



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 1PST / pdb_00001pst
Title : CRYSTALLOGRAPHIC ANALYSES OF SITE-DIRECTED MUTANTS OF
THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER
SPHAEROIDES
Authors : Chirino, A.J.; Feher, G.; Rees, D.C.
Deposited on : 1993-12-13
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **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) : 2.49

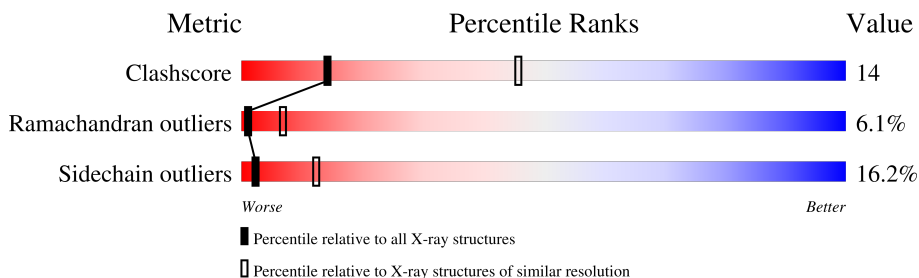
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	266	
2	M	296	
3	H	237	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	M	5	X	-	-	-
8	CRT	M	304	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6786 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	266	Total	C	N	O	S	0	0	0
			2121	1433	336	344	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	296	Total	C	N	O	S	0	0	0
			2360	1579	384	387	10			

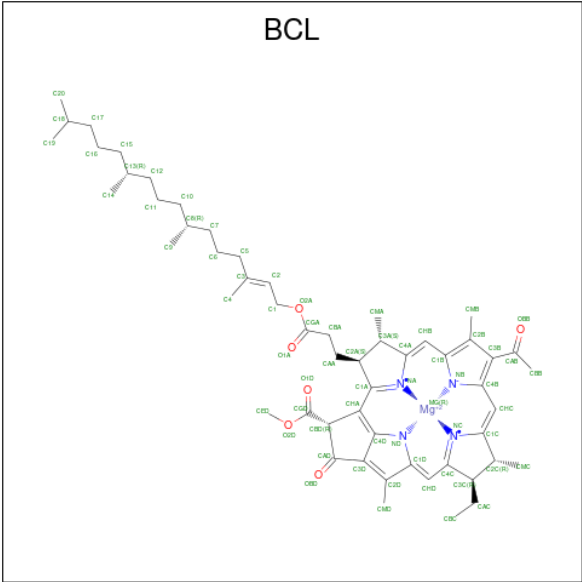
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	conflict	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

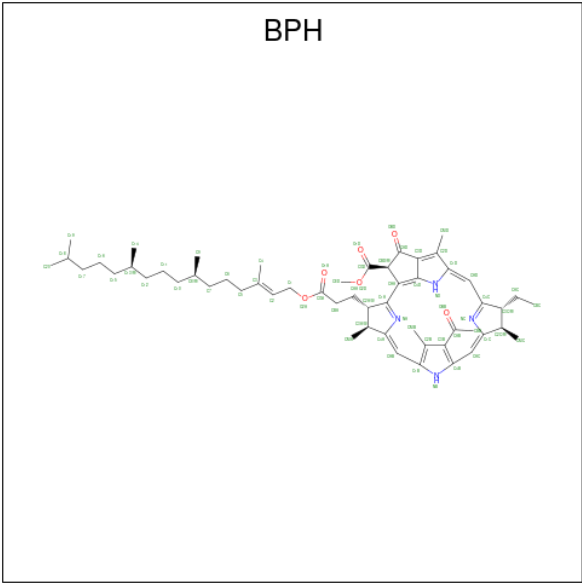
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	0	0
			1807	1156	310	332	9			

- 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
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

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



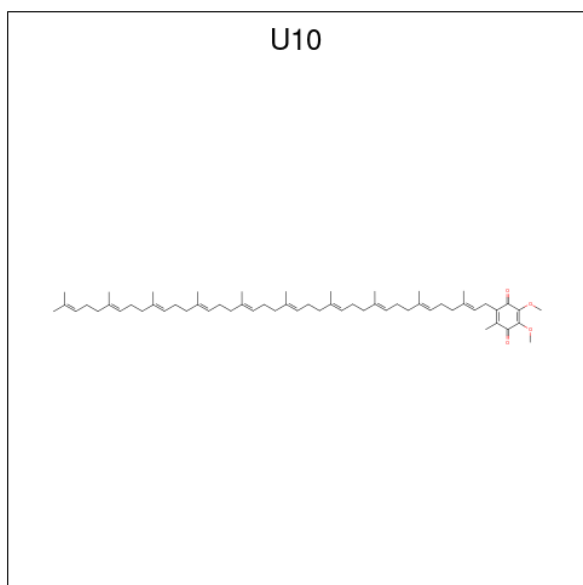
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		

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

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

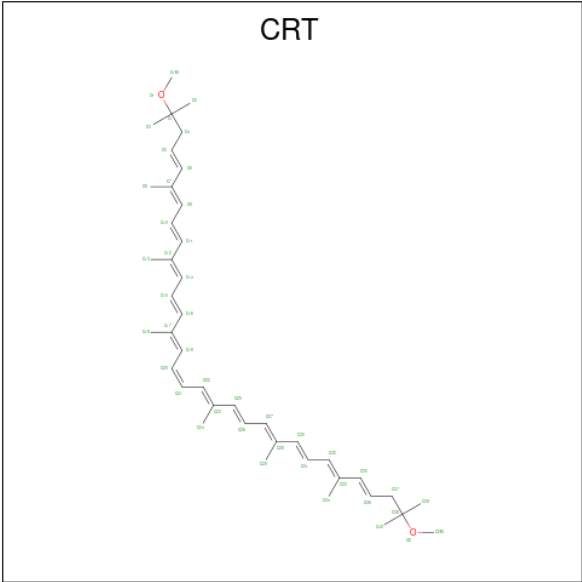


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			41	37	4		
6	M	1	Total	C	O	0	0
			51	47	4		

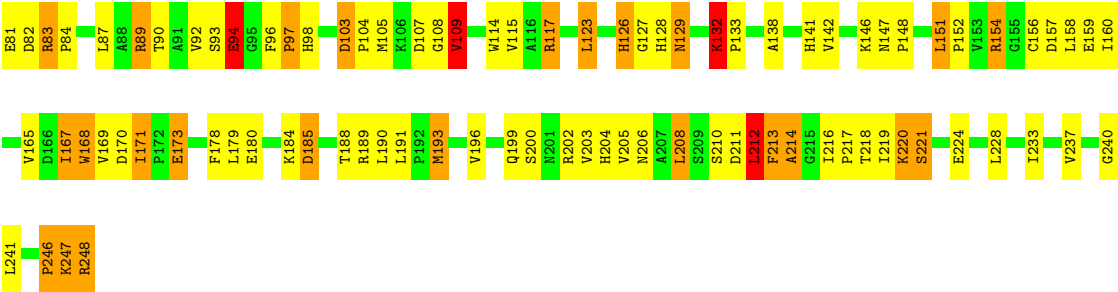
- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6786	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: U10, CRT, FE, BPH, BCL

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	0.98	9/2204 (0.4%)	1.86	58/3014 (1.9%)
2	M	1.02	10/2450 (0.4%)	1.96	77/3344 (2.3%)
3	H	0.99	6/1855 (0.3%)	1.91	62/2523 (2.5%)
All	All	1.00	25/6509 (0.4%)	1.91	197/8881 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	M	0	2
3	H	0	4
All	All	0	7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	116	HIS	CD2-NE2	-7.54	1.29	1.37
1	L	211	HIS	CD2-NE2	-7.21	1.29	1.37
1	L	153	HIS	CD2-NE2	-7.06	1.30	1.37
2	M	145	HIS	CD2-NE2	-7.06	1.30	1.37
2	M	193	HIS	CD2-NE2	-6.94	1.30	1.37
1	L	168	HIS	CD2-NE2	-6.84	1.30	1.37
3	H	68	HIS	CD2-NE2	-6.77	1.30	1.37
3	H	204	HIS	CD2-NE2	-6.73	1.30	1.37
1	L	190	HIS	CD2-NE2	-6.70	1.30	1.37
2	M	182	HIS	CD2-NE2	-6.64	1.30	1.37
2	M	301	HIS	CD2-NE2	-6.52	1.30	1.37
3	H	98	HIS	CD2-NE2	-6.34	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	173	HIS	CD2-NE2	-6.12	1.31	1.37
3	H	126	HIS	CD2-NE2	-5.98	1.31	1.37
3	H	141	HIS	CD2-NE2	-5.97	1.31	1.37
2	M	266	HIS	CG-ND1	-5.95	1.31	1.38
3	H	128	HIS	CD2-NE2	-5.85	1.31	1.37
2	M	182	HIS	CG-ND1	-5.64	1.32	1.38
1	L	230	HIS	CG-ND1	-5.58	1.32	1.38
1	L	168	HIS	CG-ND1	-5.29	1.32	1.38
2	M	219	HIS	CG-ND1	-5.06	1.32	1.38
2	M	266	HIS	CD2-NE2	-5.06	1.32	1.37
2	M	145	HIS	CG-ND1	-5.04	1.32	1.38
1	L	230	HIS	CD2-NE2	-5.04	1.32	1.37
2	M	146	THR	CA-CB	5.01	1.61	1.53

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	148	TRP	N-CA-C	-12.78	91.60	111.02
2	M	270	ILE	CB-CA-C	-11.08	97.78	111.97
1	L	5	PHE	CA-CB-CG	11.04	124.84	113.80
2	M	226	VAL	N-CA-CB	-10.71	98.19	112.22
2	M	270	ILE	N-CA-CB	10.59	122.94	110.55
1	L	153	HIS	CA-CB-CG	10.28	124.08	113.80
2	M	22	GLU	N-CA-C	10.14	132.41	110.80
1	L	183	ASN	OD1-CG-ND2	-10.00	112.60	122.60
2	M	105	PHE	CA-CB-CG	9.51	123.31	113.80
3	H	31	LEU	N-CA-C	-9.33	90.93	110.80
3	H	52	ASN	CA-CB-CG	9.10	121.70	112.60
1	L	196	SER	N-CA-C	-8.89	101.66	111.36
3	H	107	ASP	CA-CB-CG	8.63	121.23	112.60
3	H	90	THR	N-CA-C	-8.50	96.25	109.76
3	H	35	ASN	OD1-CG-ND2	-8.49	114.11	122.60
2	M	237	GLN	OE1-CD-NE2	-8.36	114.24	122.60
2	M	182	HIS	CB-CG-CD2	-8.35	120.34	131.20
1	L	268	LYS	N-CA-C	8.11	123.04	108.69
1	L	155	ASP	CA-CB-CG	8.03	120.62	112.60
1	L	103	ARG	N-CA-C	-7.80	101.88	111.40
3	H	30	TYR	N-CA-C	7.63	121.19	112.57
1	L	153	HIS	CB-CG-CD2	-7.60	121.32	131.20
3	H	49	PRO	N-CA-C	7.54	128.01	112.47
3	H	212	LEU	CA-C-O	-7.36	109.99	120.51
1	L	183	ASN	CB-CG-ND2	7.33	127.40	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	146	PHE	CA-CB-CG	7.33	121.12	113.80
2	M	148	TRP	CA-CB-CG	7.28	127.42	113.60
3	H	46	ASP	N-CA-C	-7.27	95.50	109.24
3	H	173	GLU	N-CA-C	-7.25	92.77	107.41
3	H	59	PRO	N-CA-C	7.21	123.54	113.53
2	M	38	LEU	CA-C-O	-7.14	115.19	119.55
3	H	48	THR	CA-C-N	7.02	128.61	119.84
3	H	48	THR	C-N-CA	7.02	128.61	119.84
3	H	40	TYR	N-CA-C	6.95	118.90	109.24
2	M	44	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	M	18	LEU	O-C-N	-6.88	117.17	123.50
1	L	216	PHE	CA-CB-CG	-6.86	106.94	113.80
1	L	14	GLY	N-CA-C	-6.85	101.03	111.24
2	M	145	HIS	CB-CG-CD2	-6.84	122.31	131.20
3	H	51	ALA	N-CA-C	6.79	125.26	110.80
1	L	113	ILE	N-CA-CB	-6.77	104.62	112.34
2	M	226	VAL	CB-CA-C	6.77	121.46	112.46
3	H	68	HIS	CB-CG-CD2	-6.72	122.46	131.20
1	L	116	HIS	CB-CG-CD2	-6.71	122.47	131.20
3	H	42	LEU	N-CA-C	6.71	119.41	111.02
3	H	94	GLU	N-CA-C	6.71	125.09	110.80
2	M	259	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	M	195	ASN	OD1-CG-ND2	-6.66	115.94	122.60
3	H	170	ASP	N-CA-C	-6.66	99.17	109.76
2	M	80	TRP	N-CA-C	-6.63	96.67	110.80
2	M	259	ASN	CB-CG-ND2	6.59	126.29	116.40
3	H	157	ASP	N-CA-C	-6.56	99.94	109.59
2	M	52	LEU	N-CA-C	6.52	124.68	110.80
2	M	270	ILE	N-CA-C	-6.37	104.31	110.42
3	H	157	ASP	CA-CB-CG	6.35	118.95	112.60
3	H	141	HIS	O-C-N	6.31	130.68	123.48
2	M	144	LYS	N-CA-C	6.31	124.24	110.80
2	M	269	ALA	N-CA-C	6.31	118.96	111.33
1	L	86	TRP	N-CA-C	-6.30	104.34	111.14
3	H	204	HIS	CB-CG-CD2	-6.27	123.04	131.20
3	H	203	VAL	N-CA-C	-6.25	98.63	107.75
1	L	60	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	L	68	PRO	N-CA-C	6.22	118.29	110.70
1	L	179	PHE	CA-C-O	-6.22	114.29	120.70
3	H	52	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	L	153	HIS	CB-CG-ND1	6.16	131.94	122.70
3	H	147	ASN	OD1-CG-ND2	-6.13	116.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	211	HIS	CB-CG-CD2	-6.12	123.24	131.20
3	H	117	ARG	O-C-N	-6.10	114.47	122.59
1	L	210	ASP	CA-CB-CG	6.08	118.68	112.60
2	M	98	ALA	O-C-N	-6.07	115.71	121.05
2	M	289	THR	N-CA-CB	-6.07	100.90	109.94
3	H	62	LYS	N-CA-C	-6.07	99.11	109.24
1	L	256	PHE	CA-CB-CG	6.06	119.86	113.80
3	H	103	ASP	CA-C-N	6.02	126.19	119.32
3	H	103	ASP	C-N-CA	6.02	126.19	119.32
1	L	36	VAL	N-CA-C	-5.99	104.67	110.72
1	L	227	LEU	N-CA-C	-5.96	104.69	111.07
3	H	22	ILE	N-CA-C	-5.96	104.81	110.42
1	L	60	ASN	CA-C-N	5.93	125.55	119.56
1	L	60	ASN	C-N-CA	5.93	125.55	119.56
3	H	68	HIS	CA-CB-CG	5.91	119.71	113.80
3	H	211	ASP	CA-C-O	5.87	129.12	122.37
1	L	269	LEU	N-CA-C	5.84	122.72	109.81
2	M	294	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	L	167	PHE	CA-CB-CG	5.81	119.61	113.80
3	H	52	ASN	CB-CG-ND2	5.79	125.09	116.40
2	M	175	VAL	CA-C-N	5.79	125.77	120.03
2	M	175	VAL	C-N-CA	5.79	125.77	120.03
2	M	171	TRP	CG-CD2-CE3	5.75	139.65	133.90
3	H	30	TYR	CA-CB-CG	-5.75	103.56	113.90
1	L	159	ASN	OD1-CG-ND2	-5.73	116.87	122.60
3	H	109	VAL	N-CA-CB	-5.71	101.24	111.92
3	H	141	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	L	213	ASP	CA-CB-CG	5.69	118.29	112.60
2	M	104	SER	N-CA-C	5.68	122.89	110.80
3	H	81	GLU	N-CA-C	-5.67	99.49	108.73
1	L	170	ASN	CA-C-N	5.65	124.85	118.97
1	L	170	ASN	C-N-CA	5.65	124.85	118.97
1	L	259	TRP	CG-CD2-CE3	5.65	139.55	133.90
2	M	57	VAL	N-CA-C	-5.65	105.02	110.72
1	L	173	HIS	CA-CB-CG	5.64	119.44	113.80
2	M	182	HIS	CB-CG-ND1	5.64	131.16	122.70
2	M	201	PHE	CA-C-O	-5.62	114.91	120.70
2	M	171	TRP	CE2-CD2-CG	-5.58	100.51	107.20
3	H	126	HIS	CB-CG-CD2	-5.57	123.95	131.20
2	M	33	GLY	CA-C-N	5.57	126.81	119.84
2	M	33	GLY	C-N-CA	5.57	126.81	119.84
1	L	51	TRP	O-C-N	-5.57	116.34	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	PHE	CA-CB-CG	-5.55	108.25	113.80
2	M	39	LEU	N-CA-C	5.54	118.84	111.75
3	H	40	TYR	CA-C-N	5.54	126.76	119.84
3	H	40	TYR	C-N-CA	5.54	126.76	119.84
2	M	248	ALA	N-CA-C	-5.54	105.16	111.14
2	M	240	ASP	CA-CB-CG	5.53	118.13	112.60
2	M	105	PHE	N-CA-C	5.53	122.58	110.80
2	M	6	ILE	N-CA-C	-5.53	95.52	111.00
3	H	221	SER	N-CA-C	-5.53	102.66	110.29
2	M	222	THR	N-CA-CB	5.53	118.08	110.07
2	M	166	ILE	N-CA-C	-5.52	104.99	111.00
3	H	211	ASP	O-C-N	5.51	129.02	122.46
2	M	252	TRP	CG-CD2-CE3	5.51	139.41	133.90
2	M	164	ARG	O-C-N	-5.50	116.03	120.38
2	M	66	TRP	CG-CD2-CE3	5.50	139.40	133.90
2	M	199	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	L	190	HIS	CA-CB-CG	-5.49	108.31	113.80
1	L	190	HIS	CB-CG-CD2	-5.48	124.07	131.20
2	M	28	ASN	CA-CB-CG	-5.47	107.13	112.60
2	M	26	LEU	N-CA-C	-5.46	105.34	112.23
2	M	268	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	L	170	ASN	CA-CB-CG	5.44	118.04	112.60
1	L	146	PHE	CA-C-N	5.44	125.20	119.76
1	L	146	PHE	C-N-CA	5.44	125.20	119.76
1	L	59	TRP	CG-CD2-CE3	5.41	139.31	133.90
2	M	193	HIS	CB-CG-CD2	-5.40	124.18	131.20
2	M	75	TRP	CA-C-O	-5.39	115.16	120.82
2	M	103	LEU	CA-C-N	5.39	131.83	121.54
2	M	103	LEU	C-N-CA	5.39	131.83	121.54
1	L	130	THR	N-CA-C	-5.38	105.10	110.97
1	L	86	TRP	CE2-CD2-CG	-5.38	100.75	107.20
1	L	166	ASN	CA-CB-CG	5.37	117.97	112.60
3	H	180	GLU	N-CA-C	-5.36	99.99	108.73
2	M	293	ASN	CA-CB-CG	5.35	117.95	112.60
1	L	258	GLN	OE1-CD-NE2	-5.34	117.26	122.60
3	H	168	TRP	N-CA-C	-5.34	100.47	109.07
3	H	28	ILE	N-CA-C	5.33	115.95	110.36
2	M	185	TRP	CE2-CD2-CG	-5.33	100.81	107.20
3	H	171	ILE	CA-C-N	5.31	124.76	119.24
3	H	171	ILE	C-N-CA	5.31	124.76	119.24
2	M	10	VAL	N-CA-C	-5.29	100.86	108.48
3	H	211	ASP	CA-C-N	5.29	131.64	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	211	ASP	C-N-CA	5.29	131.64	121.54
1	L	100	TRP	CE2-CD2-CG	-5.27	100.87	107.20
2	M	171	TRP	CB-CG-CD1	-5.26	119.00	126.90
3	H	167	ILE	N-CA-C	-5.26	100.90	108.53
1	L	54	VAL	N-CA-CB	-5.26	104.39	110.55
3	H	72	THR	N-CA-C	-5.25	99.10	108.13
1	L	59	TRP	CB-CG-CD1	-5.22	119.06	126.90
2	M	75	TRP	N-CA-C	-5.22	105.49	111.07
1	L	25	TRP	CG-CD2-CE3	5.21	139.11	133.90
2	M	182	HIS	CA-CB-CG	5.21	119.01	113.80
2	M	81	ASN	CA-CB-CG	-5.21	107.39	112.60
2	M	185	TRP	CG-CD2-CE3	5.19	139.09	133.90
3	H	41	PRO	N-CA-C	5.19	123.15	112.47
1	L	115	TYR	O-C-N	-5.18	115.69	122.59
2	M	95	GLU	CA-C-N	5.18	125.72	120.38
2	M	95	GLU	C-N-CA	5.18	125.72	120.38
1	L	142	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	L	142	TRP	CG-CD2-CE3	5.16	139.06	133.90
1	L	114	GLY	CA-C-O	5.15	125.71	121.18
3	H	37	ARG	CA-C-N	5.15	128.91	120.63
3	H	37	ARG	C-N-CA	5.15	128.91	120.63
1	L	25	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	L	151	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	M	185	TRP	CB-CG-CD1	-5.14	119.19	126.90
3	H	78	PRO	N-CA-C	-5.14	101.88	112.47
2	M	294	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	L	255	TRP	CB-CG-CD1	-5.13	119.20	126.90
2	M	146	THR	N-CA-C	-5.13	105.60	111.14
1	L	155	ASP	N-CA-C	-5.12	105.59	111.07
2	M	268	TRP	CE2-CD2-CG	-5.11	101.07	107.20
2	M	145	HIS	N-CA-C	5.11	121.68	110.80
2	M	23	ASP	CA-CB-CG	5.09	117.69	112.60
2	M	104	SER	N-CA-CB	-5.08	101.90	110.49
2	M	297	TRP	CE2-CD2-CG	-5.07	101.11	107.20
3	H	208	LEU	N-CA-C	5.07	117.51	109.50
2	M	25	ASN	CA-C-O	5.05	127.74	120.51
3	H	212	LEU	N-CA-C	-5.05	100.03	110.80
2	M	41	TRP	CE2-CD2-CG	-5.05	101.14	107.20
3	H	168	TRP	CE2-CD2-CG	-5.05	101.14	107.20
2	M	252	TRP	CE2-CD2-CG	-5.05	101.14	107.20
3	H	132	LYS	O-C-N	-5.05	117.96	121.65
2	M	155	TRP	CB-CG-CD1	-5.04	119.33	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	193	HIS	CA-CB-CG	-5.04	108.76	113.80
3	H	190	LEU	O-C-N	-5.03	117.30	123.19
1	L	100	TRP	CD1-CG-CD2	5.02	114.33	106.30
3	H	129	ASN	N-CA-C	5.01	118.06	110.64

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	TYR	Peptide
3	H	56	PHE	Peptide
3	H	58	LEU	Peptide
3	H	83	ARG	Peptide
1	L	269	LEU	Peptide
2	M	81	ASN	Peptide
2	M	96	PRO	Peptide

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	2121	0	2077	56	0
2	M	2360	0	2285	79	0
3	H	1807	0	1814	64	0
4	L	117	0	115	10	0
4	M	51	0	41	6	0
5	L	65	0	76	6	0
5	M	130	0	152	8	0
6	L	41	0	52	4	0
6	M	51	0	68	5	0
7	M	1	0	0	0	0
8	M	42	0	57	2	0
All	All	6786	0	6737	192	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 14.

All (192) 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)
3:H:154:ARG:HD2	3:H:160:ILE:HG12	1.52	0.92
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.58	0.84
1:L:205:GLU:HA	3:H:65:ILE:HG13	1.63	0.79
2:M:261:THR:HG22	3:H:40:TYR:HD1	1.49	0.76
2:M:27:ALA:HB2	2:M:51:TYR:HD1	1.50	0.74
4:M:1:BCL:HBB3	5:M:3:BPH:H4C1	1.69	0.73
2:M:20:MET:SD	2:M:22:GLU:HG2	2.29	0.73
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.71	0.72
3:H:89:ARG:HE	3:H:89:ARG:H	1.38	0.72
2:M:236:GLU:HG3	3:H:117:ARG:HH21	1.55	0.71
2:M:97:PRO:HA	2:M:111:GLU:O	1.92	0.70
2:M:27:ALA:HB2	2:M:51:TYR:CD1	2.27	0.69
5:L:271:BPH:HED1	6:M:303:U10:H171	1.74	0.67
5:M:3:BPH:HBB2	5:M:3:BPH:HHC	1.77	0.67
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.78	0.66
1:L:100:TRP:HZ3	6:M:303:U10:H33	1.61	0.66
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.78	0.65
3:H:158:LEU:HD23	3:H:202:ARG:HH22	1.62	0.64
1:L:52:SER:OG	1:L:85:LEU:HD23	1.97	0.63
3:H:39:GLY:HA2	3:H:42:LEU:HG	1.81	0.63
3:H:154:ARG:HG3	3:H:202:ARG:NE	2.14	0.63
2:M:107:ALA:HB3	2:M:112:GLY:HA3	1.80	0.63
2:M:144:LYS:HZ3	2:M:148:TRP:HB2	1.62	0.63
3:H:132:LYS:HE3	3:H:171:ILE:HD11	1.81	0.62
1:L:229:ILE:HG21	6:L:272:U10:H3M2	1.80	0.62
2:M:204:LEU:HB2	2:M:279:THR:HG21	1.82	0.62
2:M:130:TRP:CZ3	2:M:151:LEU:HG	2.35	0.61
2:M:12:VAL:HG11	3:H:169:VAL:HG11	1.81	0.61
2:M:271:TRP:HA	2:M:274:VAL:HG22	1.82	0.61
2:M:27:ALA:HA	2:M:51:TYR:HA	1.81	0.61
2:M:89:LEU:HD11	8:M:304:CRT:H81	1.83	0.60
2:M:63:GLY:HA3	5:M:5:BPH:H5C2	1.84	0.59
3:H:63:THR:HA	3:H:73:LEU:O	2.02	0.59
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.83	0.59
2:M:110:LYS:HD2	2:M:114:LEU:HD13	1.84	0.58
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.86	0.58
3:H:60:LYS:O	3:H:76:PRO:HD3	2.04	0.57
1:L:215:PHE:HB2	2:M:142:MET:HE2	1.86	0.57
4:L:2:BCL:H122	5:L:271:BPH:HBA1	1.87	0.57
4:L:4:BCL:O1A	2:M:207:ALA:HA	2.05	0.57
2:M:145:HIS:O	2:M:148:TRP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:HB	2:M:27:ALA:CB	2.35	0.56
1:L:173:HIS:HB2	1:L:247:CYS:SG	2.46	0.56
3:H:30:TYR:OH	3:H:56:PHE:HB3	2.06	0.56
1:L:187:LEU:HD23	2:M:273:ALA:HB2	1.88	0.55
3:H:154:ARG:HG3	3:H:202:ARG:HE	1.69	0.55
2:M:226:VAL:HG13	2:M:244:ALA:HB1	1.87	0.55
4:L:2:BCL:HAA2	4:L:4:BCL:HBC1	1.87	0.55
1:L:117:ILE:HD11	2:M:222:THR:HG23	1.88	0.55
2:M:94:LEU:HD13	2:M:114:LEU:HG	1.87	0.55
1:L:41:PHE:HB3	1:L:96:ALA:HB2	1.88	0.55
1:L:15:THR:HG21	1:L:19:GLY:O	2.06	0.55
3:H:93:SER:HB2	3:H:96:PHE:CZ	2.43	0.54
1:L:60:ASN:O	1:L:64:ILE:HG13	2.08	0.54
2:M:228:ARG:HD2	2:M:228:ARG:H	1.72	0.54
1:L:170:ASN:O	1:L:173:HIS:HB3	2.07	0.54
2:M:21:THR:HB	2:M:27:ALA:HB3	1.88	0.54
4:M:1:BCL:HHC	4:M:1:BCL:HBB2	1.89	0.53
6:L:272:U10:H121	6:L:272:U10:H1M3	1.90	0.53
2:M:164:ARG:HH21	2:M:288:GLY:HA3	1.73	0.53
4:L:2:BCL:H171	5:L:271:BPH:H2	1.90	0.53
3:H:62:LYS:HG2	3:H:75:VAL:HG23	1.91	0.53
2:M:236:GLU:HG3	3:H:117:ARG:NH2	2.22	0.52
1:L:75:LEU:HG	1:L:140:GLY:O	2.10	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.09	0.52
2:M:35:PHE:HB2	2:M:47:LEU:HD21	1.91	0.51
3:H:105:MET:HE1	3:H:240:GLY:HA2	1.91	0.51
1:L:131:LEU:HD22	1:L:156:TRP:HH2	1.76	0.51
2:M:249:ALA:HB3	3:H:40:TYR:CE2	2.46	0.51
1:L:174:MET:HB3	4:M:1:BCL:O1D	2.10	0.51
3:H:59:PRO:HB2	3:H:60:LYS:HD3	1.93	0.50
2:M:275:LEU:CD1	2:M:278:LEU:HD23	2.41	0.50
3:H:241:LEU:HA	3:H:247:LYS:HE2	1.94	0.50
2:M:179:ILE:HG23	4:M:1:BCL:HED1	1.93	0.50
4:L:2:BCL:HBA1	4:L:2:BCL:O2D	2.12	0.49
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.93	0.49
1:L:135:ARG:NH1	1:L:251:THR:HG22	2.28	0.49
1:L:218:ASP:HB3	2:M:136:ARG:HD3	1.94	0.49
2:M:22:GLU:CB	2:M:139:ALA:HB1	2.43	0.49
3:H:133:PRO:HA	3:H:168:TRP:HA	1.94	0.49
3:H:29:TYR:HB3	3:H:30:TYR:CE2	2.48	0.49
1:L:215:PHE:CZ	2:M:146:THR:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:272:U10:H3M3	6:L:272:U10:H4M2	1.95	0.49
2:M:285:LEU:O	2:M:289:THR:HB	2.13	0.48
1:L:73:TYR:HE2	1:L:82:LYS:HD2	1.78	0.48
3:H:37:ARG:HH21	3:H:43:GLU:H	1.61	0.48
1:L:107:ILE:HD13	2:M:255:THR:CG2	2.44	0.48
5:M:3:BPH:HHC	5:M:3:BPH:CBB	2.44	0.48
2:M:22:GLU:HB3	2:M:139:ALA:HB1	1.95	0.48
1:L:113:ILE:HD13	2:M:247:ARG:HG3	1.96	0.47
2:M:165:PRO:HG2	2:M:174:ALA:HB2	1.96	0.47
1:L:113:ILE:CD1	2:M:247:ARG:HG3	2.44	0.47
3:H:50:ALA:HB1	3:H:55:PRO:HG2	1.94	0.47
2:M:22:GLU:HG3	2:M:139:ALA:O	2.14	0.47
1:L:201:GLU:O	1:L:204:LYS:HE2	2.15	0.47
1:L:208:THR:OG1	1:L:211:HIS:HD2	1.98	0.47
2:M:219:HIS:HA	6:M:303:U10:O2	2.14	0.47
2:M:205:SER:HB3	5:M:3:BPH:HMA3	1.97	0.47
3:H:220:LYS:HG2	3:H:221:SER:N	2.30	0.47
1:L:13:GLY:H	1:L:110:LYS:HZ3	1.62	0.47
1:L:267:VAL:O	2:M:87:ARG:HD2	2.15	0.46
4:L:2:BCL:H112	4:L:4:BCL:HBB2	1.97	0.46
2:M:140:LEU:HB2	2:M:142:MET:HG2	1.97	0.46
3:H:212:LEU:O	3:H:214:ALA:N	2.46	0.46
3:H:129:ASN:ND2	3:H:224:GLU:HB2	2.29	0.46
3:H:247:LYS:HG2	3:H:248:ARG:N	2.31	0.46
2:M:252:TRP:HB3	2:M:256:MET:HE2	1.97	0.46
3:H:68:HIS:HE1	3:H:123:LEU:HB2	1.80	0.46
2:M:170:SER:HB3	2:M:172:SER:OG	2.16	0.46
1:L:174:MET:HE3	2:M:183:LEU:HD11	1.98	0.45
1:L:178:SER:HA	4:M:1:BCL:O1A	2.16	0.45
1:L:238:LEU:HD23	5:L:271:BPH:HBC1	1.97	0.45
5:L:271:BPH:HHC	5:L:271:BPH:OBB	2.15	0.45
2:M:242:GLY:HA2	3:H:115:VAL:HG11	1.98	0.45
2:M:280:GLY:HA2	5:M:3:BPH:HED3	1.99	0.45
3:H:154:ARG:HB2	3:H:202:ARG:HH21	1.81	0.45
3:H:210:SER:HA	3:H:213:PHE:HD2	1.82	0.45
1:L:131:LEU:HD13	4:L:4:BCL:HMC2	1.99	0.45
1:L:153:HIS:CE1	5:L:271:BPH:H191	2.51	0.45
3:H:191:LEU:HD21	3:H:205:VAL:HG21	1.98	0.45
2:M:163:ILE:HA	2:M:166:ILE:HG12	1.98	0.45
1:L:48:LEU:HD12	1:L:85:LEU:HD11	2.00	0.44
3:H:48:THR:HA	3:H:49:PRO:HD2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:33:GLY:H	2:M:34:PRO:HD3	1.82	0.44
2:M:188:ASN:HA	2:M:191:LEU:HD22	1.99	0.44
3:H:104:PRO:HB3	3:H:109:VAL:HG12	1.99	0.44
3:H:152:PRO:HB2	3:H:154:ARG:HD3	1.98	0.44
1:L:268:LYS:O	1:L:269:LEU:HB2	2.16	0.44
6:M:303:U10:H3M3	6:M:303:U10:H4M2	1.99	0.44
3:H:247:LYS:HE3	3:H:247:LYS:HB3	1.95	0.44
1:L:214:THR:HG21	2:M:20:MET:O	2.18	0.44
2:M:96:PRO:HA	2:M:115:TRP:CG	2.52	0.44
2:M:82:PRO:O	2:M:84:VAL:N	2.51	0.43
2:M:94:LEU:HD22	2:M:94:LEU:HA	1.84	0.43
2:M:261:THR:HA	3:H:40:TYR:CD1	2.53	0.43
2:M:160:LEU:HD23	2:M:284:ILE:HG21	1.98	0.43
2:M:109:LEU:O	2:M:114:LEU:HD22	2.18	0.43
3:H:64:PHE:HB2	3:H:73:LEU:HB3	2.00	0.43
1:L:25:TRP:HZ3	3:H:97:PRO:HG3	1.84	0.43
1:L:107:ILE:HG23	2:M:254:TRP:HE3	1.83	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.44	0.43
2:M:148:TRP:HZ2	2:M:271:TRP:CH2	2.36	0.43
4:L:2:BCL:HBB3	4:L:2:BCL:HMB1	2.01	0.43
1:L:213:ASP:HA	1:L:223:SER:OG	2.19	0.43
6:L:272:U10:H172	6:L:272:U10:H101	2.01	0.43
1:L:56:GLN:HG3	1:L:58:THR:HG22	2.00	0.43
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.78	0.43
3:H:104:PRO:O	3:H:108:GLY:N	2.52	0.42
3:H:179:LEU:HD21	3:H:193:MET:HE3	2.00	0.42
5:M:3:BPH:HBC2	5:M:3:BPH:H2C	1.90	0.42
3:H:199:GLN:CD	3:H:200:SER:H	2.27	0.42
4:L:4:BCL:HBB2	4:L:4:BCL:HMB3	2.01	0.42
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.84	0.42
3:H:148:PRO:HA	3:H:151:LEU:HD23	1.99	0.42
1:L:107:ILE:HD13	2:M:255:THR:HG23	2.01	0.42
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.01	0.42
3:H:103:ASP:HA	3:H:104:PRO:HD3	1.73	0.42
4:L:2:BCL:H2C	5:M:3:BPH:HBC2	2.00	0.42
2:M:201:PHE:HA	2:M:204:LEU:HD12	2.02	0.42
1:L:38:THR:HG21	1:L:100:TRP:CE3	2.55	0.42
2:M:22:GLU:HB3	2:M:23:ASP:H	1.63	0.42
2:M:242:GLY:HA3	3:H:117:ARG:HD2	2.01	0.42
3:H:82:ASP:O	3:H:84:PRO:HA	2.20	0.42
2:M:261:THR:HG22	3:H:40:TYR:CD1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:PRO:O	2:M:254:TRP:HA	2.20	0.42
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.84	0.42
2:M:35:PHE:HB3	2:M:39:LEU:HB2	2.02	0.42
3:H:210:SER:HA	3:H:213:PHE:CD2	2.55	0.42
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.55	0.41
2:M:152:SER:O	2:M:155:TRP:HB3	2.20	0.41
2:M:66:TRP:NE1	2:M:70:ILE:HD11	2.35	0.41
1:L:141:ALA:HB3	1:L:144:TYR:CE2	2.56	0.41
4:M:1:BCL:C3B	8:M:304:CRT:H20	2.50	0.41
1:L:69:PRO:HG2	1:L:142:TRP:HB2	2.02	0.41
1:L:207:ARG:NH2	2:M:141:GLY:HA3	2.34	0.41
2:M:259:ASN:ND2	3:H:40:TYR:HB3	2.36	0.41
3:H:132:LYS:CE	3:H:171:ILE:HD11	2.47	0.41
1:L:131:LEU:HD22	1:L:156:TRP:CH2	2.56	0.41
3:H:159:GLU:O	3:H:210:SER:HB3	2.21	0.41
3:H:108:GLY:HA3	3:H:114:TRP:CE3	2.56	0.41
1:L:200:PRO:O	1:L:202:LYS:N	2.54	0.41
1:L:45:GLY:O	1:L:49:ILE:HG13	2.21	0.40
1:L:75:LEU:HA	1:L:142:TRP:CD1	2.57	0.40
1:L:263:TRP:CD1	1:L:263:TRP:H	2.38	0.40
3:H:31:LEU:HD22	3:H:31:LEU:HA	1.87	0.40
3:H:89:ARG:H	3:H:89:ARG:NE	2.11	0.40
3:H:156:CYS:HB3	3:H:206:ASN:O	2.22	0.40
6:M:303:U10:H421	6:M:303:U10:H401	1.77	0.40
3:H:184:LYS:O	3:H:185:ASP:HB3	2.21	0.40
1:L:8:LYS:HE2	1:L:9:TYR:CE2	2.57	0.40
3:H:68:HIS:CE1	3:H:123:LEU:HB2	2.55	0.40
1:L:193:LEU:O	1:L:196:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	264/266 (99%)	237 (90%)	20 (8%)	7 (3%)	4	22
2	M	294/296 (99%)	242 (82%)	30 (10%)	22 (8%)	1	4
3	H	235/237 (99%)	188 (80%)	28 (12%)	19 (8%)	1	3
All	All	793/799 (99%)	667 (84%)	78 (10%)	48 (6%)	1	7

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	LEU
1	L	115	TYR
1	L	201	GLU
1	L	269	LEU
2	M	22	GLU
2	M	52	LEU
2	M	54	SER
2	M	99	PRO
2	M	104	SER
2	M	105	PHE
2	M	111	GLU
2	M	144	LYS
3	H	13	ALA
3	H	51	ALA
3	H	60	LYS
3	H	94	GLU
3	H	127	GLY
3	H	138	ALA
3	H	185	ASP
3	H	212	LEU
2	M	37	THR
2	M	83	ALA
2	M	287	SER
3	H	44	ASN
3	H	57	PRO
3	H	68	HIS
3	H	92	VAL
3	H	142	VAL
3	H	214	ALA
1	L	15	THR
2	M	82	PRO
2	M	96	PRO
3	H	32	GLN
3	H	39	GLY

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Mol	Chain	Res	Type
3	H	49	PRO
2	M	30	SER
2	M	33	GLY
2	M	80	TRP
3	H	31	LEU
3	H	246	PRO
1	L	31	VAL
1	L	202	LYS
2	M	24	VAL
2	M	195	ASN
2	M	97	PRO
2	M	112	GLY
2	M	15	PRO
2	M	32	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	210/210 (100%)	181 (86%)	29 (14%)	3	17
2	M	232/232 (100%)	197 (85%)	35 (15%)	3	14
3	H	192/192 (100%)	153 (80%)	39 (20%)	1	7
All	All	634/634 (100%)	531 (84%)	103 (16%)	2	12

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	PHE
1	L	6	GLU
1	L	8	LYS
1	L	48	LEU
1	L	54	VAL
1	L	72	GLU
1	L	82	LYS
1	L	103	ARG

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Mol	Chain	Res	Type
1	L	113	ILE
1	L	129	LEU
1	L	133	LEU
1	L	138	MET
1	L	158	SER
1	L	185	LEU
1	L	193	LEU
1	L	196	SER
1	L	204	LYS
1	L	208	THR
1	L	216	PHE
1	L	227	LEU
1	L	232	LEU
1	L	234	LEU
1	L	235	LEU
1	L	247	CYS
1	L	249	ILE
1	L	251	THR
1	L	253	THR
1	L	257	ASP
1	L	269	LEU
2	M	20	MET
2	M	24	VAL
2	M	25	ASN
2	M	28	ASN
2	M	32	VAL
2	M	35	PHE
2	M	37	THR
2	M	38	LEU
2	M	60	LEU
2	M	64	LEU
2	M	72	ILE
2	M	81	ASN
2	M	94	LEU
2	M	99	PRO
2	M	100	GLU
2	M	103	LEU
2	M	109	LEU
2	M	111	GLU
2	M	135	LEU
2	M	148	TRP
2	M	154	ILE

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Mol	Chain	Res	Type
2	M	175	VAL
2	M	222	THR
2	M	226	VAL
2	M	227	SER
2	M	228	ARG
2	M	258	PHE
2	M	259	ASN
2	M	262	MET
2	M	267	ARG
2	M	270	ILE
2	M	271	TRP
2	M	272	MET
2	M	275	LEU
2	M	286	LEU
3	H	14	SER
3	H	15	LEU
3	H	24	LEU
3	H	35	ASN
3	H	38	GLU
3	H	52	ASN
3	H	53	GLN
3	H	68	HIS
3	H	70	ARG
3	H	75	VAL
3	H	79	GLU
3	H	83	ARG
3	H	87	LEU
3	H	89	ARG
3	H	94	GLU
3	H	97	PRO
3	H	109	VAL
3	H	123	LEU
3	H	126	HIS
3	H	132	LYS
3	H	146	LYS
3	H	151	LEU
3	H	154	ARG
3	H	165	VAL
3	H	173	GLU
3	H	188	THR
3	H	193	MET
3	H	196	VAL

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Mol	Chain	Res	Type
3	H	208	LEU
3	H	212	LEU
3	H	213	PHE
3	H	217	PRO
3	H	218	THR
3	H	219	ILE
3	H	220	LYS
3	H	228	LEU
3	H	246	PRO
3	H	247	LYS
3	H	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	173	HIS
1	L	211	HIS
2	M	11	GLN
2	M	28	ASN
2	M	77	GLN
3	H	141	HIS
3	H	147	ASN
3	H	204	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	2	1	69,74,74	1.19	7 (10%)	79,115,115	1.82	17 (21%)
6	U10	M	303	-	51,51,63	1.60	13 (25%)	63,64,79	1.61	13 (20%)
4	BCL	M	1	2	54,59,74	1.21	4 (7%)	61,97,115	2.14	21 (34%)
4	BCL	L	4	1	54,59,74	1.32	8 (14%)	61,97,115	2.31	20 (32%)
6	U10	L	272	-	41,41,63	1.78	10 (24%)	51,52,79	1.52	12 (23%)
5	BPH	M	3	-	59,70,70	1.64	8 (13%)	59,101,101	2.55	19 (32%)
5	BPH	M	5	-	59,70,70	1.62	8 (13%)	59,101,101	2.51	19 (32%)
5	BPH	L	271	-	59,70,70	1.54	7 (11%)	59,101,101	2.64	19 (32%)
8	CRT	M	304	-	40,41,43	3.95	23 (57%)	47,50,54	3.00	17 (36%)

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	2	1	-	8/41/137/137	-
6	U10	M	303	-	-	15/49/73/87	0/1/1/1
4	BCL	M	1	2	-	5/23/119/137	-
4	BCL	L	4	1	-	3/23/119/137	-
6	U10	L	272	-	-	8/37/61/87	0/1/1/1
5	BPH	M	5	-	2/2/18/22	3/37/105/105	0/5/6/6
5	BPH	M	3	-	-	10/37/105/105	0/5/6/6
5	BPH	L	271	-	-	7/37/105/105	0/5/6/6
8	CRT	M	304	-	-	26/47/47/51	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C6-C5	8.47	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	5	BPH	C3A-C2A	-8.21	1.47	1.54
5	L	271	BPH	C3A-C2A	-7.91	1.47	1.54
8	M	304	CRT	C26-C25	7.90	1.55	1.34
8	M	304	CRT	C10-C11	7.64	1.54	1.34
8	M	304	CRT	C31-C30	7.62	1.54	1.34
8	M	304	CRT	C15-C16	7.46	1.54	1.34
5	M	3	BPH	C2C-C3C	-7.28	1.48	1.54
8	M	304	CRT	C35-C36	6.99	1.51	1.32
8	M	304	CRT	C21-C20	6.73	1.54	1.36
5	M	3	BPH	C3D-CAD	-5.14	1.37	1.47
8	M	304	CRT	C25-C23	-4.29	1.36	1.46
8	M	304	CRT	C30-C28	-4.13	1.37	1.46
5	L	271	BPH	C3D-CAD	-4.09	1.39	1.47
8	M	304	CRT	C11-C12	-4.03	1.37	1.46
5	M	5	BPH	C3D-CAD	-4.00	1.40	1.47
6	L	272	U10	C7-C8	-3.96	1.44	1.50
8	M	304	CRT	C31-C32	3.94	1.55	1.43
8	M	304	CRT	C15-C14	3.92	1.55	1.43
8	M	304	CRT	C20-C19	3.86	1.55	1.43
4	L	2	BCL	O2D-CGD	-3.86	1.23	1.33
4	L	2	BCL	C1D-C2D	-3.83	1.37	1.45
8	M	304	CRT	C21-C22	3.73	1.54	1.43
5	M	3	BPH	C3A-C2A	-3.71	1.51	1.54
8	M	304	CRT	C26-C27	3.67	1.54	1.43
5	L	271	BPH	O2D-CGD	-3.63	1.24	1.33
6	L	272	U10	C6-C1	3.57	1.41	1.35
4	L	4	BCL	C1D-C2D	-3.56	1.38	1.45
8	M	304	CRT	C16-C17	-3.53	1.38	1.46
4	L	4	BCL	O2D-CGD	-3.51	1.24	1.33
4	M	1	BCL	O2D-CGD	-3.50	1.24	1.33
4	L	4	BCL	O2A-CGA	-3.47	1.23	1.33
8	M	304	CRT	C35-C33	3.44	1.53	1.46
5	M	5	BPH	C3B-CAB	-3.43	1.40	1.49
5	M	5	BPH	O2D-CGD	-3.41	1.24	1.33
5	M	5	BPH	O2A-CGA	-3.39	1.23	1.33
8	M	304	CRT	C10-C9	3.38	1.53	1.43
5	M	3	BPH	O2D-CGD	-3.33	1.25	1.33
8	M	304	CRT	C6-C7	-3.31	1.38	1.46
5	M	3	BPH	O2A-CGA	-3.25	1.23	1.33
6	L	272	U10	C23-C24	3.18	1.40	1.33
8	M	304	CRT	C4-C5	3.17	1.54	1.50
4	L	2	BCL	O2A-CGA	-3.16	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	303	U10	C6-C1	3.12	1.40	1.35
6	M	303	U10	C3-C2	-3.12	1.39	1.48
4	M	1	BCL	O2A-CGA	-3.11	1.24	1.33
6	M	303	U10	C4-C5	-3.06	1.40	1.48
6	L	272	U10	C18-C19	3.03	1.40	1.33
5	L	271	BPH	O2A-CGA	-3.02	1.24	1.33
6	M	303	U10	C7-C8	-3.00	1.45	1.50
4	M	1	BCL	C1D-C2D	-2.91	1.39	1.45
6	L	272	U10	C3-C2	-2.90	1.40	1.48
6	L	272	U10	C28-C29	2.89	1.39	1.33
6	M	303	U10	C33-C34	2.85	1.39	1.33
6	L	272	U10	C4-C5	-2.80	1.40	1.48
4	L	2	BCL	C2-C3	2.79	1.39	1.33
6	L	272	U10	C34-C33	2.78	1.47	1.29
6	M	303	U10	C18-C19	2.66	1.39	1.33
6	L	272	U10	C13-C14	2.64	1.39	1.33
5	M	3	BPH	C3B-CAB	-2.63	1.42	1.49
6	M	303	U10	C28-C29	2.60	1.39	1.33
6	M	303	U10	C23-C24	2.59	1.39	1.33
4	L	2	BCL	C1D-ND	-2.57	1.34	1.37
6	M	303	U10	C38-C39	2.57	1.39	1.33
5	M	3	BPH	C1D-C2D	-2.56	1.36	1.39
6	M	303	U10	C44-C43	2.54	1.45	1.29
5	L	271	BPH	C2-C3	2.52	1.38	1.33
6	M	303	U10	C13-C14	2.51	1.38	1.33
5	M	5	BPH	C2C-C3C	-2.49	1.52	1.54
6	L	272	U10	C8-C9	2.46	1.38	1.33
5	L	271	BPH	C3B-CAB	-2.43	1.42	1.49
5	L	271	BPH	C2C-C3C	-2.39	1.52	1.54
5	M	5	BPH	C2-C3	2.37	1.38	1.33
4	L	2	BCL	CAA-C2A	-2.36	1.49	1.54
8	M	304	CRT	C8-C7	2.35	1.55	1.50
4	L	4	BCL	C2-C3	2.27	1.39	1.32
5	M	3	BPH	C2-C3	2.21	1.38	1.33
4	L	4	BCL	CMC-C2C	-2.21	1.48	1.53
6	M	303	U10	C8-C9	2.21	1.38	1.33
5	M	5	BPH	C3B-C4B	-2.17	1.38	1.41
4	L	4	BCL	C3D-CAD	-2.14	1.38	1.45
4	M	1	BCL	C3D-CAD	-2.14	1.38	1.45
4	L	2	BCL	C3A-C2A	-2.12	1.48	1.54
4	L	4	BCL	C1B-C2B	-2.08	1.38	1.43
4	L	4	BCL	C1D-ND	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C4-C1	2.06	1.56	1.52
6	M	303	U10	C1-C2	-2.03	1.40	1.47
8	M	304	CRT	C3-C1	2.02	1.57	1.52

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	271	BPH	O2D-CGD-CBD	9.32	121.19	110.95
8	M	304	CRT	C37-C36-C35	-9.20	106.03	125.93
5	M	5	BPH	C4D-CHA-CBD	-7.71	104.76	108.45
5	M	3	BPH	C4D-CHA-CBD	-7.70	104.76	108.45
5	M	3	BPH	C3D-C4D-ND	7.52	117.34	107.71
5	M	3	BPH	C4D-ND-C1D	-7.32	100.10	108.87
5	M	5	BPH	C3D-C4D-ND	7.31	117.08	107.71
5	L	271	BPH	C4D-CHA-CBD	-7.09	105.05	108.45
4	L	4	BCL	C1C-NC-C4C	6.88	109.82	106.68
8	M	304	CRT	C36-C35-C33	-6.74	115.70	125.89
4	M	1	BCL	C1C-NC-C4C	6.49	109.64	106.68
5	M	3	BPH	O2D-CGD-CBD	6.45	118.03	110.95
5	M	5	BPH	O2D-CGD-CBD	6.45	118.03	110.95
5	L	271	BPH	O1D-CGD-CBD	-6.37	115.06	124.72
8	M	304	CRT	C26-C27-C28	-6.32	118.41	127.28
8	M	304	CRT	C5-C6-C7	-6.16	116.58	125.89
5	L	271	BPH	C3D-C4D-ND	5.95	115.33	107.71
5	M	5	BPH	C4D-ND-C1D	-5.91	101.79	108.87
8	M	304	CRT	C38-C37-C36	5.59	133.23	114.10
4	L	2	BCL	C1C-NC-C4C	5.52	109.20	106.68
4	M	1	BCL	O2D-CGD-CBD	5.16	120.25	111.23
4	L	4	BCL	O2D-CGD-CBD	5.09	120.14	111.23
5	M	5	BPH	O1D-CGD-CBD	-5.09	117.01	124.72
4	L	4	BCL	C1D-ND-C4D	-5.01	102.80	106.31
5	L	271	BPH	C4D-ND-C1D	-4.94	102.95	108.87
8	M	304	CRT	C20-C19-C17	-4.83	120.51	127.28
8	M	304	CRT	C21-C22-C23	-4.70	120.69	127.28
5	M	3	BPH	C2D-C1D-ND	4.69	112.82	109.43
4	L	4	BCL	C4D-CHA-C1A	4.55	126.68	121.24
4	L	4	BCL	O1D-CGD-CBD	-4.54	115.57	124.52
4	L	4	BCL	C4A-NA-C1A	4.43	108.70	106.68
4	M	1	BCL	C4D-C3D-CAD	-4.39	103.34	108.11
5	L	271	BPH	C3D-CAD-CBD	4.35	113.33	107.61
4	L	2	BCL	C4D-C3D-CAD	-4.33	103.41	108.11
5	L	271	BPH	C2B-C1B-NB	4.29	112.53	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	BCL	C4D-CHA-C1A	4.26	126.32	121.24
8	M	304	CRT	C34-C33-C35	-4.18	111.70	118.09
4	L	4	BCL	C4D-C3D-CAD	-4.12	103.63	108.11
5	M	3	BPH	C2B-C1B-NB	4.10	112.39	109.43
4	L	2	BCL	C4D-CHA-C1A	4.10	126.14	121.24
6	M	303	U10	C7-C6-C5	3.99	123.15	118.52
5	M	5	BPH	C3D-CAD-CBD	3.91	112.75	107.61
5	M	5	BPH	CMC-C2C-C1C	-3.86	106.29	114.61
4	L	2	BCL	CBC-CAC-C3C	3.86	121.60	113.41
4	L	2	BCL	C1D-ND-C4D	-3.83	103.63	106.31
4	M	1	BCL	C1D-ND-C4D	-3.80	103.65	106.31
4	L	4	BCL	C3D-C4D-ND	3.72	116.04	109.99
5	L	271	BPH	CMC-C2C-C1C	-3.67	106.70	114.61
5	M	5	BPH	CBA-CAA-C2A	3.65	124.52	113.78
6	M	303	U10	C7-C6-C1	-3.62	118.68	124.89
8	M	304	CRT	C8-C7-C9	-3.62	116.95	122.82
4	M	1	BCL	C3D-C4D-ND	3.62	115.87	109.99
4	L	2	BCL	C3D-C4D-ND	3.59	115.83	109.99
8	M	304	CRT	C39-C38-C37	3.59	124.69	110.46
5	M	5	BPH	C2B-C1B-NB	3.56	112.01	109.43
5	M	3	BPH	C3D-CAD-CBD	3.54	112.27	107.61
6	L	272	U10	C20-C19-C21	3.50	121.30	115.23
8	M	304	CRT	C9-C10-C11	-3.49	113.09	123.20
6	M	303	U10	C30-C29-C28	-3.46	114.73	123.63
5	L	271	BPH	CMB-C2B-C3B	3.44	131.56	124.68
4	L	4	BCL	CAA-CBA-CGA	3.42	122.93	113.21
5	L	271	BPH	OBD-CAD-C3D	-3.33	122.69	127.89
4	M	1	BCL	C1-C2-C3	-3.33	121.37	126.76
5	L	271	BPH	C1B-NB-C4B	-3.32	103.98	108.82
4	L	2	BCL	C3D-C2D-C1D	3.32	110.36	105.83
4	L	2	BCL	CBA-CAA-C2A	-3.30	103.97	113.79
8	M	304	CRT	C40-C38-C37	3.23	123.28	110.46
4	M	1	BCL	O1D-CGD-CBD	-3.15	118.31	124.52
6	M	303	U10	C40-C39-C41	3.14	120.68	115.23
6	M	303	U10	C30-C29-C31	3.13	120.67	115.23
8	M	304	CRT	C15-C14-C12	-3.11	122.92	127.28
4	L	2	BCL	C1-O2A-CGA	3.09	124.14	116.65
5	M	5	BPH	C1B-NB-C4B	-3.06	104.36	108.82
6	L	272	U10	C10-C9-C11	3.05	120.51	115.23
4	L	2	BCL	C4A-NA-C1A	2.96	108.03	106.68
4	M	1	BCL	C4A-NA-C1A	2.93	108.02	106.68
5	M	3	BPH	C1B-NB-C4B	-2.91	104.57	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	271	BPH	C3B-C4B-NB	2.91	112.28	108.05
5	M	3	BPH	CED-O2D-CGD	2.88	122.46	115.92
6	L	272	U10	C10-C9-C8	-2.85	116.30	123.63
6	L	272	U10	C7-C8-C9	-2.84	121.94	126.83
5	L	271	BPH	CBA-CAA-C2A	2.80	122.03	113.78
5	L	271	BPH	C1-C2-C3	-2.80	121.62	126.20
4	L	2	BCL	OBD-CAD-C3D	-2.77	121.93	128.42
5	M	3	BPH	C1C-C2C-C3C	2.77	105.48	102.84
5	L	271	BPH	C17-C16-C15	-2.76	100.92	113.28
5	L	271	BPH	C4A-C3A-C2A	2.76	105.46	102.84
4	L	4	BCL	OBD-CAD-C3D	-2.75	121.98	128.42
5	M	5	BPH	C2D-C1D-ND	2.74	111.41	109.43
6	L	272	U10	C30-C29-C31	2.74	119.98	115.23
4	L	4	BCL	C2A-C3A-C4A	2.73	106.28	101.87
5	M	3	BPH	C1-O2A-CGA	2.70	123.18	116.65
6	M	303	U10	C40-C39-C38	-2.69	116.73	123.63
4	L	4	BCL	CHA-C4D-ND	-2.68	127.01	132.55
4	M	1	BCL	C3D-C2D-C1D	2.68	109.49	105.83
6	L	272	U10	C15-C14-C13	-2.66	116.80	123.63
4	L	4	BCL	CAA-C2A-C3A	-2.66	105.82	113.00
4	M	1	BCL	OBD-CAD-C3D	-2.62	122.29	128.42
4	M	1	BCL	CHA-C4D-ND	-2.61	127.17	132.55
5	M	3	BPH	CMA-C3A-C4A	-2.59	109.02	114.61
5	M	3	BPH	CGD-CBD-CAD	-2.59	102.46	110.85
6	L	272	U10	C20-C19-C18	-2.59	116.98	123.63
4	L	4	BCL	C2B-C1B-NB	2.58	113.01	110.33
4	L	2	BCL	C3A-C2A-C1A	2.57	105.19	101.34
5	M	5	BPH	C3B-C4B-NB	2.57	111.79	108.05
4	L	2	BCL	CAA-C2A-C3A	-2.57	106.07	113.00
4	L	2	BCL	CHA-C4D-ND	-2.54	127.30	132.55
4	L	4	BCL	C3D-C2D-C1D	2.42	109.14	105.83
6	M	303	U10	C10-C9-C8	-2.40	117.45	123.63
5	M	3	BPH	C4-C3-C5	2.40	119.40	115.23
4	M	1	BCL	C2B-C1B-NB	2.38	112.80	110.33
6	M	303	U10	C1M-C1-C6	-2.36	120.58	124.45
5	M	3	BPH	CMB-C2B-C3B	2.35	129.39	124.68
5	M	3	BPH	C4A-C3A-C2A	2.35	105.07	102.84
4	M	1	BCL	C2C-C3C-C4C	2.34	104.84	101.34
6	M	303	U10	C20-C19-C18	-2.34	117.62	123.63
8	M	304	CRT	C18-C17-C16	-2.34	114.52	118.09
8	M	304	CRT	C30-C28-C27	-2.32	115.36	119.01
5	M	3	BPH	O1D-CGD-CBD	-2.31	121.21	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4	BCL	C5-C3-C4	2.31	119.91	114.59
5	M	5	BPH	CMB-C2B-C3B	2.30	129.28	124.68
4	M	1	BCL	CAB-C3B-C2B	-2.27	123.02	127.74
5	M	5	BPH	CMA-C3A-C4A	-2.24	109.78	114.61
8	M	304	CRT	C32-C31-C30	-2.23	116.73	123.20
5	M	5	BPH	OBD-CAD-CBD	-2.23	122.55	125.82
5	M	5	BPH	C1-O2A-CGA	2.23	122.04	116.65
4	M	1	BCL	CAA-C2A-C3A	-2.19	107.08	113.00
4	L	4	BCL	CMB-C2B-C1B	-2.19	122.09	125.42
5	M	5	BPH	CBC-CAC-C3C	-2.18	109.50	113.78
8	M	304	CRT	C10-C9-C7	2.17	130.32	127.28
6	L	272	U10	C15-C14-C16	2.15	118.97	115.23
4	L	4	BCL	CHC-C4B-NB	-2.15	120.83	124.05
6	L	272	U10	C30-C29-C28	-2.15	118.12	123.63
4	L	4	BCL	CMB-C2B-C3B	2.14	132.43	125.67
5	M	3	BPH	OBD-CAD-C3D	-2.14	124.55	127.89
4	L	4	BCL	CHA-C1A-NA	-2.13	121.57	126.39
6	L	272	U10	C3-C2-C1	2.13	122.31	118.10
5	M	5	BPH	OBD-CAD-C3D	-2.13	124.57	127.89
6	M	303	U10	C25-C24-C23	-2.13	118.17	123.63
4	M	1	BCL	CAA-CBA-CGA	2.12	119.24	113.21
4	M	1	BCL	CHC-C4B-NB	-2.12	120.87	124.05
4	L	2	BCL	CED-O2D-CGD	2.11	120.71	115.92
6	M	303	U10	C15-C14-C13	-2.11	118.21	123.63
6	L	272	U10	C1M-C1-C6	-2.11	120.99	124.45
6	M	303	U10	C25-C24-C26	2.10	118.88	115.23
4	M	1	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
5	L	271	BPH	CMA-C3A-C2A	-2.07	106.13	114.13
4	M	1	BCL	C5-C3-C4	2.06	119.33	114.59
4	L	2	BCL	C2A-C1A-CHA	2.05	127.43	123.87
6	L	272	U10	C22-C21-C19	2.05	119.97	113.19
5	M	5	BPH	CED-O2D-CGD	2.05	120.56	115.92
6	M	303	U10	C35-C34-C36	2.04	118.77	115.23
4	M	1	BCL	CHA-C1A-NA	-2.04	121.77	126.39
4	L	2	BCL	C2B-C1B-NB	2.04	112.44	110.33
5	L	271	BPH	OBB-CAB-CBB	-2.02	115.88	120.19
5	M	3	BPH	CMC-C2C-C1C	-2.01	110.27	114.61
5	L	271	BPH	C2D-C1D-ND	2.00	110.88	109.43

All (2) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
5	M	5	BPH	C8
5	M	5	BPH	C13

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	BCL	CHA-CBD-CGD-O1D
4	M	1	BCL	CHA-CBD-CGD-O2D
5	L	271	BPH	C4C-C3C-CAC-CBC
5	M	3	BPH	C2C-C3C-CAC-CBC
6	L	272	U10	C29-C31-C32-C33
6	M	303	U10	C25-C24-C26-C27
8	M	304	CRT	C19-C20-C21-C22
8	M	304	CRT	C21-C22-C23-C24
8	M	304	CRT	C23-C25-C26-C27
8	M	304	CRT	C26-C27-C28-C29
8	M	304	CRT	C29-C28-C30-C31
8	M	304	CRT	C28-C30-C31-C32
8	M	304	CRT	C31-C32-C33-C34
8	M	304	CRT	C34-C33-C35-C36
8	M	304	CRT	C36-C37-C38-C39
4	L	2	BCL	O1D-CGD-O2D-CED
4	L	2	BCL	CBD-CGD-O2D-CED
5	M	3	BPH	CBD-CGD-O2D-CED
4	M	1	BCL	CBD-CGD-O2D-CED
5	L	271	BPH	C3-C5-C6-C7
4	L	4	BCL	CBD-CGD-O2D-CED
5	M	3	BPH	O1D-CGD-O2D-CED
6	L	272	U10	C20-C19-C21-C22
6	M	303	U10	C35-C34-C36-C37
6	L	272	U10	C18-C19-C21-C22
6	M	303	U10	C23-C24-C26-C27
6	M	303	U10	C33-C34-C36-C37
4	M	1	BCL	O1D-CGD-O2D-CED
6	M	303	U10	C40-C39-C41-C42
6	M	303	U10	C38-C39-C41-C42
6	L	272	U10	C9-C11-C12-C13
6	L	272	U10	C19-C21-C22-C23
6	L	272	U10	C24-C26-C27-C28
6	M	303	U10	C39-C41-C42-C43
8	M	304	CRT	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	M	304	CRT	C15-C16-C17-C19
5	M	3	BPH	CBA-CGA-O2A-C1
4	L	4	BCL	O1D-CGD-O2D-CED
6	M	303	U10	C9-C11-C12-C13
6	M	303	U10	C24-C26-C27-C28
5	M	3	BPH	O1A-CGA-O2A-C1
5	L	271	BPH	C15-C16-C17-C18
8	M	304	CRT	C18-C17-C19-C20
5	L	271	BPH	C10-C11-C12-C13
4	L	2	BCL	C3A-C2A-CAA-CBA
4	L	2	BCL	O1A-CGA-O2A-C1
5	L	271	BPH	C2C-C3C-CAC-CBC
4	L	2	BCL	C1A-C2A-CAA-CBA
8	M	304	CRT	C2-C1-C4-C5
8	M	304	CRT	C3-C1-C4-C5
8	M	304	CRT	C35-C36-C37-C38
4	L	2	BCL	CBA-CGA-O2A-C1
6	M	303	U10	C19-C21-C22-C23
8	M	304	CRT	C30-C31-C32-C33
5	M	3	BPH	C3-C5-C6-C7
4	L	2	BCL	C2C-C3C-CAC-CBC
5	M	3	BPH	C4C-C3C-CAC-CBC
6	M	303	U10	C5-C4-O4-C4M
8	M	304	CRT	C20-C21-C22-C23
6	M	303	U10	C18-C19-C21-C22
8	M	304	CRT	C2-C1-O1-C1M
8	M	304	CRT	C3-C1-O1-C1M
8	M	304	CRT	C1-C4-C5-C6
5	M	5	BPH	C3A-C2A-CAA-CBA
8	M	304	CRT	C8-C7-C9-C10
8	M	304	CRT	C17-C19-C20-C21
5	L	271	BPH	CBD-CGD-O2D-CED
8	M	304	CRT	C6-C7-C9-C10
8	M	304	CRT	C31-C32-C33-C35
6	M	303	U10	C15-C14-C16-C17
6	L	272	U10	C30-C29-C31-C32
6	L	272	U10	C2-C3-O3-C3M
6	M	303	U10	C29-C31-C32-C33
6	M	303	U10	C20-C19-C21-C22
4	M	1	BCL	C2B-C3B-CAB-CBB
5	M	3	BPH	C5-C6-C7-C8
8	M	304	CRT	O1-C1-C4-C5

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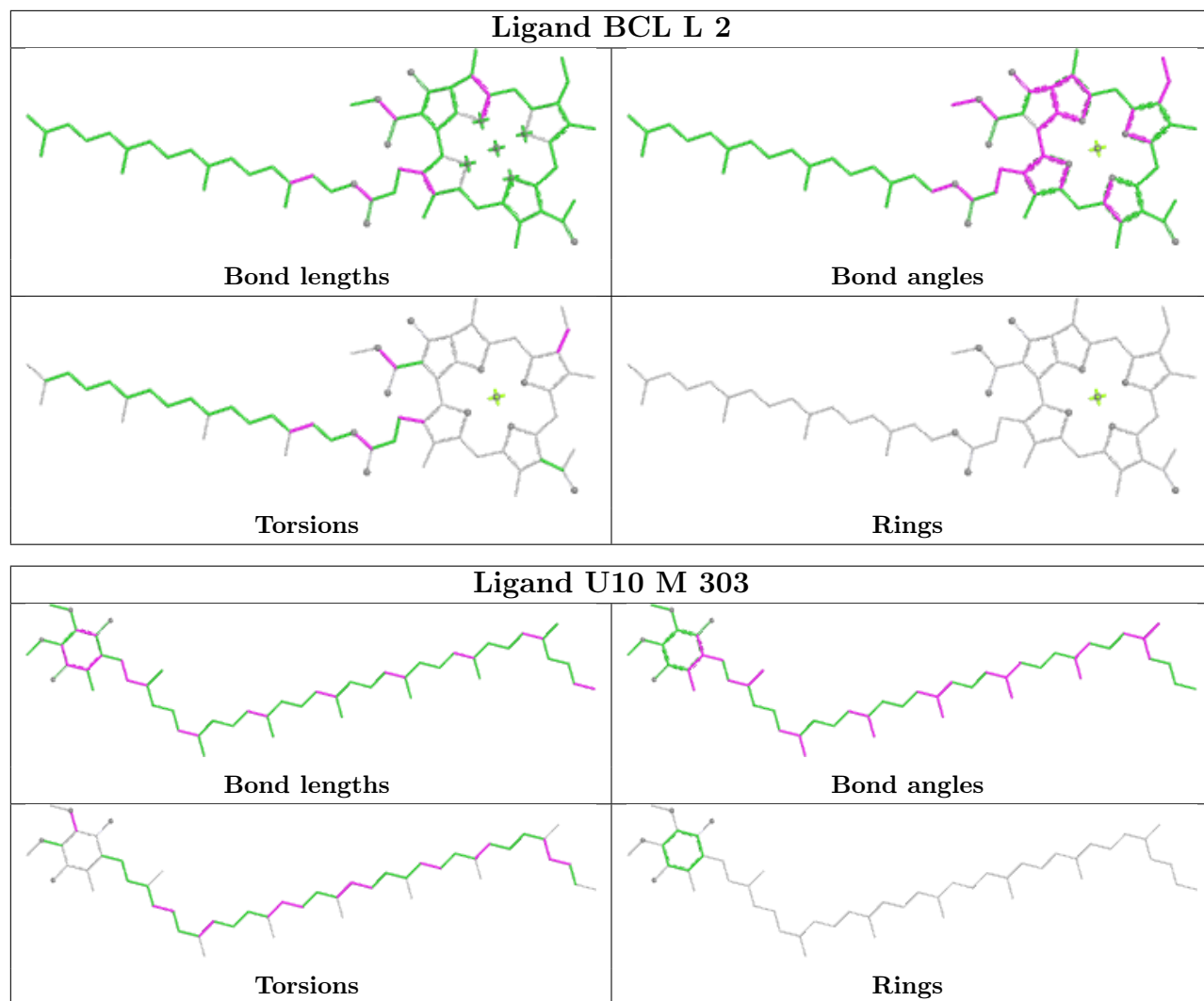
Mol	Chain	Res	Type	Atoms
5	M	3	BPH	CAA-CBA-CGA-O2A
4	L	4	BCL	C2-C1-O2A-CGA
5	M	3	BPH	CAA-CBA-CGA-O1A
5	M	5	BPH	C14-C13-C15-C16
5	M	5	BPH	O1D-CGD-O2D-CED
8	M	304	CRT	C4-C1-O1-C1M
5	L	271	BPH	C2-C1-O2A-CGA
4	L	2	BCL	C1-C2-C3-C4

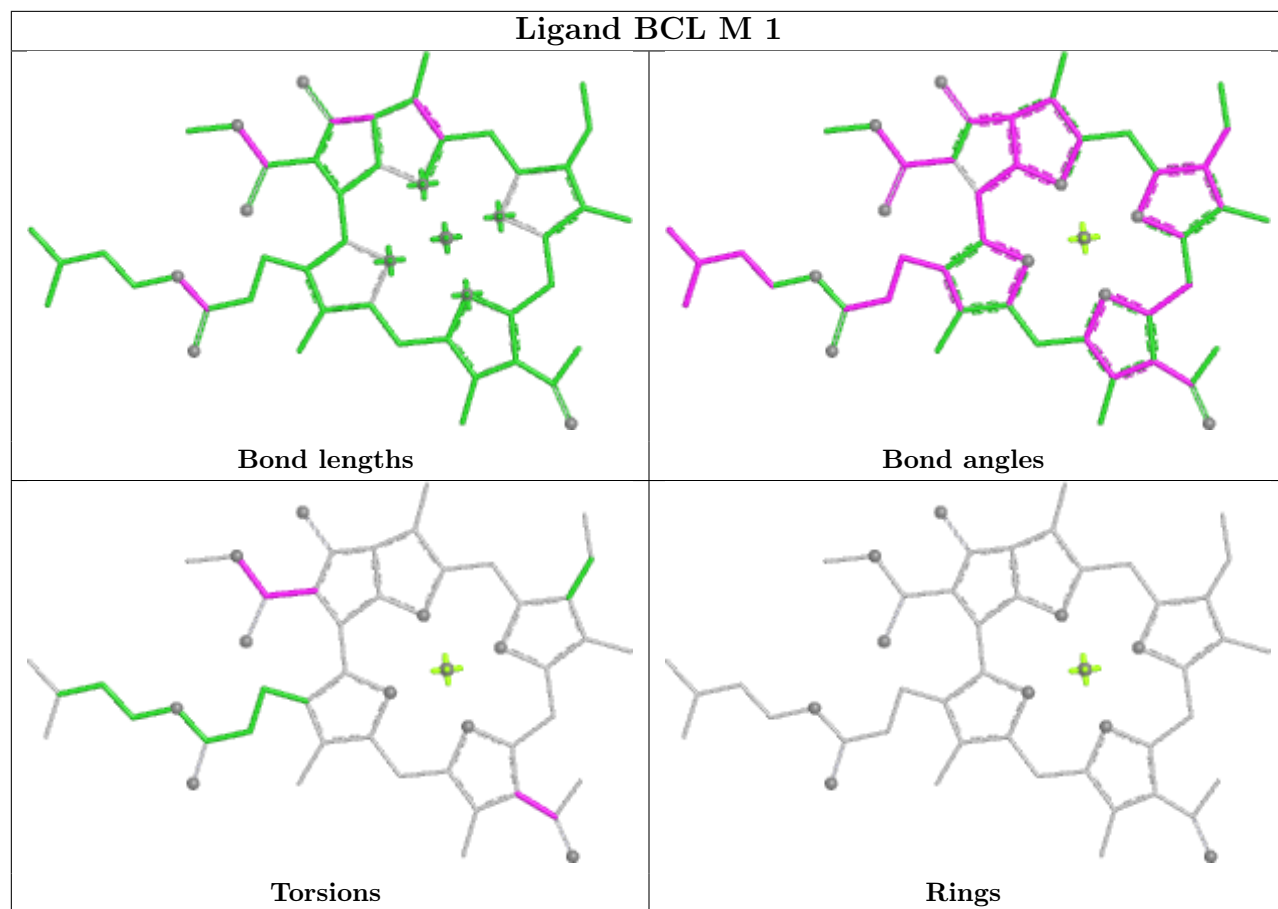
There are no ring outliers.

9 monomers are involved in 35 short contacts:

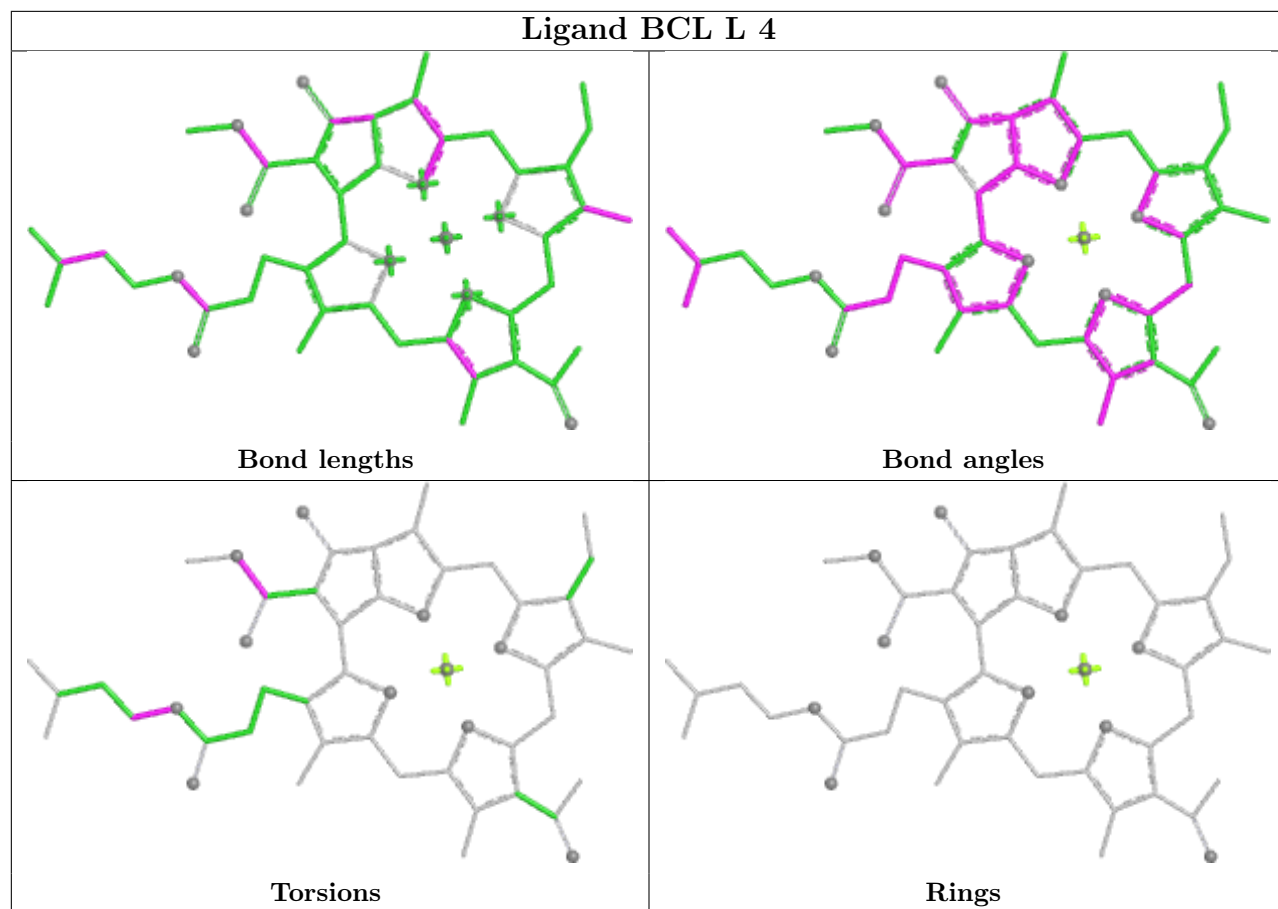
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	2	BCL	7	0
6	M	303	U10	5	0
4	M	1	BCL	6	0
4	L	4	BCL	5	0
6	L	272	U10	4	0
5	M	3	BPH	7	0
5	M	5	BPH	1	0
5	L	271	BPH	6	0
8	M	304	CRT	2	0

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.

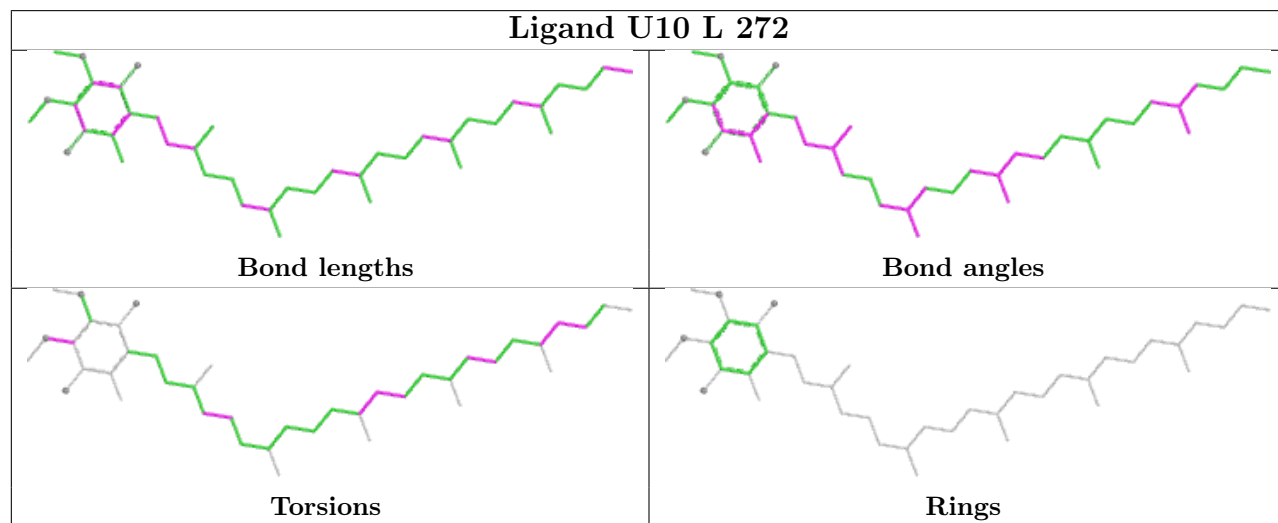




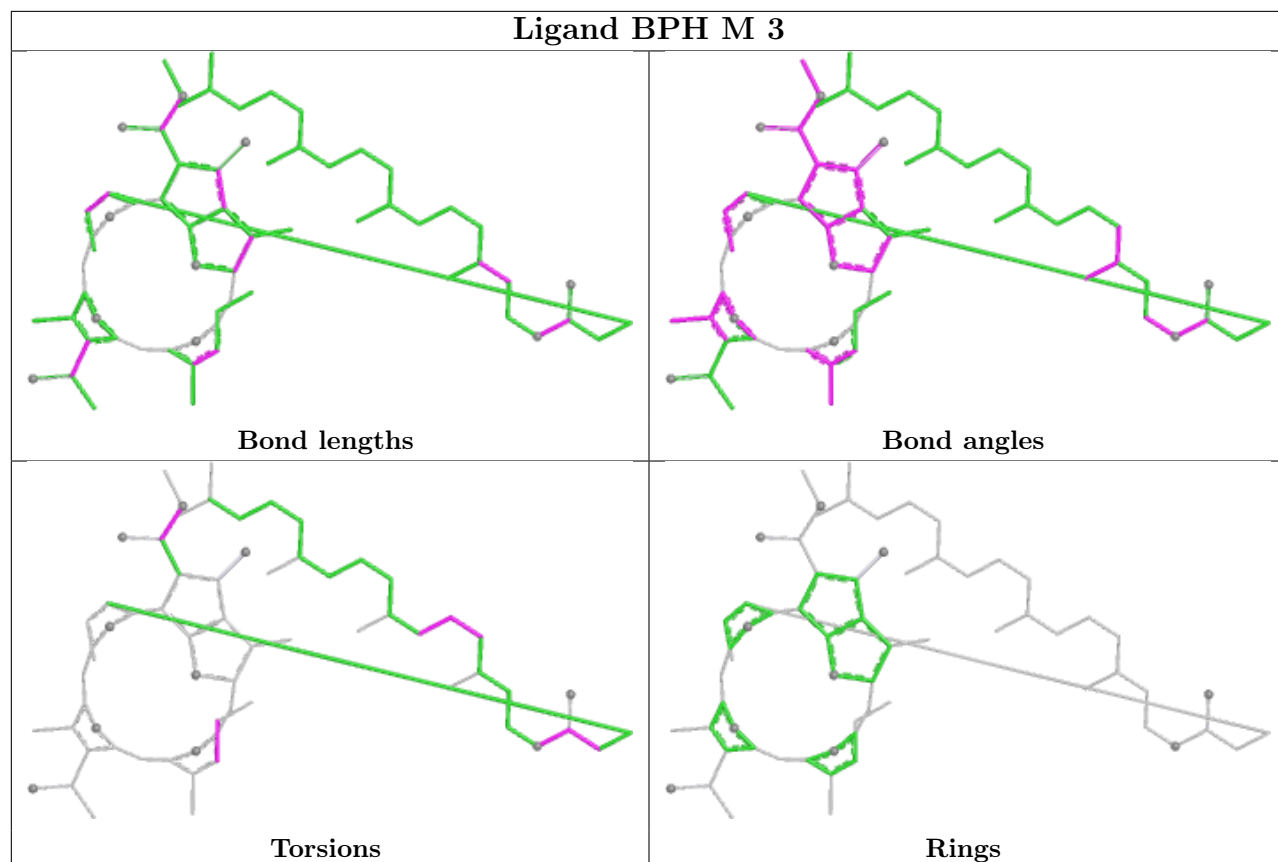
Ligand BCL L 4



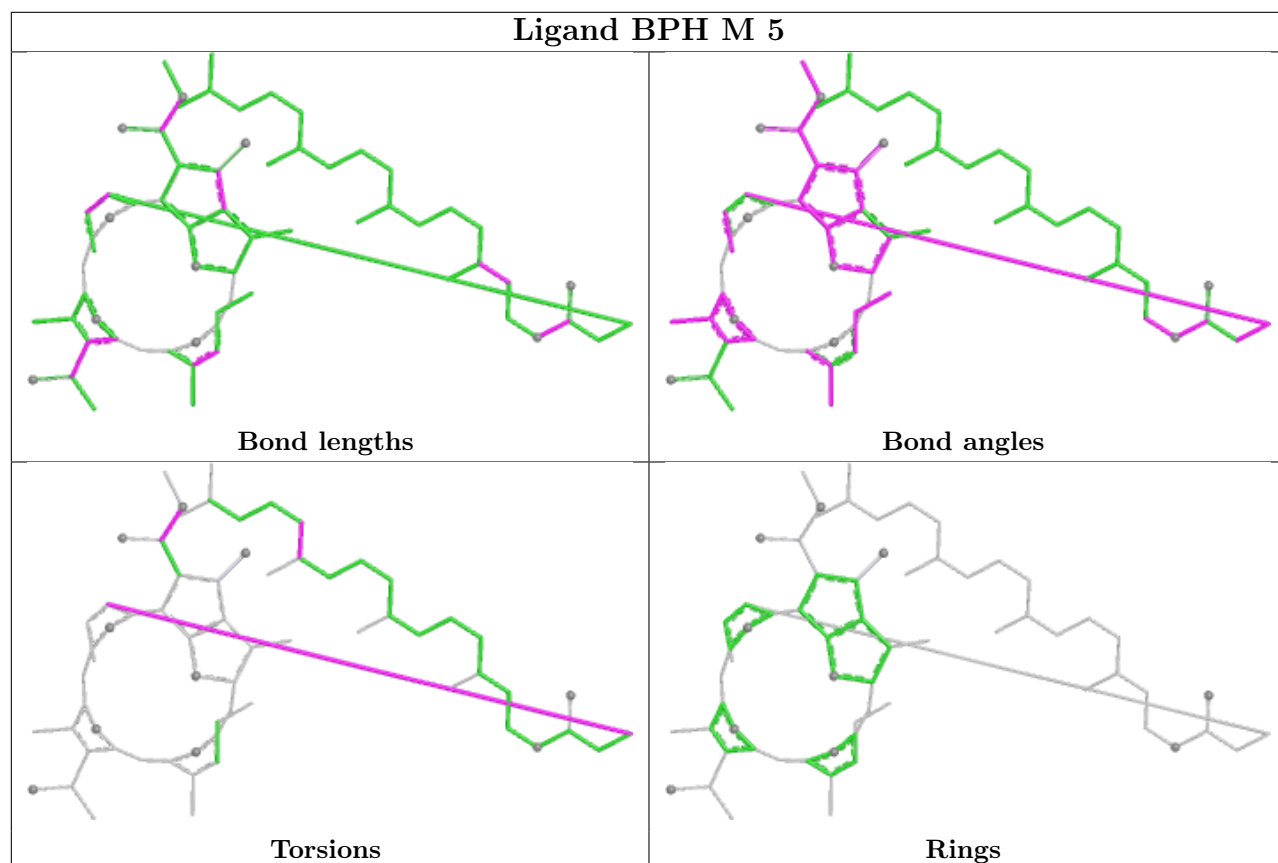
Ligand U10 L 272

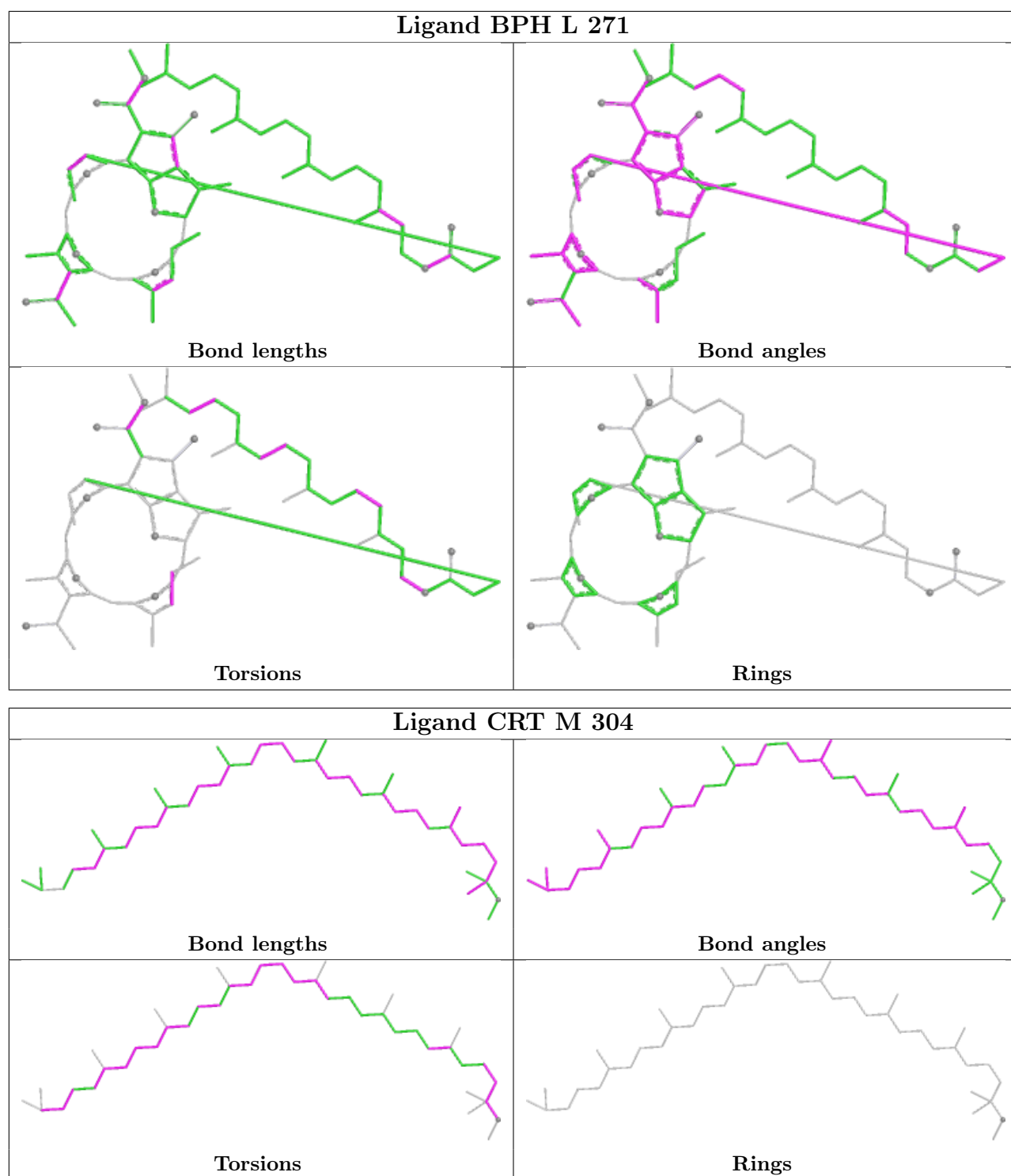


Ligand BPH M 3



Ligand BPH M 5





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.