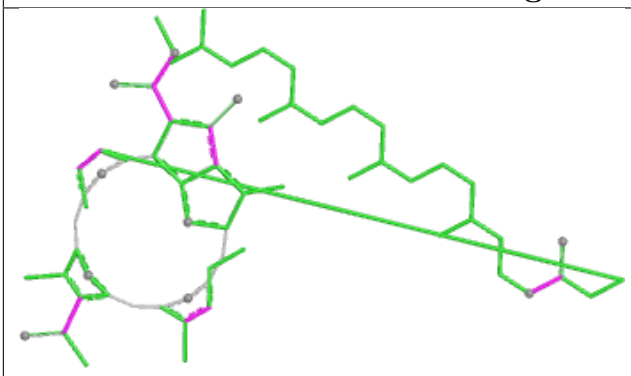
Ligand BCL N 284



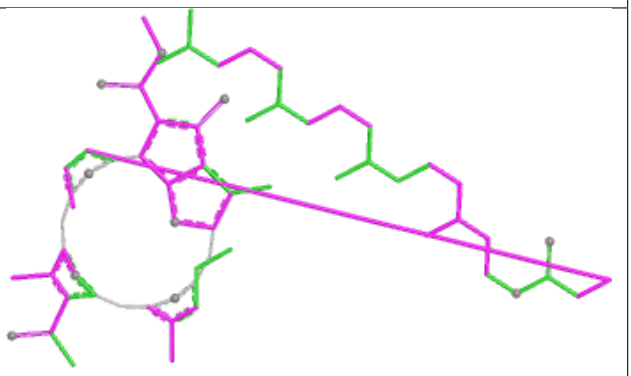
Ligand BCL L 283



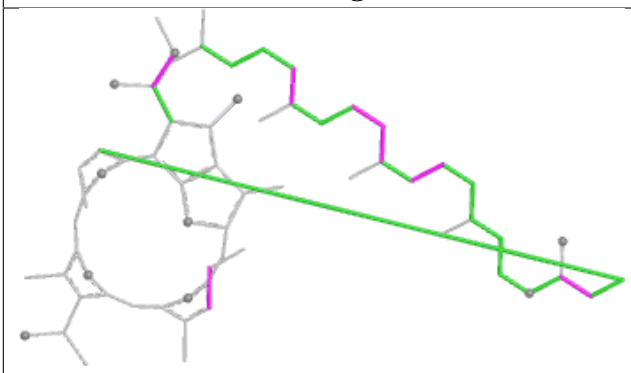
Ligand BPH L 285



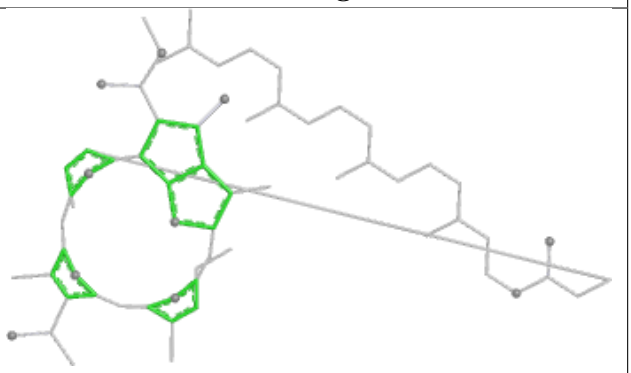
Bond lengths



Bond angles

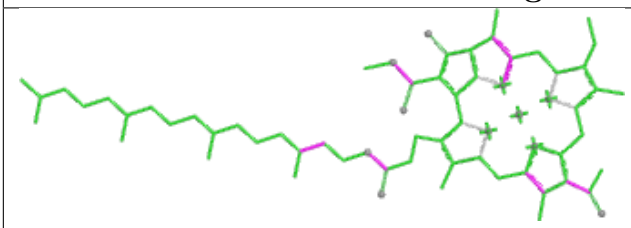


Torsions

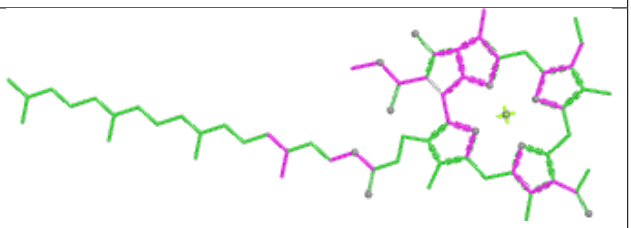


Rings

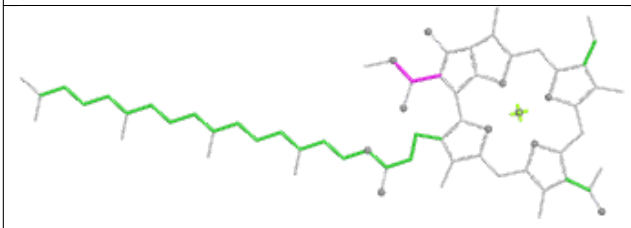
Ligand BCL O 309



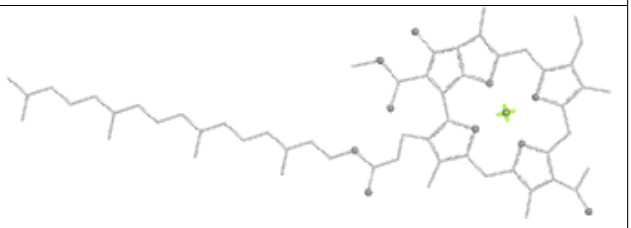
Bond lengths



Bond angles

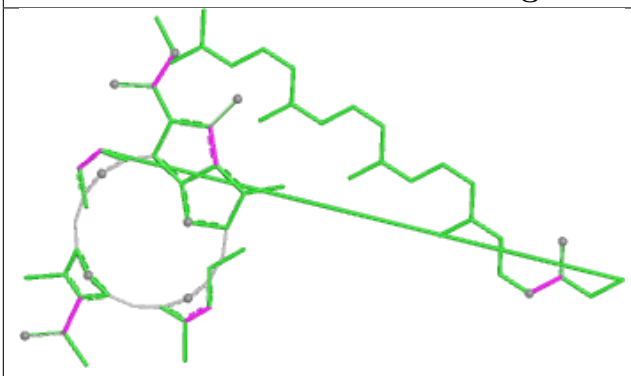


Torsions



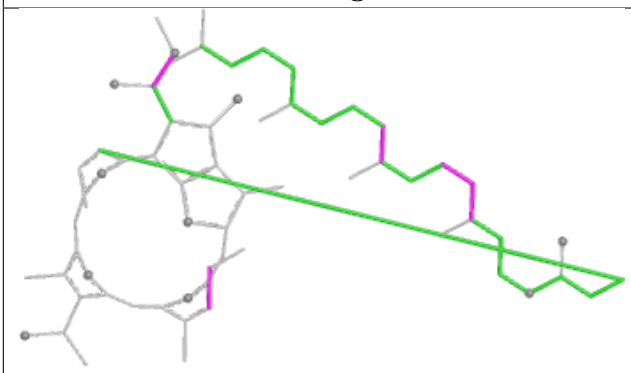
Rings

Ligand BPH N 285

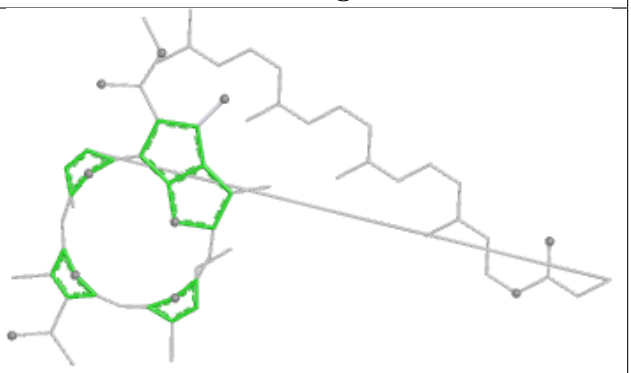


Bond lengths

Bond angles

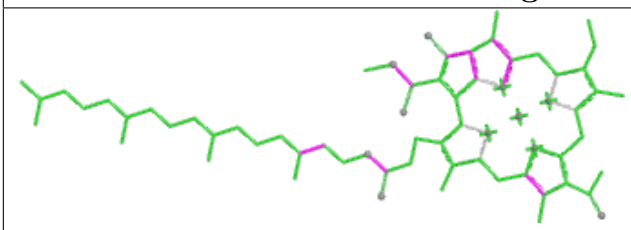


Torsions

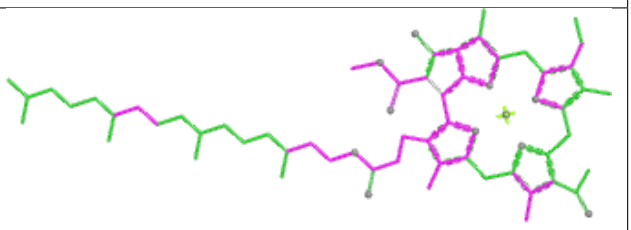


Rings

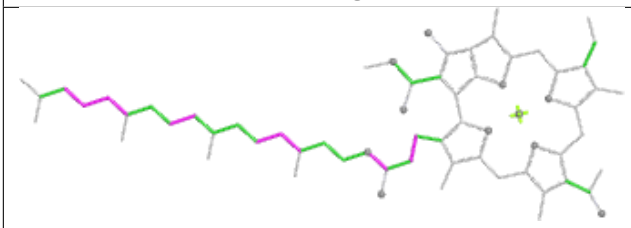
Ligand BCL M 309



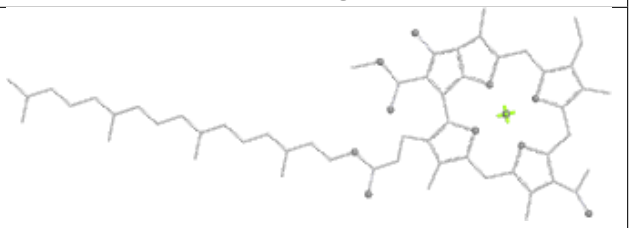
Bond lengths



Bond angles

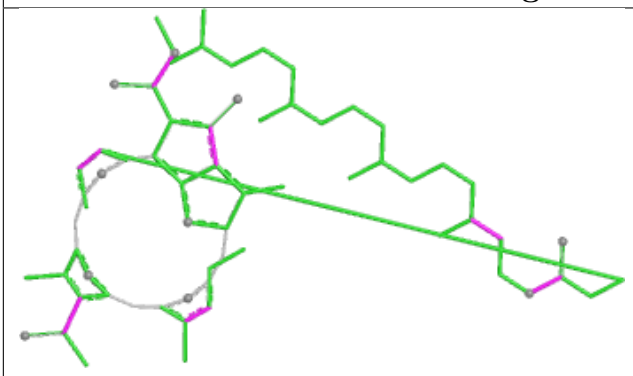


Torsions

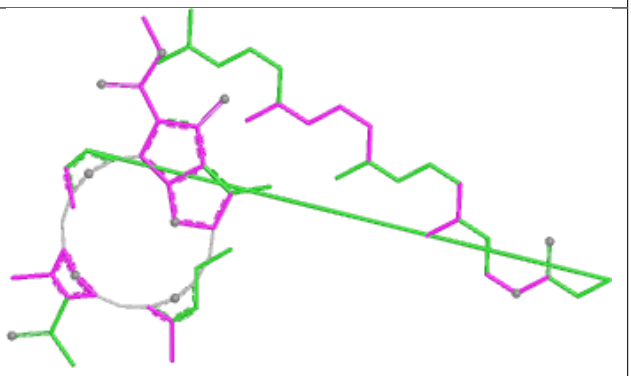


Rings

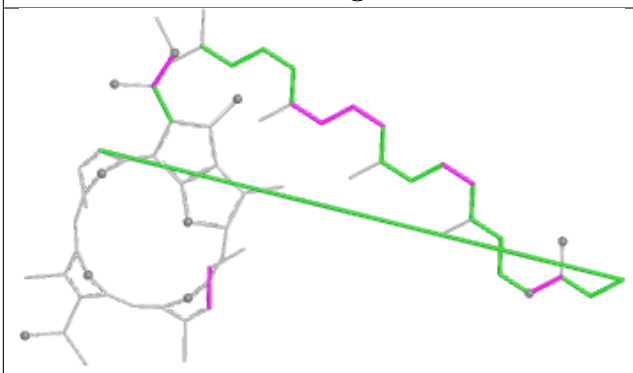
Ligand BPH O 310



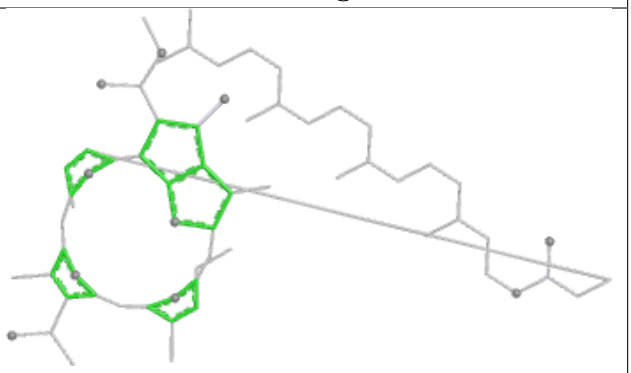
Bond lengths



Bond angles

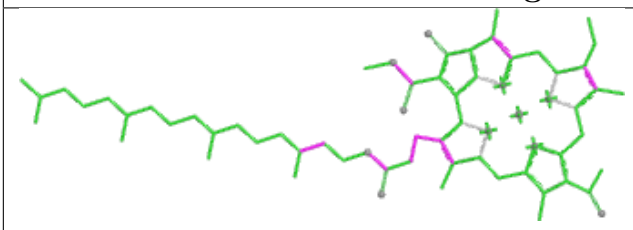


Torsions



Rings

Ligand BCL N 282



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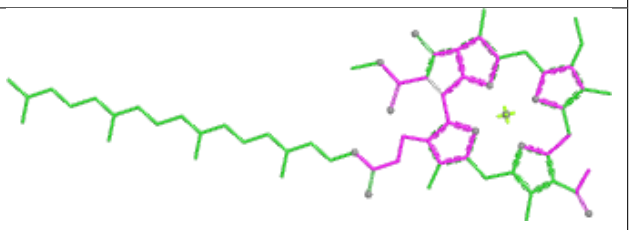
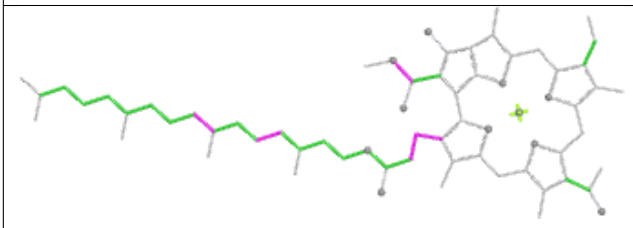
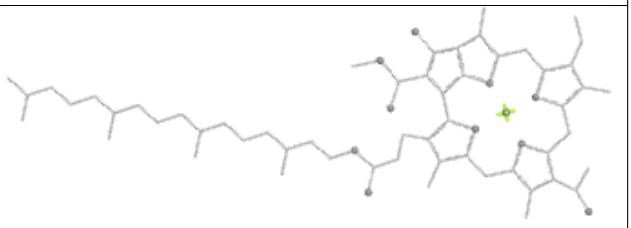


Bond angles

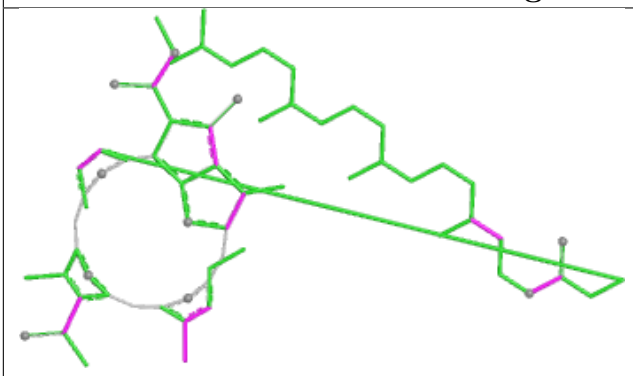


Torsions



Rings

Ligand BPH L 284



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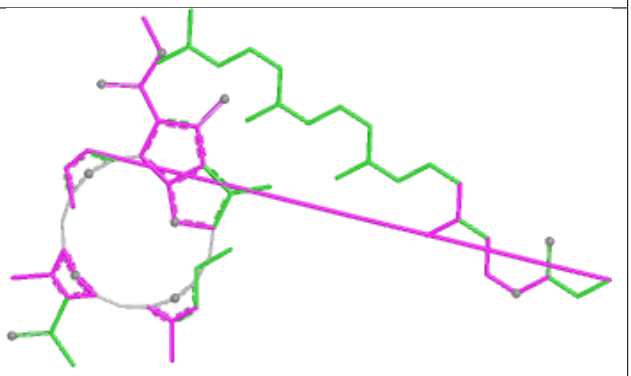
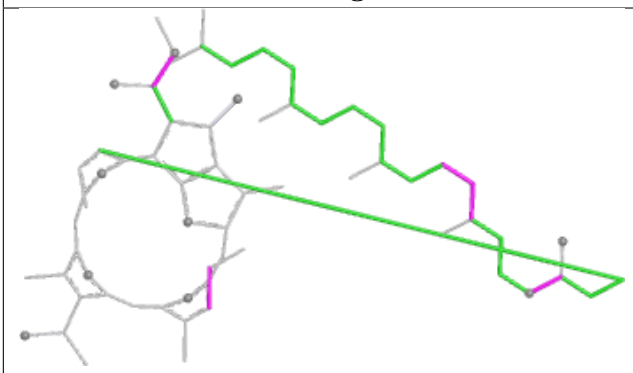
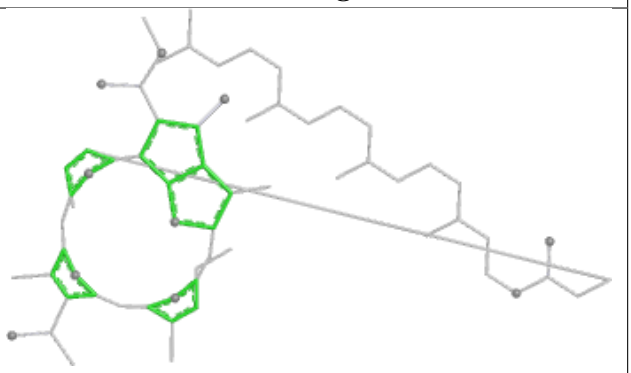


Bond angles

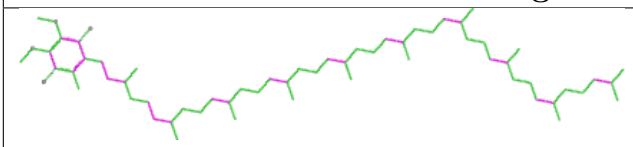


Torsions



Rings

Ligand U10 L 286



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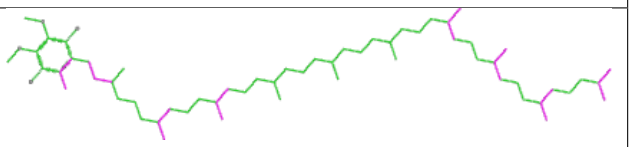
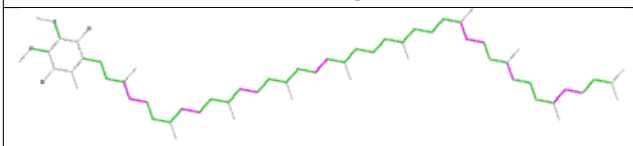
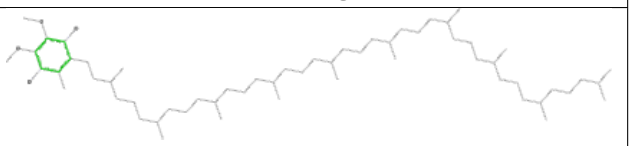


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.