



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:52 AM UTC

PDB ID : 1UMX / pdb_00001umx
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ARG M267
REPLACED WITH LEU (CHAIN M, R267L)
Authors : Fyfe, P.K.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on : 2003-09-02
Resolution : 2.80 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

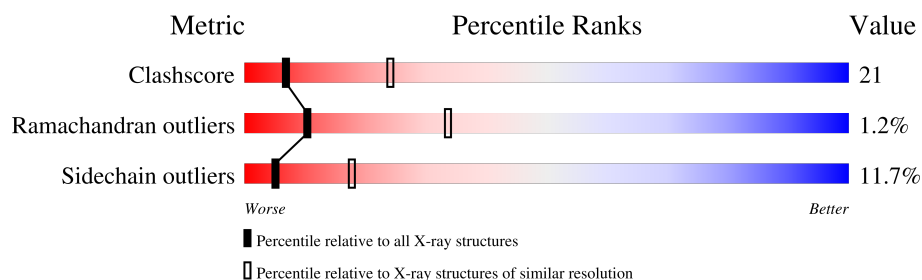
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	H	260	
2	L	281	
3	M	307	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7007 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 REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	14	0	1
			1830	1169	315	337	9			

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	10	0	0
			2232	1507	355	362	8			

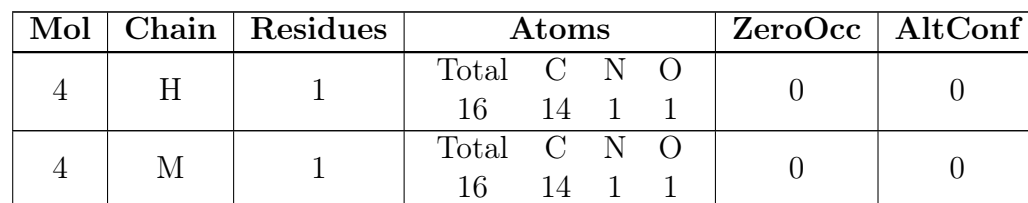
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2406	1607	392	397	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	267	LEU	ARG	engineered mutation	UNP P02953

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



- # BCL

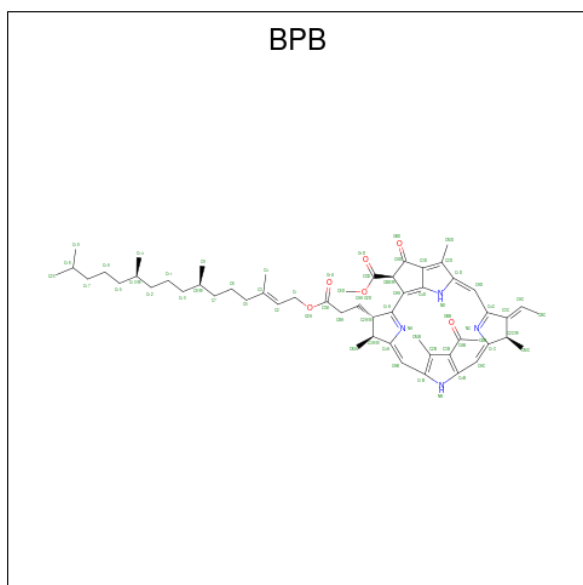
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0



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

- Molecule 6 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).

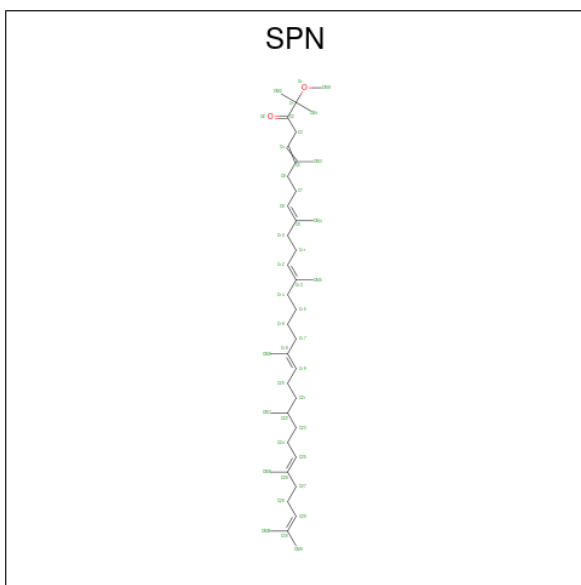


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

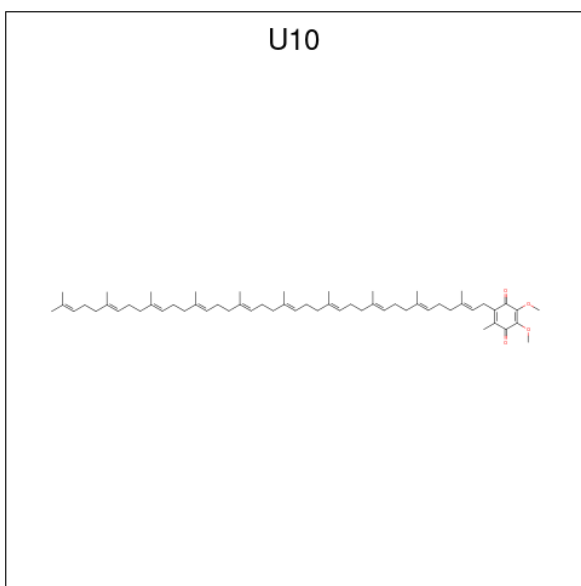
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is water.

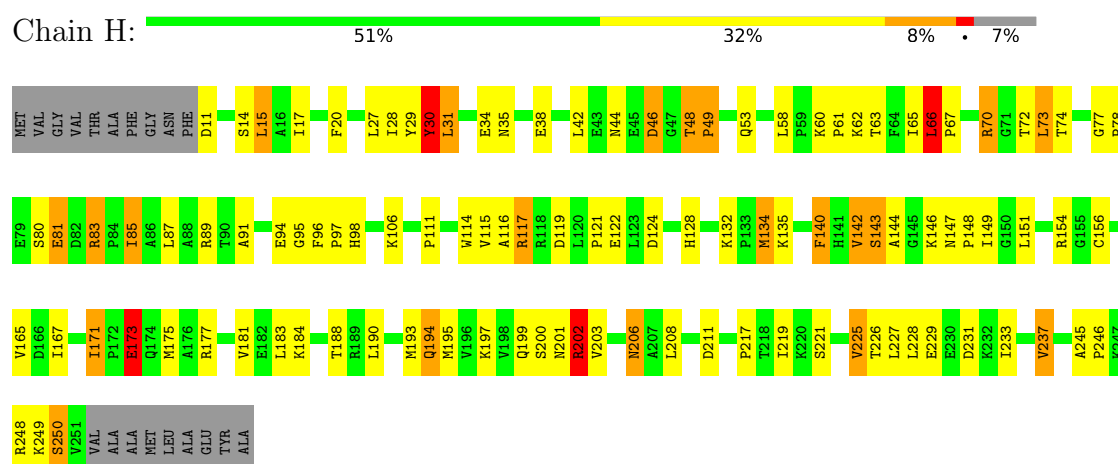
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	6	Total	O	0	0
			6	6		
11	L	6	Total	O	0	0
			6	6		
11	M	4	Total	O	0	0
			4	4		

3 Residue-property plots

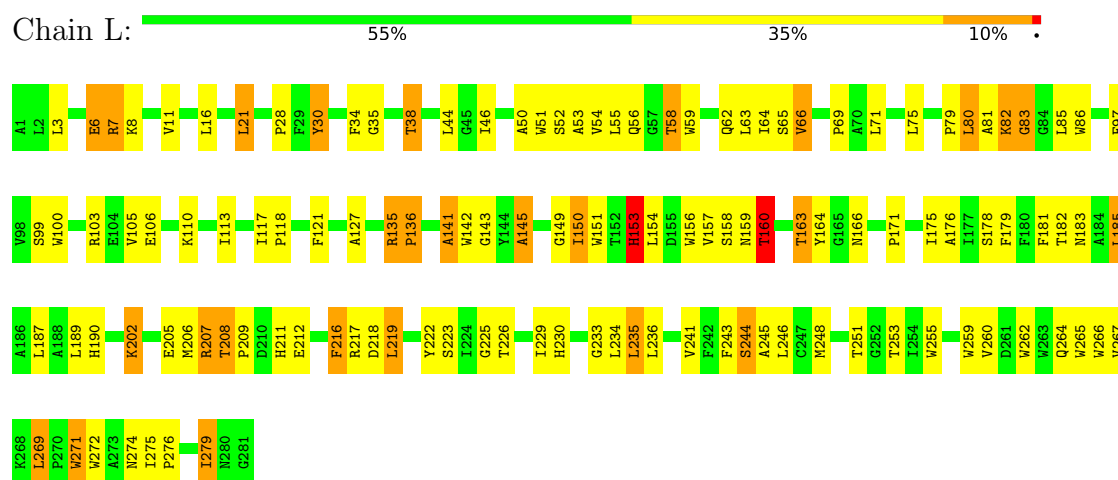
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

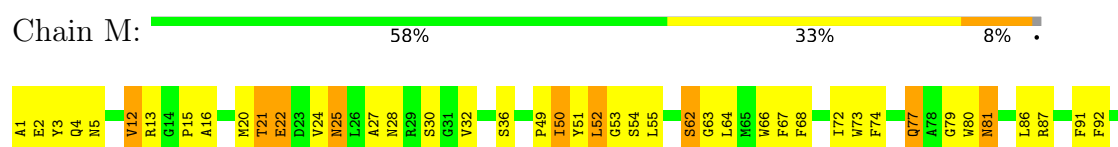
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



H301	Y210	P97
G302	G211	A98
M303	S212	P99
ALA	A213	E100
PRO	L214	
LEU	L215	P108
ASN	F216	
	V226	E111
	S227	G112
	R228	G113
	F229	
		L116
	E232	A125
	R233	
	E234	R132
		T133
	T238	Y134
	A239	L135
	D240	R136
	R241	
	G242	W148
	T243	
	E246	T154
	R247	
		W157
	F251	F162
	G252	T163
	R253	R164
	G254	P165
	T255	T166
		L167
	A260	M168
	T261	G169
	E262	S170
	G263	W171
	G264	
	T265	T179
	H266	
	L267	L183
	W268	
		N188
	M272	F189
	A273	
	V274	V192
	L275	H193
		G194
	L278	N195
	T279	L196
	G280	
	G281	N199
	L282	P200
		F201
	T289	L204
	W297	S205
	G298	T206
	G299	
	N200	T208

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.64Å 141.64Å 187.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.5 (29.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.224 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: BPB, SPN, BCL, U10, FE, LDA, PO4

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	H	1.42	12/1878 (0.6%)	1.70	28/2555 (1.1%)
2	L	1.52	11/2320 (0.5%)	1.46	22/3175 (0.7%)
3	M	1.29	12/2498 (0.5%)	1.43	25/3412 (0.7%)
All	All	1.41	35/6696 (0.5%)	1.52	75/9142 (0.8%)

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	H	1	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	202	LYS	CG-CD	-28.21	0.67	1.52
2	L	202	LYS	CD-CE	25.11	2.27	1.52
3	M	21	THR	CA-C	-8.44	1.44	1.52
1	H	34	GLU	C-O	-7.92	1.14	1.24
1	H	250	SER	C-N	-7.32	1.23	1.33
1	H	31	LEU	CA-C	7.17	1.62	1.52
3	M	302	GLY	C-N	-6.38	1.24	1.33
2	L	164	TYR	CA-C	-6.33	1.44	1.52
1	H	116	ALA	CA-C	-6.24	1.46	1.53
1	H	171	ILE	CA-CB	6.10	1.62	1.54
2	L	208	THR	CA-CB	5.99	1.61	1.53
2	L	226	THR	N-CA	-5.78	1.39	1.46
2	L	185	LEU	CA-C	5.56	1.60	1.52
2	L	248	MET	SD-CE	-5.55	1.65	1.79
2	L	30	TYR	C-O	-5.52	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	140	PHE	C-O	-5.48	1.17	1.23
1	H	49	PRO	C-O	-5.37	1.17	1.23
3	M	188	ASN	N-CA	-5.36	1.39	1.46
1	H	38	GLU	CA-C	-5.35	1.46	1.52
3	M	261	THR	N-CA	-5.29	1.39	1.45
2	L	179	PHE	N-CA	-5.27	1.40	1.46
1	H	140	PHE	N-CA	-5.25	1.39	1.46
1	H	144	ALA	CA-CB	-5.24	1.44	1.53
3	M	253	ARG	NE-CZ	5.22	1.38	1.33
3	M	234	GLU	C-O	5.22	1.30	1.24
3	M	168	MET	SD-CE	-5.18	1.66	1.79
3	M	227	SER	C-O	-5.15	1.16	1.24
1	H	85	ILE	CA-CB	-5.12	1.47	1.53
1	H	81	GLU	C-O	5.12	1.30	1.23
3	M	272	MET	C-O	-5.11	1.18	1.24
3	M	297	TRP	C-O	-5.07	1.18	1.24
2	L	105	VAL	N-CA	-5.04	1.40	1.46
3	M	36	SER	C-O	-5.03	1.17	1.24
3	M	209	LEU	C-O	-5.03	1.18	1.24
2	L	135	ARG	N-CA	5.01	1.50	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	202	LYS	CB-CG-CD	-19.75	65.86	111.30
1	H	31	LEU	N-CA-C	-19.64	68.97	110.80
1	H	65	ILE	CA-C-N	12.52	144.24	121.70
1	H	65	ILE	C-N-CA	12.52	144.24	121.70
1	H	30	TYR	O-C-N	-10.40	108.75	122.59
1	H	65	ILE	O-C-N	-10.15	112.52	123.18
1	H	65	ILE	N-CA-C	-9.21	95.28	108.17
2	L	83	GLY	N-CA-C	8.98	127.23	115.47
1	H	31	LEU	N-CA-CB	8.83	125.41	110.49
3	M	253	ARG	N-CA-C	-8.80	101.64	111.14
3	M	289	THR	N-CA-C	-8.49	102.85	113.55
1	H	30	TYR	CA-C-N	8.48	137.74	121.54
1	H	30	TYR	C-N-CA	8.48	137.74	121.54
1	H	66	LEU	CB-CA-C	8.24	125.75	110.10
3	M	81	ASN	N-CA-C	8.13	121.41	109.04
2	L	202	LYS	CD-CE-NZ	8.01	137.54	111.90
1	H	66	LEU	N-CA-CB	7.92	123.96	110.50
2	L	82	LYS	N-CA-CB	7.54	126.49	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	81	GLU	N-CA-C	-7.50	99.17	110.28
2	L	35	GLY	N-CA-C	-7.42	103.51	112.49
3	M	212	SER	CA-C-N	-7.39	109.80	120.29
3	M	212	SER	C-N-CA	-7.39	109.80	120.29
3	M	170	SER	N-CA-C	7.34	119.54	108.46
1	H	46	ASP	CA-C-N	-7.28	114.92	123.08
1	H	46	ASP	C-N-CA	-7.28	114.92	123.08
1	H	95	GLY	N-CA-C	7.21	124.59	114.85
3	M	213	ALA	N-CA-C	-7.07	103.65	111.36
1	H	83	ARG	N-CA-C	6.95	114.39	108.13
1	H	30	TYR	CB-CA-C	6.86	124.08	110.42
2	L	158	SER	N-CA-C	6.58	119.29	111.33
3	M	268	TRP	N-CA-C	-6.57	104.04	111.07
2	L	219	LEU	N-CA-C	6.47	118.00	111.07
3	M	266	HIS	N-CA-C	-6.46	104.87	112.89
2	L	225	GLY	N-CA-C	6.40	120.75	112.68
3	M	234	GLU	N-CA-C	6.21	118.13	111.36
3	M	204	LEU	N-CA-C	-6.20	103.83	111.40
1	H	142	VAL	CB-CA-C	-6.19	102.04	111.69
2	L	6	GLU	N-CA-C	6.19	119.00	111.82
1	H	206	ASN	N-CA-C	6.18	118.10	111.36
1	H	67	PRO	CA-C-N	-6.14	114.72	123.20
1	H	67	PRO	C-N-CA	-6.14	114.72	123.20
2	L	253	THR	CA-C-N	-6.10	114.59	121.85
2	L	253	THR	C-N-CA	-6.10	114.59	121.85
1	H	173	GLU	N-CA-C	-6.01	105.25	113.30
3	M	80	TRP	CA-C-N	-5.99	112.48	121.83
3	M	80	TRP	C-N-CA	-5.99	112.48	121.83
2	L	141	ALA	N-CA-C	5.98	118.13	108.32
1	H	58	LEU	N-CA-C	-5.97	101.53	110.24
3	M	229	PHE	N-CA-C	-5.95	103.56	112.54
3	M	299	GLN	N-CA-C	-5.87	104.24	111.40
3	M	79	GLY	N-CA-C	-5.73	102.70	114.16
1	H	165	VAL	N-CA-C	-5.70	108.30	113.71
3	M	132	ARG	N-CA-C	-5.69	104.98	111.07
3	M	193	HIS	N-CA-C	-5.68	104.93	112.94
1	H	74	THR	OG1-CB-CG2	-5.53	98.24	109.30
2	L	160	THR	CB-CA-C	5.50	121.22	110.67
1	H	237	VAL	N-CA-C	5.45	116.94	111.00
2	L	230	HIS	N-CA-C	-5.43	105.01	111.69
3	M	251	PHE	N-CA-C	-5.30	105.50	111.28
3	M	282	ILE	N-CA-C	-5.26	105.59	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	210	TYR	N-CA-C	-5.23	105.66	111.36
1	H	65	ILE	CA-C-O	-5.21	114.96	120.48
3	M	241	ARG	CG-CD-NE	-5.21	100.55	112.00
2	L	244	SER	N-CA-C	-5.16	105.34	110.97
2	L	58	THR	CB-CA-C	-5.13	99.02	109.94
2	L	75	LEU	CA-C-N	-5.12	117.04	122.67
2	L	75	LEU	C-N-CA	-5.12	117.04	122.67
2	L	66	VAL	N-CA-C	5.09	115.09	107.51
3	M	240	ASP	CA-C-N	5.04	128.25	121.05
3	M	240	ASP	C-N-CA	5.04	128.25	121.05
2	L	59	TRP	N-CA-C	-5.02	107.19	113.72
1	H	48	THR	N-CA-C	-5.02	102.92	110.24
3	M	81	ASN	CB-CA-C	5.01	115.56	109.85
2	L	121	PHE	N-CA-C	-5.00	105.96	111.71
2	L	153	HIS	CB-CA-C	5.00	119.09	110.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	66	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	30	TYR	Mainchain,Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1830	0	1836	71	0
2	L	2232	0	2187	100	0
3	M	2406	0	2319	111	0
4	H	16	0	31	4	0
4	M	16	0	31	5	0
5	L	132	0	148	12	0
5	M	132	0	148	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	65	0	74	6	0
6	M	65	0	74	11	0
7	M	1	0	0	0	0
8	M	43	0	69	8	0
9	M	48	0	63	2	0
10	M	5	0	0	0	0
11	H	6	0	0	1	0
11	L	6	0	0	1	0
11	M	4	0	0	0	0
All	All	7007	0	6980	296	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 21.

All (296) 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:M:50:ILE:HD13	3:M:51:TYR:N	1.67	1.09
4:H:1251:LDA:H121	4:M:1305:LDA:H91	1.14	1.07
3:M:50:ILE:HD13	3:M:51:TYR:H	1.16	1.07
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.36	1.05
2:L:271:TRP:H	2:L:271:TRP:CD1	1.80	0.98
4:H:1251:LDA:H121	4:M:1305:LDA:C9	1.94	0.98
3:M:108:PRO:HG2	3:M:111:GLU:HG3	1.51	0.93
1:H:98:HIS:CD2	2:L:7:ARG:HH21	1.88	0.90
3:M:25:ASN:ND2	3:M:27:ALA:H	1.69	0.89
4:H:1251:LDA:C12	4:M:1305:LDA:H91	2.02	0.88
3:M:199:ASN:C	3:M:199:ASN:HD22	1.80	0.87
2:L:156:TRP:O	2:L:160:THR:HG23	1.75	0.86
6:L:1284:BPB:HBBA	3:M:210:TYR:HB3	1.57	0.86
5:M:1303:BCL:H51	6:M:1307:BPB:HMBB	1.59	0.85
2:L:205:GLU:O	2:L:207:ARG:NH2	2.10	0.84
2:L:56:GLN:HE22	2:L:65:SER:H	1.23	0.84
2:L:266:TRP:O	2:L:269:LEU:HD22	1.78	0.82
3:M:25:ASN:HD21	3:M:27:ALA:CB	1.92	0.82
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.61	0.81
2:L:156:TRP:O	2:L:160:THR:CG2	2.29	0.80
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.62	0.80
2:L:11:VAL:O	2:L:110:LYS:HE3	1.82	0.80
1:H:42:LEU:H	1:H:53:GLN:HE22	1.31	0.79
5:M:1303:BCL:H51	6:M:1307:BPB:CMB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LYS:HE2	3:M:1:ALA:O	1.82	0.78
2:L:30:TYR:O	2:L:103:ARG:NH1	2.17	0.77
2:L:159:ASN:O	2:L:163:THR:HG22	1.85	0.76
5:L:1282:BCL:HMB1	5:L:1282:BCL:HBB3	1.68	0.74
2:L:272:TRP:HA	2:L:275:ILE:CD1	2.15	0.74
5:M:1303:BCL:H102	5:M:1304:BCL:H171	1.69	0.74
1:H:98:HIS:CD2	2:L:7:ARG:NH2	2.56	0.74
2:L:272:TRP:CA	2:L:275:ILE:HD12	2.17	0.73
6:M:1307:BPB:HHC	6:M:1307:BPB:HBBB	1.69	0.73
1:H:132:LYS:HG3	1:H:171:ILE:CD1	2.18	0.72
2:L:38:THR:HG22	2:L:99:SER:HB3	1.70	0.72
2:L:271:TRP:CD1	2:L:271:TRP:N	2.56	0.72
2:L:181:PHE:HB3	6:M:1307:BPB:HBBA	1.70	0.71
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.75	0.68
5:M:1303:BCL:C5	6:M:1307:BPB:HMBB	2.23	0.68
1:H:35:ASN:HD22	3:M:261:THR:H	1.41	0.67
2:L:182:THR:HG22	2:L:236:LEU:HD13	1.75	0.67
5:M:1303:BCL:H102	5:M:1304:BCL:C17	2.25	0.66
5:M:1304:BCL:OBB	5:M:1304:BCL:HHC	1.95	0.66
3:M:157:TRP:NE1	8:M:1308:SPN:H202	2.10	0.66
1:H:148:PRO:HA	1:H:151:LEU:CD1	2.27	0.65
3:M:199:ASN:C	3:M:199:ASN:ND2	2.55	0.65
1:H:197:LYS:CE	3:M:1:ALA:O	2.44	0.65
5:M:1303:BCL:C3B	8:M:1308:SPN:H152	2.27	0.65
1:H:35:ASN:ND2	3:M:264:GLY:HA3	2.12	0.64
3:M:108:PRO:HD2	3:M:111:GLU:HB2	1.80	0.64
1:H:70:ARG:NH1	1:H:121:PRO:O	2.31	0.64
2:L:181:PHE:HB3	6:M:1307:BPB:CBB	2.28	0.64
3:M:199:ASN:HD22	3:M:200:PRO:N	1.95	0.64
2:L:208:THR:HB	2:L:209:PRO:HD2	1.81	0.63
1:H:202:ARG:HG2	1:H:203:VAL:N	2.11	0.63
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.13	0.63
2:L:274:ASN:O	2:L:275:ILE:C	2.40	0.63
2:L:34:PHE:O	2:L:38:THR:HG23	1.99	0.62
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.80	0.61
3:M:21:THR:O	3:M:24:VAL:HG23	2.01	0.61
3:M:113:GLY:HA2	3:M:116:LEU:HD12	1.81	0.61
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.82	0.61
3:M:195:ASN:C	3:M:195:ASN:OD1	2.44	0.60
1:H:156:CYS:HB3	1:H:206:ASN:O	2.02	0.60
2:L:103:ARG:NH2	3:M:255:THR:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1303:BCL:CAB	8:M:1308:SPN:H162	2.31	0.60
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.83	0.60
2:L:100:TRP:CZ2	9:M:1309:U10:H251	2.36	0.60
3:M:108:PRO:CG	3:M:111:GLU:HG3	2.29	0.59
3:M:189:PHE:O	3:M:193:HIS:HD2	1.85	0.59
1:H:35:ASN:ND2	3:M:260:ALA:HB1	2.18	0.59
3:M:192:VAL:O	3:M:192:VAL:CG1	2.50	0.59
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.83	0.59
3:M:25:ASN:HD21	3:M:27:ALA:HB3	1.66	0.58
5:M:1303:BCL:CBB	5:M:1303:BCL:HMB1	2.33	0.58
2:L:269:LEU:HD23	2:L:272:TRP:CZ2	2.38	0.58
3:M:25:ASN:HD21	3:M:27:ALA:HB2	1.69	0.58
1:H:42:LEU:N	1:H:53:GLN:HE22	2.00	0.58
3:M:243:THR:OG1	3:M:247:ARG:HD3	2.04	0.57
2:L:150:ILE:HD13	2:L:150:ILE:N	2.20	0.57
1:H:27:LEU:O	1:H:31:LEU:HB2	2.04	0.57
3:M:28:ASN:HB3	3:M:52:LEU:O	2.04	0.57
3:M:192:VAL:O	3:M:192:VAL:HG12	2.04	0.56
3:M:162:PHE:O	3:M:166:ILE:HD13	2.04	0.56
5:M:1303:BCL:C14	8:M:1308:SPN:H112	2.36	0.56
2:L:217:ARG:O	2:L:218:ASP:C	2.48	0.56
3:M:21:THR:O	3:M:22:GLU:C	2.47	0.56
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.86	0.56
6:L:1284:BPB:HHC	6:L:1284:BPB:HBBB	1.88	0.56
3:M:97:PRO:HA	3:M:111:GLU:O	2.05	0.55
2:L:150:ILE:HD13	2:L:150:ILE:H	1.72	0.55
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.41	0.55
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.37	0.55
1:H:87:LEU:HD11	2:L:8:LYS:HA	1.87	0.55
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.88	0.55
1:H:122:GLU:OE1	3:M:233:ARG:NH2	2.35	0.55
2:L:38:THR:HG22	2:L:99:SER:CB	2.37	0.55
2:L:66:VAL:HG12	2:L:86:TRP:HB2	1.88	0.55
5:L:1283:BCL:H192	6:L:1284:BPB:H11A	1.88	0.54
6:L:1284:BPB:HMC	3:M:213:ALA:HB3	1.89	0.54
2:L:79:PRO:O	2:L:80:LEU:C	2.49	0.54
1:H:194:GLN:H	1:H:194:GLN:NE2	2.05	0.54
2:L:181:PHE:CD2	6:M:1307:BPB:HBB	2.42	0.54
3:M:194:GLY:O	3:M:195:ASN:HB3	2.07	0.54
2:L:269:LEU:HD23	2:L:272:TRP:HZ2	1.72	0.54
1:H:197:LYS:NZ	3:M:1:ALA:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1282:BCL:H2C	5:M:1304:BCL:HBC2	1.90	0.54
1:H:201:ASN:O	1:H:202:ARG:HB3	2.07	0.53
1:H:89:ARG:HD3	1:H:91:ALA:O	2.09	0.53
2:L:52:SER:HB2	2:L:85:LEU:HD12	1.90	0.53
3:M:157:TRP:CD1	8:M:1308:SPN:H202	2.44	0.53
1:H:175:MET:HE1	3:M:232:GLU:OE2	2.08	0.53
4:H:1251:LDA:H121	4:M:1305:LDA:C10	2.39	0.52
2:L:175:ILE:O	2:L:178:SER:HB2	2.09	0.52
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.44	0.52
3:M:21:THR:C	3:M:22:GLU:O	2.51	0.52
2:L:208:THR:O	2:L:209:PRO:C	2.52	0.52
6:M:1307:BPB:HBBB	6:M:1307:BPB:CHC	2.37	0.52
2:L:156:TRP:O	2:L:160:THR:HG22	2.07	0.52
5:M:1303:BCL:H8	5:M:1304:BCL:C20	2.39	0.52
1:H:96:PHE:N	1:H:96:PHE:CD1	2.77	0.52
2:L:145:ALA:O	2:L:156:TRP:NE1	2.43	0.52
3:M:21:THR:O	3:M:22:GLU:O	2.28	0.51
3:M:204:LEU:HD13	4:M:1305:LDA:HM13	1.91	0.51
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.92	0.51
2:L:209:PRO:O	2:L:212:GLU:HB2	2.11	0.51
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.91	0.51
2:L:279:ILE:HG21	3:M:91:PHE:HB3	1.92	0.51
1:H:117:ARG:HD2	3:M:242:GLY:CA	2.41	0.51
2:L:166:ASN:OD1	2:L:166:ASN:C	2.51	0.51
2:L:6:GLU:OE1	3:M:253:ARG:NH1	2.44	0.51
3:M:62:SER:O	3:M:63:GLY:C	2.54	0.51
1:H:121:PRO:HB3	1:H:225:VAL:O	2.10	0.51
1:H:206:ASN:O	1:H:248:ARG:NH1	2.44	0.50
3:M:234:GLU:O	3:M:238:ILE:HG13	2.12	0.50
2:L:113:ILE:CG2	3:M:226:VAL:HG12	2.41	0.50
3:M:50:ILE:CD1	3:M:51:TYR:N	2.57	0.50
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.93	0.50
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.75	0.50
2:L:149:GLY:O	2:L:153:HIS:HB3	2.12	0.50
2:L:244:SER:O	2:L:245:ALA:C	2.55	0.50
3:M:241:ARG:HD2	3:M:246:GLU:OE2	2.12	0.50
2:L:271:TRP:H	2:L:271:TRP:HD1	1.51	0.49
2:L:156:TRP:CE2	2:L:160:THR:HG21	2.46	0.49
2:L:117:ILE:N	2:L:118:PRO:HD2	2.28	0.49
1:H:132:LYS:HG3	1:H:171:ILE:HD11	1.93	0.49
1:H:140:PHE:HA	3:M:13:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:205:SER:HB3	5:M:1304:BCL:HMA3	1.93	0.49
3:M:25:ASN:OD1	3:M:27:ALA:HB3	2.13	0.49
3:M:64:LEU:HB3	3:M:68:PHE:CE2	2.47	0.49
5:M:1303:BCL:H3A	5:M:1303:BCL:HBA1	1.48	0.49
2:L:160:THR:O	2:L:163:THR:HG23	2.12	0.48
3:M:25:ASN:ND2	3:M:27:ALA:HB3	2.27	0.48
2:L:69:PRO:HD3	2:L:83:GLY:O	2.13	0.48
1:H:14:SER:HA	1:H:17:ILE:HG22	1.94	0.48
1:H:142:VAL:HG21	1:H:147:ASN:ND2	2.29	0.48
5:M:1303:BCL:H141	8:M:1308:SPN:CM4	2.44	0.48
1:H:201:ASN:O	1:H:202:ARG:CB	2.62	0.48
1:H:35:ASN:HD21	3:M:264:GLY:HA3	1.78	0.47
2:L:153:HIS:CE1	2:L:154:LEU:CD1	2.97	0.47
2:L:246:LEU:HD12	2:L:246:LEU:HA	1.64	0.47
5:L:1282:BCL:HMC3	5:M:1304:BCL:CBC	2.44	0.47
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.95	0.47
3:M:300:ASN:O	3:M:301:HIS:HB2	2.14	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.49	0.47
3:M:297:TRP:O	3:M:301:HIS:N	2.47	0.47
1:H:248:ARG:HB2	1:H:248:ARG:CZ	2.45	0.47
3:M:199:ASN:ND2	3:M:201:PHE:H	2.12	0.47
5:M:1304:BCL:H161	5:M:1304:BCL:H192	1.55	0.47
1:H:154:ARG:NH1	1:H:202:ARG:NH2	2.63	0.47
3:M:243:THR:OG1	3:M:247:ARG:CD	2.62	0.47
5:M:1303:BCL:H8	5:M:1304:BCL:H203	1.96	0.47
2:L:190:HIS:CD2	3:M:266:HIS:CD2	3.03	0.47
1:H:156:CYS:SG	1:H:248:ARG:HA	2.55	0.46
1:H:199:GLN:OE1	1:H:202:ARG:HD3	2.15	0.46
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.13	0.46
1:H:83:ARG:HD2	1:H:114:TRP:CH2	2.50	0.46
1:H:135:LYS:HB3	1:H:135:LYS:HE3	1.73	0.46
2:L:16:LEU:H	2:L:106:GLU:CD	2.23	0.46
2:L:141:ALA:HB1	11:L:2003:HOH:O	2.16	0.46
5:M:1303:BCL:HMB1	5:M:1303:BCL:HBB3	1.98	0.46
5:M:1304:BCL:HBC2	5:M:1304:BCL:H2C	1.53	0.46
3:M:232:GLU:OE1	3:M:232:GLU:N	2.41	0.46
9:M:1309:U10:H28	9:M:1309:U10:H322	1.46	0.46
2:L:233:GLY:O	2:L:234:LEU:C	2.57	0.46
5:L:1282:BCL:CBB	5:L:1282:BCL:CMB	2.94	0.46
3:M:135:LEU:HD23	3:M:135:LEU:HA	1.78	0.46
1:H:35:ASN:ND2	3:M:261:THR:H	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:GLU:O	1:H:233:ILE:HD12	2.15	0.46
2:L:50:ALA:O	2:L:53:ALA:HB3	2.15	0.45
2:L:156:TRP:O	2:L:157:VAL:C	2.58	0.45
1:H:245:ALA:N	1:H:246:PRO:CD	2.79	0.45
2:L:113:ILE:HG21	3:M:226:VAL:HG12	1.98	0.45
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.98	0.45
6:M:1307:BPB:HBAA	6:M:1307:BPB:H44	1.42	0.45
2:L:235:LEU:HD12	2:L:235:LEU:HA	1.72	0.45
3:M:2:GLU:HG3	3:M:4:GLN:NE2	2.30	0.45
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.51	0.45
3:M:53:GLY:O	3:M:54:SER:C	2.59	0.45
3:M:25:ASN:HD21	3:M:27:ALA:H	1.57	0.45
2:L:55:LEU:HD13	2:L:81:ALA:HB2	1.99	0.45
3:M:25:ASN:ND2	3:M:27:ALA:N	2.51	0.45
3:M:15:PRO:O	3:M:16:ALA:C	2.57	0.45
2:L:171:PRO:HD2	2:L:259:TRP:CZ3	2.52	0.44
2:L:182:THR:HG22	2:L:236:LEU:CD1	2.45	0.44
5:L:1282:BCL:HMB1	5:L:1282:BCL:CBB	2.42	0.44
1:H:63:THR:HA	1:H:73:LEU:O	2.18	0.44
2:L:63:LEU:O	2:L:64:ILE:C	2.59	0.44
3:M:73:TRP:NE1	3:M:77:GLN:NE2	2.65	0.44
3:M:98:ALA:O	3:M:99:PRO:C	2.59	0.44
3:M:279:THR:O	3:M:280:GLY:C	2.59	0.44
2:L:28:PRO:O	3:M:254:TRP:HA	2.17	0.44
3:M:25:ASN:ND2	3:M:25:ASN:C	2.76	0.44
3:M:72:ILE:O	3:M:73:TRP:C	2.60	0.44
1:H:15:LEU:HA	1:H:15:LEU:HD22	1.71	0.44
1:H:181:VAL:O	1:H:188:THR:HA	2.17	0.44
3:M:73:TRP:O	3:M:74:PHE:C	2.58	0.44
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	2.00	0.44
1:H:119:ASP:OD1	1:H:226:THR:HG21	2.18	0.44
2:L:127:ALA:CB	5:L:1282:BCL:H43	2.48	0.44
2:L:176:ALA:HB2	2:L:243:PHE:HB3	2.00	0.44
5:M:1303:BCL:HMB1	5:M:1303:BCL:HBB2	2.00	0.44
1:H:173:GLU:OE1	1:H:177:ARG:NH1	2.51	0.44
2:L:183:ASN:OD1	3:M:213:ALA:HA	2.17	0.43
5:M:1303:BCL:CBB	5:M:1303:BCL:CMB	2.95	0.43
6:M:1307:BPB:H14A	6:M:1307:BPB:H10	2.00	0.43
2:L:265:TRP:CG	2:L:266:TRP:N	2.86	0.43
2:L:219:LEU:O	3:M:132:ARG:NH1	2.40	0.43
2:L:229:ILE:HG13	2:L:229:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:51:TYR:CD1	3:M:51:TYR:C	2.96	0.43
2:L:69:PRO:HG2	2:L:142:TRP:HB2	2.01	0.43
2:L:259:TRP:O	2:L:260:VAL:C	2.60	0.43
5:L:1282:BCL:HBB3	5:L:1282:BCL:CMB	2.42	0.43
2:L:51:TRP:O	2:L:52:SER:C	2.58	0.43
2:L:80:LEU:HD13	2:L:85:LEU:HD21	1.99	0.43
3:M:77:GLN:HB3	3:M:92:PHE:CD1	2.53	0.43
3:M:243:THR:O	3:M:247:ARG:HG2	2.18	0.43
2:L:3:LEU:HD23	2:L:3:LEU:HA	1.85	0.42
2:L:135:ARG:O	2:L:136:PRO:C	2.62	0.42
1:H:245:ALA:HB3	1:H:246:PRO:HD3	2.01	0.42
5:M:1303:BCL:H102	5:M:1304:BCL:C20	2.49	0.42
1:H:44:ASN:C	1:H:46:ASP:N	2.76	0.42
1:H:195:MET:HE3	1:H:195:MET:HB3	1.89	0.42
3:M:212:SER:O	3:M:213:ALA:C	2.57	0.42
5:M:1303:BCL:H141	8:M:1308:SPN:HM43	2.02	0.42
8:M:1308:SPN:HMA3	8:M:1308:SPN:C3	2.50	0.42
1:H:29:TYR:O	1:H:30:TYR:C	2.62	0.42
1:H:147:ASN:OD1	1:H:149:ILE:N	2.52	0.42
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.51	0.42
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.55	0.42
2:L:219:LEU:HA	3:M:132:ARG:HH12	1.85	0.42
5:L:1283:BCL:H3A	5:L:1283:BCL:HBA1	1.72	0.42
1:H:20:PHE:CE1	3:M:279:THR:HG22	2.55	0.42
5:L:1282:BCL:OBB	5:L:1282:BCL:HHC	2.20	0.42
6:L:1284:BPB:HBB	3:M:210:TYR:CD2	2.55	0.42
5:M:1303:BCL:H141	5:M:1303:BCL:H162	1.85	0.42
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.85	0.42
3:M:280:GLY:O	5:M:1304:BCL:HED3	2.20	0.42
2:L:222:TYR:CG	2:L:223:SER:N	2.87	0.41
3:M:228:ARG:H	3:M:228:ARG:HG2	1.72	0.41
1:H:124:ASP:OD2	1:H:128:HIS:HB2	2.20	0.41
1:H:143:SER:OG	3:M:13:ARG:HB2	2.20	0.41
1:H:117:ARG:O	1:H:228:LEU:HB2	2.20	0.41
6:L:1284:BPB:ND	6:L:1284:BPB:NC	2.68	0.41
6:M:1307:BPB:H6	6:M:1307:BPB:H9A	1.63	0.41
1:H:77:GLY:O	1:H:78:PRO:C	2.61	0.41
3:M:183:LEU:HA	3:M:183:LEU:HD23	1.84	0.41
3:M:204:LEU:O	3:M:205:SER:C	2.62	0.41
1:H:60:LYS:HA	1:H:61:PRO:HD3	1.89	0.41
5:L:1282:BCL:H2C	5:L:1282:BCL:HBC2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:73:TRP:HE1	3:M:77:GLN:HE22	1.69	0.41
3:M:206:ILE:CG2	3:M:210:TYR:CE2	3.04	0.41
1:H:48:THR:HA	1:H:49:PRO:HD3	1.91	0.41
3:M:12:VAL:O	3:M:12:VAL:HG12	2.21	0.41
3:M:32:VAL:HG22	3:M:49:PRO:HD3	2.02	0.41
1:H:134:MET:O	1:H:135:LYS:C	2.64	0.41
2:L:97:PHE:CE1	5:L:1282:BCL:H121	2.56	0.41
2:L:150:ILE:N	2:L:150:ILE:CD1	2.83	0.41
2:L:219:LEU:C	3:M:132:ARG:HH12	2.27	0.41
2:L:275:ILE:HA	2:L:276:PRO:HD3	1.87	0.41
5:M:1303:BCL:H111	5:M:1303:BCL:H91	1.34	0.41
1:H:111:PRO:O	3:M:247:ARG:NH1	2.53	0.41
1:H:183:LEU:O	1:H:184:LYS:C	2.62	0.41
2:L:50:ALA:O	2:L:51:TRP:C	2.64	0.41
2:L:255:TRP:CZ2	2:L:262:TRP:HB2	2.56	0.41
2:L:265:TRP:CD2	2:L:266:TRP:N	2.90	0.40
5:M:1304:BCL:H121	5:M:1304:BCL:H162	1.91	0.40
2:L:30:TYR:HB2	3:M:254:TRP:HB3	2.03	0.40
2:L:160:THR:HA	2:L:163:THR:CG2	2.51	0.40
3:M:99:PRO:O	3:M:100:GLU:C	2.64	0.40
1:H:201:ASN:C	1:H:201:ASN:OD1	2.63	0.40
2:L:135:ARG:HB3	2:L:136:PRO:CD	2.48	0.40
3:M:66:TRP:O	3:M:67:PHE:C	2.64	0.40
1:H:227:LEU:HA	1:H:227:LEU:HD23	1.76	0.40
1:H:89:ARG:HG2	11:H:2002:HOH:O	2.22	0.40
2:L:21:LEU:HD13	2:L:21:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/260 (92%)	221 (92%)	14 (6%)	4 (2%)	7	25
2	L	279/281 (99%)	251 (90%)	26 (9%)	2 (1%)	18	47
3	M	301/307 (98%)	267 (89%)	30 (10%)	4 (1%)	9	31
All	All	819/848 (97%)	739 (90%)	70 (8%)	10 (1%)	10	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
2	L	145	ALA
3	M	22	GLU
3	M	301	HIS
2	L	80	LEU
3	M	100	GLU
1	H	66	LEU
3	M	30	SER
1	H	202	ARG
1	H	211	ASP

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	H	195/208 (94%)	166 (85%)	29 (15%)	3	10
2	L	220/220 (100%)	196 (89%)	24 (11%)	6	21
3	M	236/240 (98%)	213 (90%)	23 (10%)	8	25
All	All	651/668 (98%)	575 (88%)	76 (12%)	5	18

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	15	LEU
1	H	28	ILE

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Mol	Chain	Res	Type
1	H	62	LYS
1	H	66	LEU
1	H	70	ARG
1	H	72	THR
1	H	73	LEU
1	H	80	SER
1	H	94	GLU
1	H	106	LYS
1	H	115	VAL
1	H	117	ARG
1	H	134	MET
1	H	143	SER
1	H	146	LYS
1	H	173	GLU
1	H	190	LEU
1	H	193	MET
1	H	194	GLN
1	H	200	SER
1	H	202	ARG
1	H	208	LEU
1	H	217	PRO
1	H	221	SER
1	H	225	VAL
1	H	231	ASP
1	H	237	VAL
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	44	LEU
2	L	46	ILE
2	L	54	VAL
2	L	58	THR
2	L	82	LYS
2	L	136	PRO
2	L	150	ILE
2	L	153	HIS
2	L	160	THR
2	L	163	THR
2	L	185	LEU
2	L	202	LYS
2	L	206	MET

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Mol	Chain	Res	Type
2	L	207	ARG
2	L	216	PHE
2	L	235	LEU
2	L	241	VAL
2	L	251	THR
2	L	269	LEU
2	L	271	TRP
2	L	279	ILE
3	M	12	VAL
3	M	25	ASN
3	M	50	ILE
3	M	52	LEU
3	M	55	LEU
3	M	62	SER
3	M	77	GLN
3	M	81	ASN
3	M	86	LEU
3	M	133	THR
3	M	136	ARG
3	M	154	ILE
3	M	166	ILE
3	M	179	ILE
3	M	196	LEU
3	M	199	ASN
3	M	204	LEU
3	M	214	LEU
3	M	247	ARG
3	M	262	MET
3	M	265	ILE
3	M	267	LEU
3	M	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	35	ASN
1	H	53	GLN
1	H	98	HIS
1	H	128	HIS
1	H	194	GLN
2	L	56	GLN

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Mol	Chain	Res	Type
2	L	280	ASN
3	M	4	GLN
3	M	11	GLN
3	M	25	ASN
3	M	28	ASN
3	M	44	ASN
3	M	77	GLN
3	M	193	HIS
3	M	199	ASN
3	M	299	GLN
3	M	300	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	SPN	M	1308	-	42,42,42	3.71	18 (42%)	50,52,52	2.09	16 (32%)
5	BCL	L	1283	2	69,74,74	1.23	7 (10%)	79,115,115	2.12	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	L	1282	2	69,74,74	1.25	5 (7%)	79,115,115	1.77	21 (26%)
5	BCL	M	1304	3	69,74,74	1.30	5 (7%)	79,115,115	1.93	21 (26%)
4	LDA	H	1251	-	13,15,15	2.20	1 (7%)	14,17,17	3.26	3 (21%)
4	LDA	M	1305	-	13,15,15	2.63	1 (7%)	14,17,17	1.70	3 (21%)
10	PO4	M	1310	-	4,4,4	0.84	0	6,6,6	0.84	0
6	BPB	L	1284	-	57,70,70	1.51	7 (12%)	55,101,101	2.42	18 (32%)
6	BPB	M	1307	-	57,70,70	1.05	3 (5%)	55,101,101	2.67	17 (30%)
9	U10	M	1309	-	48,48,63	1.66	3 (6%)	60,61,79	1.81	14 (23%)
5	BCL	M	1303	3	69,74,74	1.09	3 (4%)	79,115,115	1.96	27 (34%)

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	SPN	M	1308	-	-	20/50/51/51	-
5	BCL	L	1283	2	-	7/41/137/137	-
5	BCL	L	1282	2	-	8/41/137/137	-
5	BCL	M	1304	3	-	8/41/137/137	-
4	LDA	H	1251	-	-	2/13/13/13	-
4	LDA	M	1305	-	-	8/13/13/13	-
6	BPB	L	1284	-	-	8/37/105/105	0/5/6/6
6	BPB	M	1307	-	-	20/37/105/105	0/5/6/6
9	U10	M	1309	-	-	8/45/69/87	0/1/1/1
5	BCL	M	1303	3	-	11/41/137/137	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1305	LDA	O1-N1	-9.24	1.19	1.42
8	M	1308	SPN	C3-C4	-8.63	1.37	1.50
8	M	1308	SPN	C10-C9	-8.30	1.34	1.51
8	M	1308	SPN	C17-C18	-7.80	1.35	1.51
4	H	1251	LDA	O1-N1	-7.79	1.23	1.42
8	M	1308	SPN	C6-C5	-7.32	1.36	1.51
5	M	1304	BCL	MG-NA	7.24	2.23	2.06
8	M	1308	SPN	C14-C13	-7.24	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1309	U10	C36-C34	-6.79	1.37	1.51
9	M	1309	U10	C6-C1	6.56	1.47	1.35
5	L	1282	BCL	MG-NA	6.52	2.21	2.06
8	M	1308	SPN	C4-C5	6.40	1.47	1.33
8	M	1308	SPN	C8-C9	6.25	1.47	1.33
8	M	1308	SPN	C19-C18	6.10	1.47	1.33
6	L	1284	BPB	C1B-C2B	5.71	1.45	1.39
5	L	1283	BCL	MG-NC	-5.24	1.93	2.06
8	M	1308	SPN	C20-C19	-5.06	1.35	1.50
8	M	1308	SPN	C12-C13	5.05	1.44	1.33
8	M	1308	SPN	C11-C12	-5.02	1.35	1.50
6	L	1284	BPB	C1D-C2D	4.73	1.44	1.39
8	M	1308	SPN	C7-C8	-4.51	1.36	1.50
5	M	1303	BCL	MG-NA	4.39	2.16	2.06
6	M	1307	BPB	C1B-C2B	3.80	1.43	1.39
6	L	1284	BPB	OBD-CAD	3.71	1.27	1.22
8	M	1308	SPN	C21-C22	-3.43	1.36	1.52
6	L	1284	BPB	C1-C2	3.37	1.58	1.49
6	M	1307	BPB	C1D-C2D	3.33	1.43	1.39
5	L	1282	BCL	MG-NC	3.19	2.13	2.06
8	M	1308	SPN	C1-C2	-3.13	1.50	1.53
9	M	1309	U10	C4-C3	3.06	1.47	1.36
5	L	1283	BCL	CMD-C2D	-3.06	1.44	1.50
8	M	1308	SPN	C16-C15	-2.85	1.37	1.51
5	M	1303	BCL	C3D-C4D	-2.85	1.37	1.44
5	L	1283	BCL	MG-NB	2.84	2.11	2.05
5	L	1282	BCL	MG-ND	2.75	2.11	2.05
6	M	1307	BPB	C4D-ND	-2.66	1.34	1.38
6	L	1284	BPB	C3D-CAD	-2.50	1.43	1.47
5	L	1283	BCL	C3C-C4C	-2.44	1.48	1.51
6	L	1284	BPB	C4C-C3C	2.42	1.53	1.45
5	M	1304	BCL	CBA-CGA	-2.33	1.43	1.50
5	L	1283	BCL	CHC-C1C	2.29	1.43	1.37
5	M	1304	BCL	CHC-C1C	2.29	1.43	1.37
5	L	1283	BCL	C3B-C4B	2.26	1.45	1.41
5	L	1282	BCL	O2D-CGD	2.24	1.38	1.33
5	M	1303	BCL	C1-C2	2.20	1.55	1.49
6	L	1284	BPB	C3A-C2A	-2.14	1.52	1.54
5	L	1283	BCL	C1B-C2B	2.08	1.48	1.43
5	M	1304	BCL	C3C-C4C	-2.07	1.49	1.51
5	L	1282	BCL	CHC-C1C	2.05	1.42	1.37
8	M	1308	SPN	C21-C20	-2.04	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1308	SPN	C6-C7	-2.03	1.47	1.53
8	M	1308	SPN	C10-C11	-2.03	1.47	1.53
5	M	1304	BCL	C3B-C4B	2.01	1.45	1.41

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1307	BPB	C1-C2-C3	-8.90	111.62	126.20
6	L	1284	BPB	O2D-CGD-CBD	8.25	120.01	110.95
4	H	1251	LDA	CM2-N1-C1	-7.97	93.50	110.23
6	M	1307	BPB	O2D-CGD-CBD	7.80	119.52	110.95
4	H	1251	LDA	CM1-N1-C1	-7.59	94.28	110.23
5	L	1283	BCL	C4D-CHA-C1A	6.65	129.18	121.24
6	L	1284	BPB	C4D-CHA-CBD	-6.65	105.27	108.45
6	M	1307	BPB	C4D-CHA-CBD	-5.94	105.61	108.45
5	L	1283	BCL	C2B-C1B-NB	-5.64	104.48	110.33
6	M	1307	BPB	CMA-C3A-C4A	-5.64	102.46	114.61
5	M	1304	BCL	O2D-CGD-CBD	5.55	120.93	111.23
5	M	1303	BCL	C11-C12-C13	-5.52	97.62	115.97
5	L	1283	BCL	C1C-NC-C4C	5.32	109.11	106.68
5	L	1282	BCL	CAA-C2A-C3A	-5.28	98.73	113.00
9	M	1309	U10	C30-C29-C31	5.15	124.17	115.23
5	L	1282	BCL	C2B-C1B-NB	-5.08	105.06	110.33
6	M	1307	BPB	C2B-C1B-NB	-5.05	105.78	109.43
8	M	1308	SPN	C7-C6-C5	5.00	129.74	113.19
8	M	1308	SPN	CM5-C13-C14	4.84	123.63	115.23
5	M	1304	BCL	O2D-CGD-O1D	-4.83	114.45	123.85
5	M	1304	BCL	C4D-CHA-C1A	4.75	126.91	121.24
5	L	1283	BCL	CHD-C1D-ND	-4.65	118.26	124.80
4	H	1251	LDA	O1-N1-C1	-4.63	97.93	109.27
6	L	1284	BPB	CMA-C3A-C4A	-4.48	104.95	114.61
8	M	1308	SPN	C15-C14-C13	4.44	124.29	113.47
6	L	1284	BPB	C2B-C1B-NB	-4.29	106.33	109.43
6	M	1307	BPB	C1-O2A-CGA	4.21	126.84	116.65
5	M	1303	BCL	C2B-C1B-NB	-4.20	105.97	110.33
9	M	1309	U10	C37-C36-C34	4.19	127.06	113.19
6	M	1307	BPB	C6-C5-C3	-4.17	103.30	113.47
5	M	1304	BCL	C7-C6-C5	-4.08	102.40	113.26
8	M	1308	SPN	CM6-C18-C17	3.93	122.05	115.23
9	M	1309	U10	C17-C18-C19	-3.93	118.64	127.62
5	M	1303	BCL	C4D-CHA-C1A	3.92	125.92	121.24
5	L	1283	BCL	CAC-C3C-C4C	-3.92	103.89	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CMB-C2B-C1B	-3.89	119.49	125.42
5	L	1283	BCL	CMB-C2B-C1B	-3.88	119.52	125.42
8	M	1308	SPN	CM7-C22-C21	3.86	125.03	111.27
8	M	1308	SPN	CM3-C5-C6	3.84	121.90	115.23
4	M	1305	LDA	CM1-N1-C1	-3.78	102.30	110.23
5	M	1304	BCL	C11-C10-C8	-3.71	103.64	115.97
4	M	1305	LDA	CM2-N1-C1	3.66	117.92	110.23
5	M	1303	BCL	CAA-C2A-C3A	-3.62	103.22	113.00
5	L	1283	BCL	CAA-C2A-C3A	-3.61	103.25	113.00
5	L	1283	BCL	O2D-CGD-CBD	3.60	117.52	111.23
5	M	1304	BCL	C1C-NC-C4C	3.60	108.32	106.68
6	L	1284	BPB	C7-C6-C5	-3.59	103.69	113.26
5	M	1303	BCL	C16-C15-C13	-3.57	104.10	115.97
6	L	1284	BPB	OBB-CAB-CBB	-3.56	112.60	120.19
5	L	1282	BCL	CED-O2D-CGD	3.55	123.96	115.92
5	M	1304	BCL	CHA-C1A-NA	-3.52	118.43	126.39
5	L	1282	BCL	CMA-C3A-C2A	-3.52	100.39	113.98
5	L	1283	BCL	CHC-C1C-NC	3.49	129.44	124.40
6	L	1284	BPB	C2D-C1D-ND	-3.48	106.92	109.43
5	M	1303	BCL	CHB-C1B-NB	3.46	129.25	124.05
5	L	1282	BCL	C3B-C4B-NB	-3.43	105.23	109.76
9	M	1309	U10	C35-C34-C36	3.42	121.16	115.23
6	M	1307	BPB	C2D-C1D-ND	-3.37	107.00	109.43
6	L	1284	BPB	CAA-C2A-C3A	-3.37	103.90	113.00
5	M	1303	BCL	O2A-C1-C2	3.36	121.03	108.11
5	M	1304	BCL	C2B-C1B-NB	-3.32	106.88	110.33
5	L	1282	BCL	C11-C12-C13	-3.31	104.97	115.97
9	M	1309	U10	C32-C33-C34	-3.28	120.11	127.62
5	M	1304	BCL	OBB-CAB-C3B	-3.27	114.66	120.43
6	M	1307	BPB	C5-C3-C2	3.26	128.48	121.17
5	M	1304	BCL	CGD-CBD-CAD	-3.26	100.30	110.85
6	M	1307	BPB	CMB-C2B-C3B	3.26	131.19	124.68
6	L	1284	BPB	O2A-CGA-O1A	-3.21	115.60	123.63
5	L	1283	BCL	C3C-C4C-CHD	-3.20	116.64	123.39
5	L	1283	BCL	CHB-C1B-NB	3.17	128.81	124.05
9	M	1309	U10	C26-C27-C28	-3.16	96.37	112.02
5	M	1303	BCL	CMD-C2D-C1D	3.16	130.30	124.73
8	M	1308	SPN	C16-C15-C14	3.16	124.75	113.13
5	M	1304	BCL	C3B-C4B-NB	-3.16	105.59	109.76
6	L	1284	BPB	CMA-C3A-C2A	-3.12	102.08	114.13
5	L	1283	BCL	CHD-C1D-C2D	3.11	131.95	125.49
6	M	1307	BPB	CAA-C2A-C3A	-3.11	104.61	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1309	U10	C22-C23-C24	-3.09	120.55	127.62
5	L	1283	BCL	CAA-CBA-CGA	3.08	121.94	113.21
5	L	1282	BCL	C4D-CHA-C1A	3.06	124.90	121.24
5	M	1303	BCL	C16-C17-C18	-3.06	102.29	115.94
9	M	1309	U10	C4M-O4-C4	3.04	127.16	116.47
5	M	1304	BCL	C1-C2-C3	-3.03	121.23	126.20
5	L	1282	BCL	O2A-CGA-O1A	-2.99	116.16	123.63
5	L	1282	BCL	CHC-C4B-NB	2.97	128.51	124.05
6	L	1284	BPB	C3D-CAD-CBD	-2.97	103.69	107.61
5	M	1303	BCL	O2D-CGD-CBD	2.96	116.41	111.23
6	L	1284	BPB	CBB-CAB-C3B	2.95	129.17	120.34
5	M	1304	BCL	C1D-ND-C4D	2.95	108.38	106.31
5	M	1304	BCL	CBB-CAB-C3B	2.93	126.58	120.40
5	L	1283	BCL	C1D-CHD-C4C	-2.90	119.63	126.62
4	M	1305	LDA	O1-N1-C1	-2.90	102.16	109.27
5	M	1303	BCL	C11-C10-C8	-2.85	106.50	115.97
5	M	1303	BCL	C1C-NC-C4C	-2.85	105.38	106.68
5	M	1303	BCL	CHD-C1D-C2D	2.84	131.40	125.49
5	M	1303	BCL	CMA-C3A-C2A	-2.83	103.03	113.98
8	M	1308	SPN	C16-C17-C18	2.82	120.33	113.47
5	M	1304	BCL	CHB-C1B-NB	2.82	128.27	124.05
5	M	1303	BCL	C3B-C4B-NB	-2.82	106.04	109.76
6	L	1284	BPB	OBD-CAD-C3D	2.81	132.27	127.89
5	M	1303	BCL	C1D-ND-C4D	2.79	108.27	106.31
5	L	1282	BCL	CBA-CAA-C2A	2.79	122.09	113.79
6	M	1307	BPB	C4-C3-C2	-2.78	116.48	123.63
8	M	1308	SPN	CM7-C22-C23	2.78	121.18	111.27
9	M	1309	U10	C27-C28-C29	-2.78	121.27	127.62
5	M	1304	BCL	CAA-C2A-C3A	-2.77	105.51	113.00
5	M	1303	BCL	CHA-C1A-NA	-2.76	120.13	126.39
5	M	1303	BCL	CHD-C1D-ND	-2.76	120.92	124.80
6	M	1307	BPB	O2A-C1-C2	-2.74	97.57	108.11
5	M	1304	BCL	CHD-C1D-ND	-2.71	120.99	124.80
6	M	1307	BPB	O2D-CGD-O1D	-2.69	118.62	123.85
6	M	1307	BPB	C4B-NB-C1B	2.66	112.70	108.82
5	M	1304	BCL	C11-C12-C13	-2.63	107.21	115.97
5	L	1283	BCL	C1D-ND-C4D	-2.61	104.48	106.31
5	L	1283	BCL	O1D-CGD-CBD	-2.60	119.40	124.52
5	L	1282	BCL	OBB-CAB-C3B	2.59	125.01	120.43
8	M	1308	SPN	C15-C16-C17	2.58	122.60	113.13
5	L	1283	BCL	C6-C5-C3	-2.57	107.20	113.47
5	M	1304	BCL	CMD-C2D-C1D	2.57	129.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1309	U10	C35-C34-C33	-2.57	117.03	123.63
5	M	1303	BCL	OB B-CAB-C3B	2.56	124.96	120.43
6	L	1284	BPB	O1D-CGD-CBD	-2.55	120.85	124.72
5	L	1282	BCL	C1-O2A-CGA	2.54	122.80	116.65
5	L	1282	BCL	CHA-C1A-NA	-2.51	120.71	126.39
5	L	1283	BCL	C4-C3-C5	2.50	119.57	115.23
5	M	1303	BCL	C2D-C1D-ND	-2.49	107.66	110.13
6	L	1284	BPB	C4B-NB-C1B	2.48	112.44	108.82
6	M	1307	BPB	CMA-C3A-C2A	-2.47	104.58	114.13
6	L	1284	BPB	O2D-CGD-O1D	-2.47	119.04	123.85
5	M	1304	BCL	CHD-C1D-C2D	2.45	130.59	125.49
9	M	1309	U10	C1M-C1-C6	-2.43	120.45	124.45
5	M	1303	BCL	O2D-CGD-O1D	-2.43	119.11	123.85
8	M	1308	SPN	O1-C1-C2	2.43	113.87	108.90
8	M	1308	SPN	C20-C21-C22	2.39	127.29	114.56
9	M	1309	U10	O5-C5-C6	-2.38	117.18	121.79
6	L	1284	BPB	C16-C15-C13	-2.36	108.12	115.97
5	L	1282	BCL	C17-C16-C15	-2.35	102.75	113.28
5	L	1282	BCL	C4-C3-C5	2.35	119.30	115.23
5	M	1303	BCL	CBB-CAB-C3B	-2.33	115.49	120.40
8	M	1308	SPN	CM8-C26-C27	2.30	119.23	115.23
5	L	1282	BCL	C1-C2-C3	-2.29	122.44	126.20
5	M	1303	BCL	CMA-C3A-C4A	-2.28	105.65	111.77
5	L	1282	BCL	C2D-C1D-ND	-2.28	107.87	110.13
5	L	1283	BCL	C2C-C3C-C4C	2.28	104.75	101.34
5	M	1304	BCL	C2C-C3C-C4C	2.27	104.74	101.34
5	M	1303	BCL	CBA-CAA-C2A	-2.26	107.08	113.79
9	M	1309	U10	C20-C19-C18	-2.25	117.85	123.63
5	M	1303	BCL	C2C-C3C-C4C	2.25	104.71	101.34
6	L	1284	BPB	C11-C10-C8	-2.25	108.50	115.97
8	M	1308	SPN	CM2-C1-C2	-2.24	104.75	109.43
5	L	1282	BCL	O1D-CGD-CBD	-2.22	120.14	124.52
5	L	1283	BCL	CMC-C2C-C3C	-2.21	105.43	113.98
6	M	1307	BPB	C6-C7-C8	-2.20	108.67	115.97
5	L	1283	BCL	C5-C3-C2	-2.20	116.24	121.17
8	M	1308	SPN	C23-C24-C25	-2.17	106.47	112.16
9	M	1309	U10	C7-C8-C9	-2.14	123.14	126.83
5	L	1282	BCL	C1D-ND-C4D	2.13	107.80	106.31
5	L	1282	BCL	O2A-CGA-CBA	2.12	118.31	111.83
8	M	1308	SPN	CM5-C13-C12	-2.11	118.22	123.63
5	L	1283	BCL	C3B-C4B-NB	-2.09	107.00	109.76
5	M	1303	BCL	CMB-C2B-C3B	2.06	132.17	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C2A-C3A-C4A	2.05	105.18	101.87
5	L	1283	BCL	CMA-C3A-C4A	-2.02	106.34	111.77
5	L	1283	BCL	C3D-C4D-ND	2.01	113.26	109.99

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1305	LDA	C2-C1-N1-CM1
4	M	1305	LDA	N1-C1-C2-C3
5	L	1283	BCL	CHA-CBD-CGD-O1D
5	L	1283	BCL	CHA-CBD-CGD-O2D
5	L	1283	BCL	C11-C12-C13-C14
5	M	1303	BCL	C4C-C3C-CAC-CBC
5	M	1304	BCL	C2C-C3C-CAC-CBC
5	M	1304	BCL	C4C-C3C-CAC-CBC
6	L	1284	BPB	C2C-C3C-CAC-CBC
6	M	1307	BPB	C2C-C3C-CAC-CBC
6	M	1307	BPB	C4C-C3C-CAC-CBC
8	M	1308	SPN	C20-C21-C22-CM7
6	M	1307	BPB	C4-C3-C5-C6
6	M	1307	BPB	C2-C3-C5-C6
8	M	1308	SPN	C14-C15-C16-C17
8	M	1308	SPN	CM3-C5-C6-C7
8	M	1308	SPN	C11-C10-C9-CM4
8	M	1308	SPN	CM5-C13-C14-C15
8	M	1308	SPN	C16-C17-C18-CM6
8	M	1308	SPN	C4-C5-C6-C7
8	M	1308	SPN	C11-C10-C9-C8
8	M	1308	SPN	C12-C13-C14-C15
8	M	1308	SPN	C16-C17-C18-C19
5	L	1282	BCL	C14-C13-C15-C16
5	M	1303	BCL	C11-C10-C8-C9
6	M	1307	BPB	C11-C12-C13-C14
5	M	1304	BCL	C6-C7-C8-C10
6	M	1307	BPB	C11-C10-C8-C7
6	M	1307	BPB	C12-C13-C15-C16
9	M	1309	U10	C29-C31-C32-C33
5	M	1303	BCL	C8-C10-C11-C12
5	M	1304	BCL	C15-C16-C17-C18
6	M	1307	BPB	C15-C16-C17-C18
5	M	1303	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	M	1308	SPN	CM6-C18-C19-C20
9	M	1309	U10	C34-C36-C37-C38
6	M	1307	BPB	C16-C17-C18-C19
6	M	1307	BPB	C8-C10-C11-C12
4	H	1251	LDA	C1-C2-C3-C4
4	M	1305	LDA	C3-C4-C5-C6
5	L	1282	BCL	C16-C17-C18-C20
6	M	1307	BPB	C16-C17-C18-C20
6	M	1307	BPB	C5-C6-C7-C8
5	L	1282	BCL	C12-C13-C15-C16
9	M	1309	U10	C23-C24-C26-C27
5	M	1303	BCL	C11-C12-C13-C14
9	M	1309	U10	C24-C26-C27-C28
9	M	1309	U10	C25-C24-C26-C27
6	L	1284	BPB	O2A-C1-C2-C3
6	L	1284	BPB	C4-C3-C5-C6
4	M	1305	LDA	C11-C10-C9-C8
5	L	1282	BCL	C11-C12-C13-C15
5	M	1303	BCL	C11-C12-C13-C15
5	M	1304	BCL	C13-C15-C16-C17
4	M	1305	LDA	C5-C6-C7-C8
6	M	1307	BPB	C3A-C2A-CAA-CBA
6	M	1307	BPB	C1A-C2A-CAA-CBA
5	L	1282	BCL	C16-C17-C18-C19
6	L	1284	BPB	C2-C3-C5-C6
6	M	1307	BPB	C14-C13-C15-C16
9	M	1309	U10	C14-C16-C17-C18
8	M	1308	SPN	O1-C1-C2-O2
8	M	1308	SPN	C21-C22-C23-C24
6	M	1307	BPB	C3-C5-C6-C7
5	M	1304	BCL	C16-C17-C18-C19
6	L	1284	BPB	C16-C17-C18-C19
4	M	1305	LDA	C2-C1-N1-CM2
4	H	1251	LDA	C2-C3-C4-C5
5	M	1303	BCL	C3A-C2A-CAA-CBA
5	L	1282	BCL	C11-C12-C13-C14
6	M	1307	BPB	C6-C7-C8-C9
4	M	1305	LDA	C2-C1-N1-O1
5	M	1303	BCL	C5-C6-C7-C8
5	M	1304	BCL	C16-C17-C18-C20
8	M	1308	SPN	C3-C4-C5-CM3
5	L	1283	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	M	1304	BCL	C12-C13-C15-C16
8	M	1308	SPN	CM2-C1-C2-C3
6	L	1284	BPB	C6-C7-C8-C9
6	M	1307	BPB	C11-C10-C8-C9
8	M	1308	SPN	CM8-C26-C27-C28
5	L	1283	BCL	C11-C12-C13-C15
6	M	1307	BPB	C11-C12-C13-C15
9	M	1309	U10	C5-C4-O4-C4M
9	M	1309	U10	C35-C34-C36-C37
6	L	1284	BPB	C13-C15-C16-C17
5	M	1303	BCL	C3-C5-C6-C7
5	L	1283	BCL	C13-C15-C16-C17
5	L	1282	BCL	C6-C7-C8-C9
5	M	1303	BCL	C13-C15-C16-C17
6	M	1307	BPB	C13-C15-C16-C17
5	L	1283	BCL	C11-C10-C8-C9
6	L	1284	BPB	C14-C13-C15-C16
8	M	1308	SPN	C10-C11-C12-C13
8	M	1308	SPN	C17-C18-C19-C20
8	M	1308	SPN	C18-C19-C20-C21
8	M	1308	SPN	CM2-C1-C2-O2
4	M	1305	LDA	C9-C10-C11-C12
5	L	1282	BCL	CAD-CBD-CGD-O2D
5	M	1303	BCL	CAD-CBD-CGD-O2D

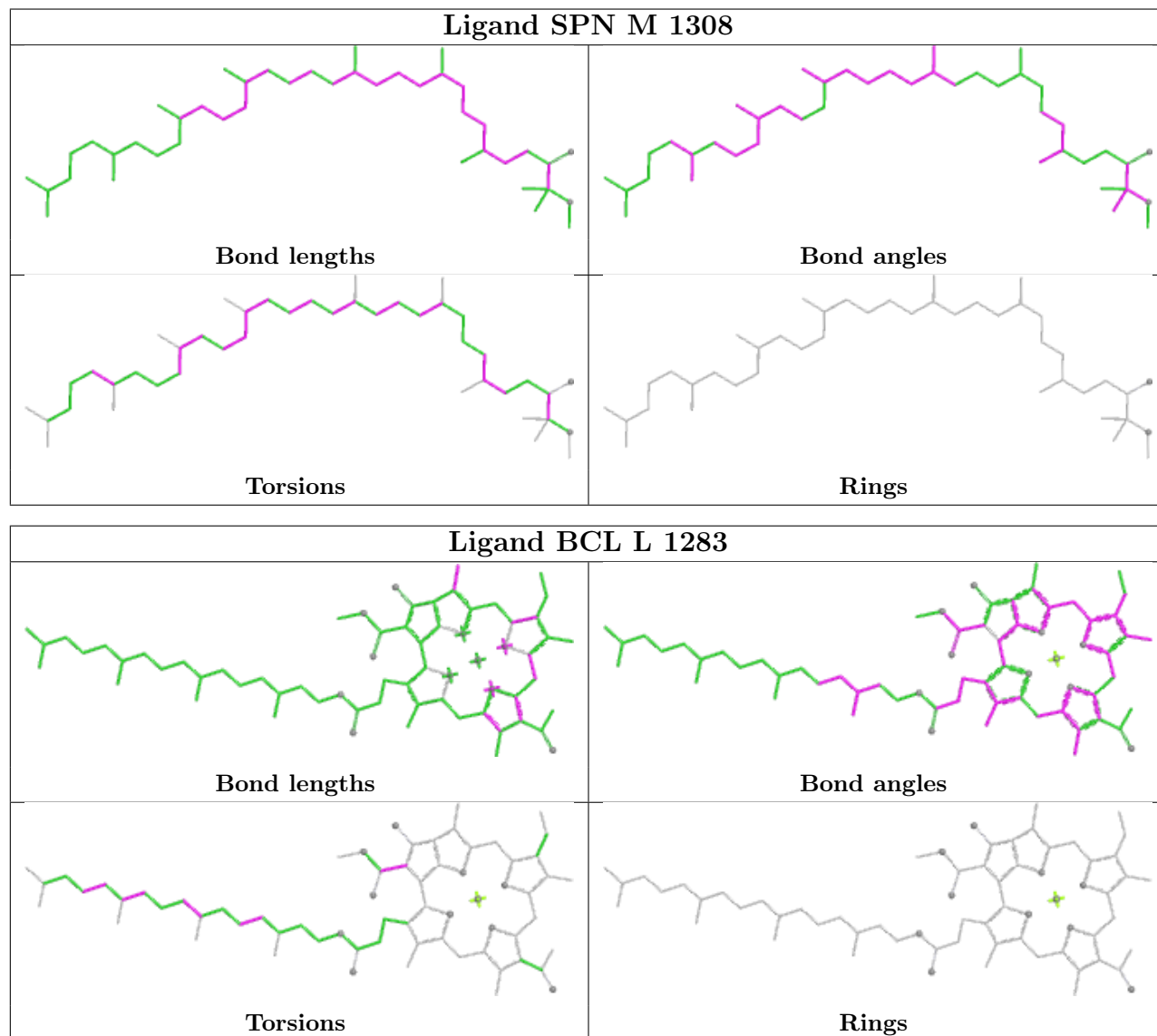
There are no ring outliers.

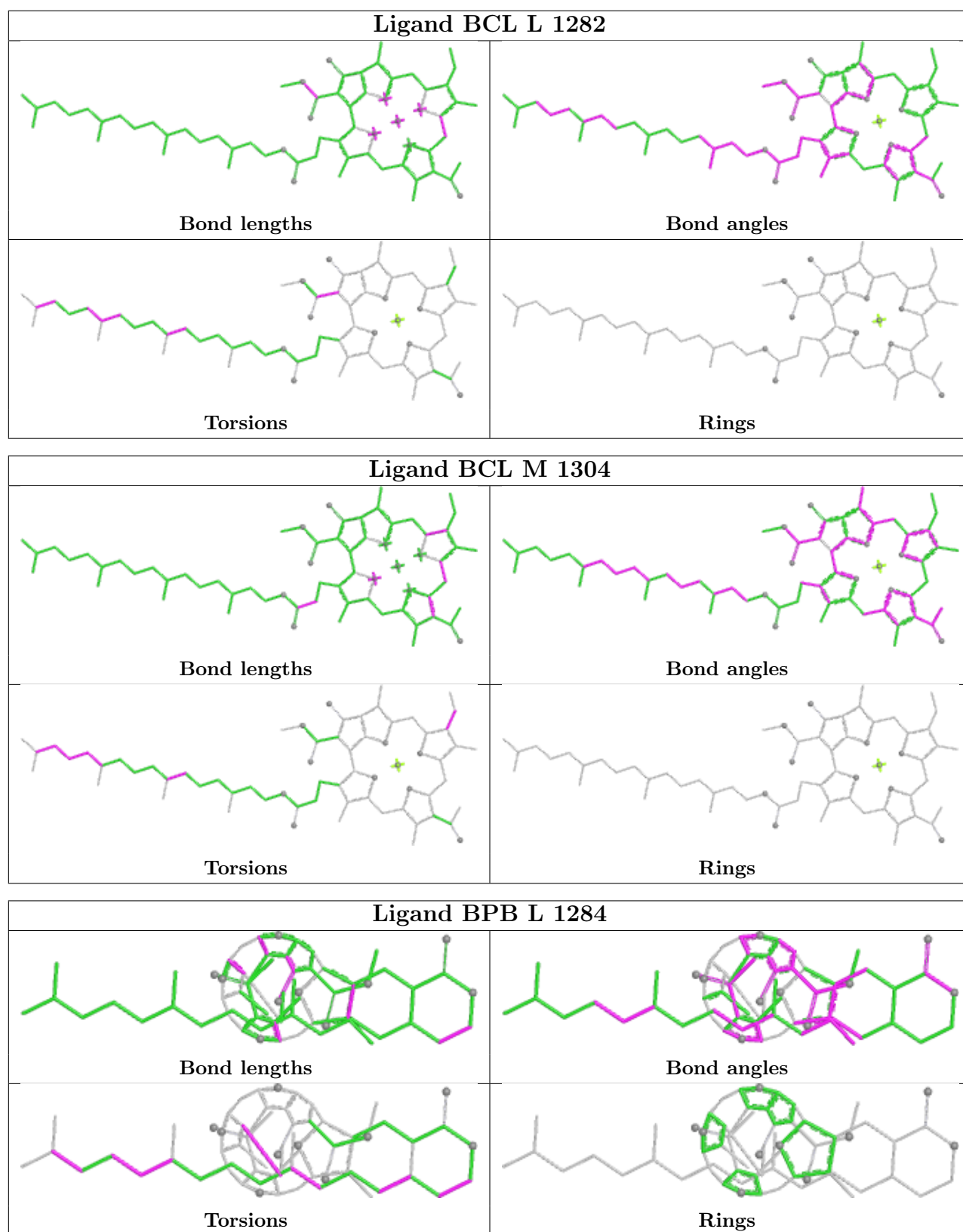
10 monomers are involved in 63 short contacts:

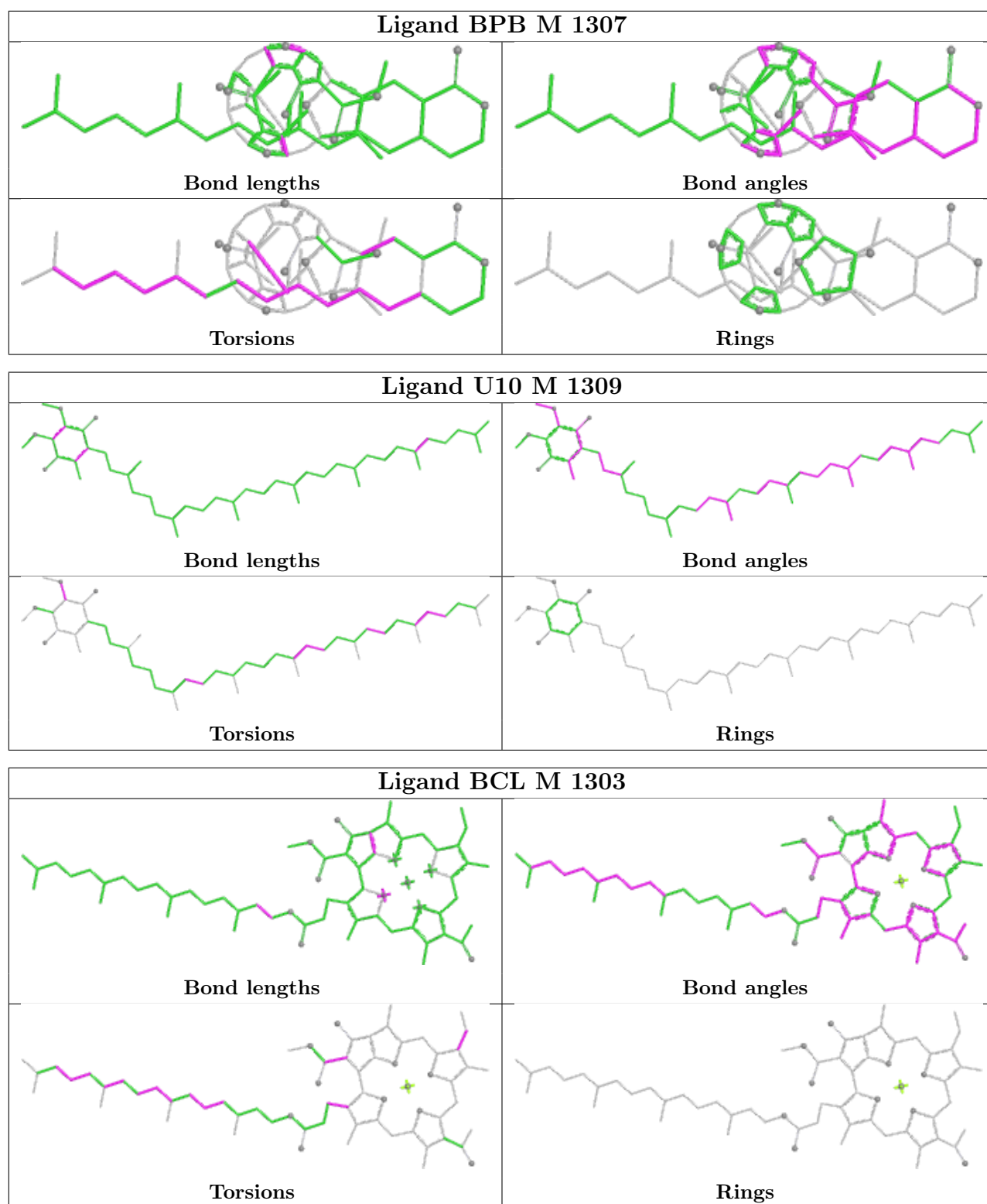
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1308	SPN	8	0
5	L	1283	BCL	2	0
5	L	1282	BCL	10	0
5	M	1304	BCL	15	0
4	H	1251	LDA	4	0
4	M	1305	LDA	5	0
6	L	1284	BPB	6	0
6	M	1307	BPB	11	0
9	M	1309	U10	2	0
5	M	1303	BCL	20	0

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.







5.7 Other polymers [i](#)

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.