



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:32 pm BST

PDB ID : 1AIJ
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER
SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE
Authors : Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Fe-
her, G.
Deposited on : 1997-04-18
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

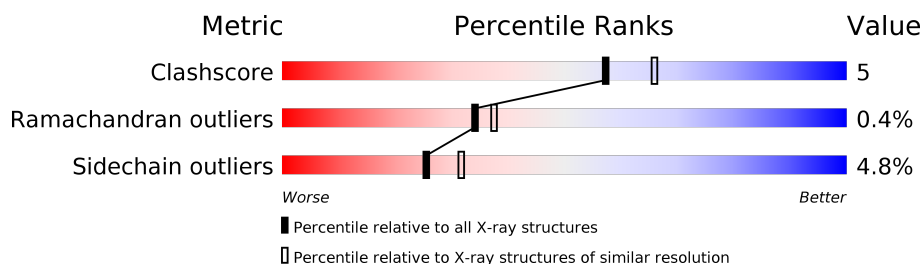
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14393 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
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
1	R	281	Total	C	N	O	S	4	0	0
			2232	1507	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2404	1605	393	396	10			
2	S	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

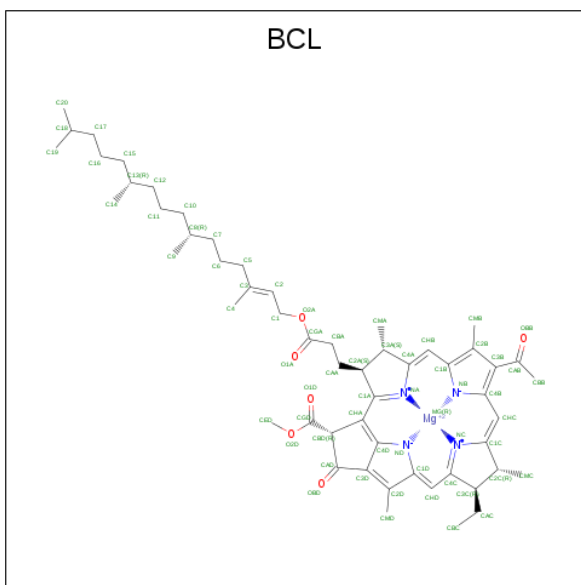
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	4	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

There are 2 discrepancies between the modelled and reference sequences:

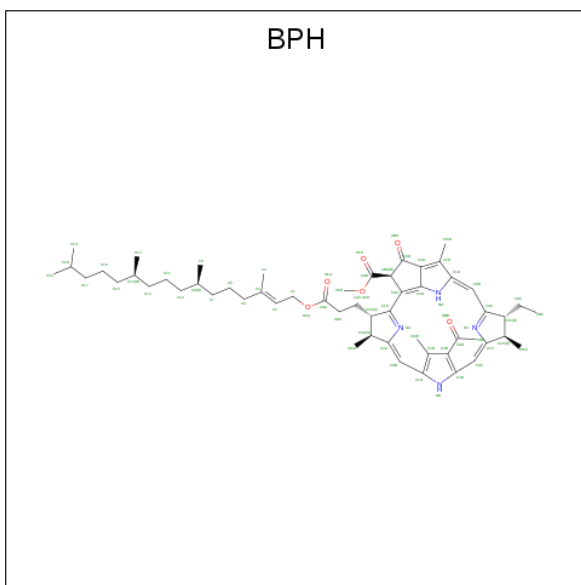
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
T	8	GLN	GLY	conflict	UNP P11846

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



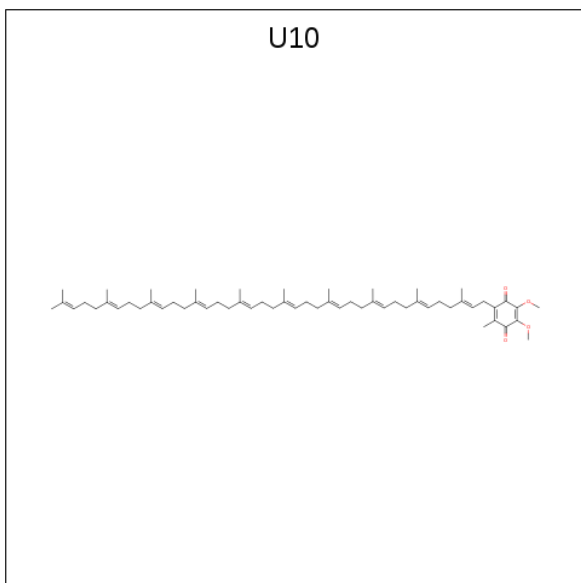
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	S	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			51	41	4	6		
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	R	1	Total	C	N	O	0	0
			65	55	4	6		
5	S	1	Total	C	N	O	0	0
			52	42	4	6		

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

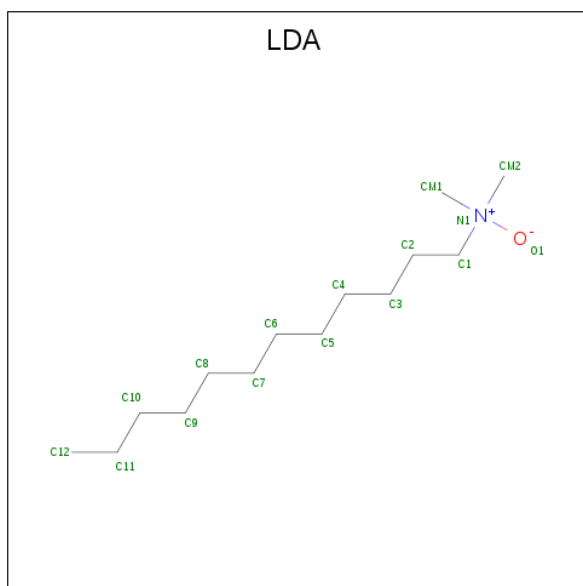


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			44	40	4		
6	M	1	Total	C	O	0	0
			38	34	4		
6	R	1	Total	C	O	0	0
			18	14	4		
6	S	1	Total	C	O	0	0
			32	28	4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



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

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

- Molecule 9 is water.

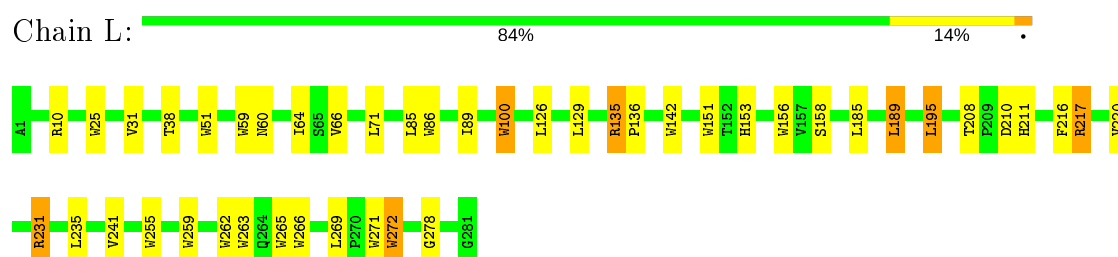
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	67	Total	O	0	0
			67	67		
9	M	91	Total	O	0	0
			91	91		
9	H	105	Total	O	0	0
			105	105		
9	R	56	Total	O	0	0
			56	56		
9	S	85	Total	O	0	0
			85	85		
9	T	64	Total	O	0	0
			64	64		

3 Residue-property plots

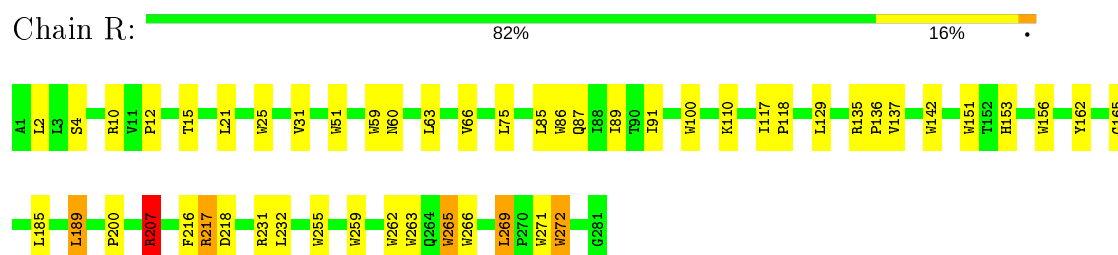
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

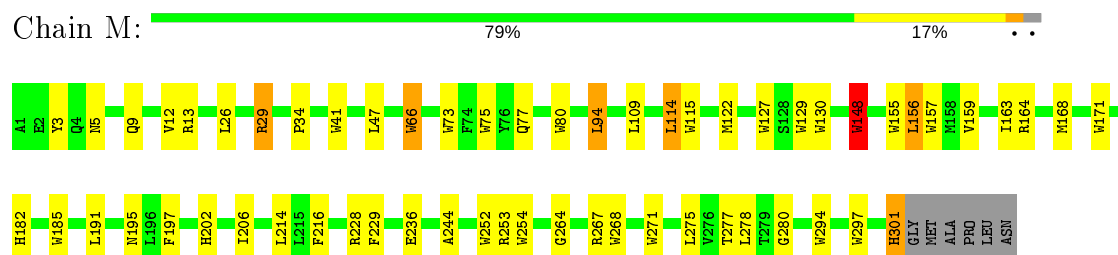
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



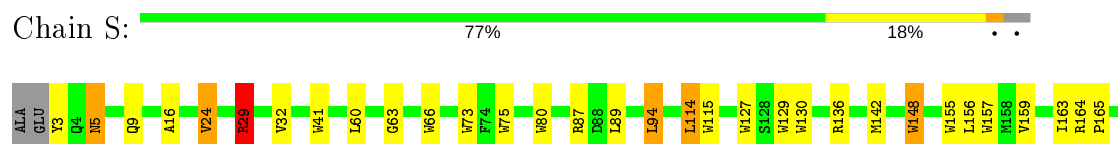
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

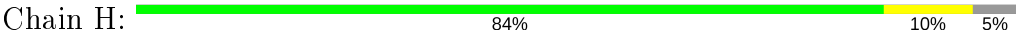


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

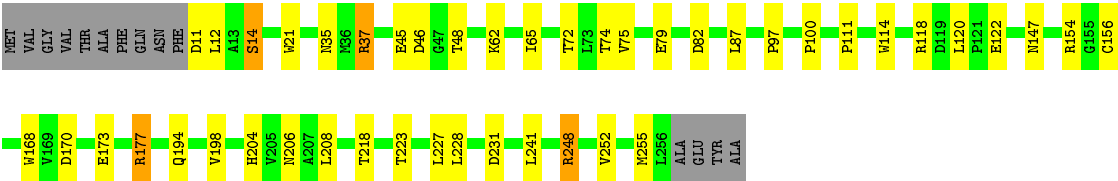




● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



4 Data and refinement statistics

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	140.08 Å 140.08 Å 271.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14393	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, LDA, FE2, U10

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	0.78	0/2320	1.48	59/3175 (1.9%)
1	R	0.78	0/2320	1.45	53/3175 (1.7%)
2	M	0.79	0/2496	1.51	67/3408 (2.0%)
2	S	0.80	0/2482	1.54	74/3389 (2.2%)
3	H	0.66	0/1917	1.21	13/2608 (0.5%)
3	T	0.66	0/1917	1.20	13/2608 (0.5%)
All	All	0.75	0/13452	1.42	279/18363 (1.5%)

There are no bond length outliers.

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	231	ARG	NE-CZ-NH1	9.91	125.26	120.30
3	H	248	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	L	10	ARG	NE-CZ-NH1	9.18	124.89	120.30
2	S	41	TRP	CD1-CG-CD2	9.09	113.57	106.30
3	T	248	ARG	NE-CZ-NH1	8.90	124.75	120.30
2	M	171	TRP	CD1-CG-CD2	8.79	113.33	106.30
2	M	80	TRP	CD1-CG-CD2	8.73	113.28	106.30
2	S	268	TRP	CD1-CG-CD2	8.69	113.25	106.30
2	M	157	TRP	CD1-CG-CD2	8.67	113.24	106.30
2	S	271	TRP	CD1-CG-CD2	8.60	113.18	106.30
2	M	41	TRP	CD1-CG-CD2	8.60	113.18	106.30
2	M	148	TRP	CE2-CD2-CG	-8.57	100.45	107.30
1	R	59	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	L	59	TRP	CD1-CG-CD2	8.49	113.09	106.30
3	T	21	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	L	25	TRP	CD1-CG-CD2	8.46	113.06	106.30
1	L	266	TRP	CD1-CG-CD2	8.38	113.01	106.30
1	L	151	TRP	CD1-CG-CD2	8.38	113.00	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	171	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	L	255	TRP	CD1-CG-CD2	8.30	112.94	106.30
3	H	168	TRP	CD1-CG-CD2	8.30	112.94	106.30
2	M	297	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	R	255	TRP	CD1-CG-CD2	8.29	112.93	106.30
2	M	75	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	L	271	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	S	157	TRP	CD1-CG-CD2	8.25	112.90	106.30
3	T	168	TRP	CD1-CG-CD2	8.24	112.89	106.30
3	T	114	TRP	CD1-CG-CD2	8.23	112.89	106.30
2	M	115	TRP	CD1-CG-CD2	8.22	112.88	106.30
3	H	21	TRP	CD1-CG-CD2	8.20	112.86	106.30
2	S	155	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	R	271	TRP	CD1-CG-CD2	8.19	112.85	106.30
2	M	185	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	L	259	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	S	148	TRP	CE2-CD2-CG	-8.18	100.76	107.30
2	M	129	TRP	CD1-CG-CD2	8.14	112.81	106.30
2	M	73	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	R	142	TRP	CD1-CG-CD2	8.11	112.79	106.30
2	S	115	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	L	51	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	L	272	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	R	262	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	L	59	TRP	CE2-CD2-CG	-8.09	100.83	107.30
2	S	297	TRP	CD1-CG-CD2	8.09	112.77	106.30
2	M	171	TRP	CE2-CD2-CG	-8.09	100.83	107.30
2	M	80	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	R	25	TRP	CD1-CG-CD2	8.04	112.73	106.30
3	H	248	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	R	266	TRP	CD1-CG-CD2	8.02	112.71	106.30
2	M	148	TRP	CG-CD2-CE3	8.01	141.11	133.90
1	L	100	TRP	CD1-CG-CD2	8.01	112.70	106.30
2	M	130	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	L	262	TRP	CD1-CG-CD2	7.99	112.70	106.30
1	R	151	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	L	86	TRP	CD1-CG-CD2	7.99	112.69	106.30
2	S	294	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	R	259	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	L	265	TRP	CD1-CG-CD2	7.96	112.67	106.30
2	M	271	TRP	CD1-CG-CD2	7.96	112.67	106.30
2	S	75	TRP	CD1-CG-CD2	7.94	112.65	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	252	TRP	CD1-CG-CD2	7.93	112.65	106.30
2	S	41	TRP	CE2-CD2-CG	-7.93	100.95	107.30
2	M	41	TRP	CE2-CD2-CG	-7.93	100.95	107.30
2	M	155	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	R	86	TRP	CD1-CG-CD2	7.92	112.64	106.30
2	S	252	TRP	CD1-CG-CD2	7.92	112.64	106.30
2	S	80	TRP	CD1-CG-CD2	7.91	112.62	106.30
1	L	142	TRP	CE2-CD2-CG	-7.90	100.98	107.30
2	S	66	TRP	CD1-CG-CD2	7.90	112.62	106.30
2	S	127	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	R	59	TRP	CE2-CD2-CG	-7.88	101.00	107.30
3	H	114	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	L	142	TRP	CD1-CG-CD2	7.87	112.59	106.30
3	T	21	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	L	266	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	S	268	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	M	294	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	R	263	TRP	CD1-CG-CD2	7.82	112.55	106.30
2	S	130	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	L	156	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	L	25	TRP	CE2-CD2-CG	-7.76	101.09	107.30
2	S	171	TRP	CE2-CD2-CG	-7.76	101.09	107.30
2	S	73	TRP	CD1-CG-CD2	7.74	112.49	106.30
2	S	129	TRP	CD1-CG-CD2	7.74	112.49	106.30
2	S	80	TRP	CE2-CD2-CG	-7.73	101.11	107.30
2	M	73	TRP	CE2-CD2-CG	-7.73	101.12	107.30
2	M	66	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	R	259	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	R	142	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	L	151	TRP	CE2-CD2-CG	-7.69	101.15	107.30
2	M	268	TRP	CD1-CG-CD2	7.68	112.45	106.30
2	M	148	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	L	263	TRP	CD1-CG-CD2	7.67	112.44	106.30
2	M	75	TRP	CE2-CD2-CG	-7.65	101.18	107.30
3	H	21	TRP	CE2-CD2-CG	-7.65	101.18	107.30
2	S	155	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	R	25	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	R	231	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	L	265	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	L	271	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	L	255	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	R	265	TRP	CD1-CG-CD2	7.58	112.36	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	129	TRP	CE2-CD2-CG	-7.57	101.24	107.30
2	S	148	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	R	51	TRP	CD1-CG-CD2	7.56	112.35	106.30
2	M	252	TRP	CE2-CD2-CG	-7.56	101.25	107.30
2	S	73	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	S	75	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	R	266	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	S	129	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	R	255	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	R	263	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	S	294	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	S	271	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	M	157	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	R	271	TRP	CE2-CD2-CG	-7.53	101.27	107.30
2	M	155	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	L	259	TRP	CE2-CD2-CG	-7.52	101.28	107.30
2	M	185	TRP	CE2-CD2-CG	-7.52	101.29	107.30
2	M	268	TRP	CE2-CD2-CG	-7.50	101.30	107.30
2	S	185	TRP	CD1-CG-CD2	7.50	112.30	106.30
2	M	254	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	R	151	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	L	100	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	L	51	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	L	86	TRP	CE2-CD2-CG	-7.45	101.34	107.30
3	H	168	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	R	272	TRP	CD1-CG-CD2	7.43	112.25	106.30
3	T	114	TRP	CE2-CD2-CG	-7.43	101.36	107.30
2	S	66	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	R	86	TRP	CE2-CD2-CG	-7.41	101.37	107.30
2	S	297	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	R	156	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	R	265	TRP	CE2-CD2-CG	-7.37	101.40	107.30
2	M	297	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	L	262	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	R	262	TRP	CE2-CD2-CG	-7.34	101.43	107.30
2	M	130	TRP	CE2-CD2-CG	-7.33	101.43	107.30
2	S	127	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	M	66	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	R	10	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	S	252	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	R	100	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	R	100	TRP	CD1-CG-CD2	7.28	112.12	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	271	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	M	254	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	L	263	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	S	115	TRP	CE2-CD2-CG	-7.24	101.51	107.30
2	M	115	TRP	CE2-CD2-CG	-7.24	101.51	107.30
2	M	294	TRP	CE2-CD2-CG	-7.21	101.53	107.30
3	H	114	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	R	51	TRP	CE2-CD2-CG	-7.21	101.53	107.30
2	S	185	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	S	130	TRP	CE2-CD2-CG	-7.18	101.55	107.30
3	T	168	TRP	CE2-CD2-CG	-7.18	101.56	107.30
2	S	29	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	L	156	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	L	272	TRP	CE2-CD2-CG	-7.13	101.60	107.30
2	S	148	TRP	CG-CD2-CE3	7.12	140.31	133.90
2	M	127	TRP	CE2-CD2-CG	-7.09	101.63	107.30
2	M	148	TRP	CB-CG-CD1	-7.08	117.80	127.00
2	S	157	TRP	CE2-CD2-CG	-7.08	101.64	107.30
2	S	254	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	M	127	TRP	CD1-CG-CD2	7.04	111.93	106.30
2	S	148	TRP	CB-CG-CD1	-7.02	117.88	127.00
3	T	248	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	R	156	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	S	254	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	R	272	TRP	CE2-CD2-CG	-6.76	101.89	107.30
2	S	136	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	R	217	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	R	153	HIS	CA-CB-CG	6.41	124.49	113.60
1	L	217	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	S	268	TRP	CG-CD2-CE3	6.16	139.44	133.90
1	L	265	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	L	59	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	L	142	TRP	CB-CG-CD1	-6.00	119.19	127.00
3	H	83	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	M	253	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	T	37	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	L	59	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	L	153	HIS	CA-CB-CG	5.89	123.62	113.60
2	M	301	HIS	CA-CB-CG	-5.83	103.70	113.60
2	S	182	HIS	CA-CB-CG	5.79	123.43	113.60
1	R	259	TRP	CG-CD2-CE3	5.78	139.11	133.90
1	L	25	TRP	CB-CG-CD1	-5.77	119.49	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	142	TRP	CG-CD2-CE3	5.77	139.09	133.90
2	S	73	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	L	25	TRP	CG-CD2-CE3	5.74	139.06	133.90
1	L	231	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	S	80	TRP	CG-CD2-CE3	5.73	139.06	133.90
1	L	266	TRP	CG-CD2-CE3	5.73	139.05	133.90
2	S	73	TRP	CG-CD2-CE3	5.71	139.04	133.90
2	S	136	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	L	142	TRP	CG-CD2-CE3	5.69	139.02	133.90
2	M	80	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	L	265	TRP	CB-CG-CD1	-5.66	119.64	127.00
2	M	80	TRP	CB-CG-CD1	-5.66	119.64	127.00
2	S	253	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	S	267	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	S	294	TRP	CG-CD2-CE3	5.64	138.98	133.90
2	M	73	TRP	CB-CG-CD1	-5.63	119.67	127.00
1	L	151	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	L	135	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	M	268	TRP	CG-CD2-CE3	5.60	138.94	133.90
1	R	142	TRP	CB-CG-CD1	-5.58	119.75	127.00
3	T	21	TRP	CG-CD2-CE3	5.57	138.91	133.90
3	H	89	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	M	294	TRP	CG-CD2-CE3	5.54	138.88	133.90
2	M	171	TRP	CG-CD2-CE3	5.53	138.88	133.90
2	S	80	TRP	CB-CG-CD1	-5.53	119.81	127.00
2	M	73	TRP	CG-CD2-CE3	5.49	138.84	133.90
2	M	155	TRP	CB-CG-CD1	-5.49	119.86	127.00
2	M	157	TRP	CG-CD1-NE1	-5.48	104.62	110.10
2	S	129	TRP	CG-CD2-CE3	5.48	138.83	133.90
2	M	41	TRP	CG-CD2-CE3	5.48	138.83	133.90
2	M	29	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	S	268	TRP	CG-CD1-NE1	-5.45	104.65	110.10
2	S	41	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	M	75	TRP	CG-CD2-CE3	5.41	138.77	133.90
2	M	254	TRP	CG-CD2-CE3	5.41	138.76	133.90
1	R	207	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	M	182	HIS	CA-CB-CG	5.38	122.75	113.60
1	L	259	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	R	262	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	S	155	TRP	CB-CG-CD1	-5.34	120.05	127.00
1	R	59	TRP	CG-CD2-CE3	5.33	138.70	133.90
2	S	297	TRP	CB-CG-CD1	-5.33	120.07	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	168	TRP	CG-CD1-NE1	-5.32	104.78	110.10
2	M	171	TRP	CG-CD1-NE1	-5.31	104.79	110.10
2	S	252	TRP	CG-CD2-CE3	5.29	138.66	133.90
2	M	66	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	R	265	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	L	151	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	L	271	TRP	CB-CG-CD1	-5.25	120.17	127.00
2	S	241	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	T	114	TRP	CG-CD1-NE1	-5.25	104.85	110.10
2	S	87	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	H	168	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	M	171	TRP	CB-CG-CD1	-5.24	120.19	127.00
2	S	75	TRP	CG-CD2-CE3	5.23	138.61	133.90
2	M	41	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	L	266	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	L	265	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	R	266	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	R	271	TRP	CG-CD2-CE3	5.18	138.56	133.90
2	S	247	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	S	268	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	R	25	TRP	CB-CG-CD1	-5.16	120.30	127.00
3	T	177	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	S	294	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	R	25	TRP	CG-CD2-CE3	5.15	138.54	133.90
2	S	171	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	L	272	TRP	CG-CD1-NE1	-5.15	104.95	110.10
2	S	271	TRP	CG-CD1-NE1	-5.14	104.96	110.10
2	S	157	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	R	255	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	S	168	MET	CA-CB-CG	-5.12	104.59	113.30
1	R	86	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	L	271	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	R	262	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	M	115	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	S	115	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	L	25	TRP	CG-CD1-NE1	-5.09	105.00	110.10
1	R	265	TRP	CB-CG-CD1	-5.08	120.39	127.00
2	S	241	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	M	129	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	R	86	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	L	271	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	L	266	TRP	CG-CD1-NE1	-5.06	105.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	L	262	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	R	271	TRP	CG-CD1-NE1	-5.03	105.07	110.10
2	M	294	TRP	CG-CD1-NE1	-5.03	105.07	110.10
3	H	70	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	M	164	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	S	252	TRP	CG-CD1-NE1	-5.01	105.09	110.10
2	S	209	LEU	CA-CB-CG	5.01	126.81	115.30
2	M	75	TRP	CG-CD1-NE1	-5.00	105.10	110.10

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	L	2232	0	2187	13	0
1	R	2232	0	2187	20	0
2	M	2404	0	2318	27	0
2	S	2390	0	2304	22	0
3	H	1869	0	1884	11	0
3	T	1869	0	1884	25	0
4	L	132	0	148	10	0
4	M	117	0	115	11	0
4	R	132	0	148	9	0
4	S	117	0	115	11	0
5	L	116	0	121	5	0
5	R	65	0	76	4	0
5	S	52	0	47	2	0
6	L	44	0	57	1	0
6	M	38	0	47	1	0
6	R	18	0	15	2	0
6	S	32	0	39	0	0
7	M	1	0	0	0	0
7	S	1	0	0	0	0
8	M	64	0	124	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	105	0	0	0	0
9	L	67	0	0	0	0
9	M	91	0	0	2	0
9	R	56	0	0	0	0
9	S	85	0	0	1	0
9	T	64	0	0	1	0
All	All	14393	0	13816	135	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 5.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:309:BCL:HBB3	4:M:310:BCL:H41	1.46	0.96
4:S:309:BCL:HBB3	4:S:310:BCL:H41	1.69	0.74
2:S:208:PHE:HD1	2:S:272:MET:HE3	1.52	0.74
5:R:284:BPH:HHC	5:R:284:BPH:HBB3	1.70	0.73
2:S:63:GLY:HA3	5:S:311:BPH:H5C2	1.70	0.73
2:M:280:GLY:HA2	4:M:310:BCL:HED3	1.76	0.67
2:S:280:GLY:HA2	4:S:310:BCL:HED3	1.78	0.66
2:S:197:PHE:HZ	4:S:310:BCL:HBB2	1.62	0.65
4:M:309:BCL:HBB2	4:M:309:BCL:HHC	1.80	0.64
1:R:200:PRO:HB3	1:R:207:ARG:HD3	1.80	0.63
3:T:11:ASP:N	3:T:14:SER:HG	1.96	0.62
3:T:37:ARG:NH2	3:T:62:LYS:HB2	2.14	0.62
2:M:94:LEU:HD21	2:M:114:LEU:HB3	1.82	0.62
3:T:206:ASN:ND2	3:T:248:ARG:HD2	2.16	0.60
3:T:206:ASN:HD21	3:T:248:ARG:HD2	1.68	0.59
2:M:197:PHE:HZ	4:M:310:BCL:HBB2	1.70	0.57
1:L:241:VAL:HG21	5:L:285:BPH:HAC1	1.87	0.56
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.88	0.56
3:T:118:ARG:HD3	3:T:120:LEU:HD12	1.89	0.54
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.72	0.54
2:S:228:ARG:HA	3:T:194:GLN:HG2	1.90	0.54
3:T:154:ARG:HE	3:T:204:HIS:HD2	1.56	0.54
2:M:197:PHE:CZ	4:M:310:BCL:HBB2	2.43	0.53
1:R:207:ARG:HG2	2:S:142:MET:HG2	1.89	0.53
4:S:309:BCL:HBB2	4:S:309:BCL:HHC	1.89	0.53
1:R:232:LEU:HD21	6:R:285:U10:H8	1.91	0.53
4:S:309:BCL:CBB	4:S:309:BCL:HHC	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:310:BCL:CBB	4:M:310:BCL:HHC	2.39	0.52
4:S:310:BCL:CBB	4:S:310:BCL:HHC	2.38	0.52
4:M:309:BCL:OBB	8:M:315:LDA:HM21	2.09	0.52
2:S:24:VAL:HG21	2:S:29:ARG:NH1	2.24	0.52
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.75	0.52
2:S:197:PHE:CZ	4:S:310:BCL:HBB2	2.42	0.52
2:M:9:GLN:HA	8:M:314:LDA:HM13	1.92	0.52
1:L:231:ARG:HD2	2:M:5:ASN:O	2.10	0.51
1:L:66:VAL:HG11	1:L:89:ILE:HD12	1.92	0.50
3:T:65:ILE:HA	3:T:72:THR:HG22	1.93	0.50
4:L:282:BCL:H122	5:L:285:BPH:H3A	1.93	0.50
4:R:282:BCL:H122	5:R:284:BPH:H3A	1.93	0.50
5:R:284:BPH:HBB2	2:S:210:TYR:HB3	1.93	0.50
1:R:218:ASP:OD1	2:S:29:ARG:HD2	2.12	0.50
3:H:206:ASN:ND2	3:H:248:ARG:HD2	2.27	0.50
5:R:284:BPH:CBB	5:R:284:BPH:HHC	2.39	0.49
2:S:228:ARG:HA	3:T:194:GLN:CG	2.42	0.49
4:L:283:BCL:HBB2	4:L:283:BCL:HMB1	1.94	0.49
1:L:189:LEU:HD13	5:L:284:BPH:HMD2	1.94	0.49
1:L:217:ARG:HD2	9:M:357:HOH:O	2.11	0.49
2:M:228:ARG:HA	3:H:194:GLN:HG2	1.94	0.49
2:M:148:TRP:CD1	8:M:312:LDA:HM11	2.48	0.49
3:T:37:ARG:HH21	3:T:62:LYS:HB2	1.78	0.49
2:M:156:LEU:HD12	2:M:277:THR:HG22	1.95	0.48
1:R:217:ARG:HD2	9:S:316:HOH:O	2.12	0.48
4:R:282:BCL:H112	4:R:283:BCL:HBB2	1.94	0.48
2:S:94:LEU:HD21	2:S:114:LEU:HB3	1.95	0.48
2:M:148:TRP:HB3	8:M:312:LDA:H51	1.96	0.48
1:R:60:ASN:HB3	1:R:63:LEU:HD12	1.95	0.48
2:S:229:PHE:HB2	2:S:244:ALA:HB2	1.96	0.48
2:S:9:GLN:HE22	3:T:198:VAL:H	1.61	0.47
4:R:282:BCL:CBB	4:R:282:BCL:HMB1	2.44	0.47
2:S:3:TYR:CZ	2:S:5:ASN:HA	2.49	0.47
1:R:265:TRP:O	1:R:269:LEU:HD13	2.14	0.47
2:M:214:LEU:HD21	6:M:311:U10:H172	1.96	0.47
2:S:264:GLY:HA3	3:T:35:ASN:OD1	2.14	0.47
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.79	0.47
3:T:122:GLU:HB2	3:T:227:LEU:HD21	1.96	0.47
1:R:117:ILE:HB	1:R:118:PRO:HD3	1.96	0.46
2:M:9:GLN:NE2	3:H:198:VAL:H	2.13	0.46
2:M:228:ARG:HA	3:H:194:GLN:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.51	0.46
1:R:75:LEU:HD21	1:R:137:VAL:HA	1.98	0.46
1:L:185:LEU:CD2	4:M:309:BCL:H43	2.46	0.45
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.51	0.45
4:L:282:BCL:CBB	4:L:282:BCL:HMB1	2.46	0.45
1:R:110:LYS:O	3:T:111:PRO:HG3	2.15	0.45
4:R:283:BCL:HBB2	4:R:283:BCL:HMB1	1.97	0.45
1:R:87:GLN:O	1:R:91:ILE:HG12	2.17	0.45
1:L:208:THR:OG1	1:L:211:HIS:HD2	1.99	0.45
2:S:16:ALA:HB1	2:S:32:VAL:HG21	1.98	0.45
4:M:310:BCL:HHC	4:M:310:BCL:HBB3	1.97	0.45
4:M:309:BCL:CBB	4:M:309:BCL:HHC	2.46	0.44
1:R:185:LEU:HD13	5:S:311:BPH:ND	2.32	0.44
2:S:202:HIS:CE1	2:S:206:ILE:HD11	2.52	0.44
3:T:62:LYS:O	3:T:74:THR:HA	2.17	0.44
4:R:282:BCL:CGA	4:R:283:BCL:HBC1	2.47	0.44
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.98	0.44
4:S:309:BCL:HBC1	4:S:310:BCL:HAA2	2.00	0.44
4:R:282:BCL:HBD	4:R:283:BCL:HAC1	1.98	0.44
4:L:282:BCL:HAA2	4:L:283:BCL:HBC1	1.98	0.44
2:S:9:GLN:NE2	3:T:198:VAL:H	2.15	0.44
2:S:164:ARG:HB3	2:S:165:PRO:HD3	2.00	0.44
4:L:282:BCL:H2C	4:M:310:BCL:H2C	2.00	0.43
1:L:278:GLY:HA2	2:M:77:GLN:O	2.18	0.43
1:L:60:ASN:O	1:L:64:ILE:HG13	2.18	0.43
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.53	0.43
4:R:283:BCL:CBB	4:R:283:BCL:HMB1	2.48	0.43
4:S:310:BCL:HBB2	4:S:310:BCL:HHC	2.00	0.43
3:T:241:LEU:HA	3:T:248:ARG:HH22	1.84	0.43
2:M:229:PHE:HB2	2:M:244:ALA:HB2	2.00	0.43
2:M:34:PRO:O	2:M:47:LEU:HB2	2.18	0.43
1:R:135:ARG:HB3	1:R:136:PRO:HD3	2.01	0.43
2:M:275:LEU:HD23	2:M:278:LEU:HD23	2.01	0.43
3:T:87:LEU:HD12	3:T:100:PRO:HA	2.01	0.43
3:T:173:GLU:HG3	9:T:292:HOH:O	2.19	0.43
1:R:4:SER:HB2	3:T:79:GLU:HG2	2.00	0.42
2:M:159:VAL:HA	2:M:163:ILE:HB	2.00	0.42
3:H:11:ASP:HB3	3:H:14:SER:OG	2.19	0.42
4:L:283:BCL:CBB	4:L:283:BCL:HMB1	2.50	0.42
1:R:85:LEU:HA	1:R:85:LEU:HD12	1.92	0.42
2:M:109:LEU:HD22	2:M:114:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:283:BCL:OBB	4:L:283:BCL:HHC	2.19	0.42
1:R:66:VAL:HG11	1:R:89:ILE:HD12	2.02	0.42
4:L:282:BCL:HBD	4:L:283:BCL:HAC1	2.02	0.42
2:M:13:ARG:O	3:H:140:PHE:HA	2.20	0.41
3:T:170:ASP:HB2	3:T:177:ARG:HG3	2.01	0.41
4:R:282:BCL:HHC	4:R:282:BCL:OBB	2.20	0.41
2:S:159:VAL:HA	2:S:163:ILE:HB	2.00	0.41
1:R:185:LEU:CD2	4:S:309:BCL:H43	2.50	0.41
4:S:310:BCL:HBC2	4:S:310:BCL:H2C	1.92	0.41
1:R:162:TYR:HA	1:R:165:GLY:O	2.21	0.41
4:R:282:BCL:HAA2	4:R:283:BCL:HBC1	2.02	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.20	0.41
1:L:189:LEU:HB3	6:L:286:U10:H4M3	2.02	0.41
4:L:282:BCL:H112	4:L:283:BCL:HBB2	2.03	0.41
1:R:12:PRO:HD3	3:T:97:PRO:HB3	2.03	0.41
3:T:241:LEU:O	3:T:248:ARG:NH2	2.54	0.41
4:L:282:BCL:HHC	4:L:282:BCL:OBB	2.20	0.41
2:S:208:PHE:HA	2:S:272:MET:CE	2.51	0.41
3:T:156:CYS:HB3	3:T:206:ASN:O	2.21	0.41
1:L:195:LEU:HD21	2:M:267:ARG:HG2	2.03	0.41
3:T:252:VAL:HA	3:T:255:MET:HG2	2.02	0.41
3:H:196:VAL:HG12	3:H:205:VAL:HG22	2.01	0.40
5:L:285:BPH:H6C1	5:L:285:BPH:H2	1.91	0.40
5:L:285:BPH:HHB	5:L:285:BPH:HMB1	1.85	0.40
2:M:236:GLU:HG2	9:M:406:HOH:O	2.22	0.40
1:R:189:LEU:HB3	6:R:285:U10:H4M3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	271 (97%)	6 (2%)	2 (1%)	22	22
1	R	279/281 (99%)	271 (97%)	6 (2%)	2 (1%)	22	22
2	M	299/307 (97%)	290 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	287 (97%)	9 (3%)	1 (0%)	41	46
3	H	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	34	37
3	T	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	34	37
All	All	1642/1696 (97%)	1592 (97%)	43 (3%)	7 (0%)	34	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	LEU
3	H	45	GLU
3	T	45	GLU
1	R	2	LEU
2	S	195	ASN
1	R	31	VAL
1	L	31	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	208 (94%)	12 (6%)	21	26
1	R	220/220 (100%)	212 (96%)	8 (4%)	35	45
2	M	236/240 (98%)	224 (95%)	12 (5%)	24	29
2	S	235/240 (98%)	223 (95%)	12 (5%)	24	29
3	H	199/209 (95%)	192 (96%)	7 (4%)	36	46
3	T	199/209 (95%)	187 (94%)	12 (6%)	19	22
All	All	1309/1338 (98%)	1246 (95%)	63 (5%)	25	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	85	LEU
1	L	126	LEU
1	L	129	LEU
1	L	158	SER
1	L	189	LEU
1	L	195	LEU
1	L	210	ASP
1	L	216	PHE
1	L	220	VAL
1	L	235	LEU
1	L	269	LEU
1	L	272	TRP
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	94	LEU
2	M	114	LEU
2	M	148	TRP
2	M	156	LEU
2	M	168	MET
2	M	191	LEU
2	M	195	ASN
2	M	216	PHE
2	M	301	HIS
3	H	12	LEU
3	H	73	LEU
3	H	82	ASP
3	H	123	LEU
3	H	208	LEU
3	H	217	PRO
3	H	231	ASP
1	R	15	THR
1	R	21	LEU
1	R	129	LEU
1	R	189	LEU
1	R	207	ARG
1	R	216	PHE
1	R	269	LEU
1	R	272	TRP
2	S	5	ASN
2	S	24	VAL
2	S	29	ARG
2	S	60	LEU

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Mol	Chain	Res	Type
2	S	89	LEU
2	S	94	LEU
2	S	114	LEU
2	S	148	TRP
2	S	156	LEU
2	S	191	LEU
2	S	216	PHE
2	S	300	ASN
3	T	12	LEU
3	T	14	SER
3	T	46	ASP
3	T	48	THR
3	T	75	VAL
3	T	82	ASP
3	T	147	ASN
3	T	208	LEU
3	T	218	THR
3	T	223	THR
3	T	228	LEU
3	T	231	ASP

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

Mol	Chain	Res	Type
1	L	211	HIS
2	M	9	GLN
2	M	195	ASN
3	H	194	GLN
3	H	206	ASN
1	R	87	GLN
1	R	211	HIS
2	S	9	GLN
3	T	147	ASN
3	T	204	HIS
3	T	206	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BCL	L	283	-	58,74,74	1.09	5 (8%)	69,115,115	2.12	14 (20%)
4	BCL	R	282	-	58,74,74	1.08	6 (10%)	69,115,115	1.96	16 (23%)
4	BCL	S	310	-	58,74,74	1.10	6 (10%)	69,115,115	2.00	15 (21%)
4	BCL	L	282	-	58,74,74	1.12	6 (10%)	69,115,115	1.92	15 (21%)
4	BCL	M	310	-	58,74,74	1.06	6 (10%)	69,115,115	1.97	16 (23%)
5	BPH	S	311	-	51,57,70	1.27	5 (9%)	60,85,101	1.77	11 (18%)
6	U10	S	312	-	32,32,63	1.66	8 (25%)	38,41,79	1.05	2 (5%)
8	LDA	M	312	-	12,15,15	2.46	1 (8%)	14,17,17	1.39	2 (14%)
6	U10	M	311	-	38,38,63	1.64	10 (26%)	46,49,79	1.10	3 (6%)
8	LDA	M	313	-	12,15,15	2.54	1 (8%)	14,17,17	1.40	4 (28%)
4	BCL	M	309	-	43,59,74	1.29	5 (11%)	51,97,115	2.28	15 (29%)
4	BCL	S	309	-	43,59,74	1.27	6 (13%)	51,97,115	2.35	14 (27%)
4	BCL	R	283	-	58,74,74	1.09	6 (10%)	69,115,115	2.13	13 (18%)
5	BPH	L	285	-	64,70,70	1.20	6 (9%)	76,101,101	1.86	14 (18%)
6	U10	R	285	-	18,18,63	1.93	5 (27%)	22,25,79	1.03	0
6	U10	L	286	-	44,44,63	1.65	10 (22%)	53,56,79	1.30	5 (9%)
5	BPH	L	284	-	50,56,70	1.29	5 (10%)	59,84,101	1.81	12 (20%)
8	LDA	M	314	-	12,15,15	2.48	1 (8%)	14,17,17	1.41	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BPH	R	284	-	64,70,70	1.13	5 (7%)	76,101,101	1.67	12 (15%)
8	LDA	M	315	-	12,15,15	2.47	1 (8%)	14,17,17	1.42	4 (28%)

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	283	-	-	3/37/137/137	-
4	BCL	R	282	-	-	7/37/137/137	-
4	BCL	S	310	-	-	8/37/137/137	-
4	BCL	L	282	-	-	3/37/137/137	-
4	BCL	M	310	-	-	5/37/137/137	-
5	BPH	S	311	-	-	11/39/90/105	0/5/6/6
6	U10	S	312	-	-	4/26/50/87	0/1/1/1
8	LDA	M	312	-	-	4/13/13/13	-
6	U10	M	311	-	-	2/33/57/87	0/1/1/1
8	LDA	M	313	-	-	6/13/13/13	-
4	BCL	M	309	-	-	3/19/119/137	-
4	BCL	S	309	-	-	3/19/119/137	-
4	BCL	R	283	-	-	2/37/137/137	-
5	BPH	L	285	-	-	9/54/105/105	0/5/6/6
6	U10	R	285	-	-	2/9/33/87	0/1/1/1
6	U10	L	286	-	-	15/41/65/87	0/1/1/1
5	BPH	L	284	-	-	9/38/89/105	0/5/6/6
8	LDA	M	314	-	-	6/13/13/13	-
5	BPH	R	284	-	-	11/54/105/105	0/5/6/6
8	LDA	M	315	-	-	6/13/13/13	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	313	LDA	O1-N1	-8.62	1.22	1.42
8	M	314	LDA	O1-N1	-8.42	1.22	1.42
8	M	315	LDA	O1-N1	-8.39	1.22	1.42
8	M	312	LDA	O1-N1	-8.34	1.22	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	285	U10	C6-C1	4.04	1.42	1.35
6	M	311	U10	C6-C1	3.93	1.42	1.35
5	L	285	BPH	C3D-CAD	-3.89	1.39	1.47
5	R	284	BPH	C3D-CAD	-3.89	1.39	1.47
6	L	286	U10	C6-C1	3.88	1.42	1.35
5	S	311	BPH	C3D-CAD	-3.81	1.39	1.47
4	R	283	BCL	O2D-CGD	-3.71	1.24	1.33
6	S	312	U10	C6-C1	3.66	1.41	1.35
4	M	310	BCL	O2D-CGD	-3.61	1.24	1.33
5	L	285	BPH	C1B-C2B	-3.60	1.38	1.45
5	L	285	BPH	O2A-CGA	-3.55	1.22	1.33
5	S	311	BPH	O2D-CGD	-3.55	1.24	1.33
5	L	284	BPH	C3D-CAD	-3.53	1.40	1.47
4	R	282	BCL	O2D-CGD	-3.50	1.24	1.33
4	L	282	BCL	O2D-CGD	-3.47	1.24	1.33
4	M	309	BCL	O2D-CGD	-3.44	1.24	1.33
5	R	284	BPH	O2D-CGD	-3.43	1.24	1.33
4	S	310	BCL	O2D-CGD	-3.42	1.24	1.33
6	R	285	U10	C7-C8	-3.42	1.45	1.50
5	R	284	BPH	O2A-CGA	-3.40	1.23	1.33
4	S	309	BCL	O2D-CGD	-3.39	1.24	1.33
4	L	283	BCL	O2D-CGD	-3.37	1.25	1.33
4	S	310	BCL	O2A-CGA	-3.36	1.23	1.33
5	L	285	BPH	O2D-CGD	-3.36	1.25	1.33
5	L	284	BPH	O2A-CGA	-3.34	1.23	1.33
5	R	284	BPH	C1B-C2B	-3.32	1.38	1.45
4	M	309	BCL	O2A-CGA	-3.32	1.23	1.33
5	L	284	BPH	C1B-C2B	-3.29	1.38	1.45
5	L	284	BPH	O2D-CGD	-3.24	1.25	1.33
5	S	311	BPH	O2A-CGA	-3.24	1.23	1.33
4	M	310	BCL	O2A-CGA	-3.20	1.24	1.33
4	S	309	BCL	O2A-CGA	-3.19	1.24	1.33
4	S	310	BCL	C4B-NB	3.12	1.38	1.35
6	S	312	U10	C4-C5	-3.10	1.39	1.48
6	S	312	U10	C7-C8	-3.09	1.46	1.50
4	L	282	BCL	C4B-NB	3.09	1.38	1.35
6	M	311	U10	C7-C8	-3.05	1.46	1.50
4	R	282	BCL	O2A-CGA	-3.05	1.24	1.33
6	L	286	U10	C8-C9	3.00	1.40	1.33
4	L	282	BCL	O2A-CGA	-2.96	1.24	1.33
4	L	283	BCL	O2A-CGA	-2.95	1.24	1.33
4	L	283	BCL	C3D-CAD	-2.95	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	285	U10	C3-C2	-2.91	1.40	1.48
6	M	311	U10	C4-C5	-2.91	1.40	1.48
5	S	311	BPH	C1B-C2B	-2.86	1.39	1.45
6	L	286	U10	C3-C2	-2.84	1.40	1.48
6	L	286	U10	C18-C19	2.84	1.39	1.33
6	L	286	U10	C28-C29	2.83	1.39	1.33
4	S	309	BCL	C3D-CAD	-2.82	1.38	1.46
4	L	283	BCL	C3B-CAB	-2.80	1.41	1.49
4	S	309	BCL	C4B-NB	2.78	1.37	1.35
6	S	312	U10	C3-C2	-2.77	1.40	1.48
6	M	311	U10	C3-C2	-2.77	1.40	1.48
6	M	311	U10	C18-C19	2.76	1.39	1.33
4	R	283	BCL	O2A-CGA	-2.74	1.25	1.33
4	M	309	BCL	C3B-CAB	-2.73	1.41	1.49
6	L	286	U10	C7-C8	-2.72	1.46	1.50
4	S	309	BCL	C3B-CAB	-2.71	1.42	1.49
4	R	282	BCL	C2-C3	2.70	1.39	1.33
6	S	312	U10	C18-C19	2.69	1.39	1.33
4	R	282	BCL	C4B-NB	2.68	1.37	1.35
6	L	286	U10	C33-C34	2.68	1.39	1.33
4	L	282	BCL	C2-C3	2.63	1.39	1.33
6	M	311	U10	C23-C24	2.63	1.39	1.33
4	R	283	BCL	C3D-CAD	-2.62	1.39	1.46
4	L	282	BCL	C3B-CAB	-2.62	1.42	1.49
4	R	282	BCL	C3D-CAD	-2.61	1.39	1.46
4	M	309	BCL	C4B-NB	2.60	1.37	1.35
4	S	310	BCL	C3D-CAD	-2.59	1.39	1.46
6	S	312	U10	C8-C9	2.58	1.39	1.33
5	L	285	BPH	C2-C3	2.58	1.39	1.33
4	S	310	BCL	C3B-CAB	-2.57	1.42	1.49
5	R	284	BPH	C2-C3	2.56	1.39	1.33
6	L	286	U10	C13-C14	2.56	1.39	1.33
4	M	310	BCL	C3B-CAB	-2.51	1.42	1.49
4	M	310	BCL	C3D-CAD	-2.51	1.39	1.46
5	L	284	BPH	C2-C3	2.51	1.39	1.33
4	M	309	BCL	C3D-CAD	-2.50	1.39	1.46
6	S	312	U10	C13-C14	2.48	1.38	1.33
4	M	310	BCL	C4B-NB	2.48	1.37	1.35
6	L	286	U10	C4-C5	-2.47	1.41	1.48
4	L	283	BCL	C2-C3	2.46	1.38	1.33
6	L	286	U10	C23-C24	2.46	1.38	1.33
4	L	282	BCL	C3D-CAD	-2.45	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	285	U10	C4-C5	-2.44	1.41	1.48
4	R	283	BCL	C2-C3	2.43	1.38	1.33
6	M	311	U10	C28-C29	2.42	1.39	1.32
4	R	282	BCL	C3B-CAB	-2.40	1.42	1.49
6	R	285	U10	C8-C9	2.39	1.39	1.32
5	S	311	BPH	C2-C3	2.39	1.38	1.33
4	R	283	BCL	C3B-CAB	-2.38	1.42	1.49
4	S	309	BCL	C2-C3	2.34	1.39	1.32
6	M	311	U10	C8-C9	2.29	1.38	1.33
4	S	310	BCL	C2-C3	2.29	1.38	1.33
6	M	311	U10	C13-C14	2.22	1.38	1.33
5	L	285	BPH	CHC-C1C	2.20	1.41	1.36
4	M	310	BCL	C2-C3	2.10	1.38	1.33
4	R	283	BCL	C4B-NB	2.06	1.37	1.35
6	S	312	U10	C6-C5	-2.04	1.40	1.46
6	M	311	U10	C7-C6	2.03	1.54	1.51

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	310	BCL	C4D-C3D-CAD	-9.26	103.31	108.47
4	M	309	BCL	C4D-C3D-CAD	-9.12	103.38	108.47
4	S	309	BCL	C4D-C3D-CAD	-9.11	103.39	108.47
4	R	283	BCL	C4D-C3D-CAD	-9.08	103.41	108.47
4	M	310	BCL	C4D-C3D-CAD	-8.89	103.51	108.47
4	L	283	BCL	C4D-C3D-CAD	-8.58	103.69	108.47
4	L	282	BCL	C4D-C3D-CAD	-8.37	103.80	108.47
4	R	282	BCL	C4D-C3D-CAD	-8.35	103.82	108.47
5	L	285	BPH	C4D-C3D-CAD	-7.22	103.30	107.87
4	R	283	BCL	C1C-NC-C4C	7.14	109.91	106.71
4	L	283	BCL	C1C-NC-C4C	7.09	109.89	106.71
5	R	284	BPH	C4D-C3D-CAD	-6.59	103.70	107.87
4	S	309	BCL	C1C-NC-C4C	6.45	109.61	106.71
5	L	284	BPH	C4D-C3D-CAD	-6.39	103.83	107.87
5	S	311	BPH	C4D-C3D-CAD	-6.15	103.97	107.87
4	M	309	BCL	C1C-NC-C4C	6.11	109.45	106.71
5	L	285	BPH	CBC-CAC-C3C	5.87	126.53	113.47
4	R	282	BCL	C1C-NC-C4C	5.84	109.33	106.71
4	S	310	BCL	C1C-NC-C4C	5.22	109.05	106.71
4	L	282	BCL	C1C-NC-C4C	5.08	108.99	106.71
4	M	310	BCL	C1C-NC-C4C	4.93	108.92	106.71
5	L	285	BPH	C3D-CAD-CBD	4.66	113.74	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	311	BPH	O2D-CGD-CBD	4.55	119.36	111.27
4	R	283	BCL	CMB-C2B-C1B	-4.51	121.53	128.46
5	R	284	BPH	O2D-CGD-CBD	4.47	119.22	111.27
4	L	283	BCL	O2D-CGD-CBD	4.39	119.07	111.27
4	S	309	BCL	O2D-CGD-CBD	4.35	119.00	111.27
5	L	284	BPH	O2D-CGD-CBD	4.31	118.92	111.27
4	R	283	BCL	CMB-C2B-C3B	4.19	132.51	124.68
4	R	283	BCL	C3D-CAD-CBD	4.16	113.08	107.61
4	M	309	BCL	C3D-CAD-CBD	4.14	113.06	107.61
4	S	310	BCL	C3D-CAD-CBD	4.06	112.96	107.61
4	S	309	BCL	C3D-CAD-CBD	4.05	112.94	107.61
5	L	285	BPH	O2D-CGD-CBD	4.04	118.45	111.27
5	R	284	BPH	C3D-CAD-CBD	4.03	112.91	107.61
4	L	283	BCL	C4A-NA-C1A	3.96	108.49	106.71
4	L	283	BCL	CMB-C2B-C1B	-3.96	122.38	128.46
4	L	282	BCL	CMB-C2B-C1B	-3.95	122.39	128.46
4	L	283	BCL	CMB-C2B-C3B	3.94	132.05	124.68
4	M	310	BCL	C3D-CAD-CBD	3.89	112.73	107.61
4	M	310	BCL	O2D-CGD-CBD	3.86	118.13	111.27
4	L	283	BCL	C3D-CAD-CBD	3.85	112.67	107.61
4	S	310	BCL	O2D-CGD-CBD	3.84	118.10	111.27
5	S	311	BPH	C3D-CAD-CBD	3.82	112.64	107.61
4	M	309	BCL	O2D-CGD-CBD	3.76	117.94	111.27
4	R	283	BCL	C4A-NA-C1A	3.75	108.39	106.71
4	L	282	BCL	C3D-CAD-CBD	3.74	112.53	107.61
5	L	284	BPH	C3D-CAD-CBD	3.70	112.48	107.61
4	L	282	BCL	CMB-C2B-C3B	3.63	131.48	124.68
5	R	284	BPH	C1-O2A-CGA	3.61	125.91	116.44
4	R	282	BCL	CMB-C2B-C1B	-3.53	123.05	128.46
4	R	282	BCL	CMB-C2B-C3B	3.52	131.27	124.68
5	R	284	BPH	O1D-CGD-CBD	-3.51	117.31	124.48
4	R	282	BCL	C3D-CAD-CBD	3.47	112.17	107.61
4	R	282	BCL	CED-O2D-CGD	3.46	123.76	115.94
4	M	310	BCL	C4-C3-C5	3.45	121.08	115.27
5	L	285	BPH	C1-O2A-CGA	3.44	125.47	116.44
4	S	309	BCL	O1D-CGD-CBD	-3.40	117.53	124.48
5	L	285	BPH	O2A-C1-C2	-3.36	99.81	108.64
4	S	309	BCL	OBD-CAD-C3D	-3.35	122.41	127.98
5	S	311	BPH	O1D-CGD-CBD	-3.32	117.69	124.48
5	L	284	BPH	O1D-CGD-CBD	-3.30	117.74	124.48
5	L	284	BPH	C4-C3-C5	3.26	119.71	115.98
4	L	283	BCL	OBD-CAD-C3D	-3.26	122.57	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	310	BCL	C4A-NA-C1A	3.25	108.17	106.71
4	S	309	BCL	CMB-C2B-C1B	-3.24	123.48	128.46
6	L	286	U10	C25-C24-C26	3.23	120.70	115.27
4	R	282	BCL	OBD-CAD-C3D	-3.22	122.64	127.98
4	L	282	BCL	CED-O2D-CGD	3.20	123.18	115.94
5	R	284	BPH	OBD-CAD-C3D	-3.19	122.69	127.98
4	L	283	BCL	O1D-CGD-CBD	-3.18	117.97	124.48
4	M	309	BCL	C4A-NA-C1A	3.16	108.12	106.71
4	R	282	BCL	C4A-NA-C1A	3.12	108.11	106.71
4	S	309	BCL	C4A-NA-C1A	3.11	108.10	106.71
5	L	285	BPH	OBD-CAD-C3D	-3.08	122.87	127.98
4	S	309	BCL	C1-O2A-CGA	3.06	124.46	116.44
4	S	309	BCL	CMB-C2B-C3B	3.06	130.40	124.68
5	S	311	BPH	OBD-CAD-C3D	-3.03	122.95	127.98
5	L	284	BPH	C1-O2A-CGA	3.02	124.38	116.44
5	S	311	BPH	C1-O2A-CGA	3.01	124.33	116.44
4	S	310	BCL	C4A-NA-C1A	2.99	108.05	106.71
4	R	282	BCL	CBC-CAC-C3C	2.95	120.03	113.47
4	S	310	BCL	C4-C3-C5	2.89	120.13	115.27
4	R	283	BCL	C1-C2-C3	-2.88	121.07	126.04
4	R	283	BCL	OBD-CAD-C3D	-2.86	123.23	127.98
6	L	286	U10	C30-C29-C31	2.85	120.07	115.27
5	S	311	BPH	C4-C3-C5	2.84	120.05	115.27
4	R	283	BCL	CAA-CBA-CGA	2.84	121.54	113.25
4	M	309	BCL	CAA-CBA-CGA	2.83	121.53	113.25
5	L	285	BPH	C11-C10-C8	-2.82	106.80	115.92
6	L	286	U10	C35-C34-C36	2.81	119.20	115.98
5	L	285	BPH	O1D-CGD-CBD	-2.81	118.73	124.48
6	M	311	U10	C15-C14-C16	2.80	119.97	115.27
4	S	310	BCL	CMB-C2B-C1B	-2.80	124.17	128.46
4	L	282	BCL	OBD-CAD-C3D	-2.78	123.36	127.98
4	L	283	BCL	C1-C2-C3	-2.77	121.24	126.04
4	S	310	BCL	C1-O2A-CGA	2.76	123.68	116.44
5	L	285	BPH	CED-O2D-CGD	2.76	122.18	115.94
4	L	282	BCL	C7-C6-C5	-2.75	105.88	113.36
4	M	309	BCL	O1D-CGD-CBD	-2.73	118.89	124.48
4	S	310	BCL	CMB-C2B-C3B	2.71	129.75	124.68
6	L	286	U10	C7-C8-C9	-2.69	122.32	126.79
4	M	309	BCL	CAA-C2A-C3A	-2.68	105.44	112.78
4	M	309	BCL	OBD-CAD-C3D	-2.68	123.53	127.98
4	S	310	BCL	OBD-CAD-CBD	-2.68	122.07	125.89
8	M	312	LDA	O1-N1-C1	2.67	115.82	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	311	BPH	C1C-NC-C4C	-2.62	108.23	110.54
5	L	284	BPH	C2B-C1B-NB	2.62	113.74	109.79
5	L	284	BPH	CED-O2D-CGD	2.60	121.82	115.94
6	L	286	U10	C3M-O3-C3	2.58	125.62	116.47
4	M	310	BCL	OBD-CAD-C3D	-2.58	123.69	127.98
8	M	315	LDA	O1-N1-C1	2.57	115.58	109.27
4	S	310	BCL	CED-O2D-CGD	2.57	121.75	115.94
4	M	310	BCL	CMB-C2B-C1B	-2.56	124.53	128.46
8	M	314	LDA	O1-N1-C1	2.55	115.53	109.27
5	R	284	BPH	C1C-NC-C4C	-2.52	108.32	110.54
4	R	283	BCL	CAA-C2A-C3A	-2.52	105.88	112.78
4	M	310	BCL	CMB-C2B-C3B	2.51	129.38	124.68
4	L	282	BCL	CHA-C1A-NA	-2.51	120.65	126.40
8	M	313	LDA	O1-N1-C1	2.50	115.42	109.27
4	M	309	BCL	CMB-C2B-C3B	2.50	129.36	124.68
5	R	284	BPH	C11-C10-C8	-2.49	107.86	115.92
5	L	285	BPH	C2B-C1B-NB	2.49	113.55	109.79
4	L	283	BCL	CED-O2D-CGD	2.48	121.54	115.94
4	R	282	BCL	C7-C6-C5	-2.48	106.63	113.36
4	L	282	BCL	C16-C15-C13	-2.47	107.94	115.92
5	R	284	BPH	CED-O2D-CGD	2.46	121.50	115.94
4	R	282	BCL	CMA-C3A-C4A	-2.43	105.25	111.77
4	R	282	BCL	CAC-C3C-C4C	-2.41	107.23	112.58
4	R	282	BCL	CHA-C1A-NA	-2.40	120.89	126.40
4	L	282	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
4	S	309	BCL	CAA-CBA-CGA	2.38	120.21	113.25
4	S	309	BCL	CAA-C2A-C3A	-2.37	106.28	112.78
4	M	309	BCL	CMB-C2B-C1B	-2.37	124.83	128.46
5	L	284	BPH	CHD-C4C-NC	-2.36	122.40	125.20
5	R	284	BPH	C2B-C1B-NB	2.35	113.34	109.79
4	S	310	BCL	CHA-C1A-NA	-2.34	121.04	126.40
5	L	285	BPH	CHD-C4C-NC	-2.34	122.42	125.20
4	M	310	BCL	CHA-C1A-NA	-2.34	121.04	126.40
5	S	311	BPH	CED-O2D-CGD	2.33	121.21	115.94
4	L	282	BCL	OBB-CAB-CBB	-2.33	114.94	120.17
5	L	284	BPH	OBD-CAD-C3D	-2.29	124.18	127.98
5	L	285	BPH	CMB-C2B-C3B	2.29	132.87	127.61
4	R	283	BCL	C4-C3-C5	2.28	119.11	115.27
4	M	310	BCL	C16-C15-C13	2.28	123.29	115.92
4	M	310	BCL	C4-C3-C2	-2.28	117.83	123.68
4	L	283	BCL	C4-C3-C5	2.27	119.10	115.27
4	M	309	BCL	CED-O2D-CGD	2.27	121.07	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	283	BCL	CAA-C2A-C3A	-2.26	106.58	112.78
4	R	282	BCL	C4-C3-C5	2.25	119.06	115.27
6	M	311	U10	C25-C24-C26	2.25	119.05	115.27
4	M	309	BCL	C1-O2A-CGA	2.24	122.33	116.44
5	L	284	BPH	CAA-C2A-C3A	-2.24	106.64	112.78
4	M	309	BCL	CHA-C1A-NA	-2.24	121.27	126.40
5	L	284	BPH	C1C-NC-C4C	-2.22	108.59	110.54
4	S	310	BCL	O1D-CGD-CBD	-2.22	119.95	124.48
6	S	312	U10	C10-C9-C11	2.20	118.97	115.27
4	L	282	BCL	C4-C3-C5	2.19	118.95	115.27
4	R	282	BCL	OBB-CAB-CBB	-2.19	115.24	120.17
4	M	310	BCL	C1-O2A-CGA	2.19	122.18	116.44
4	R	283	BCL	CAC-C3C-C2C	-2.18	108.80	114.26
8	M	313	LDA	C6-C5-C4	-2.18	103.34	114.42
4	S	310	BCL	CAA-C2A-C3A	-2.18	106.82	112.78
8	M	315	LDA	C4-C3-C2	-2.17	103.40	114.42
8	M	315	LDA	C6-C5-C4	-2.17	103.42	114.42
8	M	314	LDA	C6-C5-C4	-2.15	103.50	114.42
6	M	311	U10	C10-C9-C11	2.14	118.87	115.27
4	S	309	BCL	CHA-C1A-NA	-2.14	121.50	126.40
4	M	310	BCL	OBB-CAB-CBB	-2.12	115.39	120.17
5	S	311	BPH	C2B-C1B-NB	2.12	112.98	109.79
8	M	313	LDA	C4-C3-C2	-2.11	103.72	114.42
4	L	282	BCL	CAC-C3C-C4C	-2.10	107.92	112.58
8	M	312	LDA	C9-C8-C7	-2.10	103.77	114.42
5	S	311	BPH	C2C-C3C-C4C	2.08	104.46	101.34
5	R	284	BPH	C4-C3-C5	2.08	118.76	115.27
4	S	310	BCL	OBB-CAB-CBB	-2.07	115.50	120.17
4	S	309	BCL	C2C-C3C-C4C	2.07	104.44	101.34
4	M	310	BCL	CED-O2D-CGD	2.07	120.63	115.94
4	R	282	BCL	C2A-C1A-CHA	2.07	127.48	123.86
8	M	314	LDA	C9-C8-C7	-2.07	103.93	114.42
8	M	313	LDA	C9-C8-C7	-2.06	103.96	114.42
8	M	314	LDA	C4-C3-C2	-2.05	104.04	114.42
8	M	315	LDA	C9-C8-C7	-2.04	104.05	114.42
4	L	283	BCL	CAA-CBA-CGA	2.04	119.22	113.25
5	R	284	BPH	CHC-C4B-NB	-2.04	120.66	124.93
6	S	312	U10	C15-C14-C16	2.03	118.69	115.27
4	M	310	BCL	C2A-C1A-CHA	2.02	127.39	123.86
5	L	285	BPH	CMB-C2B-C1B	-2.02	121.95	125.06
4	R	283	BCL	CHA-C1A-NA	-2.02	121.78	126.40
4	M	309	BCL	CMC-C2C-C1C	-2.01	106.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	282	BCL	C2A-C3A-C4A	2.00	105.11	101.87

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	313	LDA	N1-C1-C2-C3
5	L	285	BPH	C4C-C3C-CAC-CBC
4	R	282	BCL	C2C-C3C-CAC-CBC
4	R	282	BCL	C4C-C3C-CAC-CBC
5	S	311	BPH	C4C-C3C-CAC-CBC
5	S	311	BPH	C4B-C3B-CAB-CBB
5	S	311	BPH	C4B-C3B-CAB-OBB
5	S	311	BPH	C2B-C3B-CAB-CBB
5	S	311	BPH	C2B-C3B-CAB-OBB
6	L	286	U10	C28-C29-C31-C32
6	L	286	U10	C29-C31-C32-C33
5	R	284	BPH	C4C-C3C-CAC-CBC
4	S	310	BCL	CBD-CGD-O2D-CED
4	M	310	BCL	CBD-CGD-O2D-CED
6	S	312	U10	C14-C16-C17-C18
8	M	314	LDA	N1-C1-C2-C3
8	M	312	LDA	N1-C1-C2-C3
5	L	284	BPH	C4C-C3C-CAC-CBC
5	L	284	BPH	C2C-C3C-CAC-CBC
5	L	284	BPH	C4B-C3B-CAB-CBB
5	L	284	BPH	C4B-C3B-CAB-OBB
5	L	284	BPH	C2B-C3B-CAB-CBB
5	L	284	BPH	C2B-C3B-CAB-OBB
4	R	283	BCL	CBD-CGD-O2D-CED
4	M	310	BCL	O1D-CGD-O2D-CED
4	S	310	BCL	O1D-CGD-O2D-CED
6	L	286	U10	C30-C29-C31-C32
5	S	311	BPH	CBD-CGD-O2D-CED
4	R	283	BCL	O1D-CGD-O2D-CED
4	R	282	BCL	CBD-CGD-O2D-CED
6	M	311	U10	C24-C26-C27-C28
4	R	282	BCL	O1D-CGD-O2D-CED
5	S	311	BPH	O1D-CGD-O2D-CED
6	L	286	U10	C14-C16-C17-C18
6	L	286	U10	C19-C21-C22-C23
8	M	314	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	M	315	LDA	C11-C10-C9-C8
8	M	314	LDA	C2-C3-C4-C5
5	R	284	BPH	C11-C10-C8-C9
8	M	315	LDA	C4-C5-C6-C7
5	L	285	BPH	C4-C3-C5-C6
5	L	285	BPH	C2-C3-C5-C6
4	S	310	BCL	C13-C15-C16-C17
5	S	311	BPH	C2C-C3C-CAC-CBC
5	R	284	BPH	C2C-C3C-CAC-CBC
8	M	313	LDA	C7-C8-C9-C10
5	L	284	BPH	O1A-CGA-O2A-C1
6	S	312	U10	C20-C19-C21-C22
6	S	312	U10	C18-C19-C21-C22
4	S	310	BCL	C5-C6-C7-C8
5	S	311	BPH	O1A-CGA-O2A-C1
4	S	310	BCL	C12-C13-C15-C16
8	M	315	LDA	C6-C7-C8-C9
5	S	311	BPH	CBA-CGA-O2A-C1
5	L	284	BPH	CBA-CGA-O2A-C1
6	L	286	U10	C12-C11-C9-C10
8	M	314	LDA	C1-C2-C3-C4
8	M	313	LDA	C6-C7-C8-C9
8	M	314	LDA	C7-C8-C9-C10
8	M	314	LDA	C9-C10-C11-C12
8	M	312	LDA	C7-C8-C9-C10
5	L	285	BPH	O1A-CGA-O2A-C1
6	L	286	U10	C2-C3-O3-C3M
6	L	286	U10	C12-C11-C9-C8
8	M	312	LDA	C9-C10-C11-C12
4	R	282	BCL	C12-C13-C15-C16
5	L	284	BPH	CAD-CBD-CGD-O2D
5	L	285	BPH	CBA-CGA-O2A-C1
5	R	284	BPH	CBD-CGD-O2D-CED
5	R	284	BPH	C16-C17-C18-C20
6	R	285	U10	C2-C3-O3-C3M
6	L	286	U10	C33-C34-C36-C37
4	L	282	BCL	C12-C13-C15-C16
4	R	282	BCL	C2A-CAA-CBA-CGA
5	R	284	BPH	C4-C3-C5-C6
4	R	282	BCL	C14-C13-C15-C16
4	S	310	BCL	C14-C13-C15-C16
4	L	283	BCL	C13-C15-C16-C17

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	S	310	BCL	O1A-CGA-O2A-C1
4	L	282	BCL	C2A-CAA-CBA-CGA
8	M	313	LDA	C2-C3-C4-C5
5	L	285	BPH	C15-C16-C17-C18
6	S	312	U10	C5-C4-O4-C4M
6	M	311	U10	C5-C4-O4-C4M
8	M	312	LDA	C11-C10-C9-C8
6	L	286	U10	C15-C14-C16-C17
5	L	285	BPH	C11-C10-C8-C9
4	L	282	BCL	C14-C13-C15-C16
8	M	313	LDA	C1-C2-C3-C4
6	L	286	U10	C4-C3-O3-C3M
8	M	315	LDA	C2-C3-C4-C5
4	M	310	BCL	C15-C16-C17-C18
5	R	284	BPH	O1D-CGD-O2D-CED
4	S	310	BCL	C2-C1-O2A-CGA
5	R	284	BPH	C2-C3-C5-C6
8	M	315	LDA	C1-C2-C3-C4
6	L	286	U10	C35-C34-C36-C37
5	R	284	BPH	C16-C17-C18-C19
6	L	286	U10	C18-C19-C21-C22
8	M	313	LDA	C11-C10-C9-C8
6	L	286	U10	C13-C14-C16-C17
4	M	309	BCL	CAD-CBD-CGD-O2D
5	R	284	BPH	CAD-CBD-CGD-O2D
4	M	310	BCL	CAD-CBD-CGD-O2D
4	S	309	BCL	CAD-CBD-CGD-O2D
4	S	309	BCL	C1-C2-C3-C4
5	R	284	BPH	C15-C16-C17-C18
5	L	285	BPH	CHA-CBD-CGD-O1D
5	S	311	BPH	CHA-CBD-CGD-O2D
4	L	283	BCL	CHA-CBD-CGD-O1D
4	L	283	BCL	CHA-CBD-CGD-O2D
5	L	285	BPH	C2-C1-O2A-CGA
4	M	310	BCL	C14-C13-C15-C16
4	M	309	BCL	CAA-CBA-CGA-O2A
4	S	309	BCL	CAA-CBA-CGA-O2A
8	M	315	LDA	C9-C10-C11-C12
6	R	285	U10	C4-C3-O3-C3M
4	M	309	BCL	CAA-CBA-CGA-O1A
6	L	286	U10	C25-C24-C26-C27

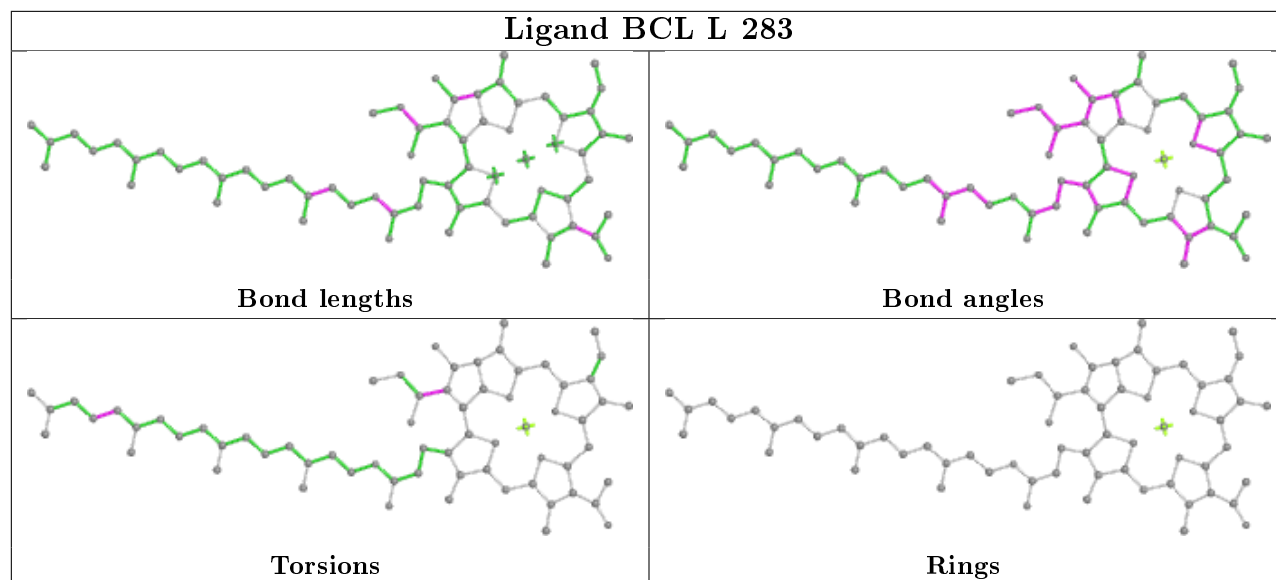
There are no ring outliers.

18 monomers are involved in 56 short contacts:

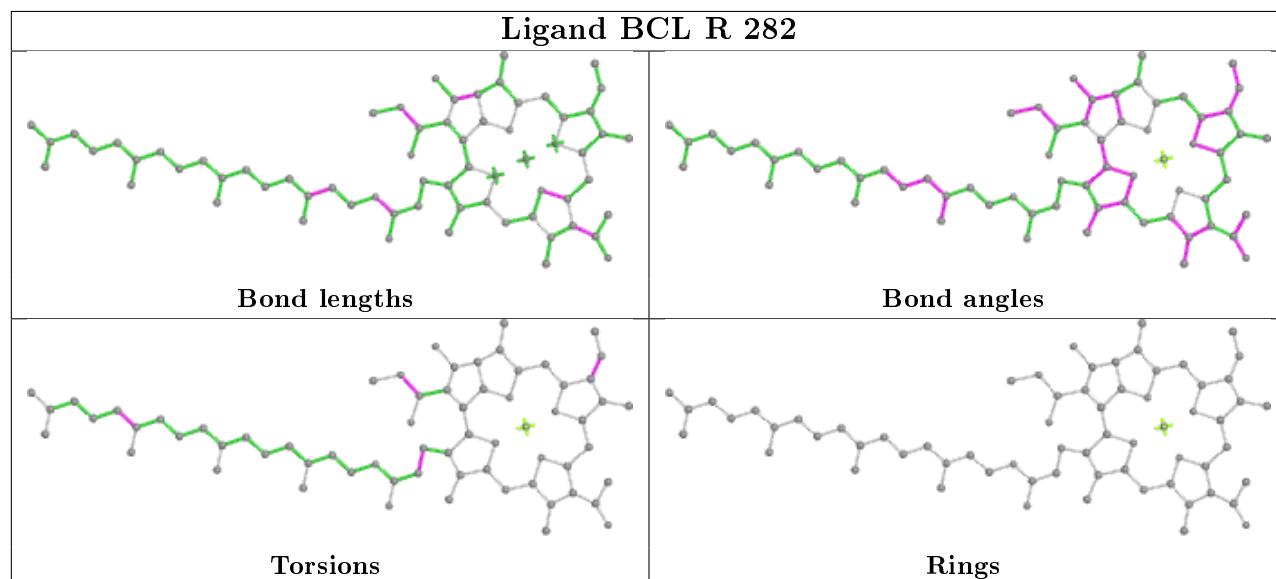
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	283	BCL	6	0
4	R	282	BCL	7	0
4	S	310	BCL	8	0
4	L	282	BCL	7	0
4	M	310	BCL	7	0
5	S	311	BPH	2	0
8	M	312	LDA	2	0
6	M	311	U10	1	0
4	M	309	BCL	5	0
4	S	309	BCL	5	0
4	R	283	BCL	6	0
5	L	285	BPH	4	0
6	R	285	U10	2	0
6	L	286	U10	1	0
5	L	284	BPH	1	0
8	M	314	LDA	1	0
5	R	284	BPH	4	0
8	M	315	LDA	1	0

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

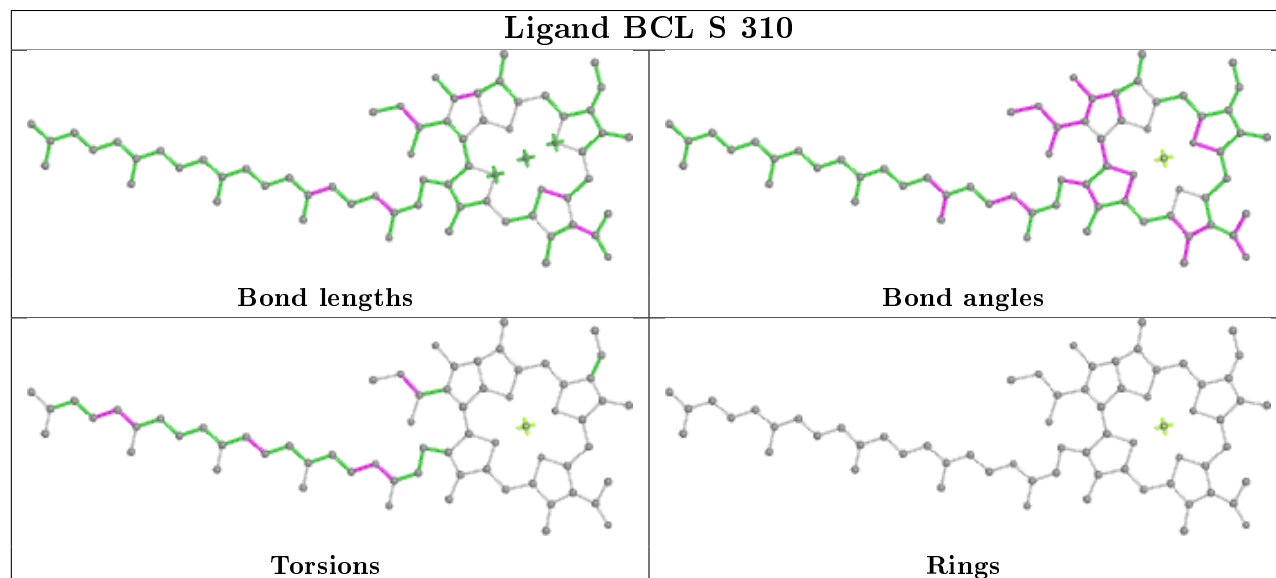
Ligand BCL L 283

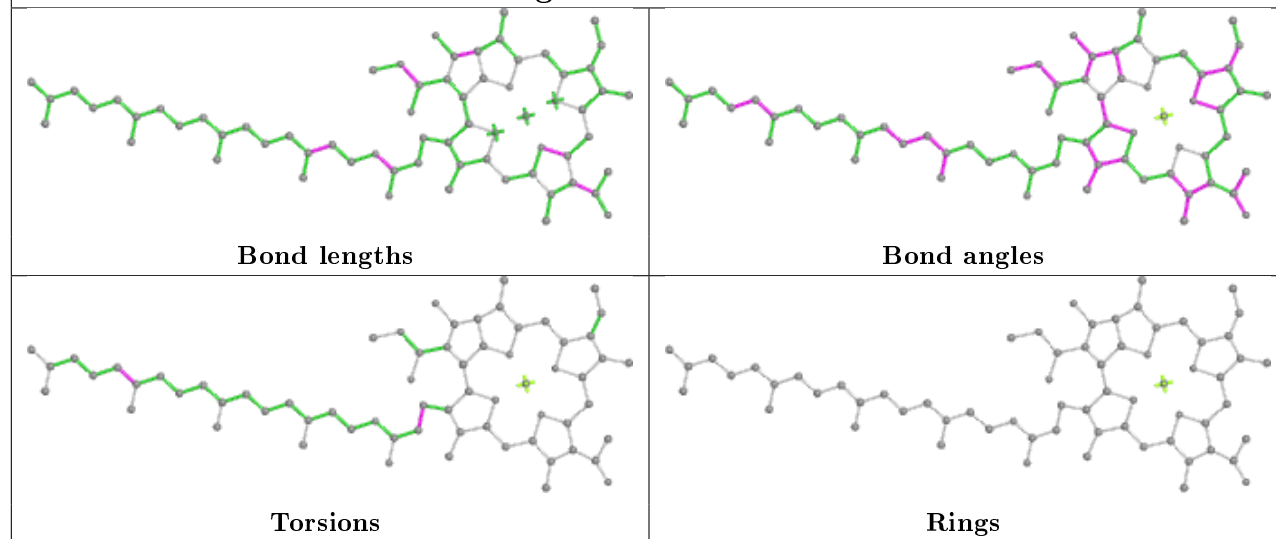
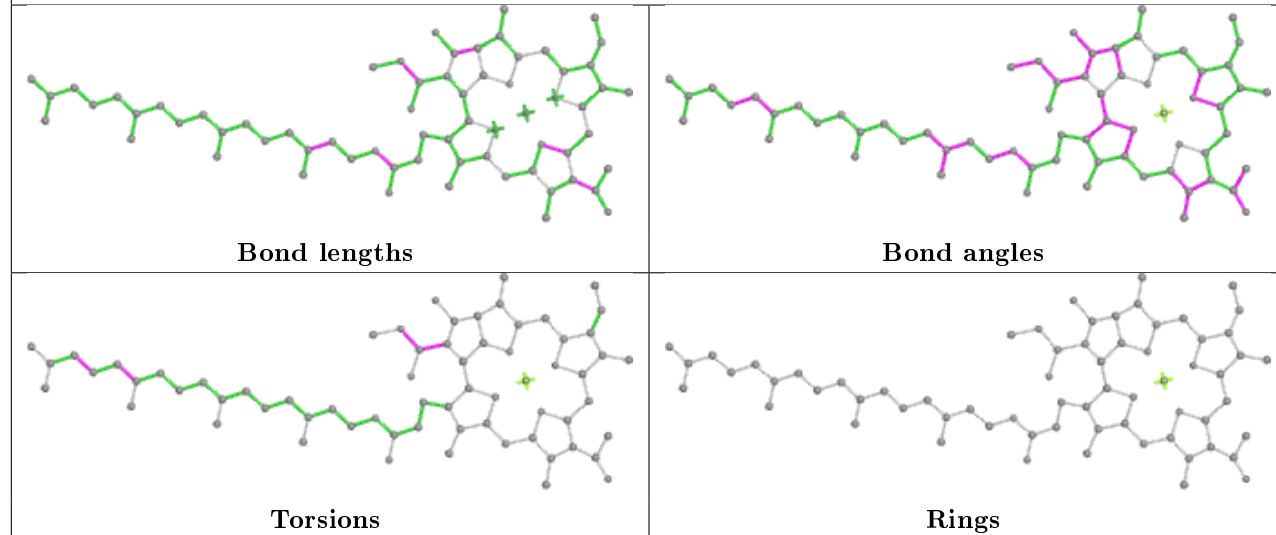


Ligand BCL R 282

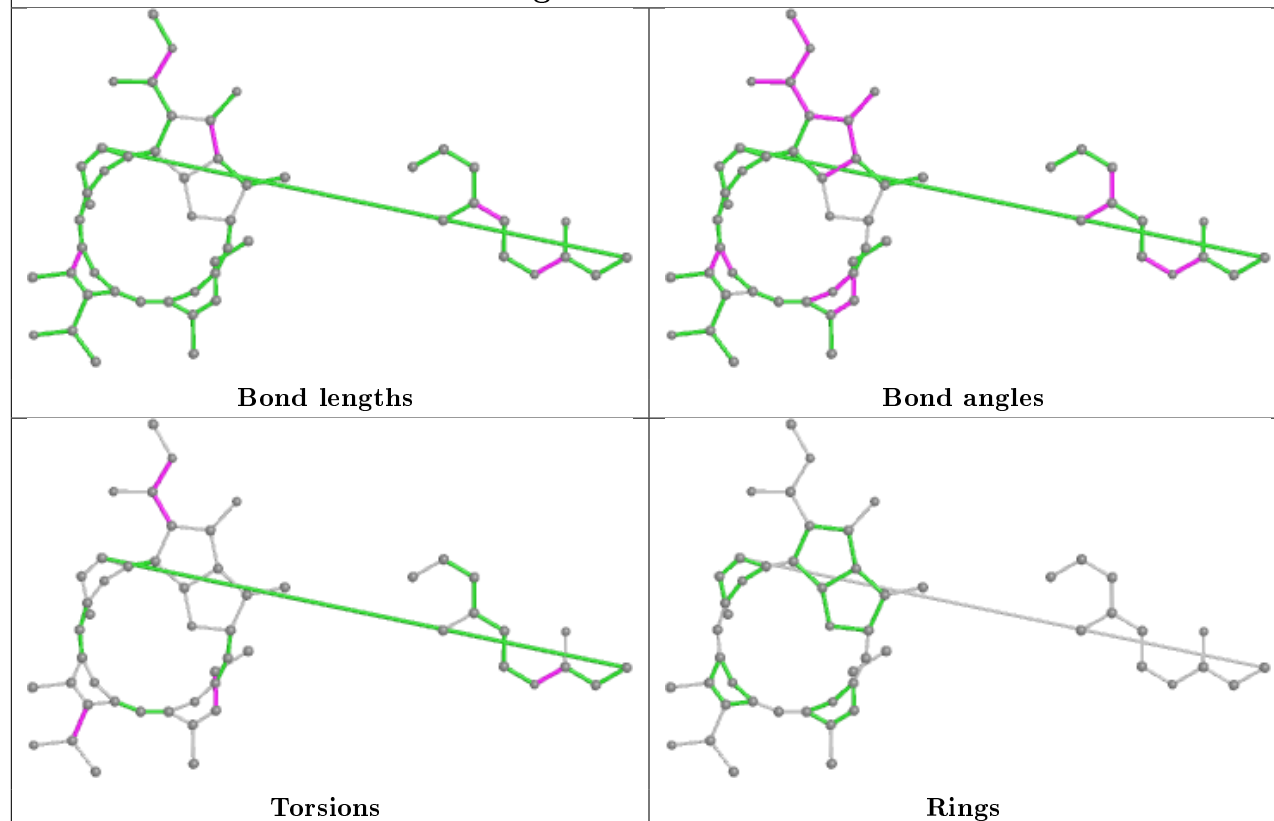


Ligand BCL S 310

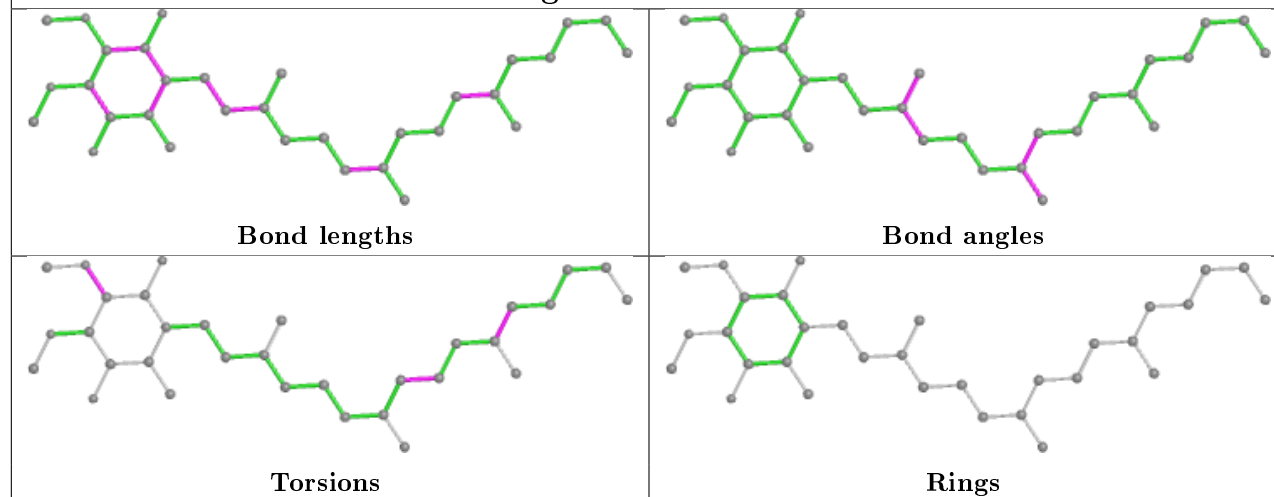


Ligand BCL L 282**Ligand BCL M 310**

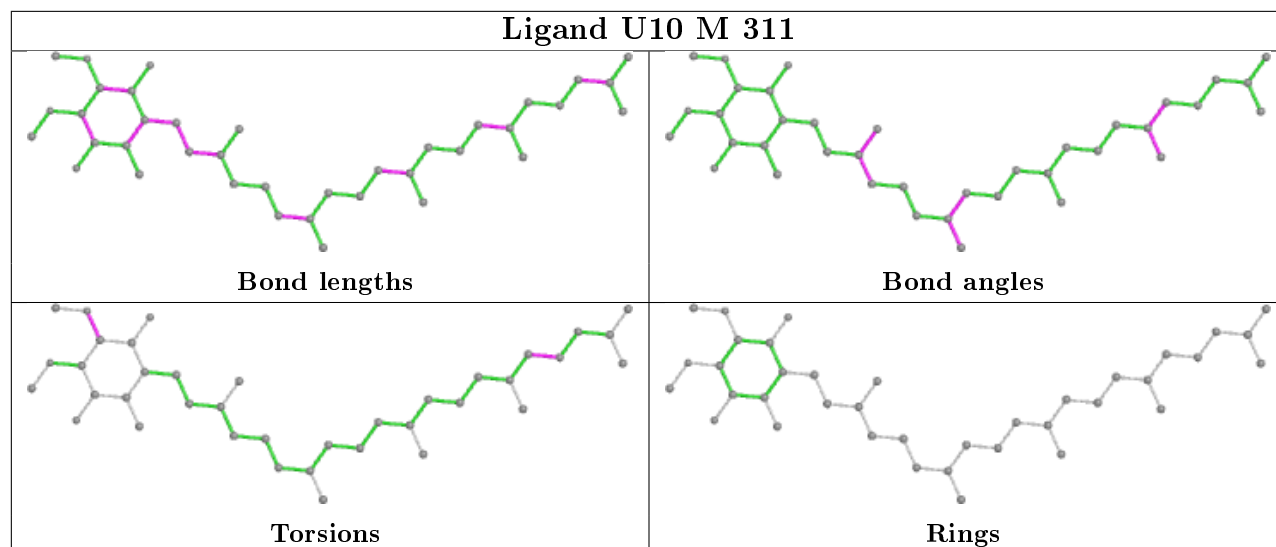
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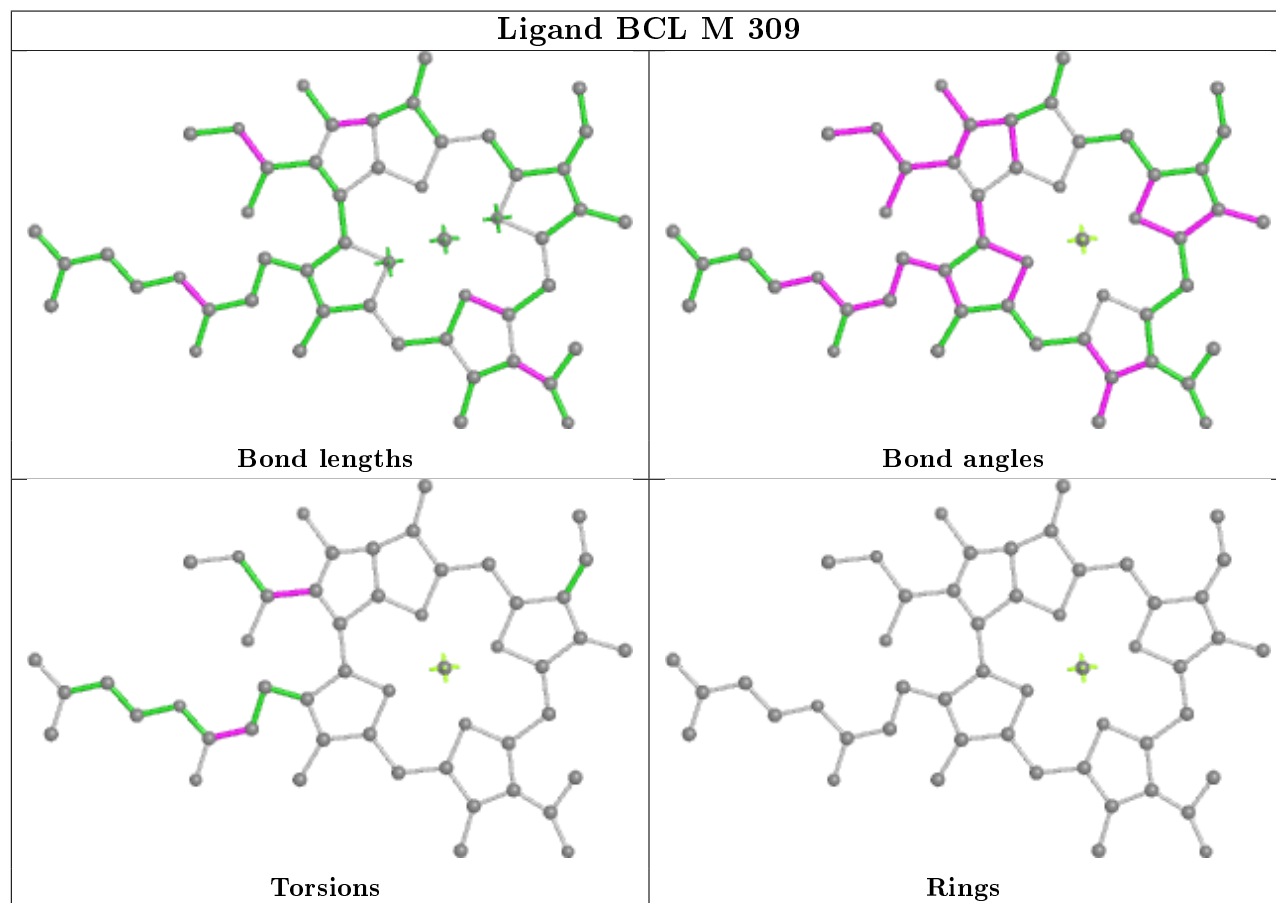
Ligand U10 S 312



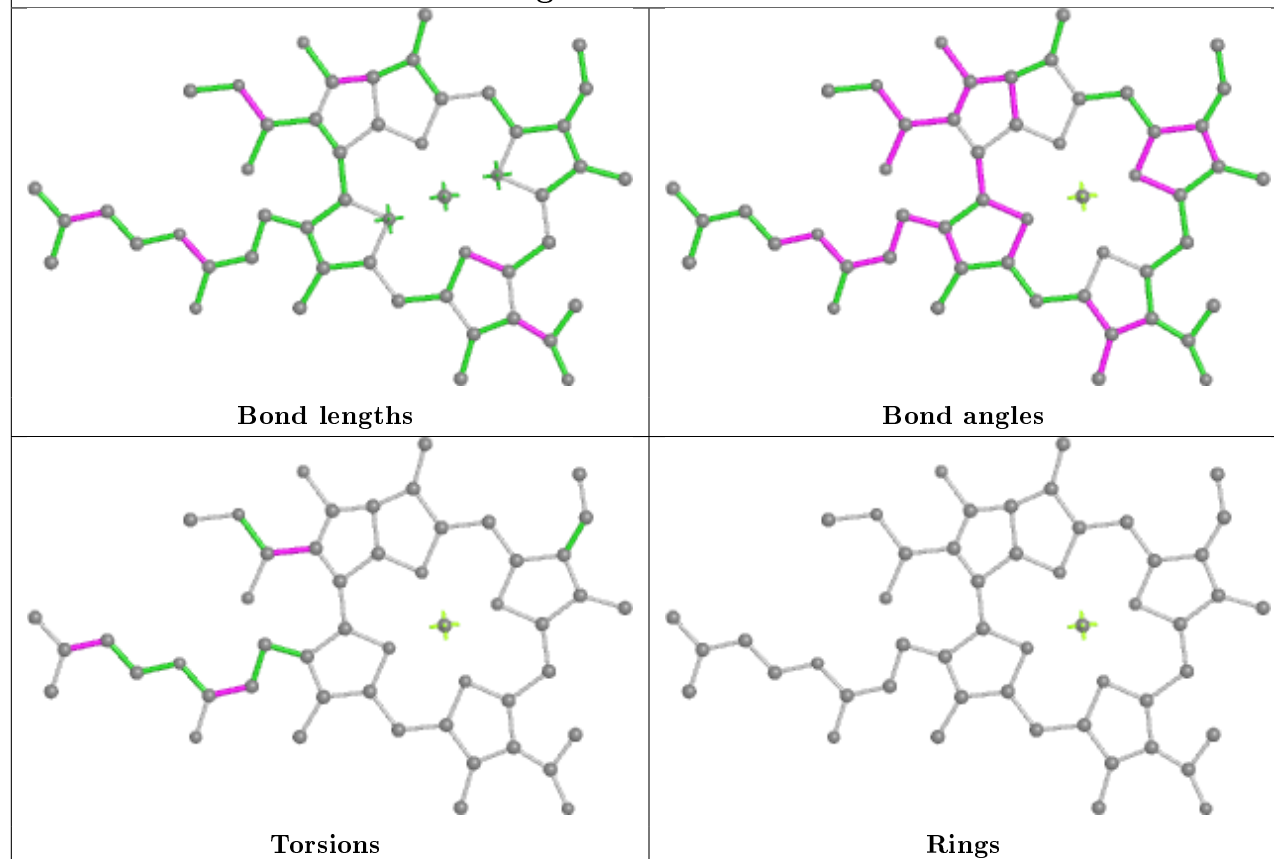
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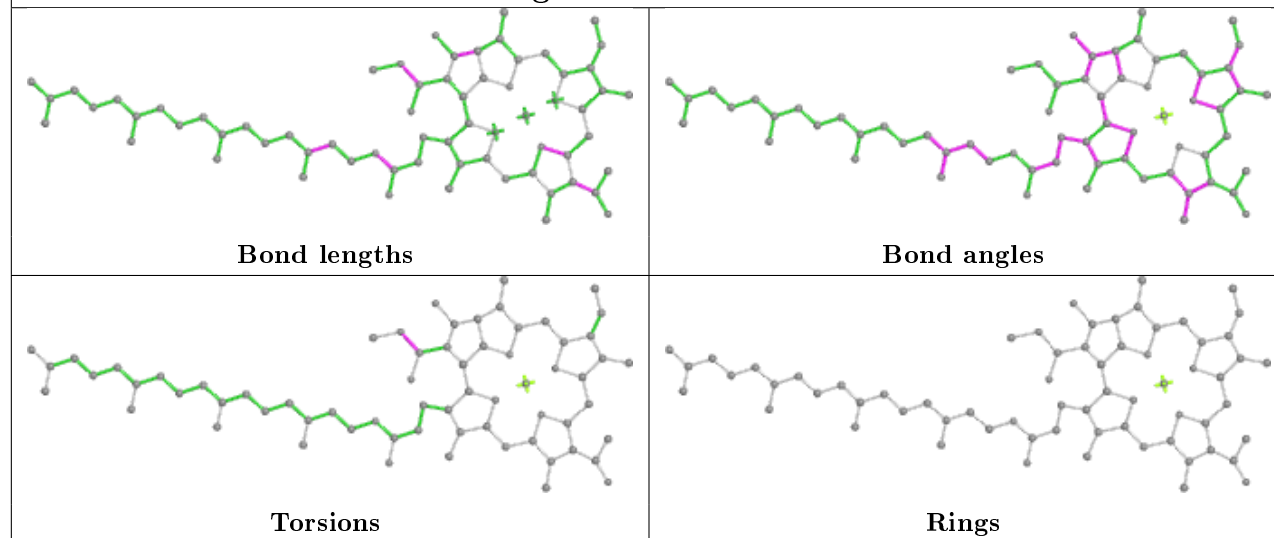
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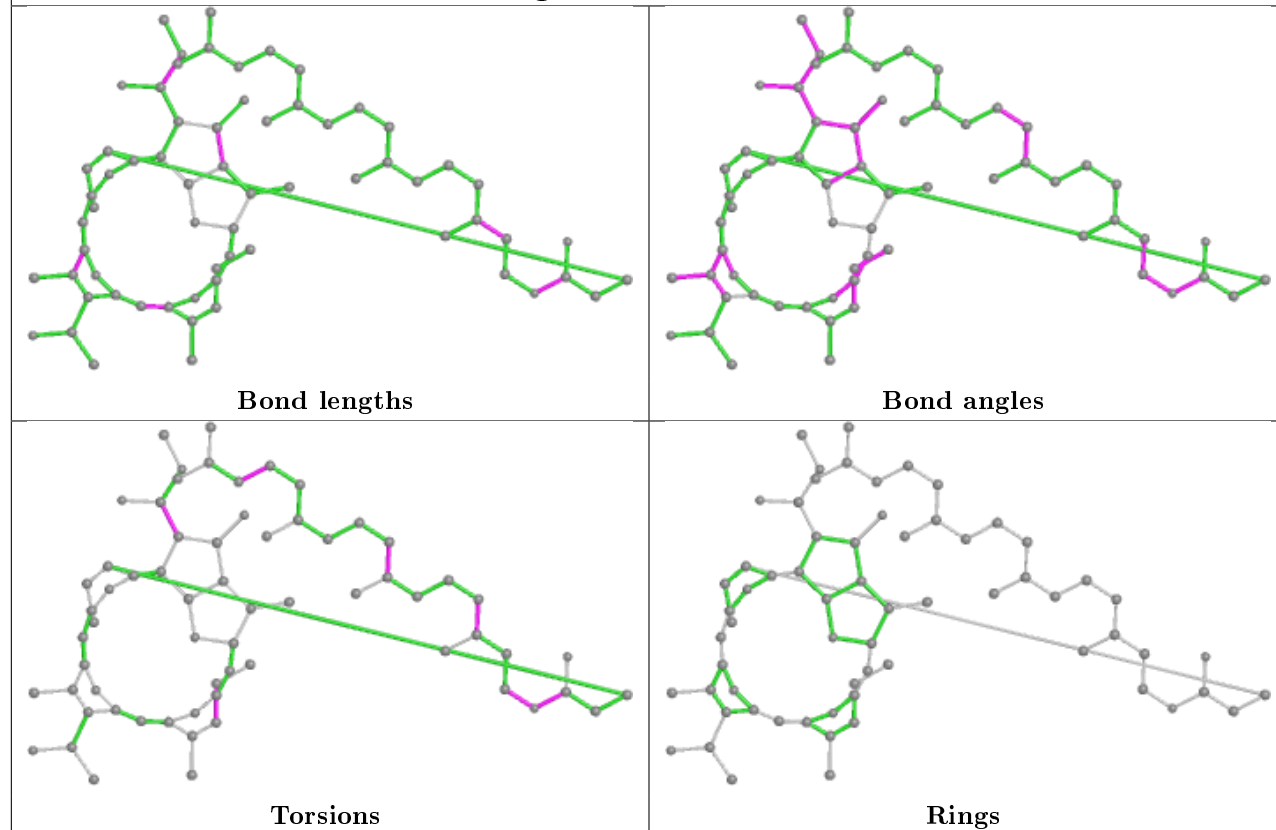
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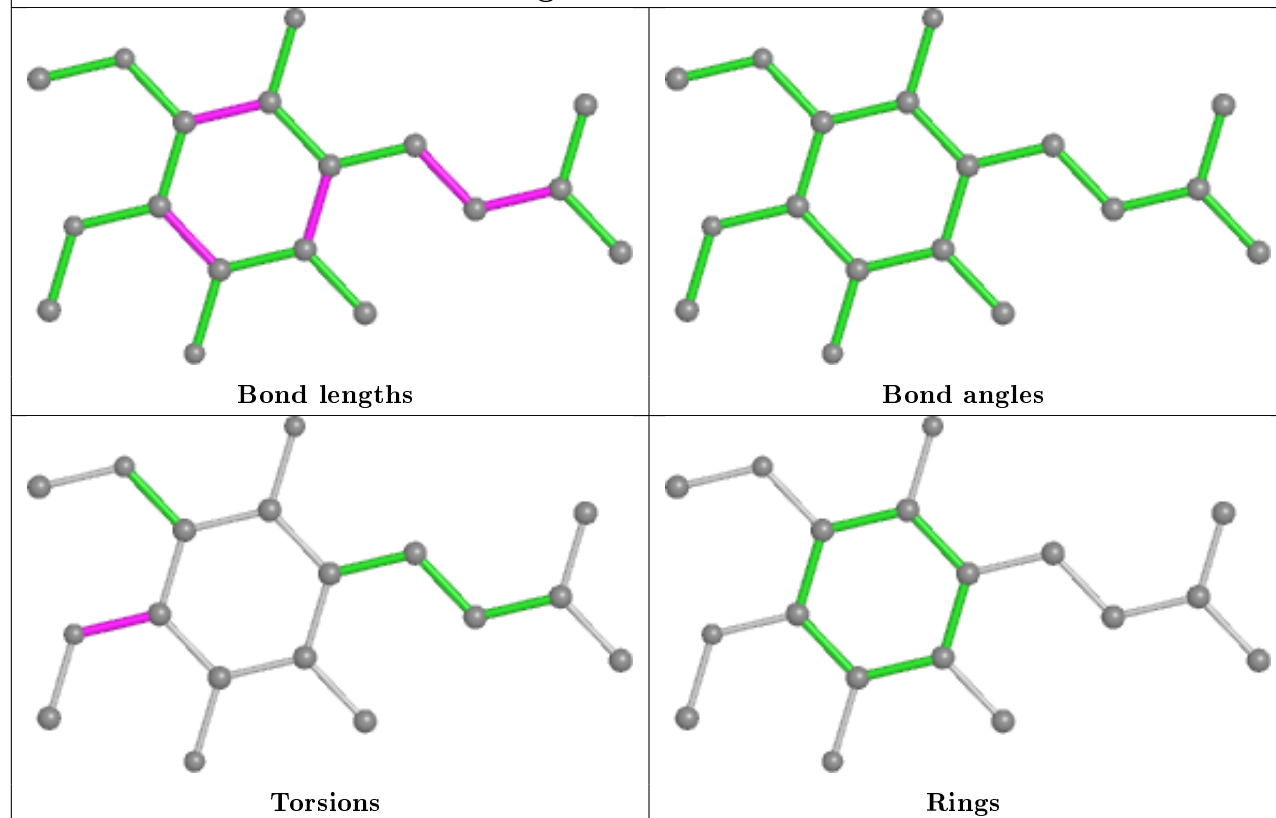
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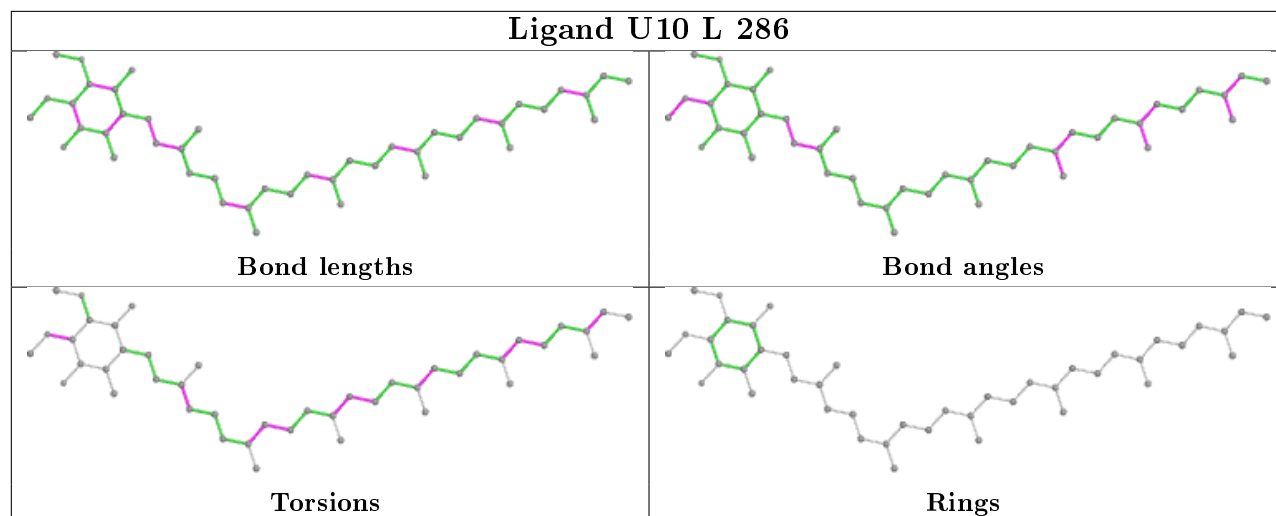
Ligand BPH L 285



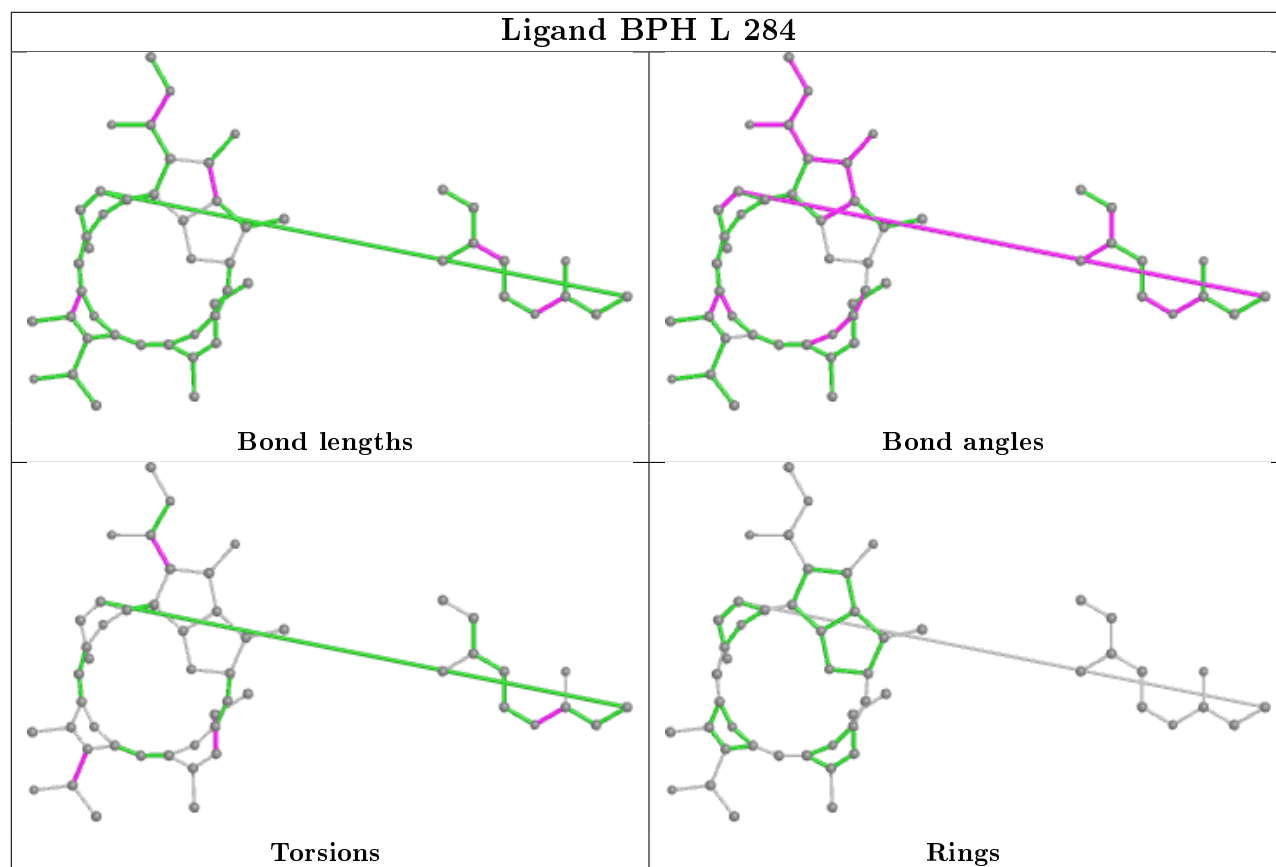
Ligand U10 R 285

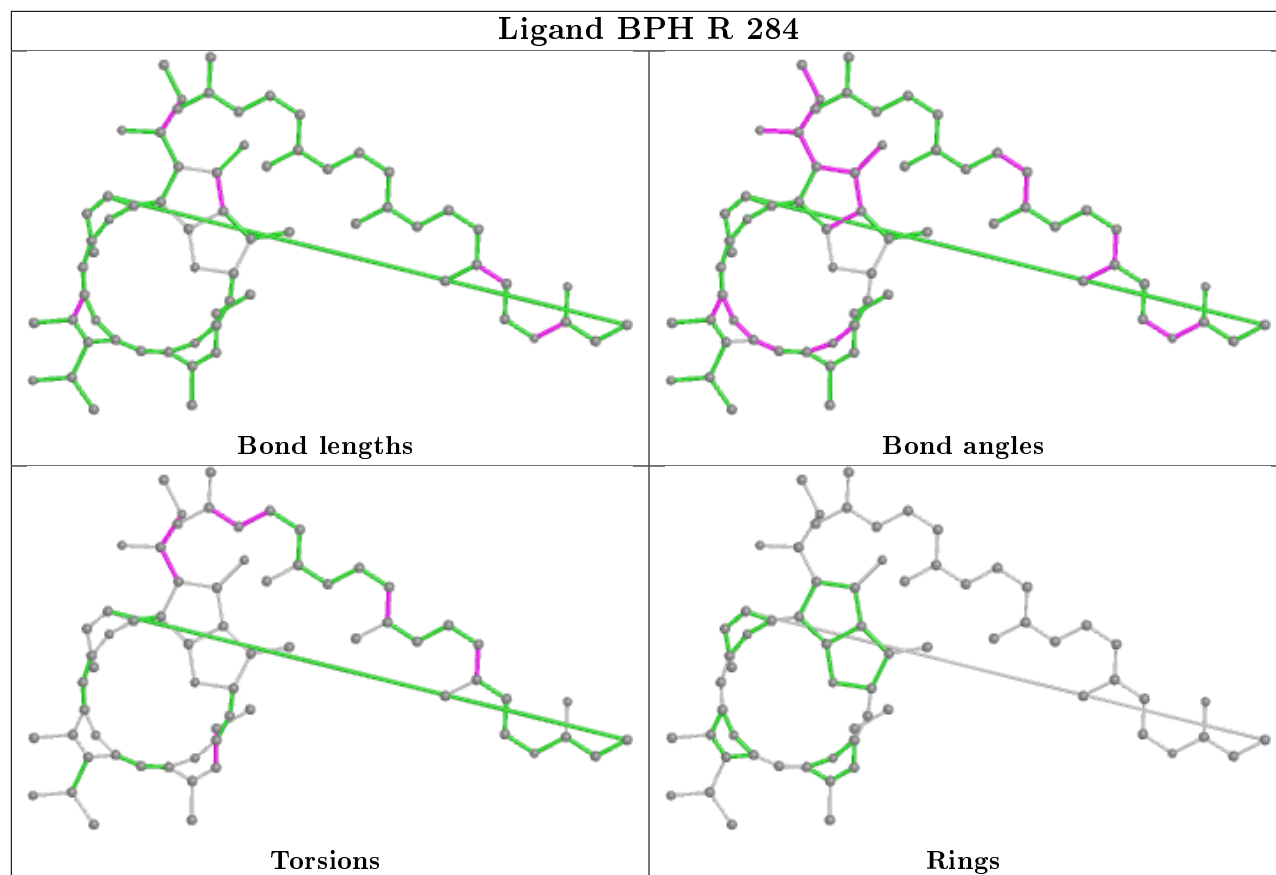


Ligand U10 L 286



Ligand BPH L 284





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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.