



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:14 PM UTC

PDB ID : 1PSS / pdb_00001pss
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

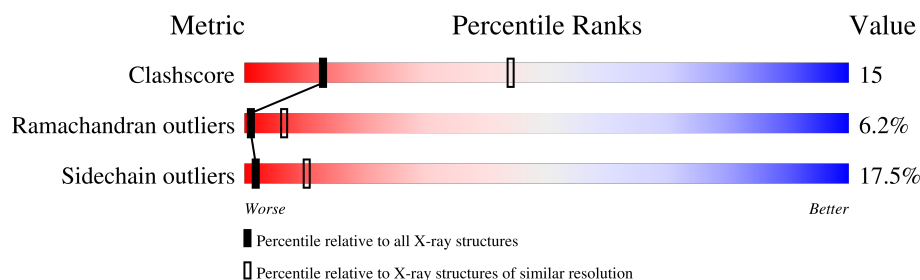
1 Overall quality at a glance

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	60% 31% 9% .
2	M	296	51% 33% 13% .
3	H	237	41% 38% 17% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	3	X	-	-	-
5	BPH	L	271	X	-	-	-

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

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6789 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			

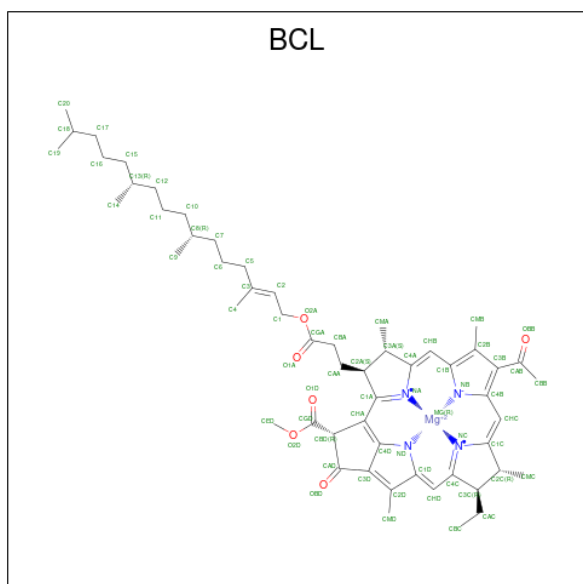
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	296	Total	C	N	O	S	0	0	0
			2362	1579	386	387	10			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

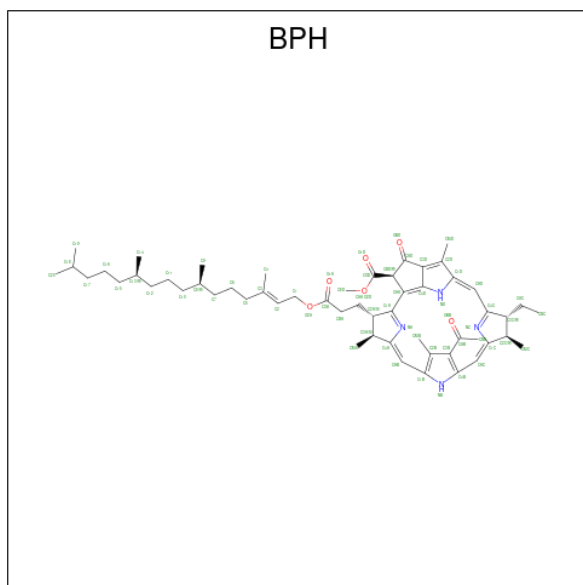
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	0	0
			1807	1156	310	332	9			

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



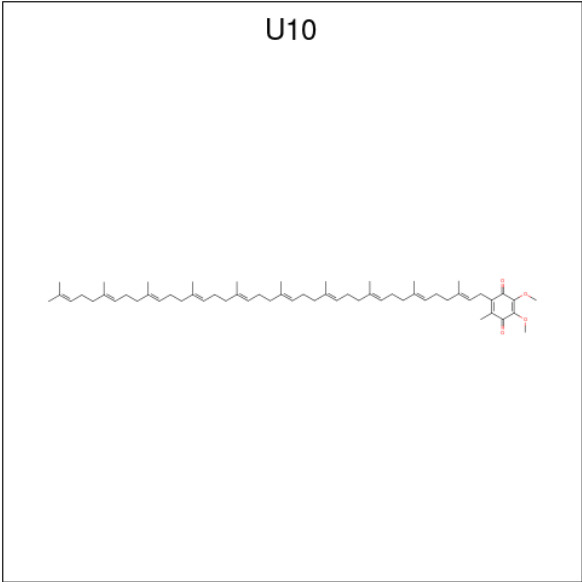
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	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: $C_{59}H_{90}O_4$).

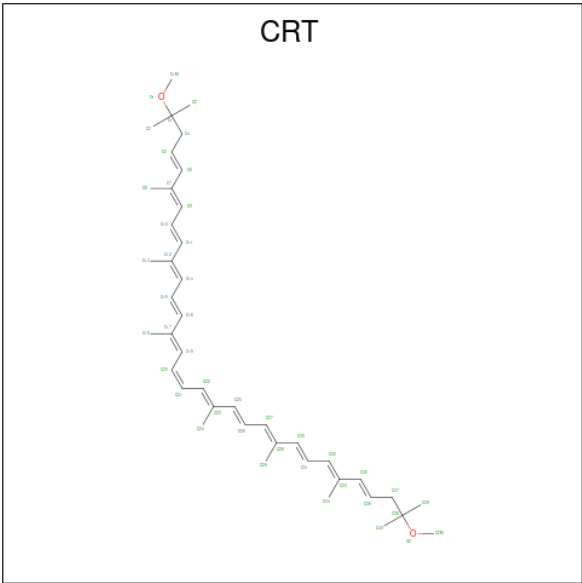


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			41	37	4		
6	M	1	Total	C	O	0	0
			51	47	4		

- 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: C₄₂H₆₀O₂).



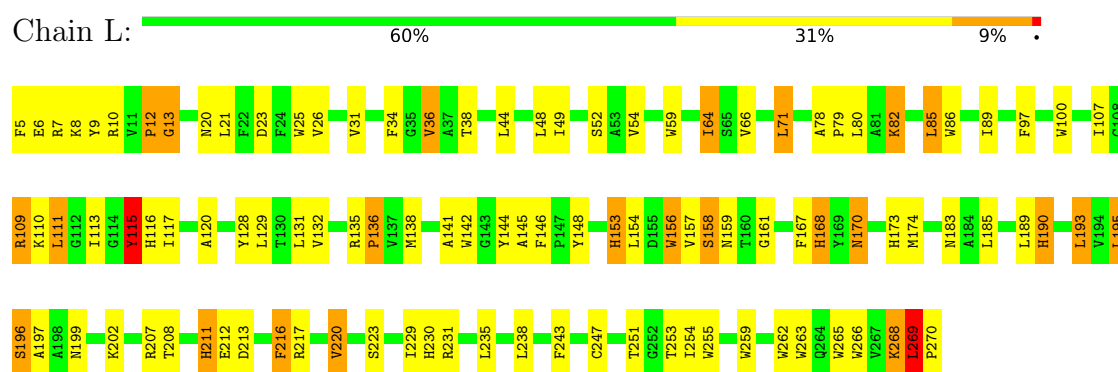
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

3 Residue-property plots

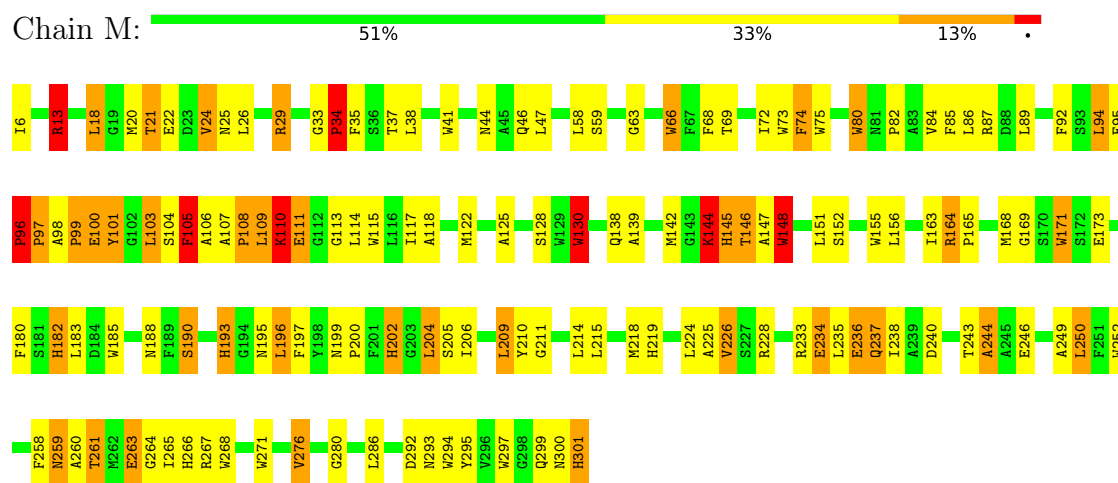
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

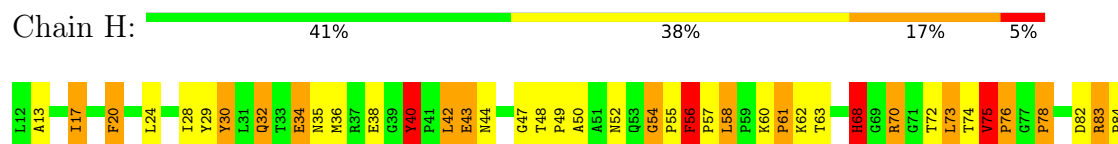
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

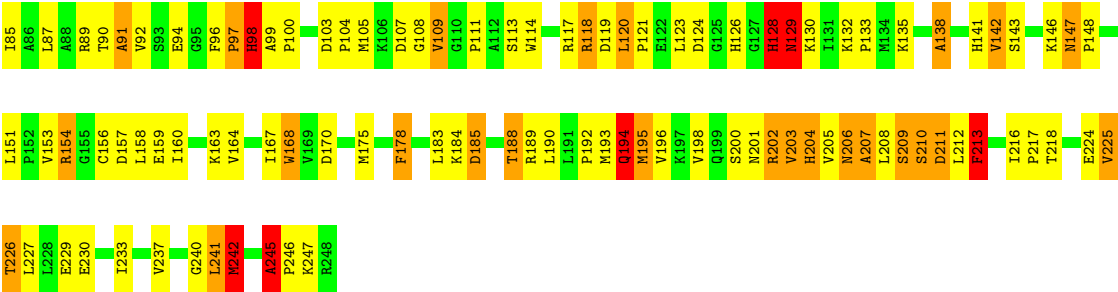


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER





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}	0.223 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6789	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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, BPH, BCL, CRT, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	1.00	13/2204 (0.6%)	1.81	41/3014 (1.4%)
2	M	1.05	9/2453 (0.4%)	1.96	78/3348 (2.3%)
3	H	1.01	6/1855 (0.3%)	2.03	68/2523 (2.7%)
All	All	1.02	28/6512 (0.4%)	1.93	187/8885 (2.1%)

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	1
3	H	0	2
All	All	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	168	HIS	CD2-NE2	-7.50	1.29	1.37
2	M	145	HIS	CD2-NE2	-6.90	1.30	1.37
3	H	68	HIS	CD2-NE2	-6.87	1.30	1.37
1	L	64	ILE	CA-CB	6.77	1.61	1.54
1	L	153	HIS	CD2-NE2	-6.70	1.30	1.37
2	M	301	HIS	CD2-NE2	-6.64	1.30	1.37
2	M	193	HIS	CD2-NE2	-6.40	1.30	1.37
1	L	211	HIS	CD2-NE2	-6.40	1.30	1.37
3	H	128	HIS	CD2-NE2	-6.38	1.30	1.37
2	M	202	HIS	CG-ND1	-6.27	1.31	1.38
3	H	126	HIS	CD2-NE2	-6.24	1.30	1.37
1	L	173	HIS	CD2-NE2	-6.18	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	98	HIS	CD2-NE2	-6.18	1.31	1.37
2	M	182	HIS	CD2-NE2	-6.09	1.31	1.37
1	L	116	HIS	CD2-NE2	-6.08	1.31	1.37
3	H	204	HIS	CD2-NE2	-6.06	1.31	1.37
2	M	266	HIS	CD2-NE2	-5.95	1.31	1.37
3	H	141	HIS	CD2-NE2	-5.92	1.31	1.37
1	L	190	HIS	CD2-NE2	-5.72	1.31	1.37
2	M	219	HIS	CG-ND1	-5.60	1.32	1.38
1	L	36	VAL	CA-CB	5.53	1.60	1.54
2	M	145	HIS	CG-ND1	-5.46	1.32	1.38
1	L	230	HIS	CG-ND1	-5.38	1.32	1.38
1	L	230	HIS	CD2-NE2	-5.37	1.31	1.37
1	L	26	VAL	CA-CB	5.35	1.59	1.53
2	M	266	HIS	CG-ND1	-5.22	1.32	1.38
1	L	190	HIS	CG-ND1	-5.19	1.32	1.38
1	L	168	HIS	CG-ND1	-5.00	1.32	1.38

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	216	PHE	CA-CB-CG	-13.38	100.42	113.80
3	H	204	HIS	N-CA-C	11.96	127.92	108.55
2	M	96	PRO	N-CA-C	10.93	124.04	110.70
2	M	105	PHE	CA-CB-CG	9.92	123.72	113.80
2	M	226	VAL	N-CA-CB	-9.90	99.25	112.22
3	H	92	VAL	N-CA-C	9.45	119.47	110.30
1	L	5	PHE	CA-CB-CG	9.34	123.14	113.80
3	H	170	ASP	CA-CB-CG	9.32	121.92	112.60
1	L	13	GLY	N-CA-C	9.07	122.31	112.33
1	L	36	VAL	N-CA-C	-8.90	101.88	110.42
2	M	101	TYR	N-CA-C	8.85	123.34	108.20
3	H	32	GLN	N-CA-C	8.61	120.58	111.03
3	H	185	ASP	CA-CB-CG	8.58	121.18	112.60
3	H	204	HIS	CA-CB-CG	-8.46	105.34	113.80
3	H	103	ASP	CA-CB-CG	8.41	121.01	112.60
1	L	146	PHE	CA-CB-CG	8.27	122.07	113.80
2	M	182	HIS	CB-CG-CD2	-8.21	120.52	131.20
3	H	91	ALA	N-CA-C	8.13	128.12	110.80
3	H	141	HIS	O-C-N	8.09	133.35	122.59
2	M	261	THR	CA-CB-OG1	-7.76	97.95	109.60
2	M	237	GLN	OE1-CD-NE2	-7.72	114.88	122.60
3	H	84	PRO	N-CA-C	7.72	123.31	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	115	TYR	N-CA-C	7.70	127.21	110.80
1	L	268	LYS	N-CA-C	7.68	122.36	109.76
1	L	199	ASN	OD1-CG-ND2	-7.67	114.93	122.60
2	M	144	LYS	N-CA-C	7.56	126.90	110.80
3	H	124	ASP	CA-CB-CG	7.55	120.15	112.60
2	M	26	LEU	N-CA-C	-7.53	104.61	113.88
2	M	148	TRP	CA-CB-CG	7.50	127.84	113.60
3	H	141	HIS	CB-CG-CD2	-7.49	121.46	131.20
2	M	145	HIS	N-CA-C	7.40	123.58	111.37
2	M	109	LEU	N-CA-C	-7.24	97.45	108.67
2	M	34	PRO	N-CA-C	7.09	127.08	112.47
1	L	153	HIS	CA-CB-CG	7.06	120.86	113.80
3	H	141	HIS	CB-CG-ND1	7.05	133.27	122.70
2	M	259	ASN	OD1-CG-ND2	-6.95	115.65	122.60
2	M	301	HIS	CB-CG-CD2	-6.89	122.24	131.20
3	H	202	ARG	N-CA-C	-6.89	99.37	109.63
2	M	46	GLN	N-CA-C	6.87	119.03	109.15
1	L	86	TRP	N-CA-C	-6.82	103.54	110.97
3	H	206	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	M	101	TYR	CA-CB-CG	6.77	126.08	113.90
3	H	211	ASP	CA-CB-CG	6.75	119.36	112.60
3	H	159	GLU	N-CA-C	6.74	125.16	110.80
3	H	90	THR	CA-C-O	6.65	127.34	119.56
2	M	261	THR	N-CA-CB	-6.64	99.19	109.48
2	M	18	LEU	N-CA-C	-6.59	99.57	108.86
3	H	32	GLN	CA-C-O	-6.57	114.14	120.90
2	M	103	LEU	N-CA-C	-6.54	103.63	112.26
3	H	156	CYS	N-CA-C	-6.53	103.37	112.25
3	H	190	LEU	N-CA-C	6.52	119.88	107.75
3	H	210	SER	N-CA-C	-6.48	97.00	110.80
3	H	194	GLN	OE1-CD-NE2	-6.47	116.13	122.60
3	H	178	PHE	CA-CB-CG	6.47	120.27	113.80
3	H	98	HIS	CB-CG-CD2	-6.45	122.82	131.20
3	H	20	PHE	N-CA-C	-6.43	104.19	111.07
2	M	226	VAL	CB-CA-C	6.40	120.98	112.46
3	H	56	PHE	N-CA-C	-6.40	97.86	109.44
1	L	23	ASP	CA-CB-CG	6.38	118.98	112.60
1	L	34	PHE	CA-CB-CG	-6.33	107.47	113.80
2	M	225	ALA	N-CA-C	-6.32	105.72	113.50
1	L	243	PHE	CA-CB-CG	-6.30	107.50	113.80
2	M	100	GLU	N-CA-C	6.30	124.21	110.80
2	M	163	ILE	N-CA-C	6.29	116.46	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	95	GLU	CA-C-N	6.29	126.86	120.38
2	M	95	GLU	C-N-CA	6.29	126.86	120.38
1	L	199	ASN	CB-CG-ND2	6.25	125.78	116.40
1	L	173	HIS	CA-CB-CG	6.23	120.03	113.80
3	H	56	PHE	CA-CB-CG	6.22	120.02	113.80
2	M	199	ASN	OD1-CG-ND2	-6.22	116.38	122.60
2	M	261	THR	CA-CB-CG2	6.18	121.00	110.50
3	H	74	THR	CA-C-O	6.17	127.34	120.92
3	H	132	LYS	O-C-N	-6.16	116.51	121.80
3	H	188	THR	N-CA-CB	-6.12	101.07	110.85
3	H	128	HIS	CB-CG-CD2	-6.08	123.29	131.20
3	H	141	HIS	CA-CB-CG	6.05	119.85	113.80
2	M	33	GLY	CA-C-N	6.02	127.36	119.84
2	M	33	GLY	C-N-CA	6.02	127.36	119.84
1	L	156	TRP	CG-CD2-CE3	6.02	139.92	133.90
3	H	83	ARG	CA-C-N	6.00	126.34	119.92
3	H	83	ARG	C-N-CA	6.00	126.34	119.92
2	M	182	HIS	CB-CG-ND1	5.99	131.68	122.70
3	H	126	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	L	116	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	M	100	GLU	CA-C-N	-5.92	115.15	122.84
2	M	100	GLU	C-N-CA	-5.92	115.15	122.84
2	M	25	ASN	CA-C-O	5.92	127.82	121.02
2	M	300	ASN	CA-C-N	5.92	132.35	121.70
2	M	300	ASN	C-N-CA	5.92	132.35	121.70
1	L	116	HIS	N-CA-C	5.90	117.71	111.28
3	H	47	GLY	N-CA-C	-5.87	102.87	110.38
1	L	170	ASN	OD1-CG-ND2	-5.86	116.75	122.60
2	M	92	PHE	CA-CB-CG	5.85	119.65	113.80
2	M	110	LYS	N-CA-C	-5.83	98.38	110.80
2	M	199	ASN	CA-CB-CG	5.83	118.42	112.60
2	M	250	LEU	CB-CA-C	-5.81	101.15	110.79
1	L	223	SER	N-CA-C	-5.76	98.10	108.48
2	M	185	TRP	N-CA-C	-5.75	104.92	111.07
3	H	52	ASN	CA-CB-CG	5.75	118.34	112.60
2	M	261	THR	CB-CA-C	5.71	118.41	109.84
3	H	82	ASP	N-CA-C	-5.71	103.67	110.41
2	M	266	HIS	CA-CB-CG	-5.70	108.10	113.80
2	M	130	TRP	CE2-CD2-CG	-5.69	100.37	107.20
2	M	66	TRP	CG-CD2-CE3	5.68	139.58	133.90
2	M	101	TYR	CA-C-O	5.67	126.44	120.54
1	L	111	LEU	N-CA-C	5.65	119.92	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	164	ARG	CA-C-N	5.65	126.03	119.47
2	M	164	ARG	C-N-CA	5.65	126.03	119.47
1	L	167	PHE	CA-CB-CG	5.64	119.44	113.80
1	L	170	ASN	CA-C-N	5.61	125.27	119.05
1	L	170	ASN	C-N-CA	5.61	125.27	119.05
2	M	145	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	L	190	HIS	CA-CB-CG	-5.59	108.21	113.80
3	H	54	GLY	CA-C-N	5.59	125.57	120.21
3	H	54	GLY	C-N-CA	5.59	125.57	120.21
3	H	241	LEU	N-CA-C	-5.58	101.59	109.96
2	M	259	ASN	CB-CG-ND2	5.57	124.76	116.40
1	L	220	VAL	N-CA-CB	-5.56	104.17	112.67
3	H	75	VAL	CA-C-O	-5.56	112.50	119.95
3	H	206	ASN	CA-CB-CG	5.55	118.15	112.60
3	H	120	LEU	O-C-N	-5.53	117.52	121.83
3	H	30	TYR	CA-CB-CG	-5.53	103.95	113.90
1	L	142	TRP	CE2-CD2-CG	-5.51	100.58	107.20
2	M	13	ARG	NE-CZ-NH1	5.51	127.01	121.50
2	M	94	LEU	N-CA-C	-5.51	97.84	107.20
2	M	252	TRP	CG-CD2-CE3	5.50	139.40	133.90
3	H	206	ASN	N-CA-C	-5.48	98.03	108.17
2	M	301	HIS	CB-CG-ND1	5.46	130.90	122.70
2	M	237	GLN	N-CA-C	-5.46	105.48	111.82
2	M	190	SER	CA-CB-OG	5.46	122.02	111.10
2	M	294	TRP	CG-CD2-CE3	5.46	139.35	133.90
1	L	211	HIS	CB-CG-CD2	-5.45	124.11	131.20
3	H	147	ASN	OD1-CG-ND2	-5.45	117.15	122.60
2	M	108	PRO	N-CA-C	5.45	119.78	111.34
3	H	183	LEU	N-CA-CB	-5.44	102.33	110.17
2	M	75	TRP	CG-CD2-CE3	5.43	139.33	133.90
3	H	42	LEU	O-C-N	5.43	128.92	122.46
2	M	297	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	L	59	TRP	CG-CD2-CE3	5.42	139.32	133.90
2	M	29	ARG	O-C-N	5.42	130.21	123.01
3	H	242	MET	CA-CB-CG	5.41	124.91	114.10
3	H	109	VAL	N-CA-CB	-5.37	101.99	111.93
3	H	68	HIS	CB-CG-CD2	-5.37	124.22	131.20
2	M	75	TRP	CE2-CD2-CG	-5.37	100.76	107.20
2	M	171	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	L	220	VAL	CB-CA-C	5.36	116.01	110.70
3	H	168	TRP	CG-CD2-CE3	5.36	139.26	133.90
2	M	294	TRP	CE2-CD2-CG	-5.34	100.79	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	213	PHE	N-CA-C	-5.34	104.34	112.04
3	H	170	ASP	N-CA-C	-5.33	100.41	108.67
3	H	245	ALA	N-CA-C	5.33	121.58	109.81
2	M	44	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	L	142	TRP	CG-CD2-CE3	5.28	139.18	133.90
2	M	41	TRP	CE2-CD2-CG	-5.27	100.87	107.20
2	M	25	ASN	CA-CB-CG	-5.26	107.34	112.60
2	M	209	LEU	N-CA-C	-5.26	105.44	111.07
2	M	182	HIS	CA-CB-CG	5.25	119.05	113.80
1	L	153	HIS	CB-CG-CD2	-5.23	124.40	131.20
3	H	30	TYR	CB-CA-C	5.21	118.55	109.65
2	M	263	GLU	CA-CB-CG	5.20	124.50	114.10
2	M	276	VAL	N-CA-C	-5.20	105.78	110.82
1	L	25	TRP	CG-CD2-CE3	5.19	139.09	133.90
3	H	164	VAL	N-CA-C	-5.17	100.89	108.54
1	L	213	ASP	CA-CB-CG	5.17	117.77	112.60
3	H	209	SER	N-CA-C	5.16	121.79	110.80
1	L	263	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	L	25	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	M	268	TRP	CG-CD2-CE3	5.14	139.04	133.90
3	H	82	ASP	CA-C-O	5.13	125.63	121.02
2	M	68	PHE	CA-CB-CG	5.12	118.92	113.80
3	H	90	THR	N-CA-CB	-5.12	103.08	110.56
1	L	263	TRP	CG-CD2-CE3	5.11	139.01	133.90
2	M	204	LEU	N-CA-C	-5.11	105.17	111.40
2	M	234	GLU	CB-CG-CD	5.10	121.27	112.60
2	M	86	LEU	N-CA-C	5.09	116.83	111.28
2	M	146	THR	CA-CB-OG1	-5.08	101.97	109.60
3	H	68	HIS	CA-CB-CG	-5.08	108.72	113.80
3	H	209	SER	CA-C-N	5.06	131.21	121.54
3	H	209	SER	C-N-CA	5.06	131.21	121.54
1	L	117	ILE	CA-C-N	5.06	126.16	119.84
1	L	117	ILE	C-N-CA	5.06	126.16	119.84
1	L	117	ILE	CA-C-O	-5.05	113.19	119.95
1	L	71	LEU	N-CA-C	5.04	121.55	110.80
3	H	138	ALA	N-CA-C	5.02	121.50	110.80
2	M	182	HIS	O-C-N	-5.01	116.36	122.22
3	H	129	ASN	N-CA-C	5.00	121.46	110.80
3	H	128	HIS	O-C-N	5.00	129.24	122.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	245	ALA	Peptide
3	H	83	ARG	Peptide
1	L	269	LEU	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	61	0
2	M	2362	0	2281	79	0
3	H	1807	0	1814	70	0
4	L	66	0	74	12	0
4	M	168	0	156	16	0
5	L	65	0	76	5	0
5	M	65	0	76	3	0
6	L	41	0	52	3	0
6	M	51	0	68	7	0
7	M	1	0	0	0	0
8	M	42	0	57	1	0
All	All	6789	0	6731	203	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 15.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:111:LEU:HD21	2:M:250:LEU:HD12	1.44	0.99
2:M:264:GLY:HA2	2:M:267:ARG:HG3	1.63	0.80
3:H:204:HIS:HB3	3:H:206:ASN:OD1	1.86	0.76
3:H:87:LEU:HG	3:H:98:HIS:HB3	1.68	0.75
3:H:61:PRO:HA	3:H:76:PRO:HG2	1.72	0.72
2:M:165:PRO:HG3	2:M:173:GLU:HB2	1.73	0.69
3:H:154:ARG:HA	3:H:160:ILE:HA	1.75	0.69
1:L:174:MET:HE2	4:M:1:BCL:HED3	1.77	0.67
2:M:13:ARG:HB2	3:H:143:SER:OG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:PHE:CE1	4:L:2:BCL:H121	2.30	0.66
3:H:189:ARG:HD3	3:H:216:ILE:HB	1.77	0.66
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.78	0.66
4:L:2:BCL:H171	5:L:271:BPH:H4C3	1.77	0.65
4:M:1:BCL:HHC	4:M:1:BCL:HBB2	1.79	0.65
2:M:260:ALA:HB2	6:M:303:U10:H103	1.79	0.65
2:M:35:PHE:HB2	2:M:47:LEU:HD11	1.80	0.63
4:M:3:BCL:HHC	4:M:3:BCL:HBB2	1.81	0.62
2:M:96:PRO:HA	2:M:115:TRP:CG	2.35	0.61
3:H:118:ARG:HB2	3:H:118:ARG:HH11	1.65	0.61
2:M:190:SER:HB2	4:M:3:BCL:H3C	1.81	0.61
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.81	0.61
1:L:6:GLU:HA	1:L:9:TYR:HD2	1.66	0.61
3:H:29:TYR:HB3	3:H:30:TYR:HD1	1.65	0.60
3:H:42:LEU:HD23	3:H:58:LEU:HG	1.82	0.60
3:H:198:VAL:HA	3:H:203:VAL:HG23	1.85	0.58
2:M:130:TRP:HZ3	2:M:147:ALA:O	1.87	0.58
1:L:13:GLY:HA3	1:L:110:LYS:HG2	1.86	0.58
3:H:133:PRO:HA	3:H:168:TRP:HA	1.84	0.58
2:M:125:ALA:HB1	5:M:5:BPH:H4C2	1.84	0.58
2:M:228:ARG:HA	3:H:194:GLN:HG3	1.85	0.57
3:H:29:TYR:HB3	3:H:30:TYR:CD1	2.39	0.57
3:H:111:PRO:HG3	3:H:242:MET:SD	2.44	0.57
4:L:2:BCL:H112	4:M:4:BCL:HBB2	1.86	0.57
2:M:215:LEU:HD11	2:M:265:ILE:HD11	1.87	0.57
4:M:1:BCL:HBC1	4:M:3:BCL:HAA2	1.85	0.56
1:L:48:LEU:HD23	1:L:89:ILE:HG13	1.87	0.56
1:L:170:ASN:OD1	1:L:247:CYS:HB2	2.05	0.56
2:M:280:GLY:HA2	4:M:3:BCL:HED3	1.87	0.56
3:H:142:VAL:HG21	3:H:147:ASN:OD1	2.05	0.56
2:M:20:MET:SD	2:M:22:GLU:HB2	2.46	0.56
2:M:235:LEU:HA	2:M:238:ILE:HD12	1.87	0.56
3:H:29:TYR:CE2	3:H:55:PRO:HA	2.41	0.55
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.88	0.55
2:M:209:LEU:HD23	2:M:276:VAL:HG11	1.88	0.55
4:L:2:BCL:HAA2	4:M:4:BCL:HBC1	1.88	0.55
3:H:178:PHE:HZ	3:H:230:GLU:HG2	1.70	0.55
3:H:154:ARG:HG3	3:H:202:ARG:HE	1.72	0.55
1:L:141:ALA:HB3	1:L:144:TYR:CE2	2.42	0.54
4:L:2:BCL:H122	5:L:271:BPH:HBA1	1.89	0.54
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:76:PRO:O	3:H:78:PRO:HD3	2.08	0.53
1:L:44:LEU:O	1:L:48:LEU:HB2	2.09	0.53
1:L:8:LYS:HZ1	3:H:113:SER:HB3	1.73	0.53
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.73	0.53
3:H:226:THR:HB	3:H:229:GLU:HG3	1.90	0.53
2:M:193:HIS:HA	2:M:292:ASP:O	2.09	0.53
3:H:213:PHE:O	3:H:216:ILE:HG13	2.08	0.53
4:L:2:BCL:HBB2	4:M:3:BCL:NB	2.24	0.53
3:H:123:LEU:HD23	3:H:128:HIS:H	1.73	0.53
3:H:68:HIS:HB3	3:H:123:LEU:HD22	1.91	0.52
1:L:128:TYR:HB2	4:L:2:BCL:H51	1.91	0.52
1:L:266:TRP:NE1	2:M:87:ARG:HA	2.24	0.52
4:M:3:BCL:HHC	4:M:3:BCL:CBB	2.39	0.52
1:L:79:PRO:HG2	1:L:82:LYS:HB2	1.89	0.52
3:H:129:ASN:HD21	3:H:224:GLU:HG3	1.75	0.52
3:H:108:GLY:HA3	3:H:114:TRP:CZ3	2.45	0.52
2:M:84:VAL:O	2:M:87:ARG:HG2	2.10	0.52
3:H:24:LEU:O	3:H:28:ILE:HG12	2.09	0.52
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.92	0.52
3:H:233:ILE:O	3:H:237:VAL:HG23	2.10	0.52
1:L:195:LEU:HB3	2:M:145:HIS:CE1	2.45	0.51
3:H:154:ARG:HD3	3:H:160:ILE:HG13	1.91	0.51
3:H:43:GLU:HB3	3:H:49:PRO:O	2.11	0.51
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.45	0.51
3:H:44:ASN:O	3:H:49:PRO:HA	2.11	0.51
3:H:29:TYR:HE2	3:H:55:PRO:HA	1.76	0.50
1:L:120:ALA:HA	1:L:238:LEU:HD21	1.93	0.50
2:M:200:PRO:HB2	3:H:17:ILE:HD12	1.93	0.50
3:H:40:TYR:O	3:H:42:LEU:HD12	2.11	0.50
1:L:7:ARG:NH1	3:H:85:ILE:HB	2.27	0.50
1:L:231:ARG:HG2	2:M:224:LEU:HD11	1.93	0.50
1:L:161:GLY:HA3	4:L:2:BCL:HAC1	1.93	0.50
2:M:22:GLU:HG2	2:M:139:ALA:O	2.12	0.49
3:H:104:PRO:HA	3:H:107:ASP:HB2	1.94	0.49
1:L:131:LEU:HD21	4:L:2:BCL:HED2	1.95	0.49
1:L:196:SER:HB2	2:M:142:MET:HB3	1.95	0.49
2:M:108:PRO:HB2	2:M:110:LYS:O	2.12	0.49
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.13	0.49
1:L:7:ARG:HH12	3:H:85:ILE:HB	1.78	0.48
2:M:110:LYS:HD3	2:M:114:LEU:HD13	1.94	0.48
2:M:197:PHE:HZ	4:M:3:BCL:HBB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:85:ILE:HG22	3:H:87:LEU:HB2	1.95	0.48
1:L:154:LEU:HD12	2:M:197:PHE:HB3	1.95	0.48
3:H:154:ARG:HB3	3:H:202:ARG:HH21	1.78	0.48
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.49	0.48
3:H:119:ASP:HA	3:H:226:THR:HG23	1.95	0.48
1:L:190:HIS:HA	6:L:272:U10:O2	2.13	0.47
2:M:59:SER:OG	2:M:128:SER:HB2	2.14	0.47
3:H:63:THR:HA	3:H:73:LEU:O	2.14	0.47
1:L:154:LEU:O	1:L:157:VAL:HB	2.14	0.47
2:M:205:SER:HB3	4:M:3:BCL:HMA3	1.97	0.47
2:M:249:ALA:HA	6:M:303:U10:H4M2	1.96	0.47
1:L:8:LYS:NZ	3:H:113:SER:HB3	2.30	0.47
6:M:303:U10:H8	6:M:303:U10:O5	2.15	0.47
1:L:109:ARG:HH22	1:L:115:TYR:HB3	1.80	0.46
2:M:144:LYS:HE3	2:M:148:TRP:HB2	1.97	0.46
2:M:260:ALA:HB1	3:H:36:MET:SD	2.55	0.46
1:L:13:GLY:CA	1:L:110:LYS:HG2	2.45	0.46
1:L:193:LEU:HD11	1:L:212:GLU:HA	1.96	0.46
2:M:190:SER:HA	2:M:196:LEU:HD23	1.98	0.46
1:L:9:TYR:CD2	2:M:250:LEU:HD11	2.50	0.46
3:H:62:LYS:O	3:H:75:VAL:HG23	2.15	0.46
1:L:174:MET:HE1	2:M:180:PHE:HE1	1.81	0.46
2:M:204:LEU:HD21	3:H:20:PHE:CD2	2.50	0.46
1:L:36:VAL:HG12	6:M:303:U10:H403	1.98	0.46
6:M:303:U10:H162	6:M:303:U10:H121	1.81	0.46
1:L:80:LEU:HB3	1:L:85:LEU:HD22	1.98	0.46
1:L:269:LEU:H	1:L:270:PRO:C	2.24	0.46
5:L:271:BPH:HBB2	2:M:210:TYR:HB3	1.97	0.46
2:M:110:LYS:H	2:M:114:LEU:HD22	1.81	0.45
3:H:38:GLU:O	3:H:42:LEU:HD11	2.17	0.45
3:H:108:GLY:HA3	3:H:114:TRP:HZ3	1.81	0.45
1:L:6:GLU:HG2	1:L:10:ARG:HD3	1.98	0.45
1:L:190:HIS:HA	6:L:272:U10:H1M3	1.99	0.45
2:M:20:MET:SD	2:M:22:GLU:OE1	2.75	0.45
2:M:37:THR:HG22	2:M:38:LEU:HG	1.98	0.45
2:M:105:PHE:HD1	2:M:106:ALA:H	1.63	0.45
2:M:73:TRP:CH2	2:M:109:LEU:HB3	2.52	0.45
2:M:63:GLY:HA3	5:M:5:BPH:H5C2	1.98	0.45
2:M:237:GLN:NE2	2:M:244:ALA:HB3	2.32	0.45
3:H:154:ARG:HG3	3:H:202:ARG:HB3	1.99	0.45
1:L:158:SER:HA	4:L:2:BCL:HBC1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:69:THR:O	2:M:72:ILE:HG13	2.16	0.44
2:M:144:LYS:NZ	2:M:148:TRP:HA	2.32	0.44
3:H:241:LEU:O	3:H:242:MET:HB3	2.17	0.44
2:M:82:PRO:HA	2:M:85:PHE:HB3	2.00	0.44
3:H:61:PRO:HA	3:H:76:PRO:CG	2.44	0.44
1:L:168:HIS:NE2	4:L:2:BCL:OBB	2.50	0.44
1:L:262:TRP:O	1:L:265:TRP:HD1	2.00	0.44
5:L:271:BPH:HBB1	2:M:210:TYR:CD2	2.51	0.44
2:M:103:LEU:HG	2:M:169:GLY:C	2.42	0.44
1:L:107:ILE:O	1:L:111:LEU:HB2	2.18	0.44
2:M:20:MET:SD	2:M:22:GLU:HA	2.58	0.44
2:M:113:GLY:O	2:M:117:ILE:HG12	2.17	0.44
1:L:174:MET:HE3	2:M:183:LEU:HD11	2.00	0.44
2:M:103:LEU:HA	2:M:171:TRP:CD1	2.52	0.44
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.44
5:M:5:BPH:HBA1	5:M:5:BPH:H3A	1.80	0.44
3:H:184:LYS:HD2	3:H:184:LYS:HA	1.88	0.44
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.00	0.43
2:M:299:GLN:C	2:M:301:HIS:H	2.26	0.43
3:H:56:PHE:O	3:H:58:LEU:N	2.51	0.43
3:H:207:ALA:O	3:H:240:GLY:HA3	2.18	0.43
1:L:157:VAL:HG11	4:M:3:BCL:HBB1	2.00	0.43
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.83	0.43
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.54	0.43
1:L:9:TYR:CE2	2:M:246:GLU:HG2	2.53	0.43
2:M:236:GLU:HB3	3:H:117:ARG:HH22	1.81	0.43
4:M:3:BCL:HBC2	4:M:3:BCL:H2C	1.83	0.43
3:H:154:ARG:O	3:H:204:HIS:CE1	2.72	0.43
2:M:74:PHE:HB3	2:M:85:PHE:HE1	1.84	0.43
3:H:54:GLY:HA2	3:H:55:PRO:HD2	1.83	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB3	2.01	0.43
5:L:271:BPH:HHC	5:L:271:BPH:HBB3	2.00	0.43
6:L:272:U10:H171	6:L:272:U10:H151	1.90	0.43
2:M:94:LEU:HD21	2:M:114:LEU:HG	2.01	0.43
3:H:87:LEU:CG	3:H:98:HIS:HB3	2.44	0.43
3:H:204:HIS:CG	3:H:205:VAL:N	2.87	0.43
1:L:109:ARG:NH2	1:L:115:TYR:H	2.17	0.42
1:L:9:TYR:CG	2:M:250:LEU:HD11	2.54	0.42
1:L:207:ARG:HG3	1:L:211:HIS:ND1	2.33	0.42
2:M:211:GLY:O	2:M:214:LEU:HB3	2.19	0.42
1:L:174:MET:HB3	4:M:1:BCL:O1D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:2:BCL:NC	4:M:3:BCL:HBB3	2.34	0.42
1:L:255:TRP:HE1	1:L:259:TRP:HA	1.84	0.42
1:L:66:VAL:HB	1:L:148:TYR:HB2	2.01	0.42
3:H:119:ASP:CG	3:H:226:THR:HG21	2.45	0.42
3:H:147:ASN:HA	3:H:148:PRO:HD3	1.87	0.42
2:M:66:TRP:HD1	2:M:118:ALA:O	2.02	0.42
8:M:304:CRT:H26	8:M:304:CRT:H241	1.83	0.42
1:L:52:SER:OG	1:L:85:LEU:HD23	2.20	0.42
3:H:34:GLU:CD	3:H:56:PHE:HD2	2.28	0.42
2:M:164:ARG:NH1	2:M:168:MET:SD	2.93	0.41
1:L:85:LEU:HD12	1:L:85:LEU:HA	1.90	0.41
2:M:35:PHE:HB2	2:M:47:LEU:CD1	2.49	0.41
1:L:153:HIS:CE1	1:L:154:LEU:HD23	2.55	0.41
2:M:103:LEU:HD21	2:M:165:PRO:O	2.20	0.41
1:L:189:LEU:HD12	2:M:146:THR:HG23	2.02	0.41
2:M:130:TRP:CZ3	2:M:147:ALA:HB1	2.55	0.41
2:M:130:TRP:CZ3	2:M:151:LEU:HG	2.56	0.41
2:M:152:SER:O	2:M:155:TRP:HB3	2.21	0.41
2:M:110:LYS:HD3	2:M:114:LEU:CD1	2.51	0.41
3:H:226:THR:CG2	3:H:229:GLU:HG3	2.51	0.41
2:M:107:ALA:HB1	2:M:111:GLU:O	2.21	0.41
6:M:303:U10:H251	6:M:303:U10:H271	1.83	0.41
3:H:119:ASP:HA	3:H:226:THR:CG2	2.51	0.41
3:H:192:PRO:HG2	3:H:195:MET:HB2	2.02	0.41
1:L:131:LEU:HD22	1:L:156:TRP:HH2	1.86	0.40
2:M:214:LEU:HG	2:M:218:MET:HE2	2.02	0.40
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.93	0.40
6:M:303:U10:H222	6:M:303:U10:H201	1.93	0.40
3:H:121:PRO:HB3	3:H:225:VAL:O	2.21	0.40
3:H:32:GLN:O	3:H:36:MET:HE2	2.22	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%)	236 (89%)	21 (8%)	7 (3%)	4	22
2	M	294/296 (99%)	245 (83%)	32 (11%)	17 (6%)	1	8
3	H	235/237 (99%)	173 (74%)	37 (16%)	25 (11%)	0	2
All	All	793/799 (99%)	654 (82%)	90 (11%)	49 (6%)	1	6

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	115	TYR
1	L	269	LEU
2	M	21	THR
2	M	24	VAL
2	M	34	PRO
2	M	96	PRO
2	M	99	PRO
2	M	105	PHE
2	M	111	GLU
2	M	144	LYS
2	M	234	GLU
2	M	244	ALA
3	H	13	ALA
3	H	70	ARG
3	H	128	HIS
3	H	138	ALA
3	H	142	VAL
3	H	185	ASP
3	H	210	SER
1	L	71	LEU
2	M	100	GLU
3	H	129	ASN
3	H	207	ALA
1	L	31	VAL
1	L	78	ALA
1	L	145	ALA
2	M	104	SER
2	M	195	ASN
3	H	68	HIS
3	H	194	GLN
3	H	242	MET

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Mol	Chain	Res	Type
3	H	247	LYS
1	L	12	PRO
2	M	80	TRP
2	M	110	LYS
3	H	50	ALA
3	H	91	ALA
3	H	203	VAL
2	M	97	PRO
3	H	40	TYR
3	H	57	PRO
3	H	200	SER
3	H	201	ASN
3	H	245	ALA
2	M	98	ALA
3	H	43	GLU
3	H	154	ARG
3	H	209	SER
3	H	76	PRO

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%)	179 (85%)	31 (15%)	3	15
2	M	232/232 (100%)	199 (86%)	33 (14%)	3	16
3	H	192/192 (100%)	145 (76%)	47 (24%)	1	4
All	All	634/634 (100%)	523 (82%)	111 (18%)	2	10

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	21	LEU
1	L	54	VAL
1	L	64	ILE

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Mol	Chain	Res	Type
1	L	82	LYS
1	L	85	LEU
1	L	109	ARG
1	L	113	ILE
1	L	129	LEU
1	L	132	VAL
1	L	136	PRO
1	L	138	MET
1	L	158	SER
1	L	159	ASN
1	L	183	ASN
1	L	185	LEU
1	L	193	LEU
1	L	195	LEU
1	L	196	SER
1	L	202	LYS
1	L	208	THR
1	L	216	PHE
1	L	217	ARG
1	L	220	VAL
1	L	229	ILE
1	L	235	LEU
1	L	251	THR
1	L	253	THR
1	L	254	ILE
1	L	268	LYS
1	L	269	LEU
2	M	6	ILE
2	M	13	ARG
2	M	18	LEU
2	M	21	THR
2	M	24	VAL
2	M	29	ARG
2	M	34	PRO
2	M	58	LEU
2	M	74	PHE
2	M	80	TRP
2	M	89	LEU
2	M	96	PRO
2	M	97	PRO
2	M	99	PRO
2	M	101	TYR

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Mol	Chain	Res	Type
2	M	130	TRP
2	M	138	GLN
2	M	148	TRP
2	M	156	LEU
2	M	182	HIS
2	M	188	ASN
2	M	196	LEU
2	M	226	VAL
2	M	233	ARG
2	M	236	GLU
2	M	240	ASP
2	M	243	THR
2	M	258	PHE
2	M	259	ASN
2	M	261	THR
2	M	263	GLU
2	M	271	TRP
2	M	286	LEU
3	H	17	ILE
3	H	34	GLU
3	H	35	ASN
3	H	40	TYR
3	H	48	THR
3	H	56	PHE
3	H	58	LEU
3	H	60	LYS
3	H	61	PRO
3	H	70	ARG
3	H	72	THR
3	H	73	LEU
3	H	75	VAL
3	H	78	PRO
3	H	89	ARG
3	H	94	GLU
3	H	96	PHE
3	H	97	PRO
3	H	98	HIS
3	H	105	MET
3	H	109	VAL
3	H	118	ARG
3	H	120	LEU
3	H	128	HIS

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Mol	Chain	Res	Type
3	H	130	LYS
3	H	135	LYS
3	H	146	LYS
3	H	153	VAL
3	H	157	ASP
3	H	158	LEU
3	H	163	LYS
3	H	175	MET
3	H	188	THR
3	H	193	MET
3	H	194	GLN
3	H	195	MET
3	H	196	VAL
3	H	208	LEU
3	H	211	ASP
3	H	212	LEU
3	H	213	PHE
3	H	217	PRO
3	H	218	THR
3	H	225	VAL
3	H	226	THR
3	H	227	LEU
3	H	246	PRO

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

Mol	Chain	Res	Type
1	L	87	GLN
1	L	153	HIS
1	L	173	HIS
1	L	258	GLN
2	M	77	GLN
2	M	193	HIS
2	M	259	ASN
3	H	32	GLN
3	H	44	ASN
3	H	53	GLN
3	H	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
8	CRT	M	304	-	40,41,43	3.93	23 (57%)	47,50,54	2.69	23 (48%)
6	U10	L	272	-	41,41,63	1.78	11 (26%)	51,52,79	2.46	15 (29%)
4	BCL	L	2	1	69,74,74	1.14	5 (7%)	79,115,115	1.75	19 (24%)
4	BCL	M	3	2	69,74,74	1.07	6 (8%)	79,115,115	1.83	20 (25%)
6	U10	M	303	-	51,51,63	1.66	13 (25%)	63,64,79	1.84	24 (38%)
5	BPH	M	5	-	59,70,70	1.74	9 (15%)	59,101,101	2.70	19 (32%)
4	BCL	M	1	2	54,59,74	1.30	8 (14%)	61,97,115	1.91	15 (24%)
4	BCL	M	4	1	54,59,74	1.28	6 (11%)	61,97,115	2.12	20 (32%)
5	BPH	L	271	-	59,70,70	1.57	6 (10%)	59,101,101	2.53	19 (32%)

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
8	CRT	M	304	-	-	19/47/47/51	-
6	U10	L	272	-	-	14/37/61/87	0/1/1/1
4	BCL	L	2	1	-	15/41/137/137	-
4	BCL	M	3	2	2/2/21/25	11/41/137/137	-
6	U10	M	303	-	-	15/49/73/87	0/1/1/1
5	BPH	M	5	-	-	11/37/105/105	0/5/6/6
4	BCL	M	1	2	-	8/23/119/137	-
4	BCL	M	4	1	-	0/23/119/137	-
5	BPH	L	271	-	1/1/18/22	6/37/105/105	0/5/6/6

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C26-C25	8.37	1.56	1.34
8	M	304	CRT	C6-C5	8.17	1.54	1.32
8	M	304	CRT	C35-C36	7.96	1.54	1.32
8	M	304	CRT	C15-C16	7.90	1.55	1.34
8	M	304	CRT	C10-C11	7.70	1.54	1.34
5	M	5	BPH	C3A-C2A	-7.67	1.48	1.54
5	L	271	BPH	C3A-C2A	-7.58	1.48	1.54
8	M	304	CRT	C31-C30	7.27	1.53	1.34
8	M	304	CRT	C21-C20	6.30	1.53	1.36
5	M	5	BPH	C2C-C3C	-5.25	1.50	1.54
5	M	5	BPH	C3D-CAD	-4.63	1.38	1.47
5	L	271	BPH	C3D-CAD	-4.42	1.39	1.47
8	M	304	CRT	C31-C32	4.08	1.55	1.43
8	M	304	CRT	C30-C28	-4.03	1.37	1.46
4	L	2	BCL	C1D-C2D	-4.03	1.37	1.45
8	M	304	CRT	C35-C33	3.95	1.54	1.46
6	M	303	U10	C3-C2	-3.86	1.37	1.48
4	L	2	BCL	O2D-CGD	-3.83	1.23	1.33
4	M	4	BCL	O2D-CGD	-3.82	1.23	1.33
8	M	304	CRT	C6-C7	-3.80	1.37	1.46
5	L	271	BPH	C3B-CAB	-3.78	1.39	1.49
6	L	272	U10	C7-C8	-3.78	1.44	1.50
8	M	304	CRT	C4-C5	3.72	1.55	1.50
4	M	1	BCL	C1D-C2D	-3.62	1.38	1.45
5	L	271	BPH	O2D-CGD	-3.62	1.24	1.33
8	M	304	CRT	C25-C23	-3.61	1.38	1.46
4	M	1	BCL	O2D-CGD	-3.60	1.24	1.33
4	M	4	BCL	C1D-C2D	-3.59	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	5	BPH	O2D-CGD	-3.58	1.24	1.33
8	M	304	CRT	C20-C19	3.51	1.54	1.43
8	M	304	CRT	C11-C12	-3.50	1.38	1.46
5	M	5	BPH	O2A-CGA	-3.48	1.23	1.33
4	M	3	BCL	C1D-C2D	-3.44	1.38	1.45
8	M	304	CRT	C10-C9	3.44	1.53	1.43
4	M	1	BCL	O2A-CGA	-3.43	1.23	1.33
5	M	5	BPH	C3B-CAB	-3.41	1.40	1.49
4	M	3	BCL	O2D-CGD	-3.34	1.25	1.33
4	M	3	BCL	O2A-CGA	-3.33	1.23	1.33
6	L	272	U10	C18-C19	3.33	1.40	1.33
5	L	271	BPH	O2A-CGA	-3.31	1.23	1.33
6	M	303	U10	C6-C1	3.24	1.41	1.35
4	M	4	BCL	O2A-CGA	-3.22	1.24	1.33
8	M	304	CRT	C26-C27	3.21	1.53	1.43
8	M	304	CRT	C16-C17	-3.20	1.39	1.46
6	M	303	U10	C4-C5	-3.15	1.39	1.48
6	M	303	U10	C38-C39	3.09	1.40	1.33
8	M	304	CRT	C21-C22	3.08	1.52	1.43
6	L	272	U10	C13-C14	3.07	1.40	1.33
8	M	304	CRT	C15-C14	3.04	1.52	1.43
6	L	272	U10	C6-C1	3.04	1.40	1.35
4	L	2	BCL	O2A-CGA	-2.92	1.24	1.33
6	L	272	U10	C34-C33	2.78	1.47	1.29
6	L	272	U10	C3-C2	-2.72	1.41	1.48
6	L	272	U10	C28-C29	2.71	1.39	1.33
6	L	272	U10	C8-C9	2.71	1.39	1.33
6	L	272	U10	C23-C24	2.70	1.39	1.33
6	M	303	U10	C33-C34	2.69	1.39	1.33
6	M	303	U10	O4-C4M	-2.69	1.39	1.45
6	M	303	U10	C28-C29	2.67	1.39	1.33
6	M	303	U10	C44-C43	2.66	1.46	1.29
6	M	303	U10	C22-C23	-2.56	1.42	1.50
5	L	271	BPH	C2-C3	2.53	1.38	1.33
4	L	2	BCL	C2-C3	2.43	1.38	1.33
4	M	1	BCL	C3A-C2A	-2.41	1.47	1.54
6	M	303	U10	C8-C9	2.41	1.38	1.33
6	M	303	U10	C18-C19	2.41	1.38	1.33
4	M	3	BCL	C2-C3	2.35	1.38	1.33
4	M	4	BCL	C1B-C2B	-2.35	1.37	1.43
4	M	1	BCL	C3B-CAB	-2.33	1.39	1.46
8	M	304	CRT	C8-C7	2.28	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	2	BCL	C1D-ND	-2.24	1.34	1.37
4	M	1	BCL	C1D-ND	-2.24	1.34	1.37
6	L	272	U10	C11-C9	2.19	1.55	1.51
5	M	5	BPH	C1D-C2D	-2.13	1.37	1.39
5	M	5	BPH	C2-C3	2.11	1.37	1.33
4	M	4	BCL	C3D-CAD	-2.11	1.38	1.45
6	L	272	U10	C4-C5	-2.10	1.42	1.48
4	M	1	BCL	C1B-C2B	-2.09	1.38	1.43
4	M	3	BCL	C1B-C2B	-2.07	1.38	1.43
6	M	303	U10	C13-C14	2.07	1.37	1.33
4	M	1	BCL	C2-C3	2.06	1.38	1.32
8	M	304	CRT	C13-C12	2.06	1.55	1.50
4	M	4	BCL	C2-C3	2.06	1.38	1.32
4	M	3	BCL	C1D-ND	-2.05	1.35	1.37
8	M	304	CRT	C18-C17	2.05	1.55	1.50
6	M	303	U10	C7-C6	2.03	1.55	1.51
5	M	5	BPH	CBD-CGD	2.00	1.55	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	272	U10	C7-C6-C5	9.57	129.64	118.52
5	M	5	BPH	O2D-CGD-CBD	8.24	120.00	110.95
6	L	272	U10	C7-C6-C1	-7.55	111.94	124.89
5	M	5	BPH	C4D-CHA-CBD	-7.52	104.85	108.45
4	M	4	BCL	C1C-NC-C4C	7.47	110.09	106.68
5	M	5	BPH	C3D-C4D-ND	7.18	116.91	107.71
5	L	271	BPH	C4D-CHA-CBD	-7.10	105.05	108.45
5	M	5	BPH	C4D-ND-C1D	-6.51	101.07	108.87
5	L	271	BPH	C3D-C4D-ND	6.25	115.73	107.71
8	M	304	CRT	C36-C35-C33	-6.02	116.79	125.89
5	L	271	BPH	C2B-C1B-NB	5.99	113.76	109.43
5	L	271	BPH	O2D-CGD-CBD	5.89	117.42	110.95
8	M	304	CRT	C38-C37-C36	5.57	133.15	114.10
8	M	304	CRT	C37-C36-C35	-5.53	113.97	125.93
4	M	3	BCL	C1C-NC-C4C	5.41	109.15	106.68
5	L	271	BPH	C4D-ND-C1D	-5.22	102.62	108.87
4	M	1	BCL	O2D-CGD-CBD	5.16	120.24	111.23
8	M	304	CRT	C10-C9-C7	-5.13	120.08	127.28
4	L	2	BCL	C1C-NC-C4C	5.10	109.01	106.68
4	M	4	BCL	C4D-C3D-CAD	-4.90	102.78	108.11
5	L	271	BPH	O1D-CGD-CBD	-4.85	117.37	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	304	CRT	C34-C33-C35	-4.82	110.73	118.09
5	M	5	BPH	C2B-C1B-NB	4.80	112.90	109.43
5	M	5	BPH	O1D-CGD-CBD	-4.70	117.59	124.72
4	M	3	BCL	C4D-CHA-C1A	4.69	126.84	121.24
4	M	4	BCL	C4D-CHA-C1A	4.68	126.82	121.24
8	M	304	CRT	C13-C12-C14	-4.63	115.32	122.82
4	M	3	BCL	C4A-NA-C1A	4.62	108.79	106.68
4	M	3	BCL	C4D-C3D-CAD	-4.56	103.15	108.11
4	L	2	BCL	C4D-C3D-CAD	-4.55	103.17	108.11
6	M	303	U10	C7-C6-C5	4.51	123.76	118.52
8	M	304	CRT	C20-C19-C17	-4.46	121.02	127.28
4	M	1	BCL	C4D-C3D-CAD	-4.34	103.39	108.11
5	L	271	BPH	C3D-CAD-CBD	4.32	113.29	107.61
4	M	1	BCL	O1D-CGD-CBD	-4.31	116.01	124.52
4	M	1	BCL	C4D-CHA-C1A	4.26	126.33	121.24
6	L	272	U10	C7-C8-C9	-4.25	119.51	126.83
5	M	5	BPH	C3D-CAD-CBD	4.20	113.14	107.61
4	L	2	BCL	C4D-CHA-C1A	4.15	126.19	121.24
5	L	271	BPH	CMC-C2C-C1C	-4.13	105.71	114.61
4	M	1	BCL	C1C-NC-C4C	4.09	108.54	106.68
4	L	2	BCL	C1D-ND-C4D	-4.07	103.46	106.31
5	M	5	BPH	OBD-CAD-C3D	-4.05	121.58	127.89
8	M	304	CRT	C10-C11-C12	-4.04	115.28	126.36
4	M	4	BCL	C4A-NA-C1A	4.00	108.50	106.68
6	L	272	U10	C1M-C1-C6	-3.96	117.94	124.45
8	M	304	CRT	C24-C23-C22	-3.95	116.42	122.82
4	M	3	BCL	O2D-CGD-CBD	3.95	118.13	111.23
5	M	5	BPH	C2D-C1D-ND	3.94	112.28	109.43
5	L	271	BPH	C1B-NB-C4B	-3.86	103.19	108.82
4	M	4	BCL	C1D-ND-C4D	-3.76	103.67	106.31
4	M	3	BCL	C3D-C4D-ND	3.76	116.09	109.99
6	L	272	U10	C8-C7-C6	3.69	121.18	112.08
4	M	3	BCL	C1D-ND-C4D	-3.65	103.75	106.31
8	M	304	CRT	C18-C17-C16	3.64	123.64	118.09
6	M	303	U10	C25-C24-C26	3.55	121.39	115.23
6	M	303	U10	C25-C24-C23	-3.53	114.57	123.63
6	M	303	U10	C1M-C1-C6	-3.50	118.70	124.45
4	M	1	BCL	C3D-C4D-ND	3.47	115.63	109.99
6	M	303	U10	C35-C34-C36	3.44	121.19	115.23
4	L	2	BCL	C3D-C4D-ND	3.43	115.57	109.99
4	L	2	BCL	C4A-NA-C1A	3.43	108.25	106.68
5	M	5	BPH	C1B-NB-C4B	-3.41	103.85	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	4	BCL	C3D-C4D-ND	3.38	115.47	109.99
6	L	272	U10	C10-C9-C11	3.35	121.04	115.23
6	M	303	U10	C30-C29-C31	3.27	120.91	115.23
6	M	303	U10	C7-C6-C1	-3.24	119.34	124.89
5	L	271	BPH	CBA-CAA-C2A	3.21	123.25	113.78
4	M	1	BCL	C3D-C2D-C1D	3.21	110.22	105.83
6	M	303	U10	C10-C9-C8	-3.20	115.42	123.63
5	M	5	BPH	C4-C3-C5	3.16	120.71	115.23
4	M	1	BCL	C1D-ND-C4D	-3.16	104.10	106.31
4	M	3	BCL	C3D-C2D-C1D	3.14	110.11	105.83
4	M	1	BCL	CBA-CAA-C2A	3.13	123.11	113.79
5	L	271	BPH	CMA-C3A-C4A	-3.13	107.86	114.61
4	M	4	BCL	C1-C2-C3	-3.13	121.70	126.76
6	L	272	U10	C30-C29-C31	3.13	120.66	115.23
8	M	304	CRT	C40-C38-C37	3.07	122.64	110.46
6	M	303	U10	C15-C14-C16	3.06	120.54	115.23
4	L	2	BCL	C1-C2-C3	-3.01	121.26	126.20
8	M	304	CRT	C39-C38-C37	2.94	122.13	110.46
5	L	271	BPH	OBD-CAD-C3D	-2.92	123.34	127.89
4	M	4	BCL	C3D-C2D-C1D	2.90	109.79	105.83
8	M	304	CRT	C30-C28-C27	-2.86	114.51	119.01
6	L	272	U10	C15-C14-C16	2.85	120.18	115.23
6	L	272	U10	C10-C9-C8	-2.84	116.33	123.63
6	M	303	U10	C1-C6-C5	-2.80	116.89	119.62
4	M	3	BCL	CHA-C4D-ND	-2.79	126.78	132.55
8	M	304	CRT	C26-C25-C23	-2.79	118.70	126.36
8	M	304	CRT	C25-C23-C22	2.78	123.39	119.01
5	M	5	BPH	CMB-C2B-C3B	2.78	130.23	124.68
4	L	2	BCL	CBC-CAC-C3C	2.76	119.28	113.41
4	L	2	BCL	CAC-C3C-C4C	-2.74	106.50	112.58
8	M	304	CRT	C11-C12-C14	2.70	123.26	119.01
4	L	2	BCL	C7-C6-C5	-2.69	106.10	113.26
5	L	271	BPH	CBB-CAB-C3B	-2.64	112.44	120.34
5	L	271	BPH	C4-C3-C5	2.60	119.75	115.23
5	L	271	BPH	C7-C6-C5	-2.60	106.33	113.26
5	M	5	BPH	CBA-CAA-C2A	2.58	121.38	113.78
4	M	4	BCL	CAA-CBA-CGA	2.58	120.52	113.21
5	M	5	BPH	CMC-C2C-C1C	-2.56	109.09	114.61
6	M	303	U10	C35-C34-C33	-2.56	117.05	123.63
6	M	303	U10	C15-C14-C13	-2.52	117.15	123.63
8	M	304	CRT	C26-C27-C28	-2.51	123.76	127.28
6	M	303	U10	C30-C29-C28	-2.49	117.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	4	BCL	CAA-C2A-C3A	-2.49	106.26	113.00
4	L	2	BCL	C3D-C2D-C1D	2.49	109.23	105.83
4	L	2	BCL	CHA-C4D-ND	-2.47	127.45	132.55
8	M	304	CRT	C4-C5-C6	-2.47	121.45	124.91
5	L	271	BPH	OBB-CAB-C3B	2.44	124.07	119.99
6	L	272	U10	C25-C24-C26	2.43	119.45	115.23
4	L	2	BCL	CBA-CAA-C2A	-2.42	106.58	113.79
6	L	272	U10	C25-C24-C23	-2.42	117.41	123.63
4	M	4	BCL	C2B-C1B-NB	2.40	112.81	110.33
5	M	5	BPH	C3B-C4B-NB	2.40	111.54	108.05
6	L	272	U10	C15-C14-C13	-2.37	117.53	123.63
4	M	1	BCL	CHA-C4D-ND	-2.37	127.66	132.55
4	L	2	BCL	CED-O2D-CGD	2.37	121.28	115.92
4	M	4	BCL	CHA-C4D-ND	-2.35	127.69	132.55
8	M	304	CRT	C18-C17-C19	-2.34	119.02	122.82
4	M	3	BCL	O1D-CGD-CBD	-2.34	119.91	124.52
6	M	303	U10	C40-C39-C38	-2.32	117.66	123.63
4	L	2	BCL	O2A-C1-C2	2.32	117.02	108.11
4	M	3	BCL	C3A-C2A-C1A	2.31	104.81	101.34
6	L	272	U10	C30-C29-C28	-2.30	117.73	123.63
5	L	271	BPH	C17-C16-C15	-2.30	102.99	113.28
6	M	303	U10	C27-C28-C29	-2.29	122.37	127.62
4	M	1	BCL	CAB-C3B-C2B	-2.29	122.98	127.74
4	M	4	BCL	CMB-C2B-C1B	-2.28	121.94	125.42
4	M	1	BCL	C3A-C2A-C1A	2.28	104.75	101.34
4	M	4	BCL	OBD-CAD-C3D	-2.28	123.09	128.42
4	L	2	BCL	OBD-CAD-C3D	-2.28	123.09	128.42
5	M	5	BPH	C1C-C2C-C3C	2.28	105.00	102.84
6	M	303	U10	C10-C9-C11	2.25	119.14	115.23
4	M	3	BCL	C7-C6-C5	-2.24	107.29	113.26
6	L	272	U10	C20-C19-C21	2.22	119.08	115.23
6	L	272	U10	C6-C1-C2	2.21	120.92	119.17
4	M	3	BCL	CGD-CBD-CAD	-2.21	103.70	110.85
6	M	303	U10	C6-C1-C2	2.21	120.91	119.17
4	M	1	BCL	CHA-C1A-NA	-2.20	121.40	126.39
4	M	3	BCL	CAA-C2A-C3A	-2.20	107.06	113.00
4	M	3	BCL	C4-C3-C5	2.19	119.03	115.23
5	L	271	BPH	C2D-C1D-ND	2.18	111.01	109.43
4	M	4	BCL	C5-C3-C4	2.18	119.60	114.59
8	M	304	CRT	C29-C28-C30	2.18	121.41	118.09
6	M	303	U10	C21-C22-C23	-2.17	101.30	112.02
5	M	5	BPH	C1-O2A-CGA	2.16	121.89	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	303	U10	C20-C19-C18	-2.16	118.08	123.63
4	M	3	BCL	CED-O2D-CGD	2.16	120.81	115.92
5	L	271	BPH	CED-O2D-CGD	2.16	120.81	115.92
4	M	4	BCL	C2C-C3C-C4C	2.16	104.57	101.34
8	M	304	CRT	C9-C10-C11	2.15	129.42	123.20
5	M	5	BPH	CAA-C2A-C3A	-2.14	107.21	113.00
8	M	304	CRT	C13-C12-C11	2.14	121.36	118.09
4	M	4	BCL	C2A-C3A-C4A	2.13	105.31	101.87
4	L	2	BCL	CHA-C1A-NA	-2.13	121.57	126.39
4	L	2	BCL	C2A-C3A-C4A	2.12	105.30	101.87
4	M	4	BCL	CHC-C4B-NB	-2.12	120.87	124.05
6	M	303	U10	O2-C2-C3	-2.11	116.57	121.03
4	M	3	BCL	CHC-C4B-NB	-2.10	120.90	124.05
4	L	2	BCL	O2A-CGA-CBA	2.08	118.17	111.83
4	M	4	BCL	CHA-C1A-NA	-2.08	121.69	126.39
4	M	3	BCL	C1-C2-C3	-2.07	122.80	126.20
4	M	1	BCL	C4A-NA-C1A	2.07	107.62	106.68
4	M	4	BCL	CMB-C2B-C3B	2.07	132.21	125.67
8	M	304	CRT	C5-C6-C7	-2.07	122.76	125.89
6	M	303	U10	O5-C5-C4	-2.07	116.65	121.03
4	M	3	BCL	CAC-C3C-C4C	-2.04	108.06	112.58
6	M	303	U10	C20-C19-C21	2.03	118.75	115.23
4	M	3	BCL	CHA-C1A-NA	-2.03	121.80	126.39
6	M	303	U10	C12-C13-C14	-2.03	122.98	127.62
6	M	303	U10	C41-C39-C38	2.02	125.70	121.17
4	M	1	BCL	C2A-C1A-CHA	2.02	127.37	123.87
5	M	5	BPH	CBB-CAB-C3B	-2.01	114.32	120.34

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	3	BCL	C13
4	M	3	BCL	C8
5	L	271	BPH	C8

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	2	BCL	C2C-C3C-CAC-CBC
4	L	2	BCL	C4C-C3C-CAC-CBC
4	M	1	BCL	CHA-CBD-CGD-O1D
4	M	1	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
4	M	3	BCL	C2C-C3C-CAC-CBC
4	M	3	BCL	C4C-C3C-CAC-CBC
4	M	3	BCL	CHA-CBD-CGD-O1D
4	M	3	BCL	CBD-CGD-O2D-CED
5	M	5	BPH	CBD-CGD-O2D-CED
5	M	5	BPH	C4C-C3C-CAC-CBC
5	M	5	BPH	C2C-C3C-CAC-CBC
6	L	272	U10	C1-C6-C7-C8
6	L	272	U10	C5-C6-C7-C8
6	M	303	U10	C5-C6-C7-C8
6	M	303	U10	C30-C29-C31-C32
8	M	304	CRT	C14-C15-C16-C17
8	M	304	CRT	C19-C20-C21-C22
8	M	304	CRT	C30-C31-C32-C33
8	M	304	CRT	C32-C33-C35-C36
8	M	304	CRT	C33-C35-C36-C37
8	M	304	CRT	C36-C37-C38-C39
4	L	2	BCL	CBD-CGD-O2D-CED
5	L	271	BPH	CBD-CGD-O2D-CED
4	L	2	BCL	O1D-CGD-O2D-CED
4	M	3	BCL	O1D-CGD-O2D-CED
4	L	2	BCL	C3-C5-C6-C7
5	M	5	BPH	O1D-CGD-O2D-CED
6	M	303	U10	C35-C34-C36-C37
6	M	303	U10	C28-C29-C31-C32
6	M	303	U10	C33-C34-C36-C37
6	L	272	U10	C15-C14-C16-C17
6	M	303	U10	C20-C19-C21-C22
6	M	303	U10	C25-C24-C26-C27
6	L	272	U10	C28-C29-C31-C32
6	M	303	U10	C23-C24-C26-C27
6	L	272	U10	C19-C21-C22-C23
6	M	303	U10	C9-C11-C12-C13
5	M	5	BPH	C5-C6-C7-C8
5	L	271	BPH	O1D-CGD-O2D-CED
8	M	304	CRT	C20-C21-C22-C23
6	L	272	U10	C30-C29-C31-C32
6	L	272	U10	C13-C14-C16-C17
6	L	272	U10	C18-C19-C21-C22
4	M	3	BCL	C11-C10-C8-C9
5	L	271	BPH	C11-C10-C8-C9
8	M	304	CRT	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
4	L	2	BCL	C8-C10-C11-C12
4	L	2	BCL	CBA-CGA-O2A-C1
4	M	3	BCL	O1A-CGA-O2A-C1
4	M	3	BCL	CBA-CGA-O2A-C1
4	L	2	BCL	O1A-CGA-O2A-C1
8	M	304	CRT	C21-C22-C23-C24
8	M	304	CRT	C26-C27-C28-C29
8	M	304	CRT	C31-C32-C33-C34
8	M	304	CRT	C29-C28-C30-C31
4	L	2	BCL	C3A-C2A-CAA-CBA
4	L	2	BCL	C5-C6-C7-C8
6	L	272	U10	C20-C19-C21-C22
6	M	303	U10	C18-C19-C21-C22
6	M	303	U10	C1-C6-C7-C8
4	L	2	BCL	C1A-C2A-CAA-CBA
5	L	271	BPH	C11-C10-C8-C7
5	L	271	BPH	C5-C6-C7-C8
4	L	2	BCL	C4B-C3B-CAB-OBB
5	M	5	BPH	C14-C13-C15-C16
6	L	272	U10	C31-C32-C33-C34
4	M	1	BCL	C2B-C3B-CAB-CBB
5	M	5	BPH	C3-C5-C6-C7
5	M	5	BPH	C12-C13-C15-C16
5	M	5	BPH	C3A-C2A-CAA-CBA
4	M	1	BCL	C4B-C3B-CAB-CBB
5	L	271	BPH	C3-C5-C6-C7
4	M	1	BCL	C2B-C3B-CAB-OBB
8	M	304	CRT	C35-C36-C37-C38
4	M	1	BCL	C1A-C2A-CAA-CBA
4	M	3	BCL	CHA-CBD-CGD-O2D
8	M	304	CRT	C17-C19-C20-C21
6	L	272	U10	C5-C4-O4-C4M
6	M	303	U10	C29-C31-C32-C33
4	L	2	BCL	C10-C11-C12-C13
8	M	304	CRT	C13-C12-C14-C15
8	M	304	CRT	C18-C17-C19-C20
6	L	272	U10	C14-C16-C17-C18
4	M	3	BCL	C1A-C2A-CAA-CBA
8	M	304	CRT	C11-C12-C14-C15
8	M	304	CRT	C16-C17-C19-C20
8	M	304	CRT	C21-C22-C23-C25
4	M	1	BCL	C4B-C3B-CAB-OBB

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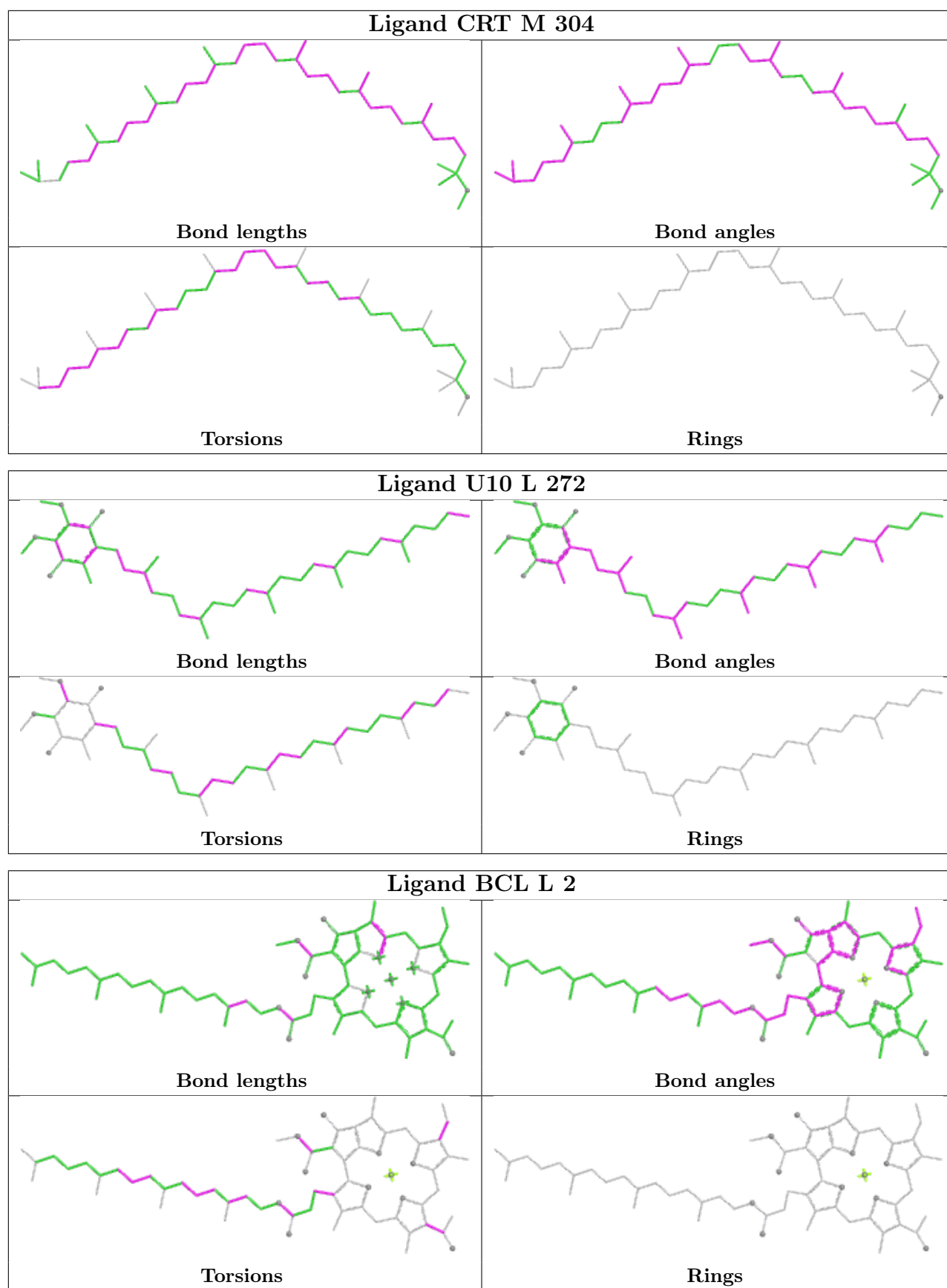
Mol	Chain	Res	Type	Atoms
6	L	272	U10	C25-C24-C26-C27
6	M	303	U10	C2-C3-O3-C3M
4	M	3	BCL	C3A-C2A-CAA-CBA
4	L	2	BCL	C2B-C3B-CAB-OB
6	L	272	U10	C9-C11-C12-C13
6	M	303	U10	C39-C41-C42-C43
5	M	5	BPH	CAA-CBA-CGA-O2A
6	M	303	U10	C34-C36-C37-C38
4	M	1	BCL	C2-C1-O2A-CGA
5	M	5	BPH	CAA-CBA-CGA-O1A
4	L	2	BCL	C1-C2-C3-C4

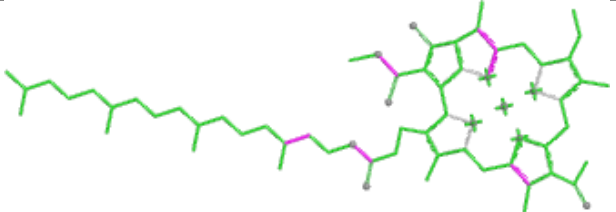
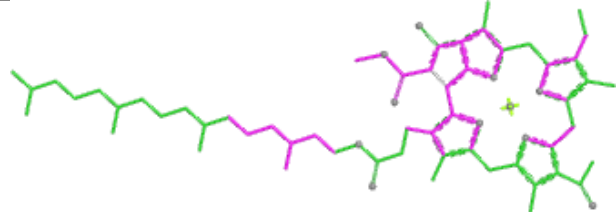
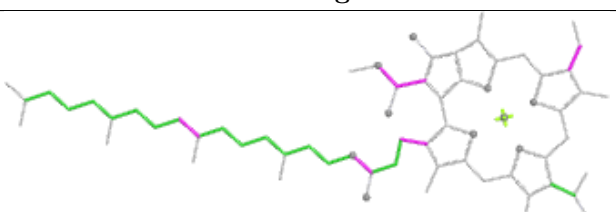
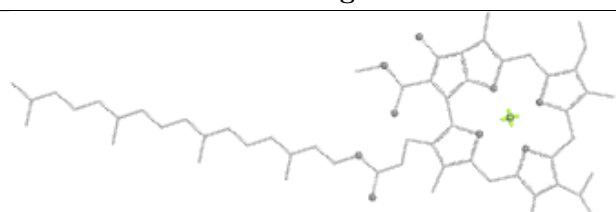
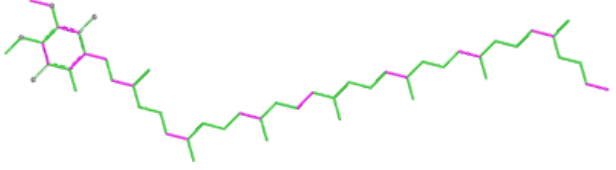
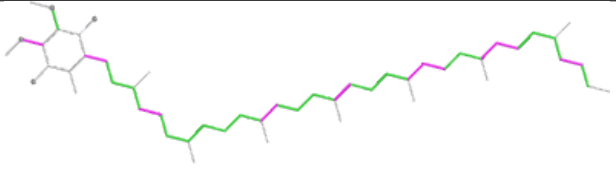
There are no ring outliers.

9 monomers are involved in 41 short contacts:

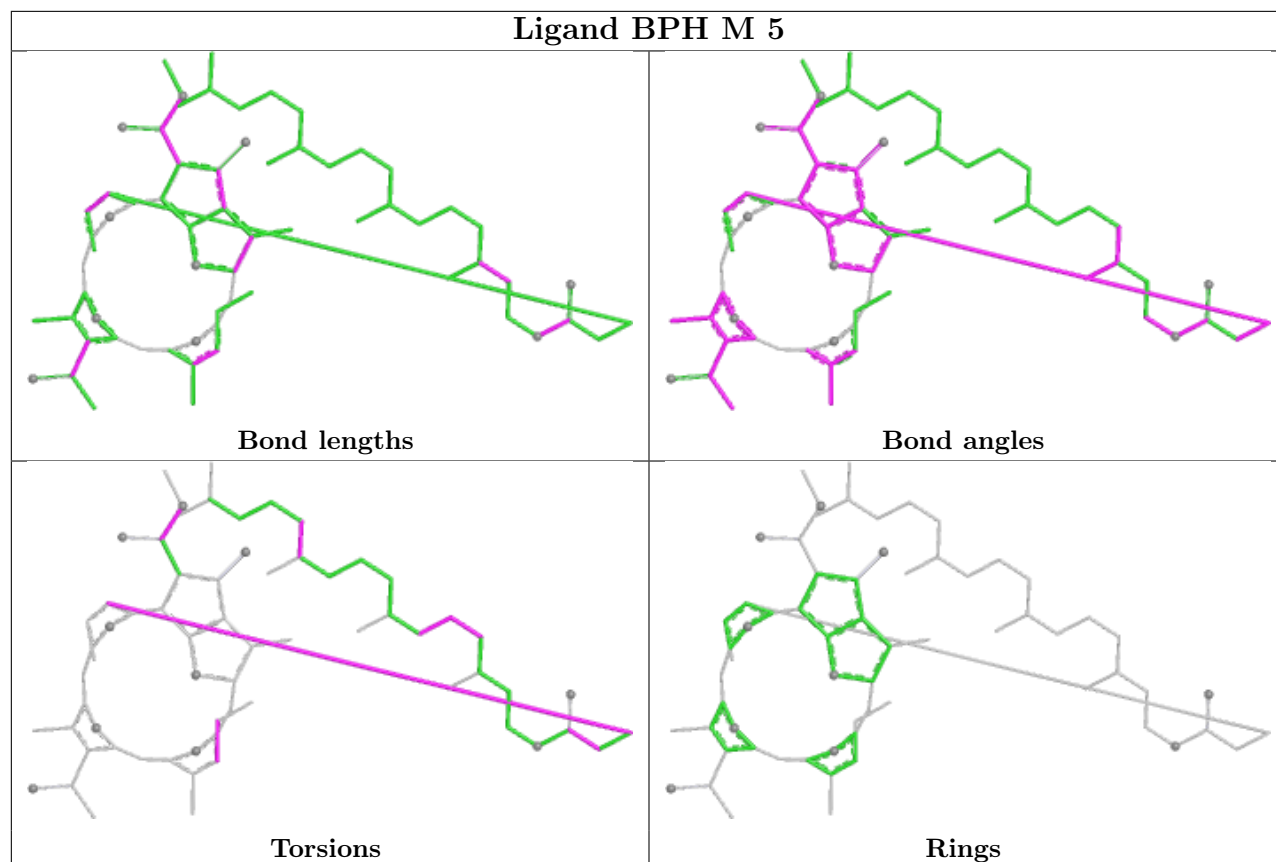
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	304	CRT	1	0
6	L	272	U10	3	0
4	L	2	BCL	12	0
4	M	3	BCL	11	0
6	M	303	U10	7	0
5	M	5	BPH	3	0
4	M	1	BCL	4	0
4	M	4	BCL	2	0
5	L	271	BPH	5	0

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.

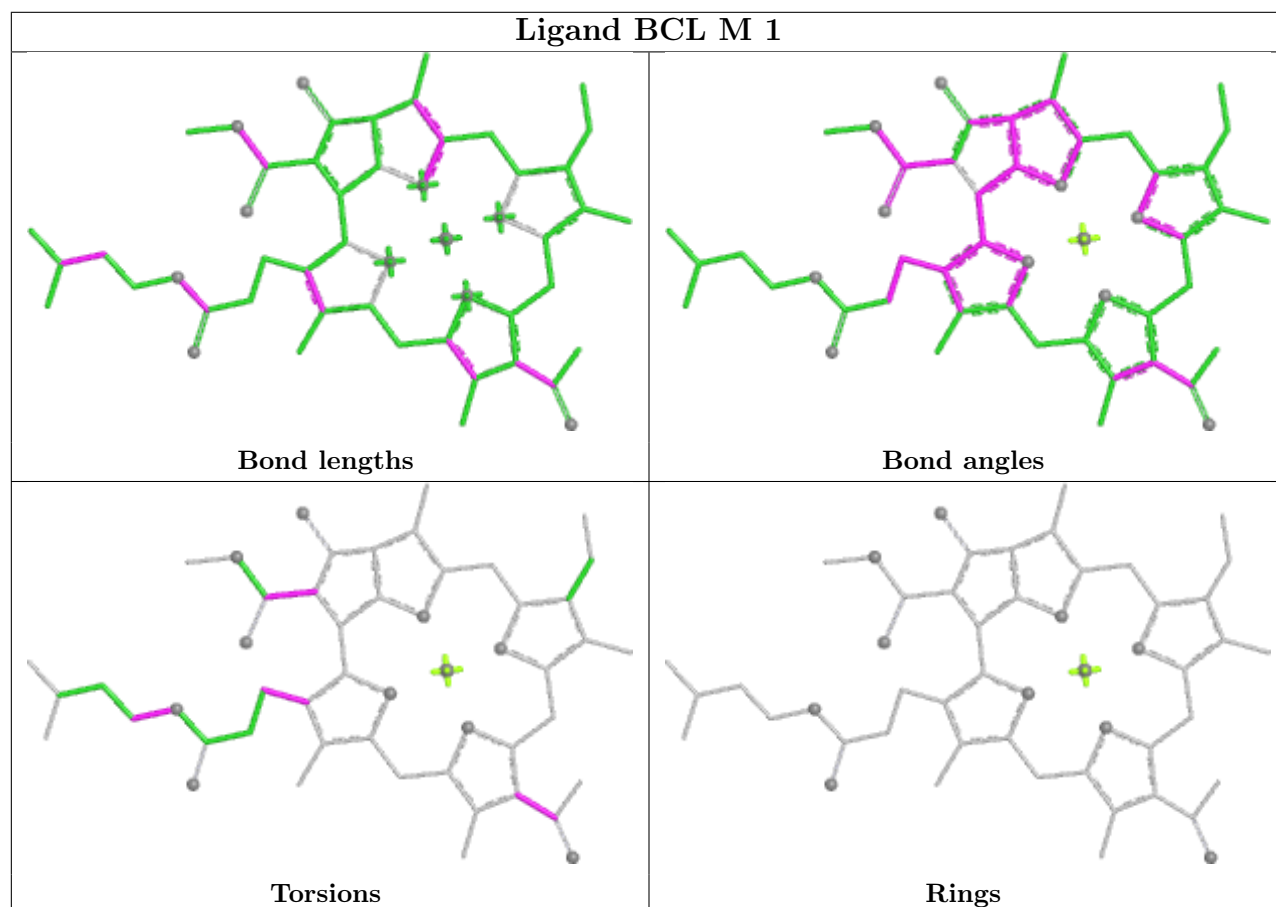


Ligand BCL M 3	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand U10 M 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

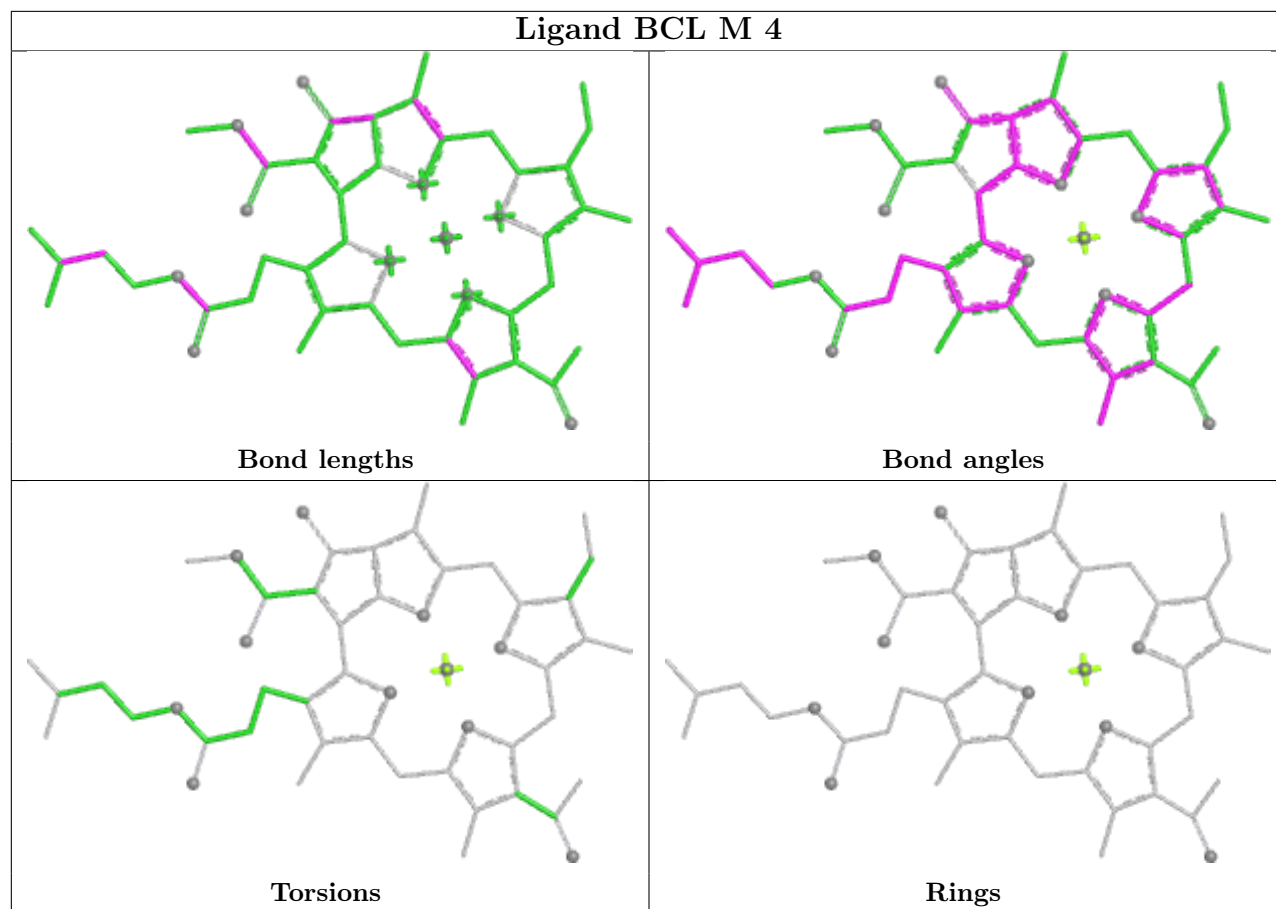
Ligand BPH M 5



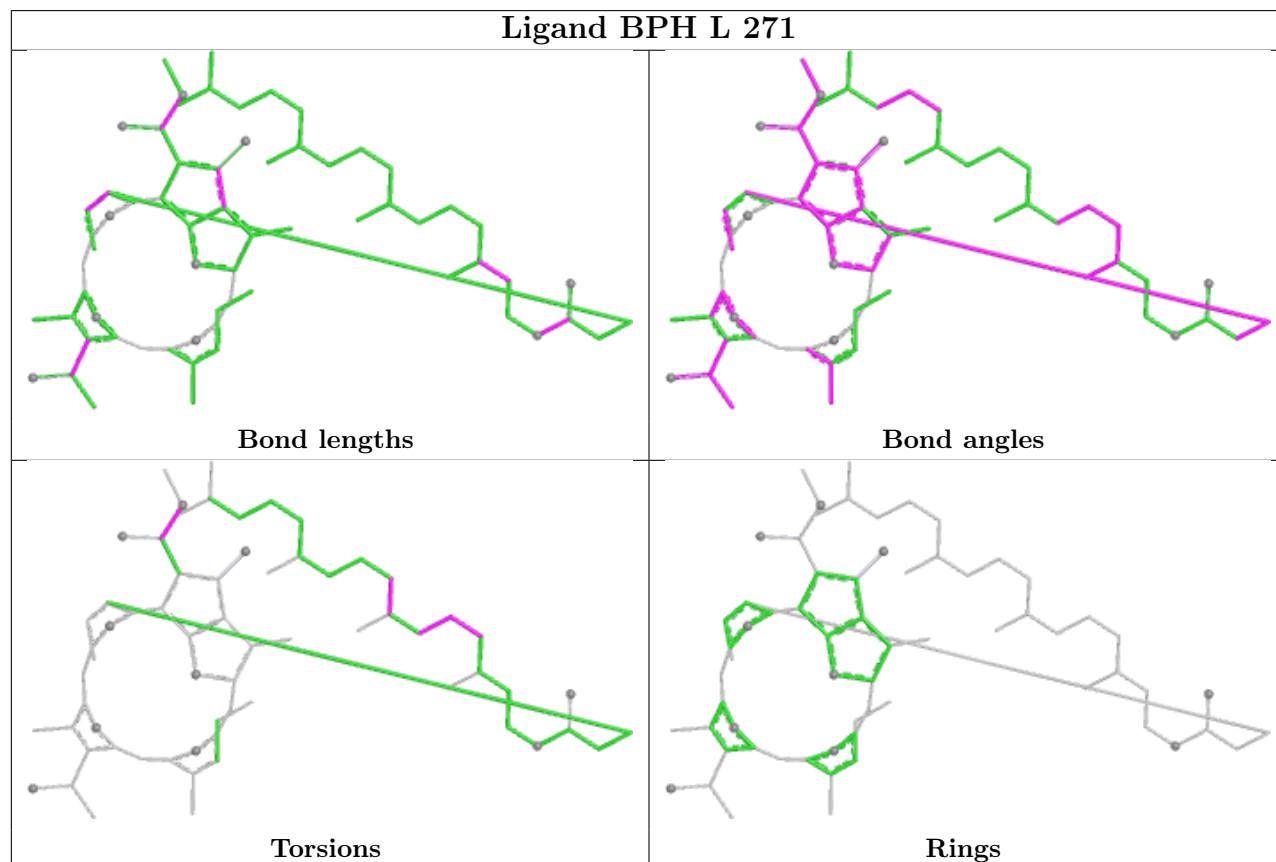
Ligand BCL M 1



Ligand BCL M 4



Ligand BPH L 271



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.