



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:51 AM EDT

PDB ID : 1AIJ / pdb_00001aij
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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

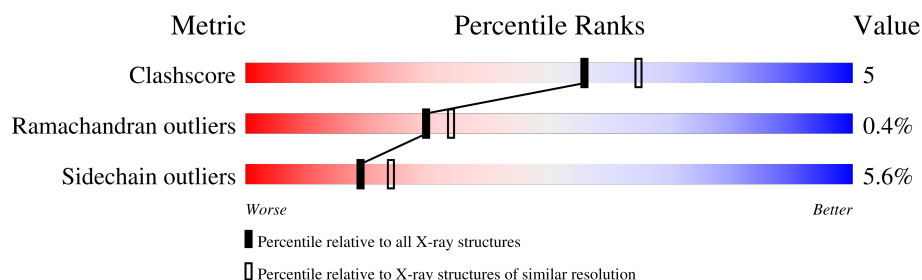
1 Overall quality at a glance

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	83% 14% .
1	R	281	80% 17% .
2	M	307	78% 17% . .
2	S	307	79% 17% . . .
3	H	260	79% 16% 5%
3	T	260	73% 19% . 5%

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			

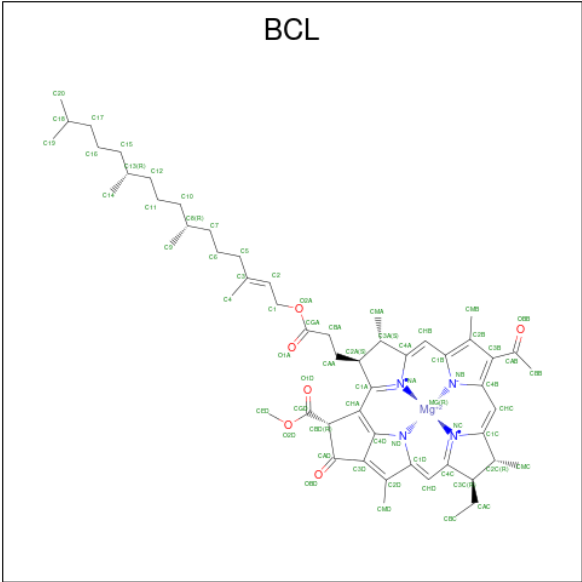
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

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:

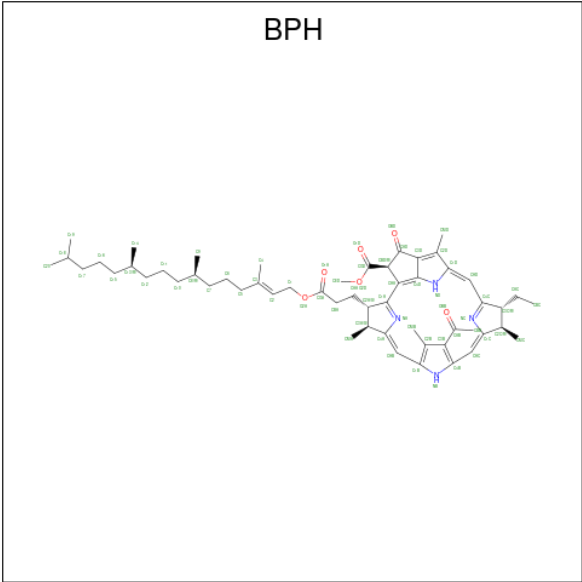
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
T	8	GLN	GLY	conflict	UNP P11846

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



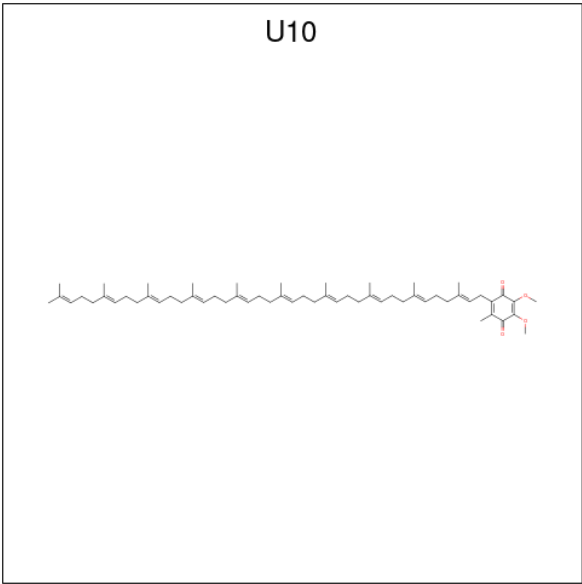
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	S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

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

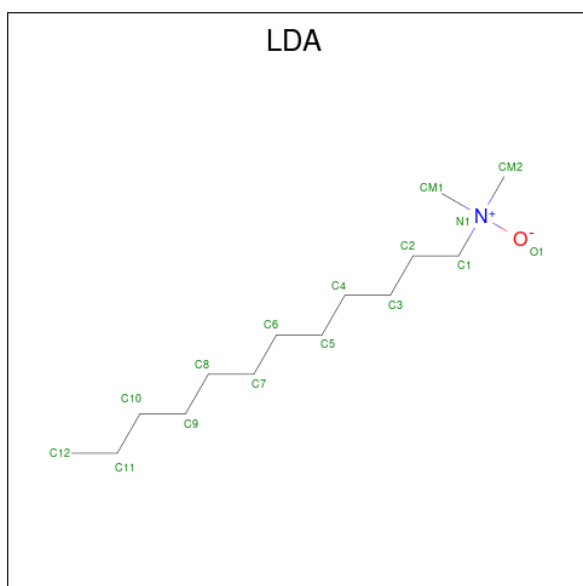


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			44	40	4		
6	M	1	Total	C	O	0	0
			38	34	4		
6	R	1	Total	C	O	0	0
			18	14	4		
6	S	1	Total	C	O	0	0
			32	28	4		

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

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

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: 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		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is water.

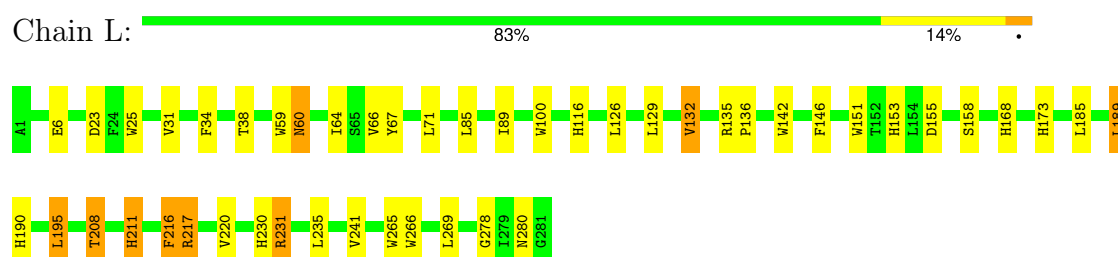
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	67	Total 67	O 67	0	0
9	M	91	Total 91	O 91	0	0
9	H	105	Total 105	O 105	0	0
9	R	56	Total 56	O 56	0	0
9	S	85	Total 85	O 85	0	0
9	T	64	Total 64	O 64	0	0

3 Residue-property plots [i](#)

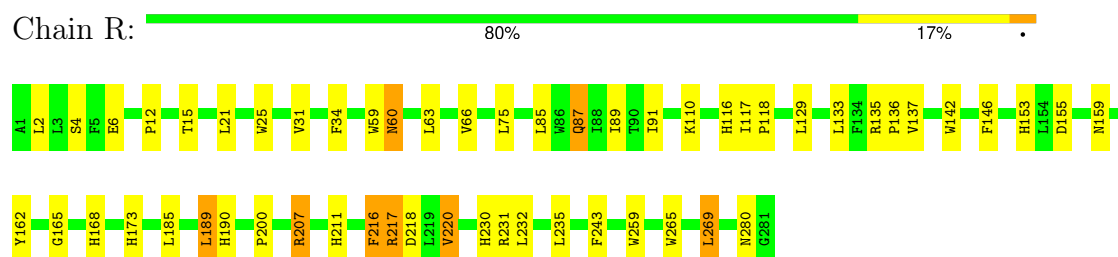
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

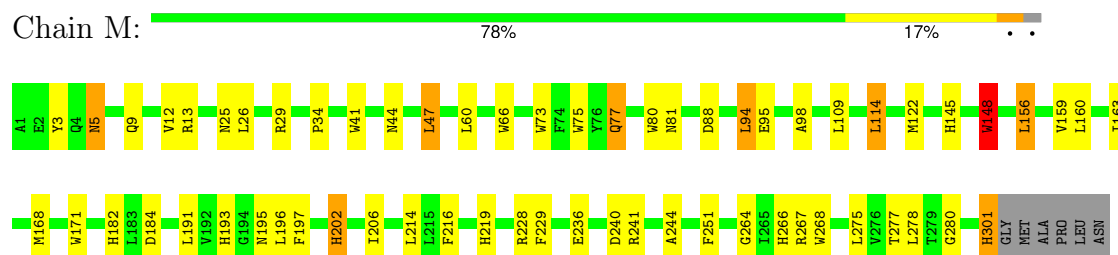
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



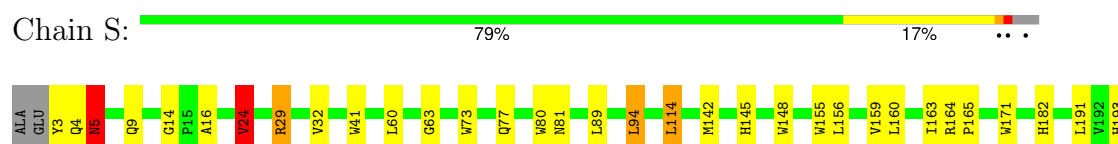
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

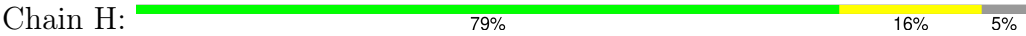


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

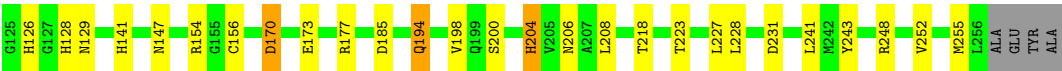




● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



● 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, U10, BCL, BPH, 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	0.86	7/2320 (0.3%)	1.55	36/3175 (1.1%)
1	R	0.86	9/2320 (0.4%)	1.55	25/3175 (0.8%)
2	M	0.85	10/2496 (0.4%)	1.54	35/3408 (1.0%)
2	S	0.86	9/2482 (0.4%)	1.58	27/3389 (0.8%)
3	H	0.79	6/1917 (0.3%)	1.46	20/2608 (0.8%)
3	T	0.80	6/1917 (0.3%)	1.45	20/2608 (0.8%)
All	All	0.84	47/13452 (0.3%)	1.53	163/18363 (0.9%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	211	HIS	CD2-NE2	-6.97	1.30	1.37
1	L	211	HIS	CD2-NE2	-6.85	1.30	1.37
3	H	128	HIS	CD2-NE2	-6.74	1.30	1.37
1	L	168	HIS	CD2-NE2	-6.68	1.30	1.37
3	T	204	HIS	CD2-NE2	-6.67	1.30	1.37
3	H	98	HIS	CD2-NE2	-6.64	1.30	1.37
3	T	126	HIS	CD2-NE2	-6.59	1.30	1.37
1	R	116	HIS	CD2-NE2	-6.57	1.30	1.37
3	T	128	HIS	CD2-NE2	-6.57	1.30	1.37
1	L	116	HIS	CD2-NE2	-6.55	1.30	1.37
2	M	301	HIS	CD2-NE2	-6.42	1.30	1.37
2	M	145	HIS	CD2-NE2	-6.38	1.30	1.37
3	T	68	HIS	CD2-NE2	-6.35	1.30	1.37
3	H	204	HIS	CD2-NE2	-6.32	1.30	1.37
3	T	98	HIS	CD2-NE2	-6.28	1.30	1.37
3	H	68	HIS	CD2-NE2	-6.25	1.30	1.37
3	T	141	HIS	CD2-NE2	-6.18	1.31	1.37
2	M	219	HIS	CD2-NE2	-6.17	1.31	1.37
1	R	190	HIS	CD2-NE2	-6.16	1.31	1.37
3	H	126	HIS	CD2-NE2	-6.14	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	193	HIS	CD2-NE2	-6.13	1.31	1.37
2	S	301	HIS	CD2-NE2	-6.02	1.31	1.37
2	M	193	HIS	CD2-NE2	-6.01	1.31	1.37
1	R	168	HIS	CD2-NE2	-5.97	1.31	1.37
2	S	145	HIS	CD2-NE2	-5.90	1.31	1.37
3	H	141	HIS	CD2-NE2	-5.88	1.31	1.37
1	L	190	HIS	CD2-NE2	-5.87	1.31	1.37
2	S	219	HIS	CD2-NE2	-5.76	1.31	1.37
2	S	266	HIS	CD2-NE2	-5.66	1.31	1.37
2	S	24	VAL	CA-CB	5.58	1.61	1.54
1	L	230	HIS	CD2-NE2	-5.36	1.31	1.37
1	R	230	HIS	CG-ND1	-5.35	1.32	1.38
2	M	202	HIS	CD2-NE2	-5.32	1.31	1.37
2	M	301	HIS	CG-ND1	-5.29	1.32	1.38
2	M	182	HIS	CD2-NE2	-5.24	1.32	1.37
1	R	173	HIS	CG-ND1	-5.21	1.32	1.38
2	S	202	HIS	CD2-NE2	-5.19	1.32	1.37
1	L	153	HIS	CD2-NE2	-5.17	1.32	1.37
1	R	153	HIS	CD2-NE2	-5.13	1.32	1.37
2	M	266	HIS	CD2-NE2	-5.10	1.32	1.37
1	L	230	HIS	CG-ND1	-5.09	1.32	1.38
2	S	182	HIS	CD2-NE2	-5.09	1.32	1.37
2	M	182	HIS	CG-ND1	-5.07	1.32	1.38
2	M	202	HIS	CG-ND1	-5.07	1.32	1.38
1	R	230	HIS	CD2-NE2	-5.06	1.32	1.37
1	R	190	HIS	CG-ND1	-5.04	1.32	1.38
2	S	202	HIS	CG-ND1	-5.02	1.32	1.38

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	153	HIS	CA-CB-CG	10.69	124.49	113.80
2	M	301	HIS	CA-CB-CG	-10.10	103.70	113.80
3	T	124	ASP	CA-CB-CG	9.82	122.42	112.60
1	L	153	HIS	CA-CB-CG	9.82	123.62	113.80
3	H	124	ASP	CA-CB-CG	9.69	122.28	112.60
2	S	182	HIS	CA-CB-CG	9.63	123.43	113.80
2	M	182	HIS	CA-CB-CG	8.96	122.75	113.80
3	T	147	ASN	OD1-CG-ND2	-8.07	114.53	122.60
2	S	77	GLN	OE1-CD-NE2	-7.73	114.87	122.60
1	L	280	ASN	CA-CB-CG	7.59	120.19	112.60
1	R	153	HIS	CB-CG-CD2	-7.46	121.51	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	153	HIS	CB-CG-CD2	-7.38	121.61	131.20
2	M	148	TRP	CG-CD2-CE3	7.21	141.11	133.90
2	S	182	HIS	CB-CG-CD2	-7.09	121.98	131.20
3	H	157	ASP	CA-CB-CG	7.03	119.63	112.60
1	R	155	ASP	CA-CB-CG	6.95	119.55	112.60
1	L	173	HIS	CA-CB-CG	6.90	120.70	113.80
1	L	146	PHE	CA-CB-CG	6.84	120.64	113.80
1	L	34	PHE	CA-CB-CG	-6.81	106.99	113.80
1	R	243	PHE	CA-CB-CG	-6.78	107.02	113.80
1	L	280	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	R	220	VAL	N-CA-CB	-6.70	104.36	112.33
1	L	155	ASP	CA-CB-CG	6.69	119.29	112.60
3	H	132	LYS	O-C-N	-6.62	117.18	121.88
1	L	211	HIS	CB-CG-CD2	-6.62	122.60	131.20
3	T	68	HIS	CB-CG-CD2	-6.55	122.69	131.20
2	M	182	HIS	CB-CG-CD2	-6.51	122.73	131.20
2	M	145	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	R	211	HIS	CB-CG-CD2	-6.46	122.80	131.20
2	S	5	ASN	N-CA-C	6.46	120.32	111.54
1	R	216	PHE	CA-CB-CG	-6.43	107.37	113.80
2	S	148	TRP	CG-CD2-CE3	6.41	140.31	133.90
1	L	116	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	L	6	GLU	N-CA-C	6.31	119.45	111.69
1	R	146	PHE	CA-CB-CG	6.29	120.09	113.80
3	H	170	ASP	CA-CB-CG	6.29	118.89	112.60
1	L	67	TYR	CA-C-N	6.24	124.21	119.66
1	L	67	TYR	C-N-CA	6.24	124.21	119.66
1	R	6	GLU	N-CA-C	6.14	118.94	111.82
2	M	148	TRP	CB-CG-CD1	-6.07	117.80	126.90
1	L	132	VAL	N-CA-CB	-6.04	101.27	111.23
3	T	96	PHE	CA-CB-CG	-6.02	107.78	113.80
2	S	148	TRP	CB-CG-CD1	-6.01	117.88	126.90
3	T	194	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	L	208	THR	CA-C-N	5.96	126.11	119.32
1	L	208	THR	C-N-CA	5.96	126.11	119.32
1	L	153	HIS	CB-CG-ND1	5.91	131.56	122.70
1	R	34	PHE	CA-CB-CG	-5.85	107.95	113.80
1	R	153	HIS	CB-CG-ND1	5.84	131.47	122.70
1	R	116	HIS	CB-CG-CD2	-5.80	123.65	131.20
1	R	280	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	R	173	HIS	CA-CB-CG	5.80	119.60	113.80
3	H	68	HIS	N-CA-C	5.80	119.42	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	5	ASN	OD1-CG-ND2	-5.76	116.84	122.60
3	H	203	VAL	N-CA-C	-5.75	100.11	108.17
3	T	52	ASN	CA-CB-CG	5.75	118.34	112.60
3	H	207	ALA	N-CA-C	5.74	118.48	111.82
3	T	126	HIS	CB-CG-CD2	-5.68	123.81	131.20
2	M	148	TRP	CE2-CD2-CG	-5.63	100.45	107.20
3	H	126	HIS	CB-CG-CD2	-5.62	123.90	131.20
3	T	147	ASN	CB-CG-ND2	5.62	124.82	116.40
3	H	135	LYS	CB-CA-C	-5.59	101.87	110.81
1	R	87	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	S	240	ASP	CA-CB-CG	5.57	118.17	112.60
2	M	160	LEU	N-CA-C	5.55	117.33	111.28
2	S	268	TRP	CG-CD2-CE3	5.54	139.44	133.90
2	M	195	ASN	OD1-CG-ND2	-5.53	117.07	122.60
3	T	185	ASP	CA-CB-CG	5.52	118.12	112.60
1	L	23	ASP	CA-CB-CG	5.51	118.11	112.60
1	L	265	TRP	CG-CD2-CE3	5.51	139.41	133.90
3	T	68	HIS	CA-CB-CG	5.47	119.27	113.80
1	L	59	TRP	CG-CD2-CE3	5.45	139.35	133.90
2	M	25	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	M	145	HIS	CB-CG-ND1	5.44	130.86	122.70
2	M	240	ASP	CA-CB-CG	5.43	118.03	112.60
2	M	251	PHE	N-CA-C	-5.42	105.06	110.97
2	M	266	HIS	CB-CG-CD2	-5.40	124.18	131.20
3	H	68	HIS	CB-CG-CD2	-5.40	124.18	131.20
3	T	68	HIS	CB-CG-ND1	5.40	130.79	122.70
3	H	44	ASN	N-CA-C	-5.39	103.57	110.53
3	T	141	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	M	77	GLN	OE1-CD-NE2	-5.39	117.21	122.60
2	M	81	ASN	CA-C-N	5.39	125.46	119.32
2	M	81	ASN	C-N-CA	5.39	125.46	119.32
1	L	211	HIS	CB-CG-ND1	5.37	130.76	122.70
2	S	148	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	L	216	PHE	CA-CB-CG	-5.36	108.44	113.80
1	R	159	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	L	59	TRP	CE2-CD2-CG	-5.31	100.83	107.20
2	M	171	TRP	CE2-CD2-CG	-5.31	100.83	107.20
3	H	141	HIS	CB-CG-CD2	-5.29	124.33	131.20
2	M	80	TRP	CE2-CD2-CG	-5.28	100.86	107.20
2	M	98	ALA	CA-C-N	5.28	125.34	119.32
2	M	98	ALA	C-N-CA	5.28	125.34	119.32
2	M	95	GLU	CA-C-N	5.26	125.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	95	GLU	C-N-CA	5.26	125.80	120.38
2	M	184	ASP	CA-CB-CG	5.26	117.86	112.60
3	T	170	ASP	N-CA-C	-5.22	100.58	108.67
1	R	259	TRP	CG-CD2-CE3	5.21	139.11	133.90
2	S	4	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	S	41	TRP	CE2-CD2-CG	-5.21	100.95	107.20
2	S	160	LEU	N-CA-C	5.21	116.64	111.07
2	M	41	TRP	CE2-CD2-CG	-5.20	100.95	107.20
3	H	204	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	R	142	TRP	CG-CD2-CE3	5.20	139.09	133.90
2	S	14	GLY	CA-C-N	5.19	125.18	119.89
2	S	14	GLY	C-N-CA	5.19	125.18	119.89
1	L	142	TRP	CE2-CD2-CG	-5.18	100.98	107.20
3	H	98	HIS	CB-CG-CD2	-5.18	124.46	131.20
3	T	243	TYR	N-CA-C	5.18	119.31	112.89
3	H	119	ASP	CA-CB-CG	5.18	117.78	112.60
3	T	204	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	R	59	TRP	CE2-CD2-CG	-5.17	101.00	107.20
3	T	120	LEU	O-C-N	-5.17	117.88	121.65
1	L	25	TRP	CG-CD2-CE3	5.16	139.06	133.90
2	S	259	ASN	OD1-CG-ND2	-5.16	117.44	122.60
3	T	21	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	R	146	PHE	CA-C-N	5.16	124.92	119.76
1	R	146	PHE	C-N-CA	5.16	124.92	119.76
2	S	80	TRP	CG-CD2-CE3	5.16	139.06	133.90
1	L	266	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	L	266	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	S	268	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	S	73	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	L	142	TRP	CB-CG-CD1	-5.14	119.19	126.90
2	M	88	ASP	CA-CB-CG	5.14	117.74	112.60
1	L	142	TRP	CG-CD2-CE3	5.12	139.02	133.90
3	T	44	ASN	N-CA-C	-5.11	102.63	110.14
2	S	81	ASN	CA-C-N	5.11	124.72	119.05
2	S	81	ASN	C-N-CA	5.11	124.72	119.05
2	M	80	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	L	25	TRP	CE2-CD2-CG	-5.09	101.09	107.20
2	S	171	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	L	59	TRP	CB-CG-CD1	-5.08	119.28	126.90
2	M	219	HIS	CB-CG-CD2	-5.08	124.59	131.20
2	S	294	TRP	CG-CD2-CE3	5.08	138.98	133.90
1	L	60	ASN	CA-C-N	5.07	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	60	ASN	C-N-CA	5.07	126.18	119.84
2	M	241	ARG	N-CA-C	5.07	117.70	110.24
3	H	249	LYS	CA-CB-CG	-5.07	103.96	114.10
2	S	80	TRP	CE2-CD2-CG	-5.07	101.11	107.20
3	T	129	ASN	OD1-CG-ND2	-5.07	117.53	122.60
2	M	73	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	S	182	HIS	CB-CG-ND1	5.07	130.30	122.70
1	R	259	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	R	142	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	L	151	TRP	CG-CD2-CE3	5.06	138.96	133.90
2	M	193	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	L	151	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	L	173	HIS	N-CA-C	-5.04	105.87	111.36
2	M	268	TRP	CG-CD2-CE3	5.04	138.94	133.90
2	M	44	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	S	219	HIS	CB-CG-CD2	-5.03	124.67	131.20
3	H	170	ASP	N-CA-C	-5.02	100.33	108.41
1	R	60	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	M	5	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	M	75	TRP	CE2-CD2-CG	-5.02	101.18	107.20
3	H	21	TRP	CE2-CD2-CG	-5.01	101.18	107.20
3	H	185	ASP	CA-CB-CG	5.01	117.61	112.60
3	T	21	TRP	CG-CD2-CE3	5.01	138.91	133.90
2	S	155	TRP	CE2-CD2-CG	-5.01	101.19	107.20
3	H	199	GLN	OE1-CD-NE2	-5.00	117.60	122.60
1	R	25	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	12	0
1	R	2232	0	2187	20	0
2	M	2404	0	2318	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	2390	0	2304	23	0
3	H	1869	0	1884	12	0
3	T	1869	0	1884	25	0
4	L	132	0	148	7	0
4	M	117	0	115	11	0
4	R	132	0	148	6	0
4	S	117	0	115	11	0
5	L	116	0	121	3	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
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	129	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 (129) 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
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:S:208:PHE:HD1	2:S:272:MET:HE3	1.54	0.70
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:HHC	4:M:309:BCL:HBB2	1.80	0.64
1:R:200:PRO:HB3	1:R:207:ARG:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:11:ASP:N	3:T:14:SER:HG	2.05	0.55
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:HHC	4:S:309:BCL:CBB	2.39	0.53
4:M:310:BCL:HHC	4:M:310:BCL:CBB	2.39	0.52
4:S:310:BCL:HHC	4:S:310:BCL:CBB	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:HHC	5:R:284:BPH:CBB	2.39	0.49
2:S:228:ARG:HA	3:T:194:GLN:CG	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:R:110:LYS:O	3:T:111:PRO:HG3	2.15	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
3:H:194:GLN:H	3:H:194:GLN:CD	2.25	0.44
4:M:309:BCL:HHC	4:M:309:BCL:CBB	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
1:L:278:GLY:HA2	2:M:77:GLN:O	2.18	0.43
4:L:282:BCL:H2C	4:M:310:BCL:H2C	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:S:211:GLY:HA3	2:S:272:MET:HE2	2.00	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
1:R:85:LEU:HD12	1:R:85:LEU:HA	1.92	0.42
2:M:109:LEU:HD22	2:M:114:LEU:HD13	2.01	0.42
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:OBB	4:R:282:BCL:HHC	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
1:L:189:LEU:HB3	6:L:286:U10:H4M3	2.02	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.20	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
5:L:285:BPH:H6C1	5:L:285:BPH:H2	1.91	0.40
3:H:196:VAL:HG12	3:H:205:VAL:HG22	2.01	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%)	18	19
1	R	279/281 (99%)	271 (97%)	6 (2%)	2 (1%)	18	19
2	M	299/307 (97%)	290 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	287 (97%)	9 (3%)	1 (0%)	36	42
3	H	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	30	34
3	T	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	30	34
All	All	1642/1696 (97%)	1592 (97%)	43 (3%)	7 (0%)	30	34

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%)	207 (94%)	13 (6%)	18	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	220/220 (100%)	208 (94%)	12 (6%)	19	24
2	M	236/240 (98%)	222 (94%)	14 (6%)	18	22
2	S	235/240 (98%)	222 (94%)	13 (6%)	19	24
3	H	199/209 (95%)	191 (96%)	8 (4%)	28	38
3	T	199/209 (95%)	186 (94%)	13 (6%)	15	18
All	All	1309/1338 (98%)	1236 (94%)	73 (6%)	19	24

All (73) 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	132	VAL
1	L	158	SER
1	L	189	LEU
1	L	195	LEU
1	L	216	PHE
1	L	217	ARG
1	L	220	VAL
1	L	231	ARG
1	L	235	LEU
1	L	269	LEU
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	47	LEU
2	M	60	LEU
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	196	LEU
2	M	216	PHE
2	M	301	HIS
3	H	12	LEU
3	H	73	LEU
3	H	82	ASP

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Mol	Chain	Res	Type
3	H	123	LEU
3	H	184	LYS
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	133	LEU
1	R	189	LEU
1	R	207	ARG
1	R	216	PHE
1	R	217	ARG
1	R	220	VAL
1	R	231	ARG
1	R	235	LEU
1	R	269	LEU
2	S	5	ASN
2	S	24	VAL
2	S	29	ARG
2	S	60	LEU
2	S	89	LEU
2	S	94	LEU
2	S	114	LEU
2	S	156	LEU
2	S	191	LEU
2	S	209	LEU
2	S	216	PHE
2	S	274	VAL
2	S	300	ASN
3	T	12	LEU
3	T	14	SER
3	T	48	THR
3	T	73	LEU
3	T	75	VAL
3	T	82	ASP
3	T	87	LEU
3	T	200	SER
3	T	208	LEU
3	T	218	THR
3	T	223	THR
3	T	228	LEU

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Mol	Chain	Res	Type
3	T	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	211	HIS
1	L	258	GLN
2	M	9	GLN
2	M	138	GLN
2	M	145	HIS
2	M	195	ASN
3	H	32	GLN
3	H	129	ASN
3	H	199	GLN
3	H	206	ASN
1	R	87	GLN
1	R	199	ASN
1	R	264	GLN
2	S	9	GLN
3	T	204	HIS
3	T	206	ASN

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 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
6	U10	R	285	-	18,18,63	1.90	5 (27%)	24,25,79	1.10	0
5	BPH	S	311	-	46,57,70	1.48	7 (15%)	42,85,101	2.98	18 (42%)
6	U10	S	312	-	32,32,63	1.66	7 (21%)	40,41,79	1.06	1 (2%)
5	BPH	R	284	-	59,70,70	1.35	7 (11%)	59,101,101	2.57	19 (32%)
4	BCL	R	283	1	69,74,74	1.06	4 (5%)	79,115,115	1.90	18 (22%)
4	BCL	S	309	2	54,59,74	1.14	4 (7%)	61,97,115	2.06	17 (27%)
8	LDA	M	313	-	13,15,15	2.53	2 (15%)	14,17,17	1.40	4 (28%)
4	BCL	S	310	2	69,74,74	1.03	4 (5%)	79,115,115	1.76	18 (22%)
6	U10	L	286	-	44,44,63	1.67	10 (22%)	54,56,79	1.29	5 (9%)
4	BCL	M	310	2	69,74,74	1.01	4 (5%)	79,115,115	1.79	20 (25%)
5	BPH	L	285	-	59,70,70	1.41	7 (11%)	59,101,101	2.65	20 (33%)
4	BCL	L	282	1	69,74,74	1.06	4 (5%)	79,115,115	1.73	19 (24%)
4	BCL	M	309	2	54,59,74	1.19	3 (5%)	61,97,115	1.98	18 (29%)
6	U10	M	311	-	38,38,63	1.65	9 (23%)	48,49,79	1.11	3 (6%)
5	BPH	L	284	-	45,56,70	1.63	7 (15%)	41,84,101	3.00	18 (43%)
4	BCL	R	282	1	69,74,74	1.02	4 (5%)	79,115,115	1.81	20 (25%)
4	BCL	L	283	1	69,74,74	1.05	4 (5%)	79,115,115	1.96	18 (22%)
8	LDA	M	312	-	13,15,15	2.47	2 (15%)	14,17,17	1.39	2 (14%)
8	LDA	M	314	-	13,15,15	2.46	2 (15%)	14,17,17	1.42	4 (28%)
8	LDA	M	315	-	13,15,15	2.47	2 (15%)	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
6	U10	R	285	-	-	1/9/33/87	0/1/1/1
5	BPH	S	311	-	-	6/22/90/105	0/5/6/6
6	U10	S	312	-	-	4/26/50/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	R	284	-	-	11/37/105/105	0/5/6/6
4	BCL	R	283	1	-	2/41/137/137	-
4	BCL	S	309	2	-	2/23/119/137	-
8	LDA	M	313	-	-	6/13/13/13	-
4	BCL	S	310	2	-	9/41/137/137	-
6	U10	L	286	-	-	14/41/65/87	0/1/1/1
4	BCL	M	310	2	-	3/41/137/137	-
5	BPH	L	285	-	-	6/37/105/105	0/5/6/6
4	BCL	L	282	1	-	3/41/137/137	-
4	BCL	M	309	2	-	2/23/119/137	-
6	U10	M	311	-	-	2/33/57/87	0/1/1/1
5	BPH	L	284	-	-	4/21/89/105	0/5/6/6
4	BCL	R	282	1	-	7/41/137/137	-
4	BCL	L	283	1	-	3/41/137/137	-
8	LDA	M	312	-	-	4/13/13/13	-
8	LDA	M	314	-	-	6/13/13/13	-
8	LDA	M	315	-	-	6/13/13/13	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	313	LDA	O1-N1	-8.23	1.22	1.42
8	M	314	LDA	O1-N1	-8.03	1.22	1.42
8	M	315	LDA	O1-N1	-8.01	1.22	1.42
8	M	312	LDA	O1-N1	-7.96	1.22	1.42
5	L	285	BPH	C3A-C2A	-5.52	1.49	1.54
5	L	284	BPH	C3A-C2A	-5.30	1.50	1.54
5	R	284	BPH	C3A-C2A	-4.84	1.50	1.54
5	L	285	BPH	C3D-CAD	-4.39	1.39	1.47
5	R	284	BPH	C3D-CAD	-4.39	1.39	1.47
5	S	311	BPH	C3D-CAD	-4.31	1.39	1.47
6	R	285	U10	C6-C1	4.11	1.42	1.35
6	M	311	U10	C6-C1	4.01	1.42	1.35
5	L	284	BPH	C3D-CAD	-4.00	1.40	1.47
6	L	286	U10	C6-C1	3.95	1.42	1.35
5	L	284	BPH	C2C-C3C	-3.81	1.51	1.54
5	S	311	BPH	C3A-C2A	-3.79	1.51	1.54
6	S	312	U10	C6-C1	3.72	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	283	BCL	O2D-CGD	-3.69	1.24	1.33
5	L	285	BPH	O2A-CGA	-3.59	1.22	1.33
4	M	310	BCL	O2D-CGD	-3.58	1.24	1.33
4	M	309	BCL	C1D-C2D	-3.54	1.38	1.45
5	S	311	BPH	O2D-CGD	-3.53	1.24	1.33
8	M	312	LDA	C1-N1	-3.52	1.47	1.51
4	R	282	BCL	O2D-CGD	-3.48	1.24	1.33
4	L	282	BCL	O2D-CGD	-3.45	1.24	1.33
8	M	315	LDA	C1-N1	-3.44	1.47	1.51
5	R	284	BPH	O2A-CGA	-3.43	1.23	1.33
4	M	309	BCL	O2D-CGD	-3.42	1.24	1.33
8	M	313	LDA	C1-N1	-3.42	1.48	1.51
5	R	284	BPH	O2D-CGD	-3.41	1.24	1.33
4	S	310	BCL	O2D-CGD	-3.40	1.24	1.33
4	S	310	BCL	O2A-CGA	-3.40	1.23	1.33
4	S	309	BCL	O2D-CGD	-3.37	1.24	1.33
5	L	284	BPH	O2A-CGA	-3.37	1.23	1.33
4	M	309	BCL	O2A-CGA	-3.35	1.23	1.33
4	L	283	BCL	O2D-CGD	-3.35	1.25	1.33
5	L	285	BPH	O2D-CGD	-3.34	1.25	1.33
8	M	314	LDA	C1-N1	-3.32	1.48	1.51
5	S	311	BPH	O2A-CGA	-3.27	1.23	1.33
4	L	282	BCL	C1D-C2D	-3.26	1.38	1.45
4	M	310	BCL	O2A-CGA	-3.23	1.24	1.33
5	L	284	BPH	O2D-CGD	-3.23	1.25	1.33
4	S	309	BCL	O2A-CGA	-3.22	1.24	1.33
4	S	310	BCL	C1D-C2D	-3.20	1.39	1.45
4	R	282	BCL	C1D-C2D	-3.19	1.39	1.45
4	R	283	BCL	C1D-C2D	-3.17	1.39	1.45
4	S	309	BCL	C1D-C2D	-3.17	1.39	1.45
5	S	311	BPH	C2C-C3C	-3.11	1.52	1.54
4	M	310	BCL	C1D-C2D	-3.10	1.39	1.45
6	L	286	U10	C8-C9	3.09	1.40	1.33
6	R	285	U10	C7-C8	-3.09	1.45	1.50
6	S	312	U10	C4-C5	-3.08	1.39	1.48
4	R	282	BCL	O2A-CGA	-3.08	1.24	1.33
4	L	283	BCL	C1D-C2D	-3.06	1.39	1.45
4	L	282	BCL	O2A-CGA	-2.99	1.24	1.33
4	L	283	BCL	O2A-CGA	-2.98	1.24	1.33
5	R	284	BPH	C3B-CAB	-2.95	1.41	1.49
6	L	286	U10	C18-C19	2.92	1.39	1.33
6	L	286	U10	C28-C29	2.92	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	285	U10	C3-C2	-2.90	1.40	1.48
6	M	311	U10	C4-C5	-2.90	1.40	1.48
5	L	284	BPH	C3B-CAB	-2.87	1.41	1.49
5	L	285	BPH	C3B-CAB	-2.84	1.41	1.49
6	M	311	U10	C18-C19	2.84	1.39	1.33
6	L	286	U10	C3-C2	-2.83	1.40	1.48
5	S	311	BPH	C3B-CAB	-2.80	1.41	1.49
6	S	312	U10	C7-C8	-2.79	1.46	1.50
4	R	282	BCL	C2-C3	2.78	1.39	1.33
4	R	283	BCL	O2A-CGA	-2.77	1.25	1.33
6	S	312	U10	C18-C19	2.76	1.39	1.33
6	S	312	U10	C3-C2	-2.76	1.40	1.48
6	L	286	U10	C33-C34	2.75	1.39	1.33
6	M	311	U10	C3-C2	-2.75	1.40	1.48
6	M	311	U10	C7-C8	-2.75	1.46	1.50
4	L	282	BCL	C2-C3	2.71	1.39	1.33
6	M	311	U10	C23-C24	2.70	1.39	1.33
6	S	312	U10	C8-C9	2.66	1.39	1.33
5	L	285	BPH	C2-C3	2.65	1.39	1.33
5	R	284	BPH	C2-C3	2.64	1.39	1.33
6	L	286	U10	C13-C14	2.63	1.39	1.33
5	L	284	BPH	C2-C3	2.58	1.39	1.33
6	S	312	U10	C13-C14	2.55	1.38	1.33
4	L	283	BCL	C2-C3	2.53	1.38	1.33
6	L	286	U10	C23-C24	2.53	1.38	1.33
4	R	283	BCL	C2-C3	2.50	1.38	1.33
5	R	284	BPH	C2C-C3C	-2.48	1.52	1.54
6	L	286	U10	C4-C5	-2.45	1.41	1.48
5	S	311	BPH	C2-C3	2.45	1.38	1.33
6	L	286	U10	C7-C8	-2.45	1.46	1.50
6	R	285	U10	C4-C5	-2.42	1.41	1.48
6	M	311	U10	C8-C9	2.35	1.38	1.33
4	S	310	BCL	C2-C3	2.35	1.38	1.33
6	M	311	U10	C28-C29	2.29	1.39	1.32
6	M	311	U10	C13-C14	2.28	1.38	1.33
6	R	285	U10	C8-C9	2.26	1.39	1.32
4	S	309	BCL	C2-C3	2.21	1.39	1.32
4	M	310	BCL	C2-C3	2.15	1.38	1.33
5	L	285	BPH	CBD-CGD	2.04	1.55	1.52

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	311	BPH	O2D-CGD-CBD	7.66	119.36	110.95
5	R	284	BPH	O2D-CGD-CBD	7.53	119.22	110.95
5	S	311	BPH	C3D-C4D-ND	7.38	117.16	107.71
5	L	284	BPH	O2D-CGD-CBD	7.26	118.92	110.95
5	L	284	BPH	C4D-CHA-CBD	-7.15	105.02	108.45
5	R	284	BPH	C4D-CHA-CBD	-7.11	105.05	108.45
4	R	283	BCL	C1C-NC-C4C	7.09	109.91	106.68
4	L	283	BCL	C1C-NC-C4C	7.04	109.89	106.68
5	R	284	BPH	C3D-C4D-ND	6.99	116.67	107.71
5	S	311	BPH	C4D-CHA-CBD	-6.93	105.13	108.45
5	L	285	BPH	O2D-CGD-CBD	6.83	118.45	110.95
5	L	284	BPH	C3D-C4D-ND	6.61	116.18	107.71
5	L	285	BPH	C3D-C4D-ND	6.56	116.11	107.71
5	L	285	BPH	CBC-CAC-C3C	6.49	126.53	113.78
4	S	309	BCL	C1C-NC-C4C	6.42	109.61	106.68
5	L	285	BPH	C4D-CHA-CBD	-6.40	105.39	108.45
4	M	309	BCL	C1C-NC-C4C	6.08	109.45	106.68
5	R	284	BPH	C4D-ND-C1D	-6.06	101.61	108.87
5	S	311	BPH	C4D-ND-C1D	-5.98	101.70	108.87
5	L	284	BPH	C2B-C1B-NB	5.96	113.74	109.43
4	R	282	BCL	C1C-NC-C4C	5.81	109.33	106.68
5	L	285	BPH	C2B-C1B-NB	5.69	113.55	109.43
5	L	285	BPH	C4D-ND-C1D	-5.61	102.16	108.87
5	L	284	BPH	C4D-ND-C1D	-5.58	102.19	108.87
5	R	284	BPH	C2B-C1B-NB	5.41	113.34	109.43
4	S	310	BCL	C1C-NC-C4C	5.20	109.05	106.68
4	L	282	BCL	C1C-NC-C4C	5.06	108.99	106.68
4	M	310	BCL	C1C-NC-C4C	4.92	108.92	106.68
5	S	311	BPH	C2B-C1B-NB	4.92	112.98	109.43
5	R	284	BPH	O1D-CGD-CBD	-4.89	117.31	124.72
4	L	283	BCL	C1D-ND-C4D	-4.83	102.92	106.31
5	L	285	BPH	C3D-CAD-CBD	4.66	113.74	107.61
5	S	311	BPH	O1D-CGD-CBD	-4.64	117.69	124.72
5	L	284	BPH	O1D-CGD-CBD	-4.61	117.74	124.72
4	S	310	BCL	C4D-CHA-C1A	4.58	126.70	121.24
4	R	283	BCL	C1D-ND-C4D	-4.52	103.14	106.31
4	L	283	BCL	O2D-CGD-CBD	4.48	119.07	111.23
4	L	283	BCL	C4D-CHA-C1A	4.45	126.55	121.24
4	S	309	BCL	O2D-CGD-CBD	4.45	119.00	111.23
4	S	309	BCL	C4D-CHA-C1A	4.44	126.55	121.24
4	S	310	BCL	C4D-C3D-CAD	-4.42	103.31	108.11
4	M	310	BCL	C4D-CHA-C1A	4.40	126.49	121.24
4	M	309	BCL	C4D-C3D-CAD	-4.35	103.38	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	309	BCL	C4D-CHA-C1A	4.35	126.43	121.24
4	S	309	BCL	C4D-C3D-CAD	-4.34	103.39	108.11
4	R	283	BCL	C4D-C3D-CAD	-4.32	103.41	108.11
4	R	282	BCL	C4D-CHA-C1A	4.31	126.39	121.24
4	M	310	BCL	C4D-C3D-CAD	-4.23	103.51	108.11
4	R	283	BCL	C4D-CHA-C1A	4.21	126.27	121.24
4	L	282	BCL	C4D-CHA-C1A	4.12	126.16	121.24
5	L	284	BPH	C1B-NB-C4B	-4.12	102.82	108.82
5	L	285	BPH	CMB-C2B-C3B	4.10	132.87	124.68
4	L	283	BCL	C4D-C3D-CAD	-4.07	103.69	108.11
5	R	284	BPH	C3D-CAD-CBD	4.03	112.91	107.61
4	L	283	BCL	C3D-C4D-ND	4.01	116.51	109.99
4	R	282	BCL	C1D-ND-C4D	-4.00	103.50	106.31
4	L	283	BCL	C4A-NA-C1A	3.97	108.49	106.68
4	L	282	BCL	C4D-C3D-CAD	-3.96	103.80	108.11
4	R	282	BCL	C4D-C3D-CAD	-3.95	103.82	108.11
5	L	285	BPH	O1D-CGD-CBD	-3.95	118.73	124.72
4	R	283	BCL	C3D-C4D-ND	3.95	116.40	109.99
4	M	310	BCL	O2D-CGD-CBD	3.95	118.13	111.23
4	S	310	BCL	O2D-CGD-CBD	3.93	118.10	111.23
4	M	309	BCL	O2D-CGD-CBD	3.84	117.94	111.23
5	S	311	BPH	C1B-NB-C4B	-3.83	103.24	108.82
5	R	284	BPH	C1-O2A-CGA	3.82	125.91	116.65
5	S	311	BPH	C3D-CAD-CBD	3.82	112.64	107.61
4	L	282	BCL	C1D-ND-C4D	-3.82	103.63	106.31
4	M	310	BCL	C1D-ND-C4D	-3.79	103.65	106.31
4	R	283	BCL	C4A-NA-C1A	3.76	108.39	106.68
5	L	284	BPH	C3D-CAD-CBD	3.70	112.48	107.61
5	L	285	BPH	C1-O2A-CGA	3.64	125.47	116.65
4	S	309	BCL	C1D-ND-C4D	-3.63	103.77	106.31
4	L	282	BCL	C3D-C4D-ND	3.62	115.86	109.99
5	R	284	BPH	CMC-C2C-C1C	-3.61	106.83	114.61
4	R	282	BCL	C3D-C4D-ND	3.61	115.85	109.99
4	M	310	BCL	C3D-C4D-ND	3.61	115.85	109.99
4	S	309	BCL	O1D-CGD-CBD	-3.54	117.53	124.52
5	S	311	BPH	C3B-C4B-NB	3.51	113.15	108.05
4	S	309	BCL	C3D-C4D-ND	3.51	115.69	109.99
5	L	285	BPH	CMC-C2C-C1C	-3.50	107.08	114.61
4	M	309	BCL	C3D-C4D-ND	3.46	115.61	109.99
4	R	282	BCL	CED-O2D-CGD	3.46	123.76	115.92
5	R	284	BPH	C1B-NB-C4B	-3.43	103.82	108.82
4	M	310	BCL	C4-C3-C5	3.37	121.08	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	310	BCL	C3D-C4D-ND	3.36	115.44	109.99
4	M	309	BCL	C1D-ND-C4D	-3.35	103.96	106.31
5	R	284	BPH	OBD-CAD-C3D	-3.34	122.69	127.89
4	L	283	BCL	O1D-CGD-CBD	-3.32	117.97	124.52
5	L	285	BPH	C1B-NB-C4B	-3.32	103.98	108.82
5	L	284	BPH	C3B-C4B-NB	3.28	112.83	108.05
5	L	284	BPH	CMB-C2B-C3B	3.28	131.25	124.68
4	M	310	BCL	C4A-NA-C1A	3.26	108.17	106.68
4	S	309	BCL	C1-O2A-CGA	3.23	124.46	116.65
5	L	285	BPH	OBD-CAD-C3D	-3.22	122.87	127.89
4	L	282	BCL	CED-O2D-CGD	3.20	123.18	115.92
5	L	284	BPH	C1-O2A-CGA	3.19	124.38	116.65
5	L	284	BPH	CMC-C2C-C1C	-3.18	107.77	114.61
5	S	311	BPH	C1-O2A-CGA	3.17	124.33	116.65
5	S	311	BPH	OBD-CAD-C3D	-3.17	122.95	127.89
4	M	309	BCL	C4A-NA-C1A	3.17	108.12	106.68
6	L	286	U10	C25-C24-C26	3.15	120.70	115.23
4	S	310	BCL	C1D-ND-C4D	-3.14	104.11	106.31
4	R	283	BCL	C1-C2-C3	-3.13	121.07	126.20
4	R	282	BCL	C4A-NA-C1A	3.13	108.11	106.68
4	S	309	BCL	C4A-NA-C1A	3.12	108.10	106.68
4	R	282	BCL	CBC-CAC-C3C	3.12	120.03	113.41
4	S	309	BCL	C3D-C2D-C1D	3.12	110.09	105.83
5	R	284	BPH	C2D-C1D-ND	3.12	111.68	109.43
5	S	311	BPH	CMB-C2B-C3B	3.09	130.85	124.68
4	M	310	BCL	C3D-C2D-C1D	3.07	110.02	105.83
5	S	311	BPH	CMA-C3A-C4A	-3.05	108.04	114.61
4	L	282	BCL	C3D-C2D-C1D	3.05	109.99	105.83
5	L	284	BPH	C4-C3-C5	3.04	119.71	116.13
4	S	310	BCL	C3D-C2D-C1D	3.04	109.98	105.83
5	L	285	BPH	CMA-C3A-C4A	-3.04	108.07	114.61
4	R	283	BCL	C3D-C2D-C1D	3.04	109.97	105.83
4	L	283	BCL	C1-C2-C3	-3.02	121.24	126.20
4	S	310	BCL	C4A-NA-C1A	3.01	108.05	106.68
4	R	282	BCL	C3D-C2D-C1D	2.98	109.90	105.83
4	M	309	BCL	C3D-C2D-C1D	2.96	109.86	105.83
4	R	283	BCL	CAA-CBA-CGA	2.93	121.54	113.21
4	M	309	BCL	CAA-CBA-CGA	2.93	121.53	113.21
4	S	310	BCL	C1-O2A-CGA	2.91	123.68	116.65
4	L	283	BCL	C3D-C2D-C1D	2.88	109.76	105.83
5	L	284	BPH	CMA-C3A-C4A	-2.87	108.43	114.61
5	S	311	BPH	CMC-C2C-C1C	-2.86	108.46	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	309	BCL	O1D-CGD-CBD	-2.85	118.89	124.52
4	S	310	BCL	C4-C3-C5	2.82	120.13	115.23
4	L	283	BCL	CHA-C4D-ND	-2.82	126.72	132.55
4	M	309	BCL	CAA-C2A-C3A	-2.80	105.44	113.00
5	R	284	BPH	CMA-C3A-C4A	-2.79	108.59	114.61
6	L	286	U10	C30-C29-C31	2.79	120.07	115.23
4	R	283	BCL	CHA-C4D-ND	-2.79	126.80	132.55
5	S	311	BPH	C4-C3-C5	2.78	120.05	115.23
4	L	282	BCL	C7-C6-C5	-2.77	105.88	113.26
5	L	285	BPH	CED-O2D-CGD	2.76	122.18	115.92
5	L	285	BPH	C11-C10-C8	-2.76	106.80	115.97
6	M	311	U10	C15-C14-C16	2.73	119.97	115.23
8	M	312	LDA	O1-N1-C1	2.67	115.82	109.27
4	R	283	BCL	CAA-C2A-C3A	-2.63	105.88	113.00
6	L	286	U10	C7-C8-C9	-2.62	122.32	126.83
6	L	286	U10	C35-C34-C36	2.61	119.20	116.13
6	L	286	U10	C3M-O3-C3	2.60	125.62	116.47
5	L	284	BPH	CED-O2D-CGD	2.60	121.82	115.92
4	S	310	BCL	CHC-C4B-NB	-2.58	120.19	124.05
8	M	315	LDA	O1-N1-C1	2.57	115.58	109.27
4	S	310	BCL	CED-O2D-CGD	2.57	121.75	115.92
4	S	309	BCL	OBD-CAD-C3D	-2.57	122.41	128.42
5	L	285	BPH	C2D-C1D-ND	2.55	111.28	109.43
4	R	283	BCL	CMB-C2B-C1B	-2.55	121.53	125.42
8	M	314	LDA	O1-N1-C1	2.55	115.53	109.27
4	R	282	BCL	CHA-C4D-ND	-2.54	127.31	132.55
4	L	282	BCL	CHA-C1A-NA	-2.53	120.65	126.39
4	R	283	BCL	C2B-C1B-NB	2.51	112.93	110.33
8	M	313	LDA	O1-N1-C1	2.50	115.42	109.27
4	L	283	BCL	OBD-CAD-C3D	-2.50	122.57	128.42
4	R	282	BCL	C7-C6-C5	-2.49	106.63	113.26
4	S	309	BCL	CAA-C2A-C3A	-2.48	106.28	113.00
4	L	283	BCL	CED-O2D-CGD	2.48	121.54	115.92
4	L	282	BCL	CHA-C4D-ND	-2.48	127.44	132.55
4	M	310	BCL	CHA-C4D-ND	-2.47	127.45	132.55
4	R	282	BCL	OBD-CAD-C3D	-2.47	122.64	128.42
4	S	309	BCL	CAA-CBA-CGA	2.47	120.21	113.21
5	R	284	BPH	CED-O2D-CGD	2.46	121.50	115.92
4	S	309	BCL	CHA-C4D-ND	-2.45	127.50	132.55
5	R	284	BPH	C11-C10-C8	-2.44	107.86	115.97
4	R	282	BCL	CHA-C1A-NA	-2.43	120.89	126.39
4	R	282	BCL	CMA-C3A-C4A	-2.43	105.25	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	282	BCL	C16-C15-C13	-2.41	107.94	115.97
4	R	282	BCL	CAC-C3C-C4C	-2.41	107.23	112.58
4	M	310	BCL	CHC-C4B-NB	-2.41	120.44	124.05
4	L	283	BCL	C2B-C1B-NB	2.40	112.82	110.33
4	M	309	BCL	CHA-C4D-ND	-2.40	127.60	132.55
4	L	282	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
5	R	284	BPH	C3B-C4B-NB	2.38	111.52	108.05
5	L	284	BPH	OBD-CAD-C3D	-2.38	124.18	127.89
4	L	283	BCL	CAA-C2A-C3A	-2.37	106.58	113.00
4	S	310	BCL	CHA-C1A-NA	-2.36	121.04	126.39
4	M	310	BCL	CHA-C1A-NA	-2.36	121.04	126.39
5	L	284	BPH	CAA-C2A-C3A	-2.35	106.64	113.00
4	M	309	BCL	C1-O2A-CGA	2.35	122.33	116.65
5	S	311	BPH	CED-O2D-CGD	2.34	121.21	115.92
5	R	284	BPH	CMB-C2B-C3B	2.32	129.31	124.68
4	S	310	BCL	O1D-CGD-CBD	-2.32	119.95	124.52
5	L	285	BPH	C3B-C4B-NB	2.31	111.42	108.05
4	S	310	BCL	CHA-C4D-ND	-2.30	127.81	132.55
4	S	310	BCL	CAA-C2A-C3A	-2.29	106.82	113.00
4	M	310	BCL	C1-O2A-CGA	2.28	122.18	116.65
4	M	309	BCL	CED-O2D-CGD	2.27	121.07	115.92
4	R	282	BCL	C2B-C1B-NB	2.26	112.67	110.33
4	M	309	BCL	CHA-C1A-NA	-2.26	121.27	126.39
4	M	310	BCL	C4-C3-C2	-2.26	117.83	123.63
5	L	285	BPH	C1C-C2C-C3C	2.25	104.98	102.84
4	R	283	BCL	CHC-C4B-NB	-2.25	120.68	124.05
4	R	283	BCL	C4-C3-C5	2.24	119.11	115.23
4	L	283	BCL	C4-C3-C5	2.23	119.10	115.23
4	R	283	BCL	OBD-CAD-C3D	-2.22	123.23	128.42
5	S	311	BPH	C4A-C3A-C2A	2.22	104.95	102.84
4	R	282	BCL	C4-C3-C5	2.21	119.06	115.23
6	M	311	U10	C25-C24-C26	2.20	119.05	115.23
4	M	310	BCL	C16-C15-C13	2.20	123.29	115.97
4	S	309	BCL	CHC-C4B-NB	-2.19	120.76	124.05
5	L	284	BPH	C2D-C1D-ND	2.18	111.01	109.43
8	M	313	LDA	C6-C5-C4	-2.18	103.34	114.37
4	R	283	BCL	CMB-C2B-C3B	2.17	132.51	125.67
8	M	315	LDA	C4-C3-C2	-2.17	103.40	114.37
8	M	315	LDA	C6-C5-C4	-2.17	103.42	114.37
4	L	282	BCL	OBD-CAD-C3D	-2.16	123.36	128.42
4	S	309	BCL	CHA-C1A-NA	-2.16	121.50	126.39
4	L	282	BCL	OBB-CAB-CBB	-2.16	114.94	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	285	BPH	O2A-C1-C2	-2.16	99.81	108.11
6	S	312	U10	C10-C9-C11	2.15	118.97	115.23
8	M	314	LDA	C6-C5-C4	-2.15	103.50	114.37
4	L	282	BCL	C4-C3-C5	2.15	118.95	115.23
4	L	282	BCL	CHC-C4B-NB	-2.14	120.84	124.05
5	R	284	BPH	C6-C5-C3	-2.12	108.29	113.47
4	L	283	BCL	CAA-CBA-CGA	2.12	119.22	113.21
8	M	313	LDA	C4-C3-C2	-2.11	103.72	114.37
4	L	282	BCL	CAC-C3C-C4C	-2.10	107.92	112.58
6	M	311	U10	C10-C9-C11	2.10	118.87	115.23
8	M	312	LDA	C9-C8-C7	-2.10	103.77	114.37
4	R	282	BCL	CHC-C4B-NB	-2.09	120.91	124.05
4	M	309	BCL	OBD-CAD-C3D	-2.09	123.53	128.42
4	S	310	BCL	C2B-C1B-NB	2.09	112.49	110.33
4	M	310	BCL	CAB-C3B-C2B	-2.08	123.41	127.74
4	R	282	BCL	C2A-C1A-CHA	2.08	127.48	123.87
4	M	310	BCL	CED-O2D-CGD	2.08	120.63	115.92
4	S	309	BCL	C2C-C3C-C4C	2.07	104.44	101.34
4	M	310	BCL	O1D-CGD-CBD	-2.07	120.43	124.52
8	M	314	LDA	C9-C8-C7	-2.06	103.93	114.37
4	L	282	BCL	CAA-C2A-C3A	-2.06	107.43	113.00
8	M	313	LDA	C9-C8-C7	-2.06	103.96	114.37
8	M	314	LDA	C4-C3-C2	-2.04	104.04	114.37
4	M	309	BCL	CHC-C4B-NB	-2.04	120.98	124.05
8	M	315	LDA	C9-C8-C7	-2.04	104.05	114.37
4	R	283	BCL	CHA-C1A-NA	-2.04	121.78	126.39
5	R	284	BPH	C4-C3-C5	2.04	118.76	115.23
4	M	310	BCL	C2A-C1A-CHA	2.03	127.39	123.87
4	L	283	BCL	CMB-C2B-C3B	2.02	132.05	125.67
4	R	282	BCL	OBB-CAB-CBB	-2.02	115.24	119.77
4	M	310	BCL	OBD-CAD-C3D	-2.02	123.69	128.42
5	S	311	BPH	C2D-C1D-ND	2.01	110.89	109.43
4	M	309	BCL	CMC-C2C-C1C	-2.01	106.37	111.77
4	L	282	BCL	C2A-C3A-C4A	2.00	105.11	101.87
4	S	310	BCL	C2A-C1A-CHA	2.00	127.34	123.87

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	283	BCL	CHA-CBD-CGD-O2D
4	M	310	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	R	282	BCL	C2C-C3C-CAC-CBC
4	R	282	BCL	C4C-C3C-CAC-CBC
4	S	310	BCL	CBD-CGD-O2D-CED
5	L	284	BPH	C4C-C3C-CAC-CBC
5	L	284	BPH	C2C-C3C-CAC-CBC
5	R	284	BPH	C4C-C3C-CAC-CBC
5	S	311	BPH	C4C-C3C-CAC-CBC
6	L	286	U10	C28-C29-C31-C32
8	M	312	LDA	N1-C1-C2-C3
8	M	313	LDA	N1-C1-C2-C3
8	M	314	LDA	N1-C1-C2-C3
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
4	R	283	BCL	O1D-CGD-O2D-CED
5	S	311	BPH	CBD-CGD-O2D-CED
6	L	286	U10	C29-C31-C32-C33
6	M	311	U10	C24-C26-C27-C28
6	S	312	U10	C14-C16-C17-C18
4	R	282	BCL	CBD-CGD-O2D-CED
6	L	286	U10	C14-C16-C17-C18
6	L	286	U10	C19-C21-C22-C23
4	R	282	BCL	O1D-CGD-O2D-CED
5	S	311	BPH	O1D-CGD-O2D-CED
8	M	314	LDA	C6-C7-C8-C9
8	M	315	LDA	C11-C10-C9-C8
8	M	315	LDA	C4-C5-C6-C7
8	M	314	LDA	C2-C3-C4-C5
4	S	310	BCL	C13-C15-C16-C17
5	R	284	BPH	C2C-C3C-CAC-CBC
5	S	311	BPH	C2C-C3C-CAC-CBC
5	L	285	BPH	C4-C3-C5-C6
5	L	284	BPH	O1A-CGA-O2A-C1
5	L	285	BPH	C2-C3-C5-C6
5	S	311	BPH	O1A-CGA-O2A-C1
8	M	313	LDA	C7-C8-C9-C10
5	L	284	BPH	CBA-CGA-O2A-C1
5	S	311	BPH	CBA-CGA-O2A-C1
4	S	310	BCL	C5-C6-C7-C8
6	L	286	U10	C12-C11-C9-C10
6	S	312	U10	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
4	S	310	BCL	C12-C13-C15-C16
5	L	285	BPH	O1A-CGA-O2A-C1
6	S	312	U10	C18-C19-C21-C22
8	M	315	LDA	C6-C7-C8-C9
8	M	313	LDA	C6-C7-C8-C9
6	L	286	U10	C2-C3-O3-C3M
6	L	286	U10	C12-C11-C9-C8
8	M	314	LDA	C9-C10-C11-C12
8	M	312	LDA	C7-C8-C9-C10
8	M	314	LDA	C7-C8-C9-C10
8	M	314	LDA	C1-C2-C3-C4
4	R	282	BCL	C12-C13-C15-C16
8	M	312	LDA	C9-C10-C11-C12
5	L	285	BPH	CBA-CGA-O2A-C1
4	R	282	BCL	C14-C13-C15-C16
5	R	284	BPH	C16-C17-C18-C20
5	R	284	BPH	C4-C3-C5-C6
6	L	286	U10	C33-C34-C36-C37
4	L	282	BCL	C12-C13-C15-C16
4	L	283	BCL	C13-C15-C16-C17
5	R	284	BPH	CBD-CGD-O2D-CED
5	L	285	BPH	C4C-C3C-CAC-CBC
4	R	282	BCL	C2A-CAA-CBA-CGA
6	R	285	U10	C2-C3-O3-C3M
4	L	283	BCL	CHA-CBD-CGD-O1D
4	S	310	BCL	O1A-CGA-O2A-C1
4	S	310	BCL	C14-C13-C15-C16
5	L	285	BPH	C15-C16-C17-C18
6	L	286	U10	C15-C14-C16-C17
4	L	282	BCL	C2A-CAA-CBA-CGA
6	M	311	U10	C5-C4-O4-C4M
6	S	312	U10	C5-C4-O4-C4M
8	M	313	LDA	C2-C3-C4-C5
5	R	284	BPH	C2-C3-C5-C6
6	L	286	U10	C35-C34-C36-C37
8	M	312	LDA	C11-C10-C9-C8
4	L	282	BCL	C14-C13-C15-C16
6	L	286	U10	C13-C14-C16-C17
6	L	286	U10	C4-C3-O3-C3M
5	R	284	BPH	C16-C17-C18-C19
8	M	315	LDA	C2-C3-C4-C5
8	M	313	LDA	C1-C2-C3-C4

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	M	310	BCL	C15-C16-C17-C18
5	R	284	BPH	O1D-CGD-O2D-CED
5	R	284	BPH	C11-C10-C8-C9
8	M	315	LDA	C1-C2-C3-C4
8	M	313	LDA	C11-C10-C9-C8
5	R	284	BPH	C15-C16-C17-C18
6	L	286	U10	C25-C24-C26-C27
4	S	310	BCL	C2-C1-O2A-CGA
4	M	309	BCL	C2B-C3B-CAB-CBB
4	S	309	BCL	C1-C2-C3-C4
4	S	310	BCL	CAD-CBD-CGD-O2D
8	M	315	LDA	C9-C10-C11-C12
4	M	309	BCL	CAA-CBA-CGA-O2A
5	R	284	BPH	C10-C11-C12-C13
4	S	309	BCL	CAA-CBA-CGA-O2A

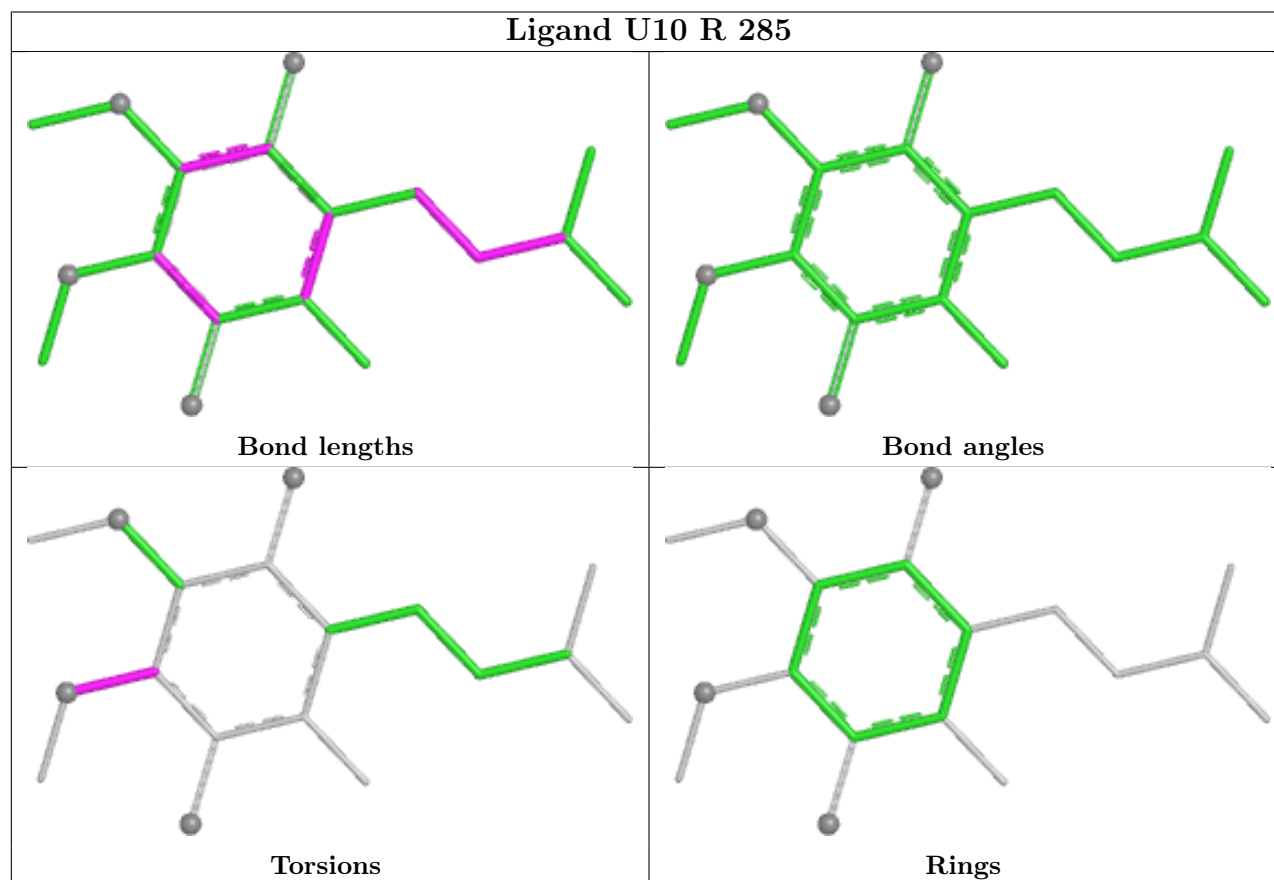
There are no ring outliers.

17 monomers are involved in 48 short contacts:

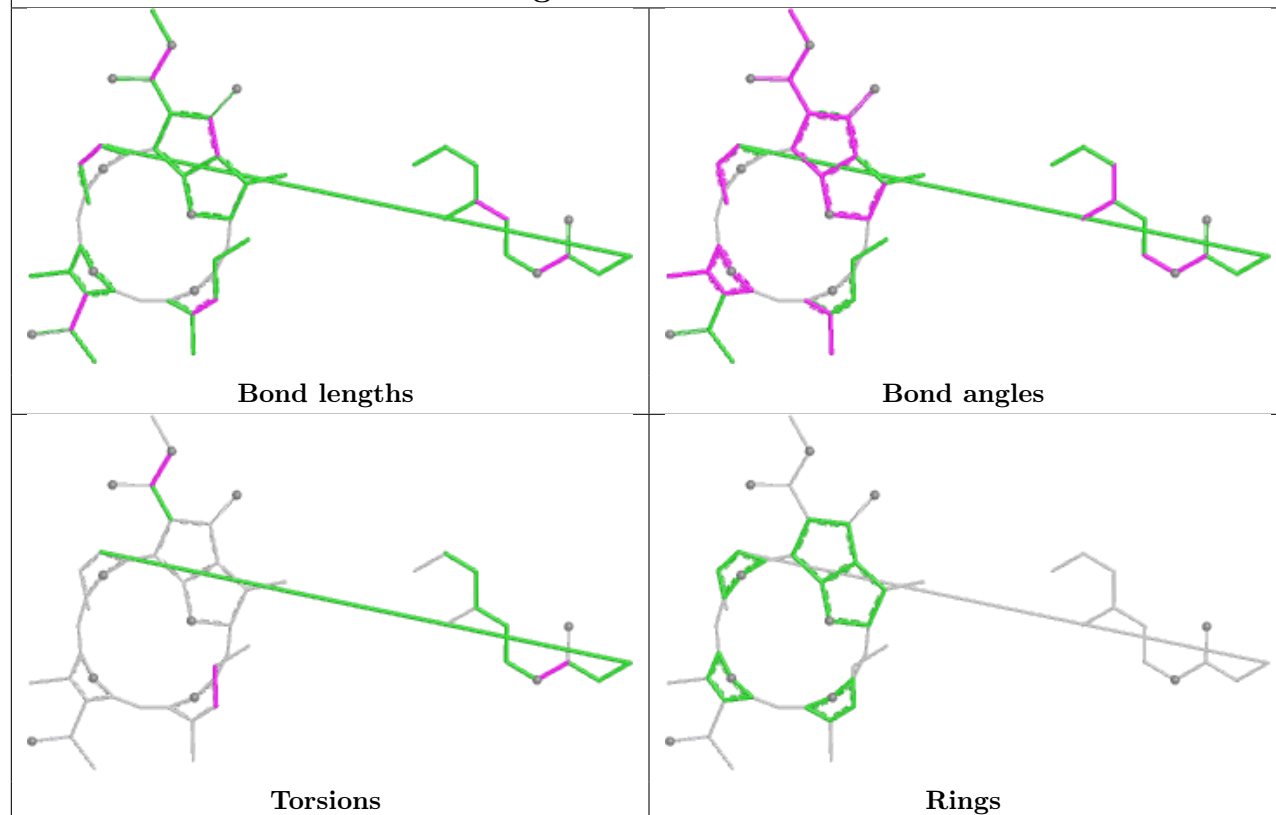
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	285	U10	2	0
5	S	311	BPH	2	0
5	R	284	BPH	4	0
4	R	283	BCL	4	0
4	S	309	BCL	5	0
4	S	310	BCL	8	0
6	L	286	U10	1	0
4	M	310	BCL	7	0
5	L	285	BPH	3	0
4	L	282	BCL	6	0
4	M	309	BCL	5	0
6	M	311	U10	1	0
4	R	282	BCL	6	0
4	L	283	BCL	4	0
8	M	312	LDA	2	0
8	M	314	LDA	1	0
8	M	315	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

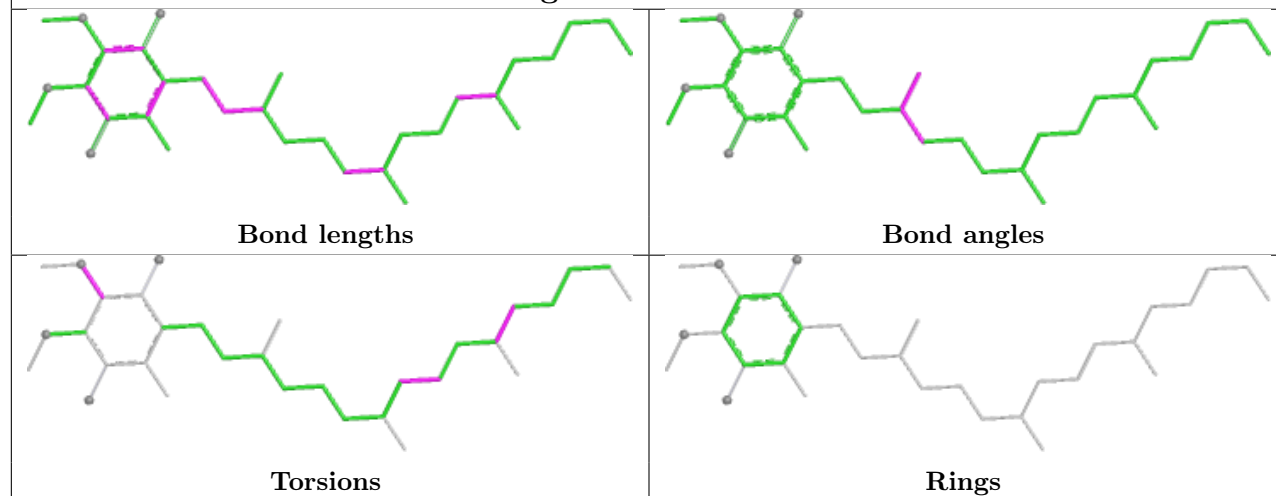
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

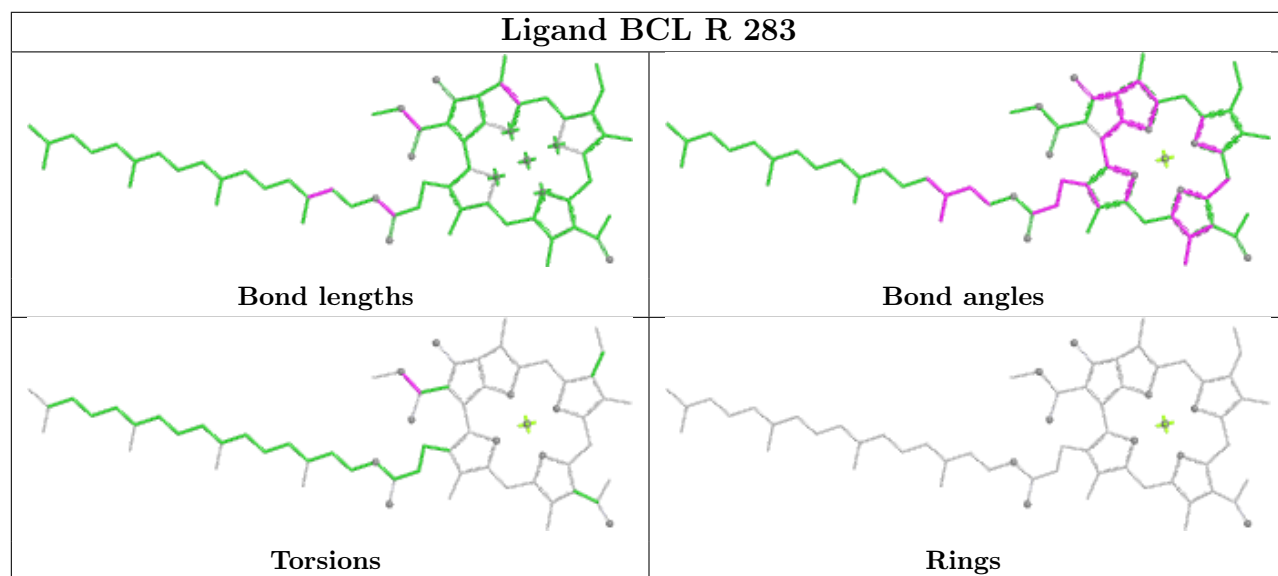
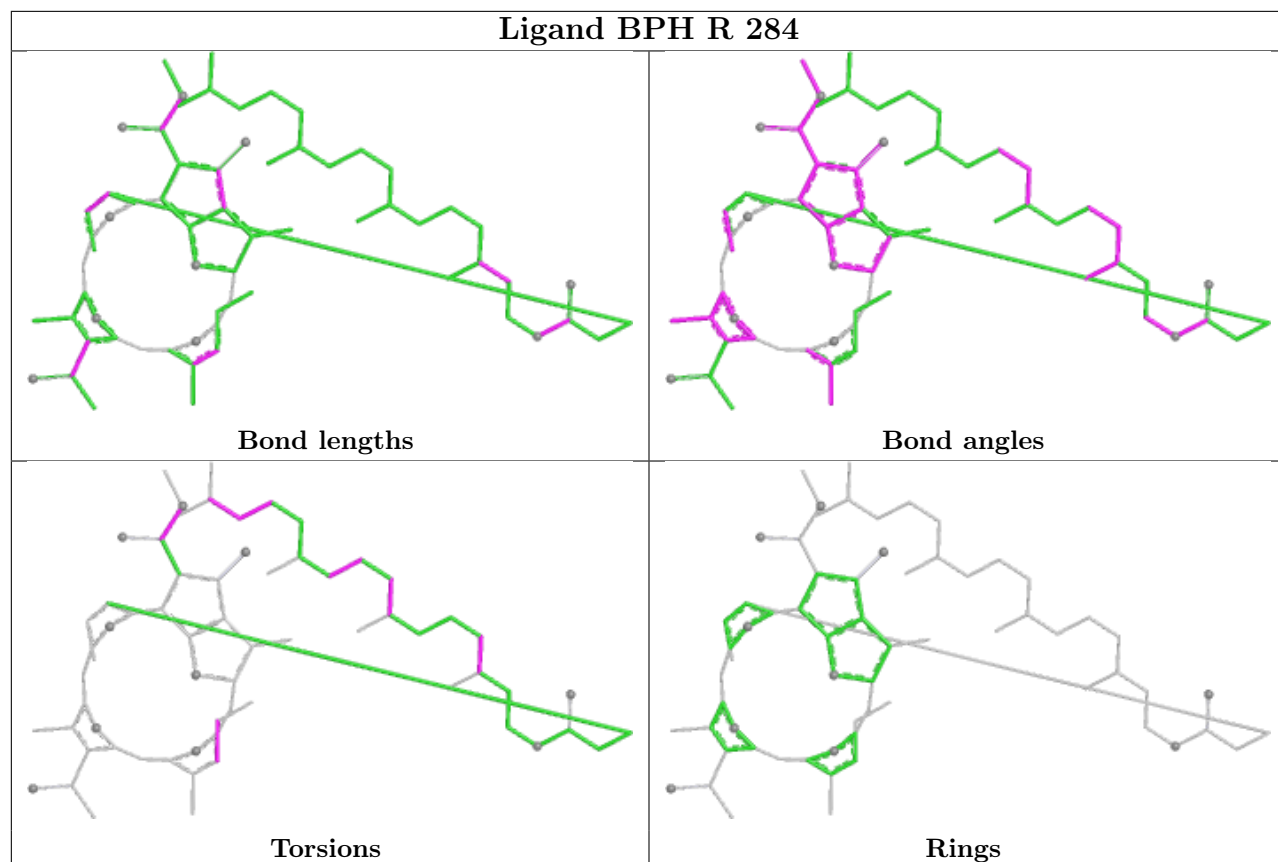


Ligand BPH S 311

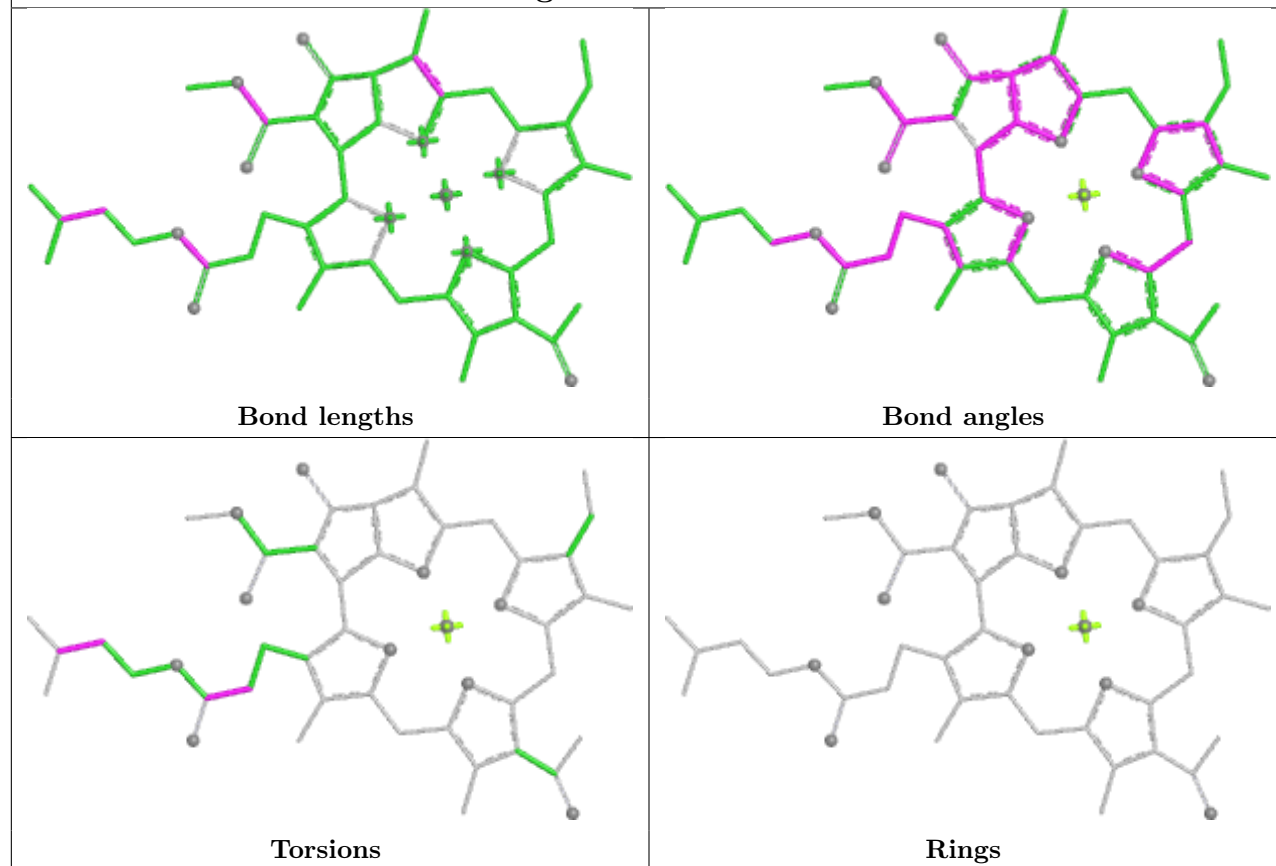


Ligand U10 S 312

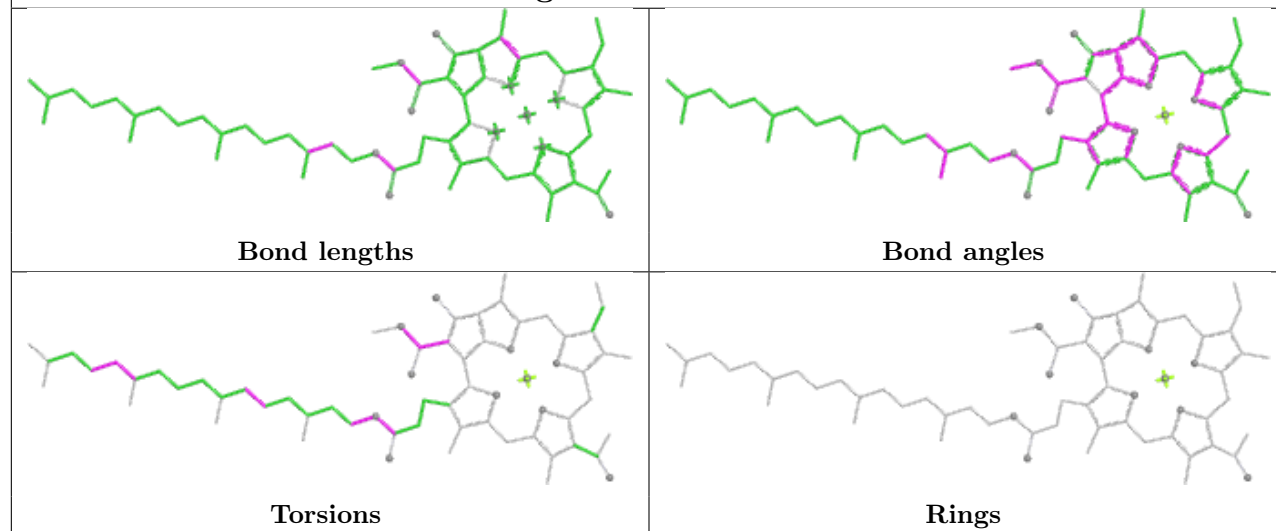


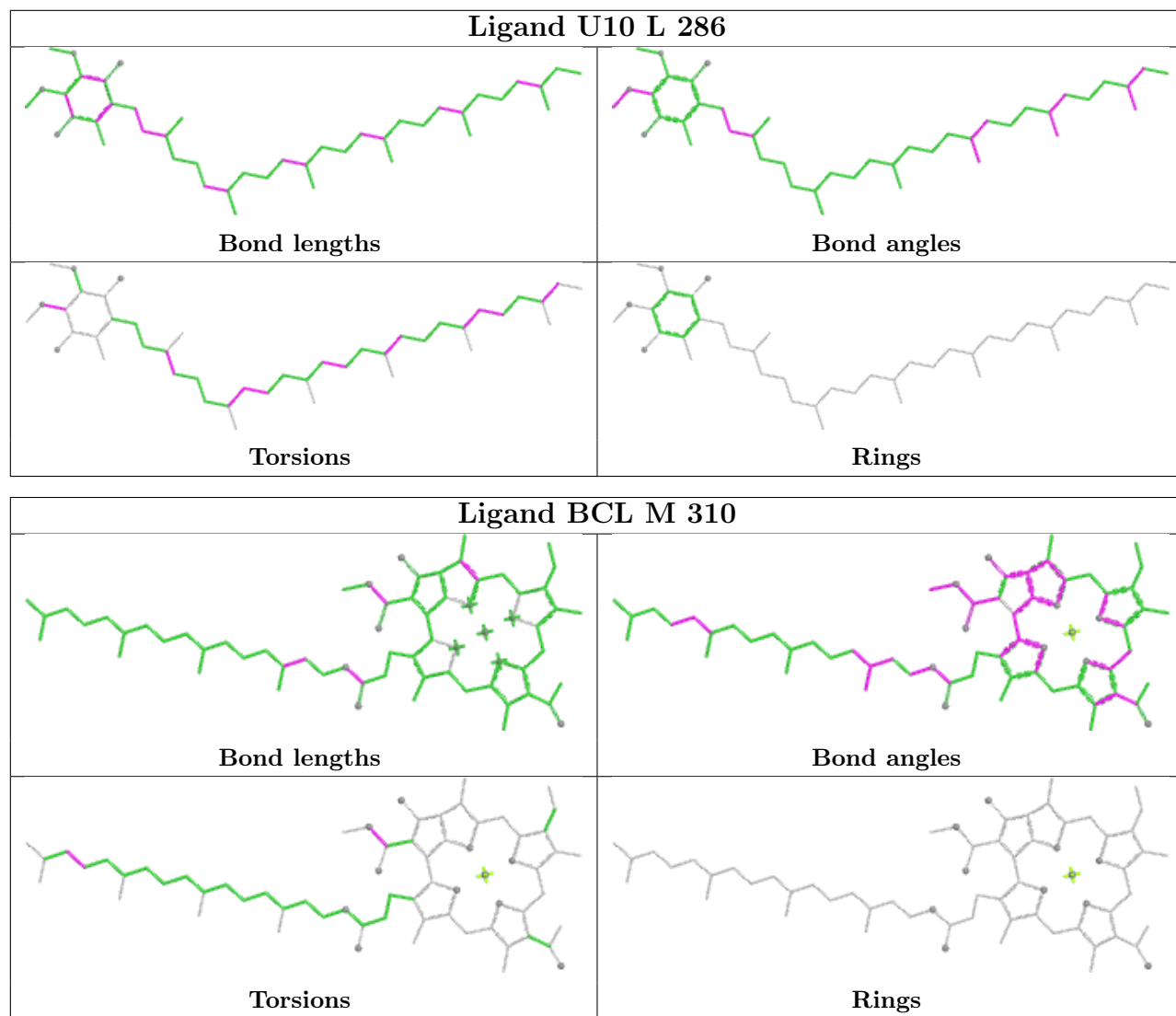


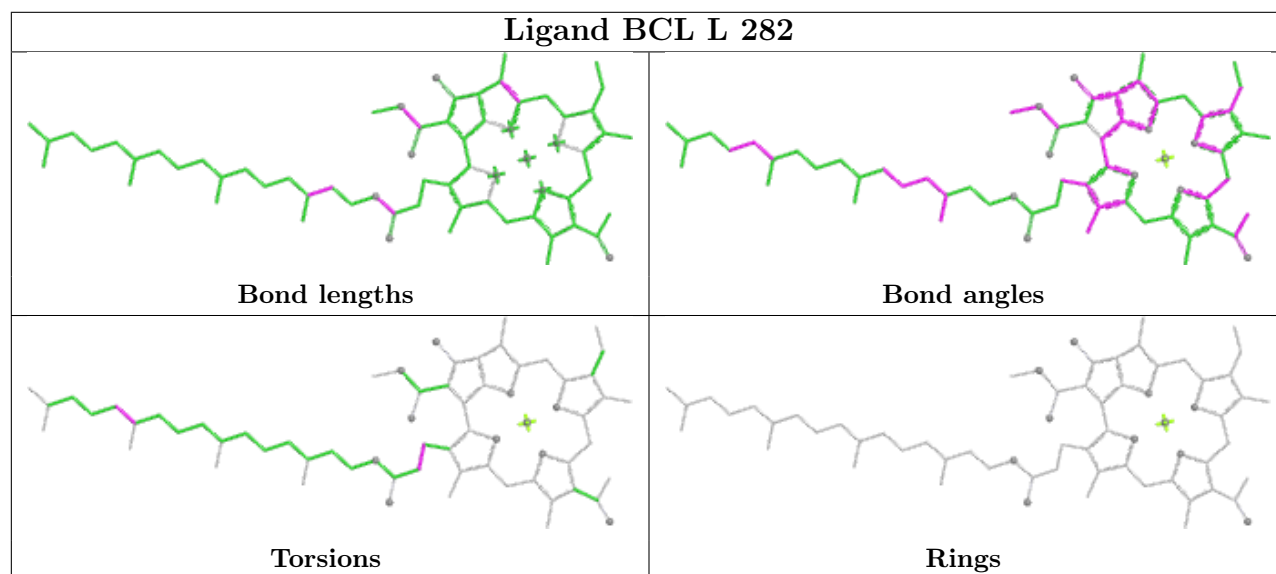
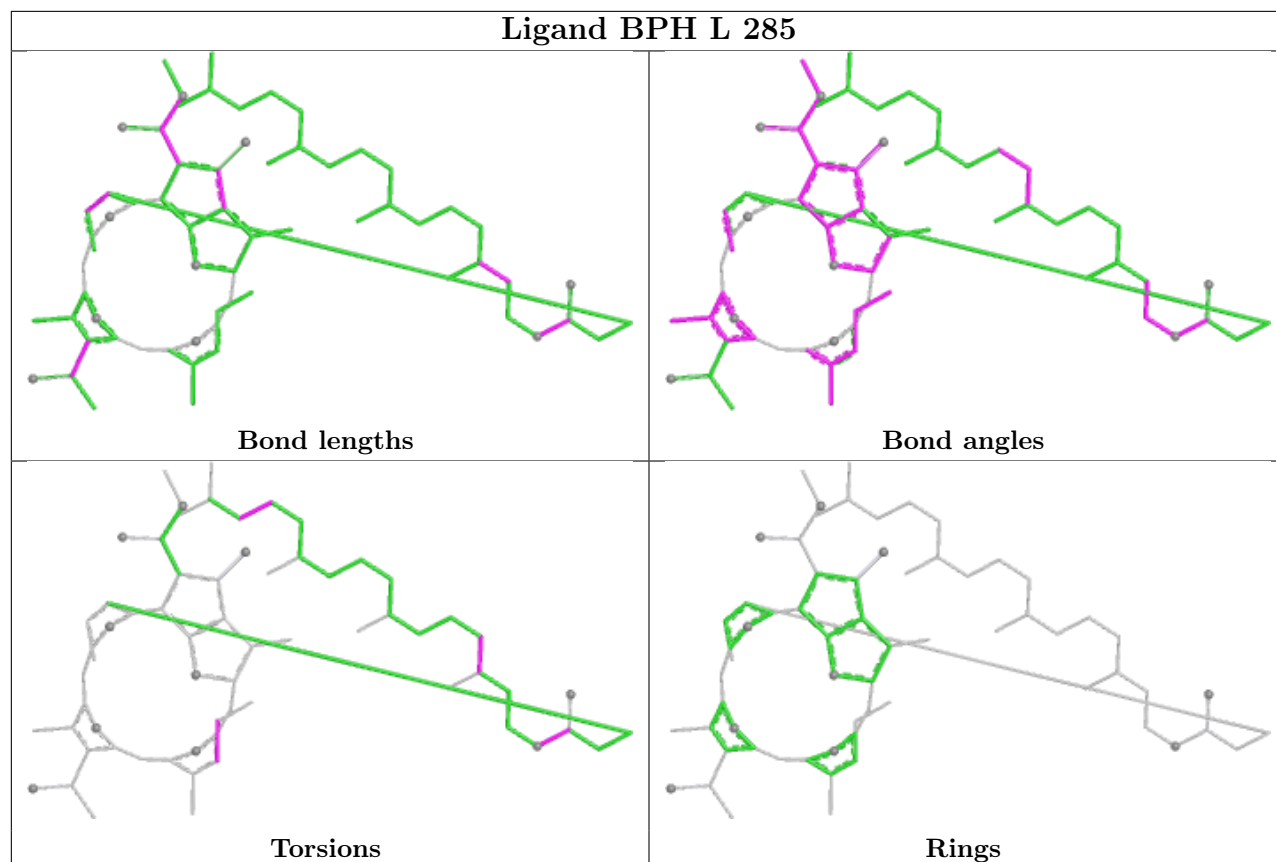
Ligand BCL S 309

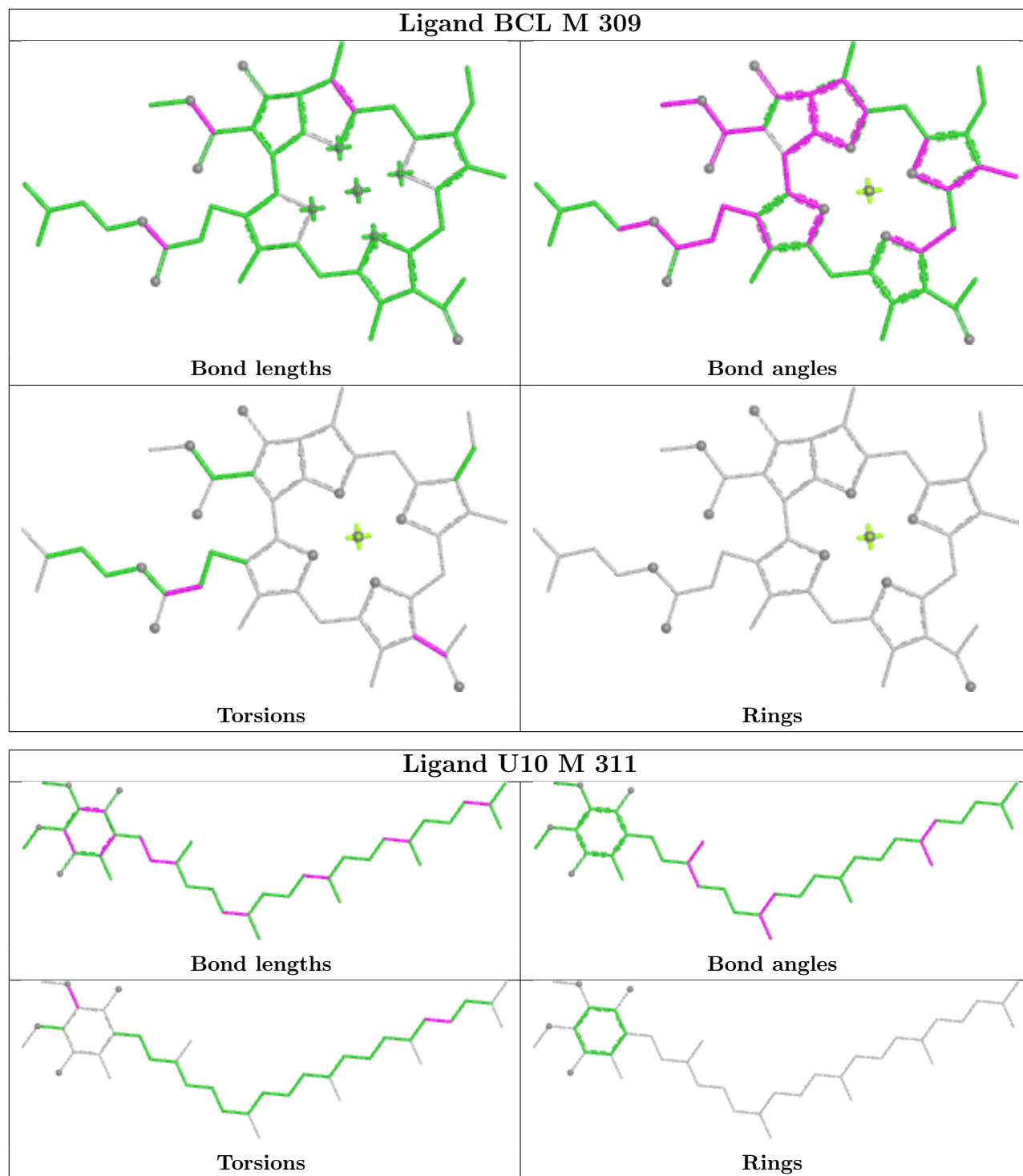


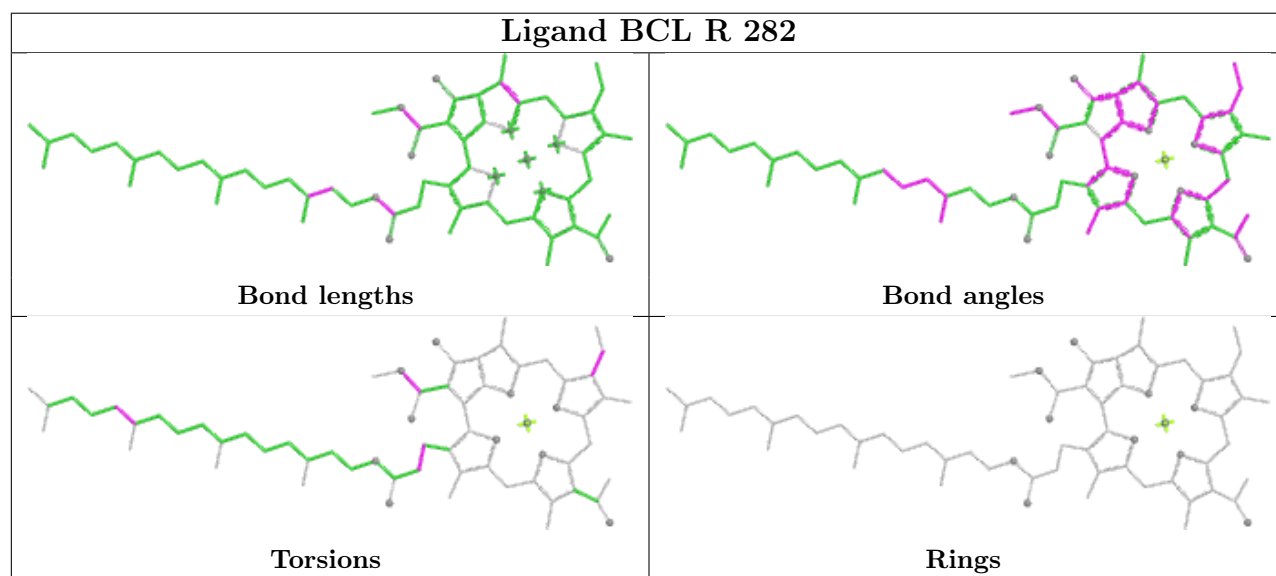
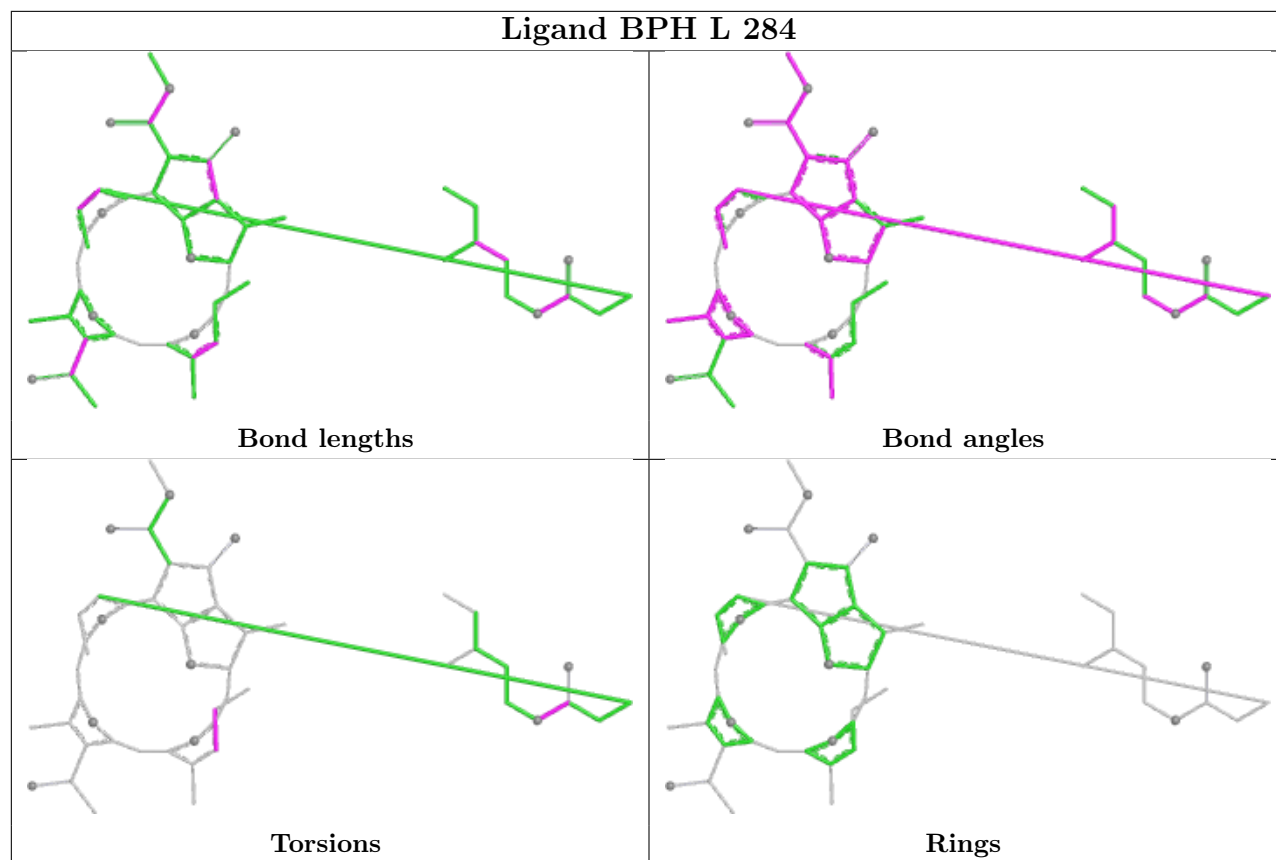
Ligand BCL S 310

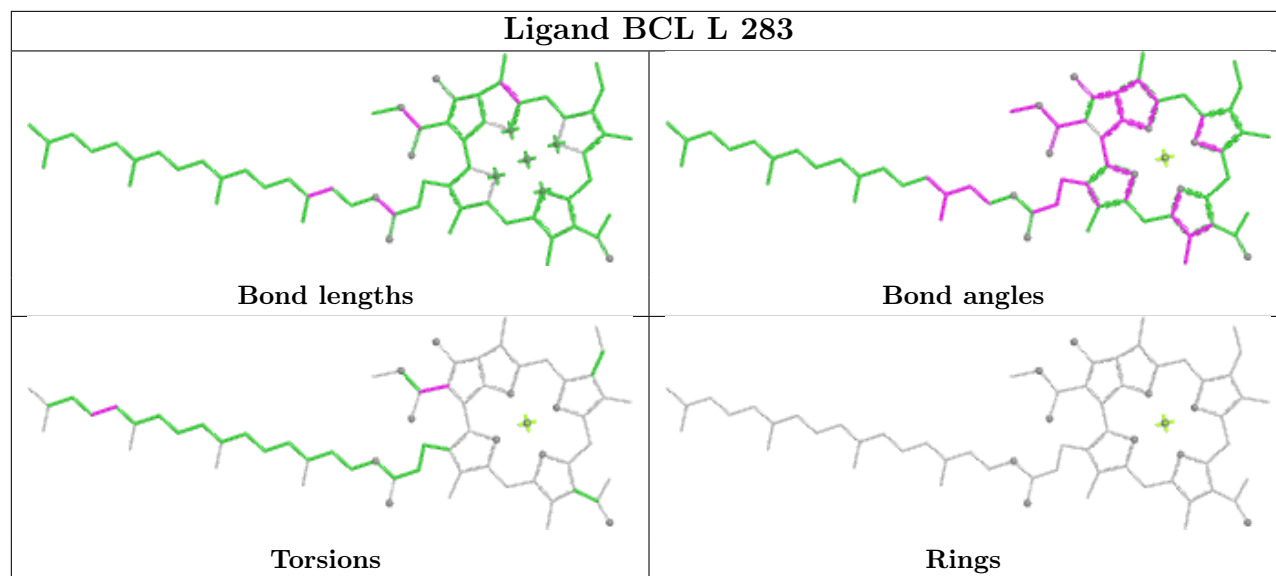












5.7 Other polymers [i](#)

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.