



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:02 AM UTC

PDB ID : 1E14 / pdb_00001e14
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197 REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 REPLACED WITH ASP (CHAIN M, GM203D)
Authors : Fyfe, P.K.; Ridge, J.P.; McAuley, K.E.; Cogdell, R.J.; Isaacs, N.W.; Jones, M.R.
Deposited on : 2000-04-18
Resolution : 2.70 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

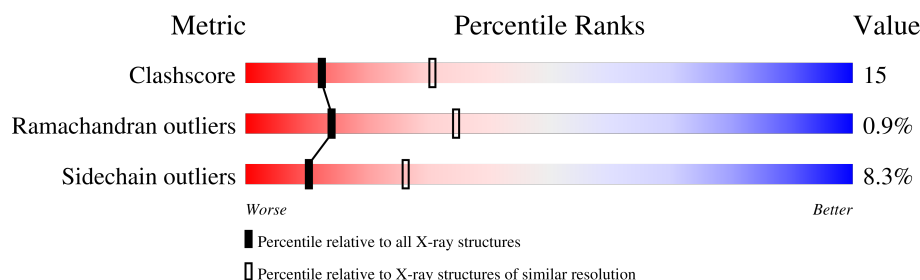
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	M	1301	X	-	-	-
6	BPH	L	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SPN	M	600	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7250 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	0	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	0	0	0
			2232	1507	355	362	8			

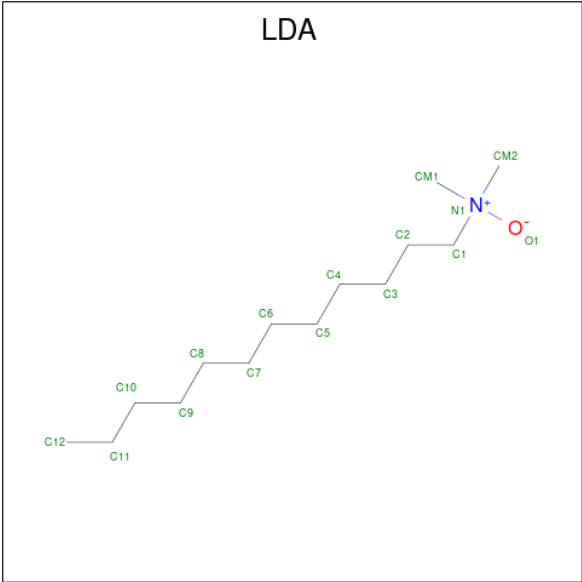
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2413	1606	398	399	10			

There are 2 discrepancies between the modelled and reference sequences:

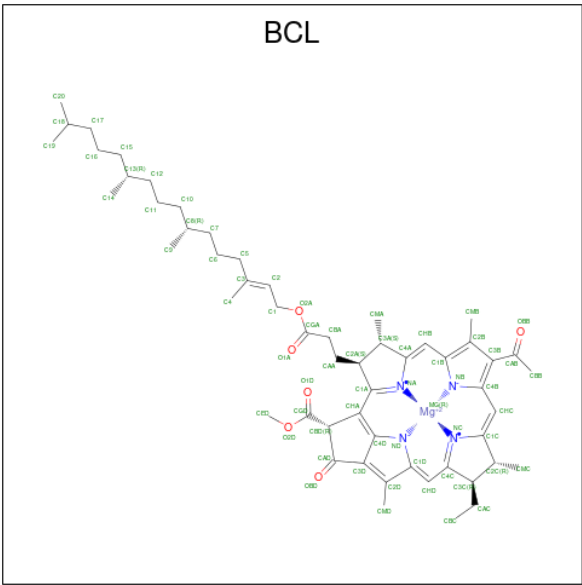
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	conflict	UNP P0C0Y9
M	203	ASP	GLY	conflict	UNP P0C0Y9

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



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

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



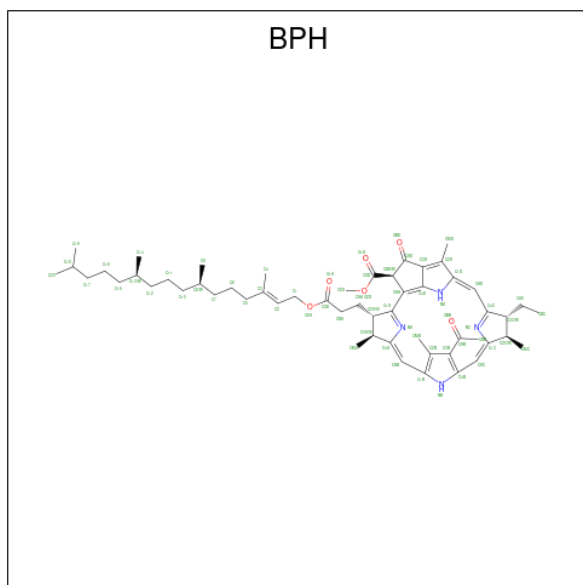
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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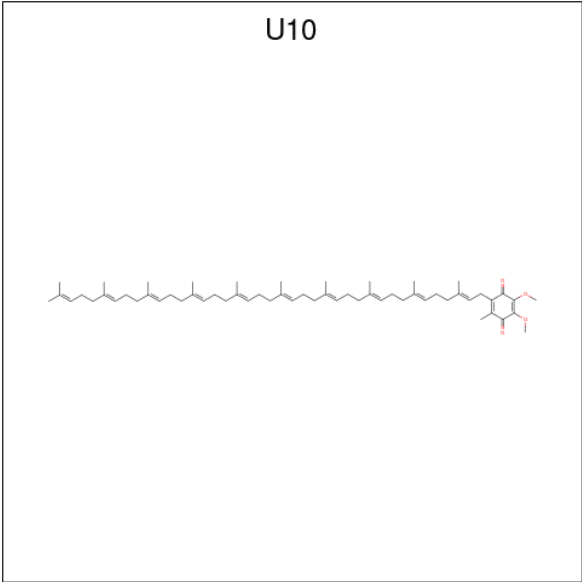
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

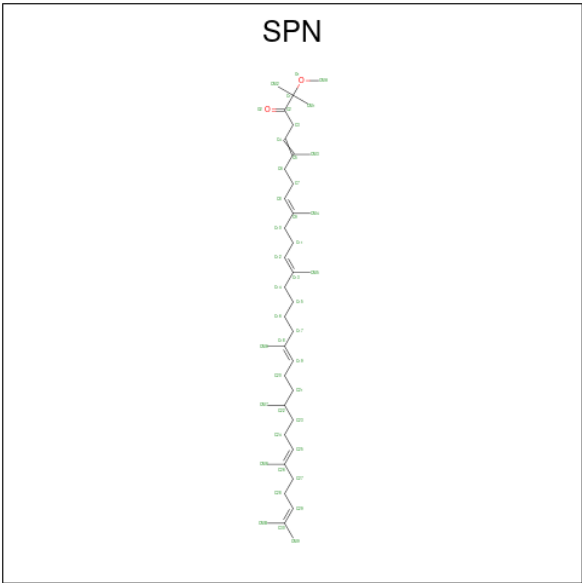


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	22	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

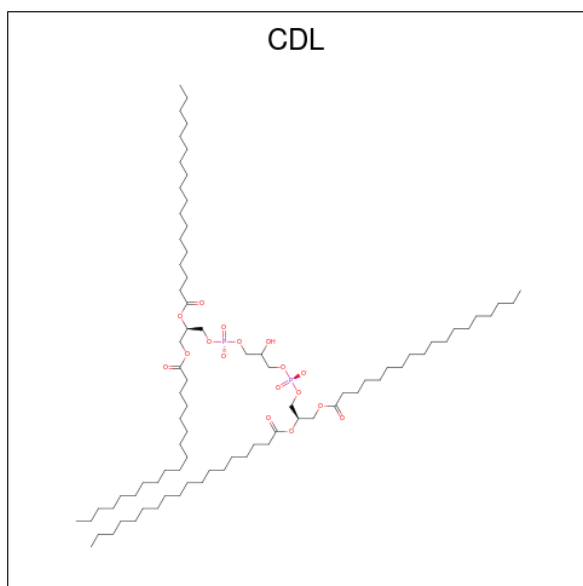
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is water.

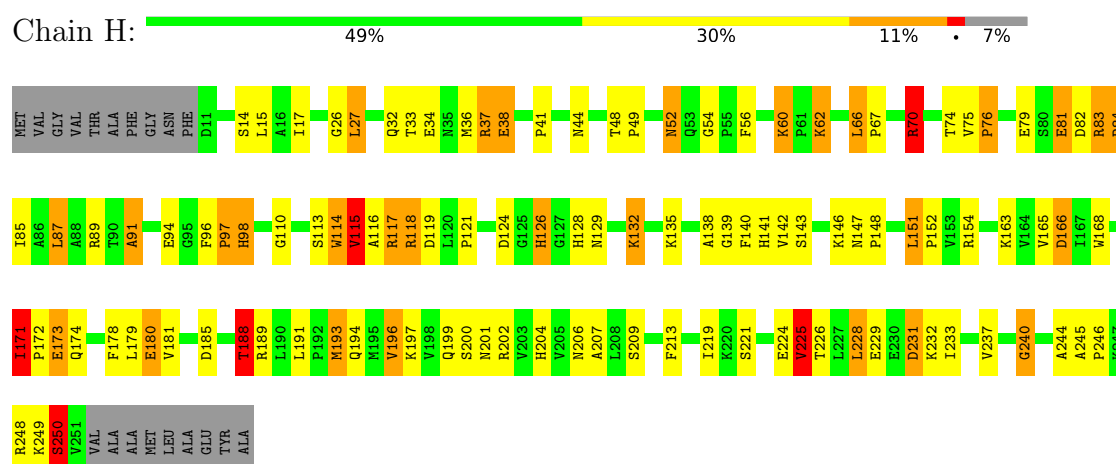
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	42	Total	O	0	0
			42	42		
11	L	28	Total	O	0	0
			28	28		
11	M	42	Total	O	0	0
			42	42		

3 Residue-property plots

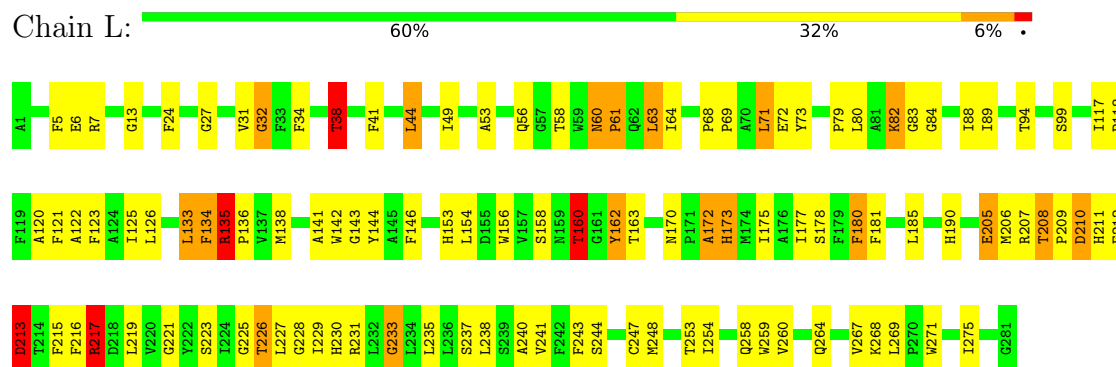
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

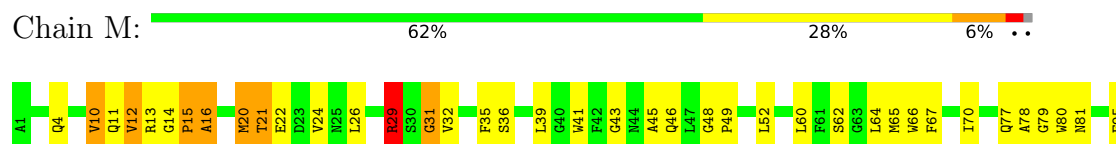
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



P96	P97	A98	P99	E100	Y101		S104	F105	A106	A107	P108	L109		G113		I117	A118	S119		M122	F123	V124		R132	T133		R136	A137		M142	G143	K144	H145		W148		L151	S152	A153	I154	W155		I163	R164	P165		S170	W171	S172		V175	P176		H182	L183	D184		M188	F189
S190	L191	V192	H193	G194	M195	L196	R197		P200		D203		A213	L214	L215	F216		R228	F229		R233	E234		A239	D240	R241	G242	T243	A244	A245	E246	R247		F251		M256	G257	F258		I270		A273	V274		I282		L285		N293	W294	Y295		H301	G302	W303	ALA	PRO	LEU	ASN

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	140.00 Å 140.00 Å 184.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: CDL, U10, BPH, BCL, SPN, FE, LDA

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	0.86	0/1878	2.10	77/2555 (3.0%)
2	L	0.81	1/2320 (0.0%)	1.93	73/3175 (2.3%)
3	M	0.77	0/2504	1.90	63/3419 (1.8%)
All	All	0.81	1/6702 (0.0%)	1.97	213/9149 (2.3%)

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	0	7
2	L	0	5
3	M	0	2
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	32	GLY	N-CA	6.85	1.52	1.45

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	188	ASN	OD1-CG-ND2	16.29	138.89	122.60
2	L	135	ARG	CD-NE-CZ	14.67	144.93	124.40
3	M	188	ASN	CA-CB-CG	-11.39	101.21	112.60
1	H	70	ARG	NE-CZ-NH2	-10.96	109.34	119.20
1	H	83	ARG	CD-NE-CZ	10.49	139.08	124.40
2	L	31	VAL	CA-C-N	-10.43	109.47	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	31	VAL	C-N-CA	-10.43	109.47	122.19
2	L	217	ARG	CD-NE-CZ	10.09	138.53	124.40
1	H	70	ARG	CD-NE-CZ	9.63	137.88	124.40
1	H	52	ASN	CA-CB-CG	9.59	122.19	112.60
3	M	182	HIS	CA-CB-CG	9.20	123.00	113.80
3	M	20	MET	CA-C-O	-8.85	111.16	121.16
2	L	134	PHE	CA-C-O	-8.80	111.63	120.70
2	L	219	LEU	CA-C-O	-8.56	111.35	120.42
1	H	37	ARG	NE-CZ-NH1	-8.32	113.18	121.50
3	M	132	ARG	NE-CZ-NH1	-8.28	113.22	121.50
1	H	231	ASP	CA-C-O	-8.16	111.90	120.55
1	H	52	ASN	OD1-CG-ND2	-8.14	114.46	122.60
1	H	166	ASP	CA-CB-CG	8.08	120.68	112.60
1	H	117	ARG	CD-NE-CZ	7.95	135.52	124.40
1	H	141	HIS	CA-C-N	7.89	132.29	120.77
1	H	141	HIS	C-N-CA	7.89	132.29	120.77
1	H	135	LYS	CA-C-O	-7.82	112.19	120.63
3	M	247	ARG	NE-CZ-NH1	7.74	129.24	121.50
2	L	254	ILE	N-CA-C	-7.73	105.23	112.96
1	H	189	ARG	CD-NE-CZ	7.70	135.18	124.40
1	H	44	ASN	OD1-CG-ND2	7.68	130.28	122.60
3	M	12	VAL	N-CA-CB	-7.67	99.15	111.58
3	M	247	ARG	CD-NE-CZ	7.59	135.03	124.40
1	H	38	GLU	CB-CG-CD	7.54	125.42	112.60
3	M	241	ARG	CD-NE-CZ	7.45	134.83	124.40
1	H	98	HIS	CA-CB-CG	-7.29	106.51	113.80
2	L	158	SER	N-CA-C	7.25	118.83	111.07
1	H	138	ALA	CA-C-O	-7.16	113.15	120.96
1	H	81	GLU	N-CA-C	-7.16	99.85	110.23
2	L	135	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	H	117	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	H	126	HIS	CA-CB-CG	-7.01	106.79	113.80
2	L	135	ARG	NE-CZ-NH1	6.92	128.42	121.50
3	M	294	TRP	CA-C-O	-6.91	113.16	120.63
2	L	60	ASN	CA-C-N	6.83	126.79	119.28
2	L	60	ASN	C-N-CA	6.83	126.79	119.28
2	L	71	LEU	CA-C-N	6.79	130.06	120.28
2	L	71	LEU	C-N-CA	6.79	130.06	120.28
1	H	152	PRO	N-CA-CB	6.76	109.62	103.33
1	H	67	PRO	N-CA-C	6.75	126.37	112.47
3	M	22	GLU	CB-CG-CD	6.75	124.07	112.60
1	H	32	GLN	OE1-CD-NE2	6.74	129.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	ARG	CA-C-O	6.71	129.36	120.16
1	H	225	VAL	CB-CA-C	-6.68	99.16	110.71
1	H	114	TRP	CA-C-N	-6.64	114.54	123.10
1	H	114	TRP	C-N-CA	-6.64	114.54	123.10
1	H	115	VAL	O-C-N	-6.62	116.39	123.14
2	L	58	THR	N-CA-C	6.61	119.92	109.81
2	L	170	ASN	CA-C-N	6.57	126.28	119.64
2	L	170	ASN	C-N-CA	6.57	126.28	119.64
1	H	225	VAL	N-CA-CB	6.55	122.19	111.45
2	L	269	LEU	CA-C-N	6.52	127.99	119.84
2	L	269	LEU	C-N-CA	6.52	127.99	119.84
3	M	39	LEU	CA-C-O	6.51	127.45	120.55
2	L	135	ARG	N-CA-CB	6.49	119.45	110.11
1	H	81	GLU	N-CA-CB	6.46	119.59	109.83
2	L	208	THR	CA-C-N	6.41	126.63	119.32
2	L	208	THR	C-N-CA	6.41	126.63	119.32
3	M	39	LEU	CA-C-N	6.39	128.18	120.13
3	M	39	LEU	C-N-CA	6.39	128.18	120.13
1	H	97	PRO	N-CA-CB	6.37	109.33	103.15
2	L	24	PHE	CA-CB-CG	6.35	120.15	113.80
2	L	213	ASP	N-CA-C	-6.32	104.47	111.36
1	H	89	ARG	CA-C-O	-6.31	114.86	121.55
1	H	163	LYS	CA-CB-CG	6.28	126.66	114.10
2	L	243	PHE	CA-CB-CG	-6.27	107.53	113.80
1	H	26	GLY	CA-C-N	6.24	128.65	120.28
1	H	26	GLY	C-N-CA	6.24	128.65	120.28
3	M	133	THR	CB-CA-C	6.22	121.06	110.74
1	H	110	GLY	CA-C-N	6.21	125.90	119.56
1	H	110	GLY	C-N-CA	6.21	125.90	119.56
2	L	38	THR	N-CA-CB	6.16	119.17	110.12
3	M	273	ALA	O-C-N	-6.15	115.14	122.15
1	H	180	GLU	CA-C-O	-6.12	113.57	120.43
2	L	143	GLY	CA-C-O	-6.08	114.25	120.45
3	M	241	ARG	NE-CZ-NH2	-6.08	113.73	119.20
3	M	184	ASP	CA-CB-CG	6.06	118.66	112.60
2	L	230	HIS	N-CA-C	-6.05	104.97	112.90
3	M	77	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	H	94	GLU	CB-CG-CD	6.04	122.87	112.60
2	L	213	ASP	CA-CB-CG	6.04	118.64	112.60
3	M	192	VAL	N-CA-CB	-6.04	102.89	112.07
3	M	195	ASN	CA-C-N	-6.04	110.64	120.72
3	M	195	ASN	C-N-CA	-6.04	110.64	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	245	ALA	CA-C-O	5.99	126.86	119.97
1	H	83	ARG	CA-C-N	5.97	126.17	119.90
1	H	83	ARG	C-N-CA	5.97	126.17	119.90
2	L	173	HIS	CA-CB-CG	5.96	119.76	113.80
2	L	27	GLY	CA-C-N	5.95	125.65	119.64
2	L	27	GLY	C-N-CA	5.95	125.65	119.64
3	M	137	ALA	CA-C-N	5.95	128.17	120.44
3	M	137	ALA	C-N-CA	5.95	128.17	120.44
2	L	228	GLY	N-CA-C	5.93	119.84	112.73
2	L	226	THR	CA-C-O	-5.91	114.25	120.63
1	H	207	ALA	N-CA-C	5.89	118.66	111.82
2	L	6	GLU	N-CA-C	5.88	119.64	112.23
1	H	142	VAL	CB-CA-C	-5.88	102.52	111.69
3	M	175	VAL	CA-C-N	5.88	125.85	120.03
3	M	175	VAL	C-N-CA	5.88	125.85	120.03
2	L	217	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	H	81	GLU	CA-C-N	-5.86	110.35	121.54
1	H	81	GLU	C-N-CA	-5.86	110.35	121.54
2	L	158	SER	CA-CB-OG	-5.86	99.39	111.10
2	L	259	TRP	O-C-N	-5.86	115.37	122.22
3	M	234	GLU	N-CA-C	5.82	117.30	111.07
2	L	158	SER	CA-C-O	5.81	126.92	120.82
1	H	84	PRO	N-CA-CB	5.80	108.47	103.36
3	M	133	THR	CA-CB-CG2	5.79	120.35	110.50
3	M	136	ARG	NH1-CZ-NH2	-5.72	111.86	119.30
3	M	15	PRO	N-CA-CB	5.71	108.28	103.25
2	L	181	PHE	CA-CB-CG	5.70	119.50	113.80
2	L	123	PHE	CA-CB-CG	5.69	119.49	113.80
1	H	209	SER	N-CA-C	-5.68	102.12	110.52
1	H	118	ARG	CD-NE-CZ	-5.65	116.48	124.40
1	H	240	GLY	O-C-N	-5.65	116.69	122.17
1	H	91	ALA	CA-C-O	-5.65	115.23	121.33
2	L	215	PHE	CA-C-O	-5.65	114.86	120.90
1	H	119	ASP	CA-C-N	5.64	136.50	122.74
1	H	119	ASP	C-N-CA	5.64	136.50	122.74
2	L	41	PHE	CA-CB-CG	5.63	119.43	113.80
1	H	79	GLU	CA-C-O	-5.63	114.69	120.54
2	L	44	LEU	N-CA-C	-5.63	104.78	111.03
3	M	31	GLY	N-CA-C	-5.63	102.65	112.55
3	M	282	ILE	CA-C-N	5.62	126.18	119.94
3	M	282	ILE	C-N-CA	5.62	126.18	119.94
3	M	246	GLU	CA-CB-CG	-5.61	102.89	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	60	LYS	CA-C-N	5.58	125.89	119.92
1	H	60	LYS	C-N-CA	5.58	125.89	119.92
1	H	41	PRO	N-CA-CB	5.57	108.73	102.60
3	M	14	GLY	CA-C-N	5.57	125.58	119.90
3	M	14	GLY	C-N-CA	5.57	125.58	119.90
2	L	31	VAL	O-C-N	-5.56	114.14	122.20
2	L	94	THR	CA-C-N	5.55	126.10	119.94
2	L	94	THR	C-N-CA	5.55	126.10	119.94
3	M	273	ALA	CA-C-N	5.54	128.28	120.42
3	M	273	ALA	C-N-CA	5.54	128.28	120.42
3	M	191	LEU	CA-C-O	5.52	126.17	119.49
1	H	132	LYS	CB-CA-C	-5.51	99.81	108.91
1	H	141	HIS	O-C-N	-5.51	116.97	123.25
3	M	153	ALA	N-CA-C	-5.51	105.19	111.14
3	M	189	PHE	CA-CB-CG	5.50	119.30	113.80
3	M	29	ARG	CD-NE-CZ	5.45	132.04	124.40
1	H	171	ILE	CA-C-N	5.45	125.27	119.28
1	H	171	ILE	C-N-CA	5.45	125.27	119.28
2	L	146	PHE	CA-C-N	5.45	126.73	120.85
2	L	146	PHE	C-N-CA	5.45	126.73	120.85
3	M	176	PRO	CA-C-O	-5.44	115.11	122.08
1	H	188	THR	N-CA-CB	-5.44	101.78	111.08
2	L	258	GLN	OE1-CD-NE2	5.43	128.03	122.60
3	M	36	SER	CA-C-N	5.43	128.56	120.31
3	M	36	SER	C-N-CA	5.43	128.56	120.31
2	L	180	PHE	CA-CB-CG	-5.42	108.38	113.80
1	H	37	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	L	88	ILE	N-CA-CB	5.39	117.47	110.57
2	L	162	TYR	CA-C-O	-5.38	112.06	119.05
3	M	81	ASN	CA-C-N	5.33	126.50	119.84
3	M	81	ASN	C-N-CA	5.33	126.50	119.84
1	H	54	GLY	CA-C-N	5.32	126.16	120.47
1	H	54	GLY	C-N-CA	5.32	126.16	120.47
2	L	13	GLY	CA-C-O	5.31	125.67	122.22
2	L	260	VAL	O-C-N	-5.31	116.51	121.87
2	L	190	HIS	CA-C-O	5.31	126.17	120.70
2	L	225	GLY	CA-C-N	5.30	127.64	120.38
2	L	225	GLY	C-N-CA	5.30	127.64	120.38
2	L	172	ALA	N-CA-C	-5.28	105.58	112.23
2	L	275	ILE	CA-C-N	5.28	125.28	120.21
2	L	275	ILE	C-N-CA	5.28	125.28	120.21
2	L	227	LEU	CA-C-N	5.26	125.82	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	227	LEU	C-N-CA	5.26	125.82	119.98
3	M	136	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	H	118	ARG	NE-CZ-NH2	-5.26	114.47	119.20
2	L	233	GLY	O-C-N	-5.25	117.15	122.19
1	H	76	PRO	N-CA-CB	5.25	108.37	102.60
3	M	21	THR	CA-CB-OG1	-5.24	101.74	109.60
1	H	224	GLU	CA-C-O	-5.24	115.63	121.23
2	L	153	HIS	N-CA-C	-5.23	105.64	112.23
3	M	132	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	M	145	HIS	O-C-N	-5.23	116.66	122.09
3	M	193	HIS	CA-C-O	5.22	126.26	119.95
2	L	120	ALA	O-C-N	-5.18	116.24	122.15
3	M	246	GLU	CG-CD-OE2	-5.16	106.53	118.40
1	H	151	LEU	CA-C-N	5.15	125.05	119.85
1	H	151	LEU	C-N-CA	5.15	125.05	119.85
3	M	43	GLY	CA-C-N	5.14	128.86	121.50
3	M	43	GLY	C-N-CA	5.14	128.86	121.50
3	M	16	ALA	CA-C-N	-5.14	115.93	122.77
3	M	16	ALA	C-N-CA	-5.14	115.93	122.77
3	M	95	GLU	CA-C-N	5.14	125.67	120.38
3	M	95	GLU	C-N-CA	5.14	125.67	120.38
1	H	81	GLU	CA-CB-CG	5.13	124.36	114.10
3	M	197	ARG	CA-CB-CG	5.12	124.34	114.10
1	H	66	LEU	CA-C-N	5.10	126.22	119.84
1	H	66	LEU	C-N-CA	5.10	126.22	119.84
1	H	147	ASN	CA-C-N	5.10	124.79	119.64
1	H	147	ASN	C-N-CA	5.10	124.79	119.64
3	M	191	LEU	N-CA-C	5.09	118.59	112.38
2	L	135	ARG	CB-CA-C	-5.09	104.23	113.49
3	M	144	LYS	CA-C-O	5.08	125.84	119.59
1	H	83	ARG	CB-CG-CD	5.07	122.96	111.30
2	L	31	VAL	CB-CA-C	-5.07	105.71	111.59
2	L	216	PHE	N-CA-CB	5.07	117.66	110.16
1	H	62	LYS	O-C-N	5.05	129.28	123.17
2	L	53	ALA	CA-C-O	-5.05	115.70	121.00
2	L	231	ARG	CA-C-N	5.05	127.00	120.44
2	L	231	ARG	C-N-CA	5.05	127.00	120.44
1	H	60	LYS	N-CA-C	-5.04	103.24	109.64
2	L	61	PRO	N-CA-CB	5.02	108.81	103.39

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	113	SER	Mainchain
1	H	114	TRP	Mainchain
1	H	115	VAL	Mainchain
1	H	185	ASP	Mainchain
1	H	250	SER	Mainchain
1	H	87	LEU	Mainchain
1	H	91	ALA	Mainchain
2	L	141	ALA	Mainchain
2	L	160	THR	Mainchain
2	L	162	TYR	Mainchain
2	L	213	ASP	Mainchain
2	L	253	THR	Mainchain
3	M	196	LEU	Mainchain
3	M	29	ARG	Mainchain

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	H	1830	0	1836	68	0
2	L	2232	0	2187	66	0
3	M	2413	0	2326	67	0
4	H	16	0	31	0	0
4	M	32	0	62	5	0
5	L	132	0	148	11	0
5	M	132	0	148	9	0
6	L	65	0	76	12	0
6	M	65	0	76	5	0
7	L	48	0	58	1	0
7	M	48	0	63	0	0
8	M	1	0	0	0	0
9	M	43	0	69	5	0
10	M	81	0	106	16	0
11	H	42	0	0	3	0
11	L	28	0	0	1	0
11	M	42	0	0	1	0
All	All	7250	0	7186	218	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 (218) 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)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HB4	10:M:800:CDL:HA61	1.10	1.10
10:M:800:CDL:HA61	10:M:800:CDL:CB4	1.83	1.08
1:H:27:LEU:HD23	10:M:800:CDL:H132	1.51	0.92
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.57	0.86
10:M:800:CDL:HB4	10:M:800:CDL:HA62	1.55	0.86
10:M:800:CDL:OB7	10:M:800:CDL:CA7	2.25	0.84
3:M:31:GLY:H	4:M:702:LDA:H92	1.40	0.84
3:M:197:ARG:HG3	3:M:197:ARG:HH11	1.44	0.81
1:H:154:ARG:HE	1:H:204:HIS:HD2	1.29	0.80
10:M:800:CDL:HA61	10:M:800:CDL:CB6	2.13	0.78
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.64	0.77
3:M:197:ARG:HG3	3:M:197:ARG:NH1	1.97	0.77
1:H:154:ARG:HE	1:H:204:HIS:CD2	2.03	0.76
2:L:154:LEU:HB3	3:M:197:ARG:HG2	1.67	0.76
10:M:800:CDL:OB7	10:M:800:CDL:C31	2.34	0.75
1:H:132:LYS:HG3	1:H:171:ILE:HD13	1.72	0.72
6:L:401:BPH:HMB1	6:L:401:BPH:HBB3	1.71	0.71
1:H:70:ARG:O	1:H:118:ARG:NH2	2.24	0.71
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.20	0.70
3:M:203:ASP:HB2	4:M:703:LDA:HM11	1.73	0.68
2:L:221:GLY:HA3	4:M:702:LDA:HM21	1.75	0.67
2:L:267:VAL:HG13	2:L:268:LYS:HD3	1.76	0.66
5:L:1302:BCL:OB	5:L:1302:BCL:HHC	1.93	0.66
2:L:208:THR:HB	2:L:209:PRO:HD2	1.77	0.66
3:M:190:SER:HA	3:M:196:LEU:HD13	1.78	0.65
1:H:171:ILE:N	1:H:172:PRO:HD2	2.11	0.65
2:L:135:ARG:HB2	2:L:136:PRO:HD3	1.78	0.65
2:L:221:GLY:HA3	4:M:702:LDA:CM2	2.26	0.65
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.44	0.64
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.16	0.63
5:L:1304:BCL:CBC	5:L:1304:BCL:C1C	2.77	0.63
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.79	0.63
1:H:36:MET:HE1	1:H:56:PHE:HB2	1.79	0.63
2:L:34:PHE:O	2:L:38:THR:HG23	1.99	0.62
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.79	0.62
2:L:71:LEU:H	2:L:71:LEU:HD12	1.64	0.62
5:L:1302:BCL:HBD	5:L:1304:BCL:HAC1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LYS:NZ	1:H:199:GLN:HE21	1.98	0.62
1:H:14:SER:HA	1:H:17:ILE:HG22	1.82	0.60
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.83	0.60
3:M:197:ARG:HH11	3:M:197:ARG:CG	2.13	0.60
5:M:1301:BCL:H51	6:M:402:BPH:HMB3	1.84	0.60
3:M:256:MET:HE3	3:M:258:PHE:CZ	2.36	0.60
1:H:132:LYS:HG3	1:H:171:ILE:CD1	2.32	0.60
5:M:1301:BCL:H61	5:M:1303:BCL:H18	1.83	0.60
3:M:101:TYR:O	3:M:104:SER:HB3	2.02	0.59
2:L:156:TRP:O	2:L:160:THR:HG23	2.02	0.59
2:L:5:PHE:CD1	3:M:246:GLU:HG2	2.37	0.59
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.84	0.59
10:M:800:CDL:OB7	10:M:800:CDL:H312	2.03	0.58
3:M:70:ILE:HD13	9:M:600:SPN:H102	1.86	0.58
5:M:1303:BCL:HMB1	5:M:1303:BCL:HBB3	1.86	0.57
5:M:1301:BCL:OBB	5:M:1301:BCL:HHC	2.04	0.57
2:L:5:PHE:CE1	3:M:246:GLU:HG2	2.40	0.57
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.86	0.56
10:M:800:CDL:HA61	10:M:800:CDL:HB61	1.86	0.56
3:M:233:ARG:HA	11:M:2031:HOH:O	2.06	0.56
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.36	0.56
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.89	0.55
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.41	0.55
1:H:121:PRO:HB3	1:H:225:VAL:O	2.06	0.55
3:M:170:SER:HG	3:M:172:SER:HG	1.53	0.55
2:L:229:ILE:HG13	2:L:229:ILE:O	2.06	0.55
1:H:34:GLU:OE1	1:H:37:ARG:NH1	2.40	0.55
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.37	0.55
2:L:156:TRP:CE2	2:L:160:THR:HG21	2.42	0.55
2:L:121:PHE:CE2	2:L:125:ILE:HD11	2.43	0.54
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.87	0.54
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.89	0.54
1:H:249:LYS:O	1:H:250:SER:HB2	2.08	0.54
6:L:401:BPH:OBB	6:L:401:BPH:HHC	2.08	0.54
3:M:65:MET:HA	3:M:65:MET:HE2	1.89	0.54
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.90	0.54
6:M:402:BPH:HBC3	6:M:402:BPH:HHD	1.90	0.53
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.44	0.53
6:M:402:BPH:HMB1	6:M:402:BPH:HBB3	1.90	0.53
1:H:146:LYS:HE2	1:H:200:SER:O	2.09	0.52
1:H:139:GLY:HA3	3:M:15:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.90	0.52
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.09	0.52
2:L:241:VAL:HG21	6:L:401:BPH:HAC2	1.92	0.52
1:H:228:LEU:O	1:H:232:LYS:HG3	2.09	0.52
3:M:119:SER:HB3	9:M:600:SPN:H232	1.91	0.52
1:H:62:LYS:HE3	11:H:2006:HOH:O	2.09	0.52
1:H:245:ALA:HB3	1:H:246:PRO:HD3	1.92	0.52
3:M:98:ALA:HB1	3:M:99:PRO:HD2	1.92	0.51
1:H:126:HIS:CE1	3:M:20:MET:HE2	2.46	0.51
2:L:60:ASN:O	2:L:64:ILE:HG13	2.10	0.51
2:L:210:ASP:HB2	3:M:20:MET:HE3	1.92	0.51
3:M:109:LEU:HA	3:M:113:GLY:HA3	1.93	0.51
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.09	0.51
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.91	0.51
1:H:83:ARG:HB2	1:H:84:PRO:HD2	1.92	0.51
2:L:135:ARG:HD3	2:L:248:MET:O	2.11	0.51
2:L:135:ARG:CB	2:L:136:PRO:HD3	2.39	0.51
3:M:67:PHE:CE1	9:M:600:SPN:H61	2.46	0.50
3:M:148:TRP:CD1	10:M:800:CDL:H511	2.46	0.50
2:L:154:LEU:HD13	3:M:197:ARG:HG2	1.94	0.50
3:M:132:ARG:O	3:M:133:THR:C	2.52	0.50
1:H:132:LYS:NZ	11:H:2028:HOH:O	2.45	0.50
1:H:197:LYS:HZ3	1:H:199:GLN:HE21	1.59	0.50
3:M:101:TYR:CG	3:M:107:ALA:HB2	2.47	0.50
2:L:69:PRO:HG2	2:L:142:TRP:CB	2.42	0.49
2:L:122:ALA:O	2:L:126:LEU:HG	2.12	0.49
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.47	0.49
2:L:210:ASP:CB	3:M:20:MET:HE3	2.43	0.49
5:L:1304:BCL:C1C	5:L:1304:BCL:HBC2	2.43	0.48
2:L:73:TYR:OH	2:L:82:LYS:HD2	2.12	0.48
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.47	0.48
1:H:34:GLU:CD	1:H:37:ARG:HH12	2.22	0.48
5:L:1302:BCL:H42	5:L:1304:BCL:HBC3	1.95	0.48
3:M:24:VAL:HG11	3:M:29:ARG:NH2	2.28	0.48
3:M:197:ARG:NH2	5:M:1303:BCL:OBB	2.46	0.48
6:L:401:BPH:HBB3	6:L:401:BPH:CMB	2.42	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
1:H:191:LEU:HD11	1:H:213:PHE:CE2	2.49	0.48
5:L:1302:BCL:OBB	5:L:1302:BCL:CHC	2.62	0.48
2:L:32:GLY:HA3	11:L:2016:HOH:O	2.13	0.48
1:H:201:ASN:O	1:H:202:ARG:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.47
1:H:33:THR:O	1:H:36:MET:HB2	2.14	0.47
1:H:140:PHE:HA	3:M:13:ARG:O	2.15	0.47
1:H:171:ILE:N	1:H:172:PRO:CD	2.78	0.47
2:L:154:LEU:HD13	3:M:197:ARG:CG	2.45	0.47
3:M:155:TRP:CD2	10:M:800:CDL:H812	2.50	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.96	0.47
2:L:172:ALA:HB3	2:L:247:CYS:HA	1.95	0.47
3:M:148:TRP:CE2	10:M:800:CDL:H511	2.50	0.47
1:H:37:ARG:HH11	1:H:37:ARG:HD2	1.46	0.46
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.46
2:L:233:GLY:HA3	3:M:216:PHE:CD1	2.50	0.46
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.97	0.46
2:L:134:PHE:O	2:L:138:MET:HG3	2.15	0.46
1:H:206:ASN:HD21	1:H:248:ARG:HD3	1.81	0.46
2:L:208:THR:O	2:L:211:HIS:HB2	2.15	0.46
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.51	0.46
1:H:121:PRO:HA	1:H:226:THR:HA	1.98	0.45
3:M:35:PHE:CE1	3:M:46:GLN:HB2	2.51	0.45
1:H:197:LYS:HD3	1:H:199:GLN:NE2	2.30	0.45
1:H:206:ASN:O	1:H:248:ARG:NH1	2.49	0.45
2:L:117:ILE:HB	2:L:118:PRO:CD	2.46	0.45
5:M:1301:BCL:H141	5:M:1301:BCL:H162	1.65	0.45
1:H:180:GLU:OE2	1:H:188:THR:HG21	2.16	0.45
2:L:175:ILE:O	2:L:178:SER:HB2	2.16	0.45
6:L:401:BPH:HMC3	3:M:213:ALA:HB3	1.97	0.45
1:H:199:GLN:HB2	1:H:202:ARG:O	2.17	0.45
1:H:66:LEU:CD2	2:L:206:MET:HE2	2.47	0.45
1:H:165:VAL:O	1:H:166:ASP:HB2	2.17	0.45
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.99	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.98	0.44
1:H:193:MET:HE2	3:M:10:VAL:HG23	1.98	0.44
3:M:48:GLY:HA2	3:M:49:PRO:C	2.42	0.44
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.47	0.44
3:M:270:ILE:HD13	10:M:800:CDL:H711	1.98	0.44
6:M:402:BPH:H9C2	6:M:402:BPH:H6C1	1.73	0.44
1:H:240:GLY:O	1:H:244:ALA:HB3	2.18	0.44
1:H:62:LYS:O	1:H:74:THR:HA	2.17	0.43
1:H:194:GLN:CD	1:H:194:GLN:H	2.26	0.43
1:H:229:GLU:O	1:H:233:ILE:HD12	2.18	0.43
2:L:241:VAL:HG21	6:L:401:BPH:H2C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:401:BPH:ND	3:M:214:LEU:HD13	2.34	0.43
5:L:1304:BCL:HMB3	5:L:1304:BCL:HBB2	1.99	0.43
2:L:209:PRO:O	2:L:212:GLU:HB2	2.19	0.43
3:M:106:ALA:O	3:M:107:ALA:C	2.61	0.43
6:L:401:BPH:H141	6:L:401:BPH:H162	1.72	0.43
3:M:200:PRO:HA	4:M:703:LDA:HM12	2.00	0.43
6:M:402:BPH:H6C1	6:M:402:BPH:H4C1	1.34	0.43
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.54	0.43
5:L:1302:BCL:H2C	5:M:1303:BCL:H2C	2.00	0.43
1:H:82:ASP:O	1:H:83:ARG:HB3	2.18	0.43
2:L:38:THR:HG22	2:L:99:SER:CB	2.49	0.43
5:M:1303:BCL:OBB	5:M:1303:BCL:HHC	2.19	0.43
10:M:800:CDL:H311	10:M:800:CDL:H522	2.00	0.43
1:H:168:TRP:CZ3	1:H:225:VAL:HG22	2.53	0.42
5:L:1304:BCL:H203	6:L:401:BPH:H112	2.00	0.42
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.19	0.42
2:L:63:LEU:O	2:L:64:ILE:C	2.62	0.42
2:L:238:LEU:HD23	6:L:401:BPH:CBC	2.50	0.42
3:M:184:ASP:O	3:M:188:ASN:HB2	2.19	0.42
2:L:68:PRO:O	2:L:69:PRO:C	2.63	0.42
1:H:173:GLU:O	1:H:174:GLN:C	2.60	0.42
2:L:226:THR:HG22	7:L:501:U10:H3M2	2.02	0.42
5:L:1302:BCL:H122	6:L:401:BPH:H3A	2.01	0.42
3:M:251:PHE:CD2	3:M:251:PHE:C	2.98	0.42
2:L:79:PRO:O	2:L:80:LEU:C	2.61	0.42
2:L:205:GLU:O	2:L:206:MET:C	2.61	0.42
2:L:247:CYS:SG	2:L:248:MET:HG2	2.59	0.42
1:H:225:VAL:HG12	1:H:229:GLU:HB2	2.01	0.42
1:H:228:LEU:HD22	1:H:232:LYS:HE3	2.01	0.42
1:H:179:LEU:HD11	1:H:196:VAL:HG21	2.01	0.41
6:L:401:BPH:CMB	6:L:401:BPH:CBB	2.98	0.41
3:M:163:ILE:HG22	3:M:285:LEU:HD11	2.03	0.41
1:H:98:HIS:HE1	11:H:2019:HOH:O	2.02	0.41
10:M:800:CDL:H312	10:M:800:CDL:C52	2.50	0.41
2:L:69:PRO:HD3	2:L:83:GLY:O	2.21	0.41
3:M:243:THR:O	3:M:247:ARG:HG2	2.20	0.41
3:M:11:GLN:NE2	3:M:41:TRP:CD2	2.88	0.41
2:L:207:ARG:HG2	3:M:142:MET:HG2	2.02	0.41
5:L:1302:BCL:H2C	5:L:1302:BCL:HBC2	1.89	0.41
2:L:133:LEU:HD12	2:L:133:LEU:O	2.20	0.41
1:H:34:GLU:CD	1:H:37:ARG:NH1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:163:THR:HG22	2:L:163:THR:O	2.21	0.41
2:L:213:ASP:O	2:L:217:ARG:HG3	2.20	0.41
3:M:241:ARG:HG3	3:M:245:ALA:HB3	2.03	0.41
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.82	0.41
2:L:248:MET:HE3	2:L:248:MET:HB3	1.92	0.41
3:M:122:MET:SD	9:M:600:SPN:H19	2.60	0.41
5:M:1301:BCL:H193	5:M:1301:BCL:H161	1.86	0.40
2:L:241:VAL:O	2:L:244:SER:HB2	2.20	0.40
3:M:78:ALA:O	3:M:79:GLY:C	2.63	0.40
1:H:128:HIS:O	1:H:129:ASN:C	2.64	0.40
1:H:48:THR:HB	1:H:49:PRO:HD2	2.02	0.40
2:L:71:LEU:HD23	2:L:144:TYR:CZ	2.56	0.40
3:M:60:LEU:HD23	3:M:64:LEU:HD11	2.04	0.40
2:L:138:MET:HE2	2:L:138:MET:HB3	1.96	0.40
3:M:35:PHE:HA	3:M:45:ALA:O	2.21	0.40
3:M:67:PHE:CZ	9:M:600:SPN:H61	2.57	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%)	224 (94%)	13 (5%)	2 (1%)	16	37
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	7	19
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER

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Mol	Chain	Res	Type
1	H	116	ALA
3	M	195	ASN
3	M	301	HIS
3	M	80	TRP
3	M	194	GLY
3	M	302	GLY

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%)	178 (91%)	17 (9%)	9	24
2	L	220/220 (100%)	203 (92%)	17 (8%)	12	30
3	M	237/241 (98%)	217 (92%)	20 (8%)	10	26
All	All	652/669 (98%)	598 (92%)	54 (8%)	10	26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	27	LEU
1	H	52	ASN
1	H	60	LYS
1	H	70	ARG
1	H	115	VAL
1	H	143	SER
1	H	171	ILE
1	H	173	GLU
1	H	188	THR
1	H	193	MET
1	H	196	VAL
1	H	221	SER
1	H	225	VAL
1	H	228	LEU
1	H	231	ASP

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Mol	Chain	Res	Type
1	H	237	VAL
2	L	38	THR
2	L	44	LEU
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	82	LYS
2	L	133	LEU
2	L	135	ARG
2	L	160	THR
2	L	185	LEU
2	L	205	GLU
2	L	210	ASP
2	L	217	ARG
2	L	223	SER
2	L	235	LEU
2	L	237	SER
2	L	271	TRP
3	M	4	GLN
3	M	10	VAL
3	M	12	VAL
3	M	52	LEU
3	M	62	SER
3	M	104	SER
3	M	109	LEU
3	M	117	ILE
3	M	124	VAL
3	M	133	THR
3	M	136	ARG
3	M	151	LEU
3	M	170	SER
3	M	182	HIS
3	M	188	ASN
3	M	192	VAL
3	M	196	LEU
3	M	197	ARG
3	M	247	ARG
3	M	274	VAL

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

Mol	Chain	Res	Type
1	H	98	HIS
1	H	126	HIS
1	H	199	GLN
1	H	204	HIS
1	H	206	ASN
2	L	87	GLN
3	M	4	GLN
3	M	299	GLN

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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	LDA	M	703	-	13,15,15	2.78	2 (15%)	14,17,17	0.80	1 (7%)
4	LDA	H	701	-	13,15,15	2.67	2 (15%)	14,17,17	0.79	1 (7%)
7	U10	L	501	-	47,47,63	2.05	14 (29%)	56,58,79	2.66	19 (33%)
7	U10	M	502	-	48,48,63	1.83	17 (35%)	60,61,79	1.49	11 (18%)
6	BPH	M	402	-	59,70,70	1.97	15 (25%)	59,101,101	3.30	21 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SPN	M	600	-	42,42,42	4.02	20 (47%)	50,52,52	2.88	19 (38%)
5	BCL	L	1302	2	69,74,74	1.49	8 (11%)	79,115,115	2.07	20 (25%)
6	BPH	L	401	-	59,70,70	2.00	15 (25%)	59,101,101	3.67	16 (27%)
5	BCL	M	1301	3	69,74,74	1.39	7 (10%)	79,115,115	2.14	24 (30%)
5	BCL	L	1304	2	69,74,74	1.36	7 (10%)	79,115,115	2.70	24 (30%)
10	CDL	M	800	-	80,80,99	0.50	0	86,92,111	0.91	3 (3%)
4	LDA	M	702	-	13,15,15	2.71	2 (15%)	14,17,17	0.84	1 (7%)
5	BCL	M	1303	3	69,74,74	1.36	7 (10%)	79,115,115	1.75	19 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	703	-	-	8/13/13/13	-
4	LDA	H	701	-	-	12/13/13/13	-
7	U10	L	501	-	-	15/41/65/87	0/1/1/1
7	U10	M	502	-	-	6/45/69/87	0/1/1/1
6	BPH	M	402	-	-	18/37/105/105	0/5/6/6
9	SPN	M	600	-	-	19/50/51/51	-
5	BCL	L	1302	2	-	8/41/137/137	-
6	BPH	L	401	-	2/2/18/22	14/37/105/105	0/5/6/6
5	BCL	M	1301	3	1/1/21/25	16/41/137/137	-
5	BCL	L	1304	2	-	9/41/137/137	-
10	CDL	M	800	-	-	35/91/91/110	-
4	LDA	M	702	-	-	12/13/13/13	-
5	BCL	M	1303	3	-	4/41/137/137	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	9.23	1.54	1.33
9	M	600	SPN	C8-C9	8.82	1.53	1.33
9	M	600	SPN	C3-C2	8.76	1.60	1.52
9	M	600	SPN	C19-C18	8.61	1.52	1.33
9	M	600	SPN	C12-C13	8.38	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	701	LDA	O1-N1	-8.10	1.22	1.42
4	M	702	LDA	O1-N1	-8.08	1.22	1.42
4	M	703	LDA	O1-N1	-7.99	1.22	1.42
9	M	600	SPN	C10-C9	-6.66	1.37	1.51
6	M	402	BPH	C2C-C3C	-6.53	1.49	1.54
9	M	600	SPN	C3-C4	-6.25	1.40	1.50
9	M	600	SPN	C6-C5	-6.18	1.38	1.51
5	L	1302	BCL	MG-NA	6.05	2.20	2.06
6	L	401	BPH	C2C-C3C	-6.04	1.49	1.54
4	M	703	LDA	C1-N1	-6.04	1.45	1.51
5	L	1304	BCL	O2D-CGD	5.82	1.47	1.33
7	L	501	U10	C20-C19	-5.81	1.25	1.49
5	L	1302	BCL	O2D-CGD	5.79	1.47	1.33
6	M	402	BPH	C1D-C2D	5.75	1.45	1.39
5	M	1301	BCL	O2D-CGD	5.63	1.47	1.33
4	M	702	LDA	C1-N1	-5.47	1.45	1.51
6	M	402	BPH	C1B-C2B	5.33	1.45	1.39
9	M	600	SPN	C17-C18	-5.31	1.40	1.51
9	M	600	SPN	C14-C13	-5.23	1.40	1.51
6	L	401	BPH	C1D-C2D	5.22	1.45	1.39
4	H	701	LDA	C1-N1	-5.17	1.46	1.51
5	M	1303	BCL	MG-NA	5.12	2.18	2.06
6	L	401	BPH	O2D-CGD	5.10	1.45	1.33
6	L	401	BPH	O2A-CGA	4.91	1.47	1.33
5	M	1303	BCL	O2D-CGD	4.65	1.44	1.33
7	L	501	U10	C7-C8	-4.57	1.43	1.50
5	M	1301	BCL	MG-NA	4.56	2.17	2.06
5	L	1304	BCL	O2A-CGA	4.30	1.45	1.33
6	L	401	BPH	C3A-C2A	-4.30	1.51	1.54
5	M	1301	BCL	O2A-CGA	4.25	1.45	1.33
6	M	402	BPH	C3A-C2A	-4.18	1.51	1.54
6	M	402	BPH	O2D-CGD	4.13	1.43	1.33
7	M	502	U10	O4-C4	4.12	1.46	1.36
7	L	501	U10	O4-C4	4.10	1.46	1.36
5	L	1304	BCL	MG-NA	4.02	2.15	2.06
9	M	600	SPN	O1-CMA	4.00	1.55	1.43
6	L	401	BPH	C1B-C2B	3.91	1.43	1.39
6	M	402	BPH	O2A-CGA	3.82	1.44	1.33
9	M	600	SPN	C20-C19	-3.75	1.39	1.50
7	L	501	U10	O3-C3	3.74	1.45	1.36
9	M	600	SPN	C11-C12	-3.72	1.39	1.50
6	L	401	BPH	O2D-CED	-3.70	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	501	U10	C13-C14	3.69	1.41	1.33
5	M	1303	BCL	O2A-CGA	3.62	1.43	1.33
7	M	502	U10	O3-C3	3.57	1.45	1.36
5	L	1302	BCL	O2A-CGA	3.51	1.43	1.33
5	L	1302	BCL	C2-C3	3.31	1.40	1.33
9	M	600	SPN	C25-C26	3.17	1.40	1.33
7	M	502	U10	C33-C34	3.16	1.40	1.33
7	M	502	U10	C13-C14	3.08	1.40	1.33
5	M	1303	BCL	C2-C3	3.07	1.40	1.33
7	M	502	U10	C8-C9	3.07	1.40	1.33
7	L	501	U10	C28-C29	3.06	1.40	1.33
6	L	401	BPH	CBD-CGD	-3.06	1.48	1.52
7	L	501	U10	C37-C38	-3.00	1.41	1.50
5	M	1301	BCL	C2-C3	2.93	1.39	1.33
5	L	1304	BCL	C2-C3	2.90	1.39	1.33
7	M	502	U10	C23-C24	2.86	1.39	1.33
9	M	600	SPN	C7-C8	-2.84	1.41	1.50
5	L	1302	BCL	C2C-C3C	-2.80	1.46	1.54
7	M	502	U10	C7-C8	-2.80	1.46	1.50
9	M	600	SPN	C21-C22	-2.80	1.39	1.52
6	M	402	BPH	CHA-CBD	2.79	1.54	1.51
6	L	401	BPH	C3D-C4D	2.76	1.45	1.41
6	M	402	BPH	O2D-CED	-2.75	1.39	1.45
7	M	502	U10	C28-C29	2.73	1.39	1.33
9	M	600	SPN	C29-C30	2.68	1.40	1.32
7	M	502	U10	C18-C19	2.63	1.39	1.33
7	L	501	U10	O3-C3M	-2.62	1.39	1.45
6	L	401	BPH	O1D-CGD	2.62	1.27	1.21
5	M	1303	BCL	MG-NC	2.58	2.12	2.06
5	M	1301	BCL	C3B-C4B	2.58	1.46	1.41
6	M	402	BPH	C4-C3	2.58	1.57	1.50
5	M	1303	BCL	C2C-C3C	-2.56	1.47	1.54
6	L	401	BPH	C2-C3	2.56	1.39	1.33
7	L	501	U10	C8-C9	2.55	1.38	1.33
6	M	402	BPH	CBD-CGD	-2.52	1.49	1.52
5	L	1302	BCL	O2D-CED	-2.52	1.39	1.45
6	M	402	BPH	C3D-C4D	2.50	1.44	1.41
6	M	402	BPH	C2-C3	2.48	1.38	1.33
7	M	502	U10	C38-C39	2.45	1.39	1.32
5	L	1302	BCL	C3B-C4B	2.45	1.45	1.41
9	M	600	SPN	C16-C15	-2.43	1.39	1.51
7	M	502	U10	O4-C4M	-2.42	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	402	BPH	C4D-ND	-2.39	1.35	1.38
9	M	600	SPN	CM4-C9	2.39	1.56	1.50
5	M	1303	BCL	O2D-CED	-2.37	1.40	1.45
5	L	1304	BCL	C3B-C4B	2.35	1.45	1.41
6	L	401	BPH	C3B-C2B	-2.29	1.35	1.39
7	L	501	U10	C42-C43	-2.25	1.43	1.50
5	L	1304	BCL	MG-ND	-2.25	2.01	2.05
5	M	1301	BCL	C3B-C2B	-2.25	1.34	1.42
7	M	502	U10	C40-C39	2.22	1.56	1.50
7	M	502	U10	C35-C34	2.22	1.56	1.50
5	L	1302	BCL	O1D-CGD	2.21	1.26	1.21
7	M	502	U10	O3-C3M	-2.21	1.40	1.45
6	L	401	BPH	OBD-CAD	2.21	1.25	1.22
7	L	501	U10	C32-C33	-2.20	1.43	1.50
5	M	1301	BCL	CAA-C2A	2.12	1.57	1.54
5	L	1304	BCL	C2C-C3C	-2.11	1.48	1.54
6	L	401	BPH	C5-C3	2.11	1.55	1.51
7	L	501	U10	C33-C34	2.10	1.37	1.33
7	M	502	U10	C17-C18	-2.09	1.44	1.50
7	L	501	U10	O4-C4M	-2.06	1.40	1.45
9	M	600	SPN	O1-C1	2.05	1.53	1.43
7	L	501	U10	C43-C44	2.03	1.38	1.32
7	M	502	U10	C22-C23	-2.02	1.44	1.50
7	M	502	U10	C12-C13	-2.01	1.44	1.50
6	M	402	BPH	C3D-C2D	-2.01	1.36	1.39
6	L	401	BPH	CHA-CBD	2.01	1.54	1.51
6	M	402	BPH	O1D-CGD	2.01	1.26	1.21

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	401	BPH	O2D-CGD-CBD	21.81	134.91	110.95
6	M	402	BPH	O2D-CGD-CBD	16.37	128.94	110.95
5	L	1304	BCL	O2D-CGD-CBD	11.39	131.15	111.23
7	L	501	U10	C37-C38-C39	10.84	152.45	127.62
5	L	1304	BCL	C1C-NC-C4C	9.28	110.92	106.68
6	L	401	BPH	O1D-CGD-CBD	-8.72	111.50	124.72
5	L	1304	BCL	C4A-NA-C1A	8.27	110.45	106.68
5	M	1301	BCL	C1C-NC-C4C	8.01	110.33	106.68
7	L	501	U10	C32-C33-C34	7.57	144.94	127.62
9	M	600	SPN	C7-C8-C9	-7.35	110.81	127.62
5	L	1302	BCL	C4A-NA-C1A	7.21	109.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	600	SPN	CM6-C18-C17	7.02	127.41	115.23
6	M	402	BPH	O2D-CGD-O1D	-6.63	110.94	123.85
9	M	600	SPN	CM5-C13-C14	6.41	126.36	115.23
6	M	402	BPH	OBD-CAD-CBD	-6.40	116.44	125.82
5	M	1303	BCL	C4A-NA-C1A	6.36	109.58	106.68
5	L	1302	BCL	C1C-NC-C4C	6.12	109.47	106.68
6	M	402	BPH	C5-C3-C2	6.00	134.63	121.17
6	M	402	BPH	C1-C2-C3	-5.75	116.77	126.20
5	L	1302	BCL	O2A-CGA-CBA	5.72	129.28	111.83
6	M	402	BPH	O1D-CGD-CBD	-5.56	116.29	124.72
5	L	1304	BCL	O2D-CGD-O1D	-5.48	113.18	123.85
6	L	401	BPH	CMA-C3A-C4A	-5.43	102.91	114.61
9	M	600	SPN	CM3-C5-C6	5.40	124.60	115.23
6	L	401	BPH	O2D-CGD-O1D	-5.39	113.36	123.85
7	L	501	U10	C42-C43-C44	5.35	145.47	127.64
6	L	401	BPH	C1-O2A-CGA	-5.28	103.87	116.65
5	M	1301	BCL	C4A-NA-C1A	5.11	109.01	106.68
5	L	1302	BCL	O2A-CGA-O1A	-4.99	111.15	123.63
5	L	1302	BCL	O2D-CGD-CBD	4.98	119.93	111.23
9	M	600	SPN	C3-C4-C5	-4.96	118.28	126.83
5	L	1304	BCL	O1D-CGD-CBD	-4.95	114.75	124.52
9	M	600	SPN	C14-C13-C12	-4.86	110.26	121.17
5	L	1304	BCL	CAC-C3C-C4C	-4.81	101.91	112.58
7	M	502	U10	C27-C28-C29	-4.76	116.74	127.62
6	L	401	BPH	O2A-CGA-O1A	-4.76	111.73	123.63
9	M	600	SPN	C6-C5-C4	-4.74	110.53	121.17
5	L	1304	BCL	O2A-CGA-O1A	-4.70	111.88	123.63
7	L	501	U10	C20-C19-C18	4.68	163.06	126.43
6	M	402	BPH	OBB-CAB-C3B	4.51	127.53	119.99
6	M	402	BPH	C4C-C3C-C2C	4.46	107.09	102.84
6	M	402	BPH	OBD-CAD-C3D	4.40	134.76	127.89
5	M	1303	BCL	C1C-NC-C4C	4.32	108.65	106.68
5	M	1301	BCL	C4-C3-C5	-4.23	107.88	115.23
9	M	600	SPN	C7-C6-C5	4.20	127.11	113.19
5	M	1301	BCL	CAA-C2A-C3A	-4.15	101.79	113.00
6	M	402	BPH	O2A-CGA-CBA	4.14	124.45	111.83
5	M	1301	BCL	CBC-CAC-C3C	-4.14	104.64	113.41
5	M	1301	BCL	O2A-CGA-CBA	4.12	124.39	111.83
9	M	600	SPN	O1-C1-C2	-4.05	100.61	108.90
5	L	1304	BCL	OBB-CAB-C3B	4.02	127.54	120.43
5	M	1301	BCL	C1-O2A-CGA	3.92	126.14	116.65
5	L	1302	BCL	CAB-C3B-C2B	3.89	135.82	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1301	BCL	CMB-C2B-C1B	-3.86	119.54	125.42
7	M	502	U10	C20-C19-C21	-3.85	108.55	115.23
5	M	1301	BCL	CAC-C3C-C4C	-3.84	104.07	112.58
9	M	600	SPN	CM4-C9-C10	3.82	121.85	115.23
7	L	501	U10	C3M-O3-C3	3.77	129.72	116.47
9	M	600	SPN	C20-C19-C18	-3.73	119.08	127.62
9	M	600	SPN	C16-C17-C18	3.68	122.43	113.47
9	M	600	SPN	CM7-C22-C21	3.64	124.27	111.27
9	M	600	SPN	C17-C18-C19	-3.60	113.09	121.17
6	L	401	BPH	C4A-C3A-C2A	3.59	106.25	102.84
7	L	501	U10	C7-C8-C9	3.58	133.00	126.83
5	M	1303	BCL	OBB-CAB-C3B	3.48	126.58	120.43
5	L	1302	BCL	O2D-CGD-O1D	-3.41	117.20	123.85
6	L	401	BPH	O2A-CGA-CBA	3.41	122.24	111.83
6	L	401	BPH	C4D-CHA-CBD	-3.40	106.82	108.45
7	L	501	U10	C35-C34-C36	-3.39	109.34	115.23
5	M	1301	BCL	CHB-C1B-NB	3.37	129.11	124.05
6	L	401	BPH	C1B-NB-C4B	-3.33	103.97	108.82
5	L	1304	BCL	C2D-C1D-ND	3.32	113.41	110.13
5	M	1301	BCL	C2C-C3C-C4C	3.30	106.29	101.34
9	M	600	SPN	C15-C14-C13	3.30	121.50	113.47
5	L	1302	BCL	C2A-C3A-C4A	3.29	107.19	101.87
5	M	1301	BCL	O2D-CGD-CBD	3.25	116.91	111.23
5	L	1302	BCL	C2C-C3C-C4C	3.25	106.20	101.34
7	L	501	U10	C31-C29-C28	3.24	128.44	121.17
6	M	402	BPH	C4-C3-C5	-3.23	109.63	115.23
5	L	1304	BCL	C1D-ND-C4D	-3.19	104.07	106.31
5	L	1302	BCL	CAC-C3C-C4C	-3.13	105.64	112.58
6	M	402	BPH	C4-C3-C2	-3.07	115.73	123.63
9	M	600	SPN	C16-C15-C14	3.06	124.37	113.13
5	L	1304	BCL	CAA-C2A-C3A	-3.04	104.79	113.00
7	L	501	U10	C1M-C1-C6	-3.02	119.49	124.45
7	M	502	U10	C12-C13-C14	3.01	134.52	127.62
7	L	501	U10	O2-C2-C3	-3.00	114.68	121.03
5	M	1303	BCL	OBB-CAB-CBB	-2.98	113.09	119.77
5	L	1302	BCL	CBA-CAA-C2A	2.95	122.56	113.79
7	L	501	U10	C40-C39-C38	-2.94	116.07	123.63
10	M	800	CDL	CA4-OA6-CA5	-2.94	110.77	117.80
5	M	1303	BCL	O2D-CGD-CBD	2.93	116.36	111.23
5	M	1303	BCL	O2A-CGA-CBA	2.91	120.71	111.83
9	M	600	SPN	C15-C16-C17	2.90	123.80	113.13
6	M	402	BPH	CAA-C2A-C3A	-2.90	105.16	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	401	BPH	C2B-C1B-NB	2.86	111.50	109.43
5	L	1302	BCL	CHC-C4B-NB	2.85	128.33	124.05
5	L	1304	BCL	C6-C5-C3	-2.85	106.52	113.47
5	M	1301	BCL	O2A-CGA-O1A	-2.83	116.54	123.63
5	M	1301	BCL	CAB-C3B-C2B	2.83	133.62	127.74
7	M	502	U10	C25-C24-C23	2.82	130.86	123.63
5	M	1303	BCL	CAC-C3C-C4C	-2.79	106.39	112.58
6	L	401	BPH	CMA-C3A-C2A	-2.73	103.57	114.13
5	L	1302	BCL	CMA-C3A-C2A	-2.70	103.53	113.98
6	M	402	BPH	CMA-C3A-C2A	-2.70	103.69	114.13
7	M	502	U10	C20-C19-C18	2.68	130.50	123.63
5	M	1303	BCL	C5-C3-C2	2.65	127.12	121.17
5	L	1304	BCL	C2A-C3A-C4A	2.65	106.15	101.87
5	M	1301	BCL	OBB-CAB-C3B	2.65	125.11	120.43
5	M	1301	BCL	C4-C3-C2	2.65	130.42	123.63
5	L	1302	BCL	CHC-C1C-NC	2.64	128.20	124.40
5	L	1304	BCL	CAA-CBA-CGA	2.62	120.66	113.21
6	M	402	BPH	C6-C5-C3	-2.62	107.10	113.47
5	M	1303	BCL	CHB-C1B-NB	2.60	127.94	124.05
7	L	501	U10	C30-C29-C28	-2.57	117.02	123.63
7	L	501	U10	C12-C13-C14	-2.56	121.76	127.62
5	L	1304	BCL	CMB-C2B-C1B	-2.56	121.52	125.42
6	L	401	BPH	OBB-CAB-C3B	2.56	124.26	119.99
7	L	501	U10	O5-C5-C6	-2.55	116.85	121.79
7	M	502	U10	C6-C1-C2	2.55	121.18	119.17
5	L	1304	BCL	CHB-C1B-NB	2.54	127.87	124.05
6	M	402	BPH	C4A-C3A-C2A	2.53	105.25	102.84
4	M	702	LDA	CM2-N1-C1	-2.53	104.93	110.23
5	L	1304	BCL	O2A-CGA-CBA	2.50	119.45	111.83
6	L	401	BPH	C1C-C2C-C3C	2.50	105.22	102.84
5	L	1304	BCL	C2C-C3C-C4C	2.50	105.08	101.34
7	L	501	U10	C36-C34-C33	2.49	126.76	121.17
5	M	1301	BCL	CMB-C2B-C3B	2.48	133.50	125.67
5	M	1303	BCL	O1D-CGD-CBD	-2.48	119.63	124.52
5	L	1304	BCL	C4D-CHA-C1A	2.46	124.18	121.24
6	M	402	BPH	C1-O2A-CGA	2.44	122.55	116.65
4	H	701	LDA	CM1-N1-C1	-2.44	105.11	110.23
5	L	1302	BCL	O1D-CGD-CBD	-2.43	119.73	124.52
5	M	1303	BCL	O2A-CGA-O1A	-2.42	117.57	123.63
6	L	401	BPH	C4D-ND-C1D	-2.41	105.99	108.87
5	L	1304	BCL	OBB-CAB-CBB	-2.37	114.45	119.77
9	M	600	SPN	C10-C9-C8	-2.37	115.85	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	800	CDL	OB8-CB7-OB9	-2.36	117.73	123.63
7	L	501	U10	C41-C39-C38	2.35	126.44	121.17
5	M	1301	BCL	CAA-CBA-CGA	2.32	119.81	113.21
6	L	401	BPH	C2D-C1D-ND	2.32	111.11	109.43
5	M	1301	BCL	CBB-CAB-C3B	-2.28	115.59	120.40
7	L	501	U10	C6-C1-C2	2.28	120.97	119.17
5	M	1303	BCL	C2A-C3A-C4A	2.27	105.54	101.87
7	M	502	U10	C25-C24-C26	-2.24	111.34	115.23
6	M	402	BPH	C1B-NB-C4B	-2.24	105.56	108.82
5	M	1303	BCL	C2C-C3C-C4C	2.23	104.69	101.34
10	M	800	CDL	OA6-CA5-C11	2.20	116.25	111.48
5	M	1303	BCL	CAA-C2A-C3A	-2.19	107.08	113.00
5	L	1302	BCL	CMA-C3A-C4A	-2.19	105.89	111.77
7	L	501	U10	C15-C14-C13	-2.19	118.01	123.63
7	M	502	U10	C27-C26-C24	-2.18	105.95	113.19
5	M	1303	BCL	C1D-ND-C4D	-2.18	104.78	106.31
5	M	1301	BCL	C2A-C3A-C4A	2.16	105.36	101.87
5	M	1303	BCL	C6-C7-C8	2.16	123.15	115.97
5	L	1302	BCL	CHC-C4B-C3B	-2.15	123.16	131.72
5	L	1302	BCL	CMC-C2C-C1C	-2.15	106.00	111.77
5	M	1301	BCL	CHA-C1A-NA	-2.13	121.57	126.39
7	M	502	U10	C22-C21-C19	-2.12	106.15	113.19
5	M	1301	BCL	C3C-C2C-C1C	2.11	105.28	101.87
5	L	1302	BCL	C3C-C2C-C1C	2.11	105.28	101.87
9	M	600	SPN	CM6-C18-C19	-2.11	118.21	123.63
5	L	1304	BCL	CAB-C3B-C2B	2.11	132.12	127.74
5	L	1302	BCL	CMD-C2D-C3D	2.10	132.50	127.69
7	L	501	U10	C4M-O4-C4	2.10	123.84	116.47
5	L	1304	BCL	CMA-C3A-C2A	-2.10	105.88	113.98
5	M	1303	BCL	C3C-C2C-C1C	2.07	105.22	101.87
5	M	1303	BCL	CHA-C1A-NA	-2.06	121.72	126.39
5	L	1304	BCL	CMC-C2C-C3C	-2.06	106.02	113.98
6	M	402	BPH	O1A-CGA-CBA	-2.06	115.73	123.78
4	M	703	LDA	CM1-N1-C1	-2.05	105.93	110.23
5	M	1303	BCL	C2D-C1D-ND	2.04	112.14	110.13
5	M	1301	BCL	CMA-C3A-C2A	-2.03	106.11	113.98
7	M	502	U10	C4M-O4-C4	2.03	123.61	116.47
6	M	402	BPH	CED-O2D-CGD	2.03	120.52	115.92
5	M	1301	BCL	CMC-C2C-C3C	-2.03	106.14	113.98
6	M	402	BPH	C11-C12-C13	-2.02	109.24	115.97
5	L	1304	BCL	CHD-C1D-ND	-2.00	121.99	124.80
7	M	502	U10	C30-C29-C31	2.00	118.70	115.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1301	BCL	C13
6	L	401	BPH	C8
6	L	401	BPH	C13

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	701	LDA	C2-C1-N1-O1
4	H	701	LDA	C2-C1-N1-CM2
4	H	701	LDA	N1-C1-C2-C3
4	M	702	LDA	C2-C1-N1-O1
4	M	702	LDA	C2-C1-N1-CM1
4	M	702	LDA	C2-C1-N1-CM2
4	M	702	LDA	N1-C1-C2-C3
4	M	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
5	L	1304	BCL	C2C-C3C-CAC-CBC
5	M	1301	BCL	C1-C2-C3-C4
5	M	1301	BCL	C1-C2-C3-C5
5	M	1301	BCL	C11-C12-C13-C15
6	L	401	BPH	C4C-C3C-CAC-CBC
6	L	401	BPH	O2A-C1-C2-C3
7	L	501	U10	C17-C18-C19-C20
7	L	501	U10	C29-C31-C32-C33
7	L	501	U10	C36-C37-C38-C39
7	L	501	U10	C41-C42-C43-C44
9	M	600	SPN	CM1-C1-O1-CMA
9	M	600	SPN	C11-C12-C13-C14
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA4
10	M	800	CDL	CA2-OA2-PA1-OA5
9	M	600	SPN	CM3-C5-C6-C7
9	M	600	SPN	C11-C10-C9-CM4
9	M	600	SPN	CM5-C13-C14-C15
9	M	600	SPN	C16-C17-C18-CM6
9	M	600	SPN	C14-C15-C16-C17
6	M	402	BPH	C4-C3-C5-C6
6	M	402	BPH	C2-C3-C5-C6
9	M	600	SPN	C4-C5-C6-C7
9	M	600	SPN	C11-C10-C9-C8
9	M	600	SPN	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	M	600	SPN	C16-C17-C18-C19
7	L	501	U10	C9-C11-C12-C13
7	L	501	U10	C34-C36-C37-C38
7	M	502	U10	C24-C26-C27-C28
5	L	1302	BCL	C6-C7-C8-C9
5	M	1301	BCL	C14-C13-C15-C16
6	L	401	BPH	C14-C13-C15-C16
6	M	402	BPH	C6-C7-C8-C9
10	M	800	CDL	C31-CA7-OA8-CA6
5	M	1301	BCL	C6-C7-C8-C10
6	L	401	BPH	C11-C10-C8-C7
6	M	402	BPH	C12-C13-C15-C16
7	M	502	U10	C29-C31-C32-C33
10	M	800	CDL	CB7-C71-C72-C73
6	M	402	BPH	C15-C16-C17-C18
10	M	800	CDL	OA9-CA7-OA8-CA6
10	M	800	CDL	CA7-C31-C32-C33
5	M	1301	BCL	C5-C6-C7-C8
5	M	1301	BCL	C8-C10-C11-C12
5	M	1301	BCL	C13-C15-C16-C17
10	M	800	CDL	CA5-C11-C12-C13
6	M	402	BPH	O1A-CGA-O2A-C1
6	M	402	BPH	CBA-CGA-O2A-C1
5	M	1301	BCL	C2-C1-O2A-CGA
10	M	800	CDL	C11-C12-C13-C14
10	M	800	CDL	C78-C79-C80-C81
10	M	800	CDL	C79-C80-C81-C82
4	M	702	LDA	C6-C7-C8-C9
6	M	402	BPH	O1D-CGD-O2D-CED
10	M	800	CDL	C51-C52-C53-C54
4	M	702	LDA	C11-C10-C9-C8
4	M	702	LDA	C7-C8-C9-C10
5	L	1304	BCL	C3-C5-C6-C7
4	M	702	LDA	C5-C6-C7-C8
10	M	800	CDL	C39-C40-C41-C42
4	H	701	LDA	C4-C5-C6-C7
10	M	800	CDL	C52-C53-C54-C55
10	M	800	CDL	C21-C22-C23-C24
4	M	703	LDA	C6-C7-C8-C9
4	H	701	LDA	C1-C2-C3-C4
9	M	600	SPN	C26-C27-C28-C29
6	L	401	BPH	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	L	501	U10	C13-C14-C16-C17
4	M	703	LDA	C3-C4-C5-C6
5	L	1302	BCL	C2A-CAA-CBA-CGA
10	M	800	CDL	C37-C38-C39-C40
7	L	501	U10	C40-C39-C41-C42
7	M	502	U10	C30-C29-C31-C32
7	M	502	U10	C28-C29-C31-C32
5	L	1304	BCL	C6-C7-C8-C9
4	M	703	LDA	C1-C2-C3-C4
4	H	701	LDA	C5-C6-C7-C8
7	L	501	U10	C15-C14-C16-C17
7	L	501	U10	C38-C39-C41-C42
5	L	1302	BCL	C15-C16-C17-C18
6	L	401	BPH	C8-C10-C11-C12
6	L	401	BPH	C10-C11-C12-C13
4	H	701	LDA	C6-C7-C8-C9
4	M	702	LDA	C2-C3-C4-C5
4	M	703	LDA	C11-C10-C9-C8
4	M	702	LDA	C9-C10-C11-C12
10	M	800	CDL	C81-C82-C83-C84
6	L	401	BPH	C5-C6-C7-C8
6	L	401	BPH	C4-C3-C5-C6
6	L	401	BPH	C2-C3-C5-C6
9	M	600	SPN	CM2-C1-C2-O2
9	M	600	SPN	CM2-C1-C2-C3
10	M	800	CDL	CB3-CB4-CB6-OB8
10	M	800	CDL	C71-C72-C73-C74
5	M	1301	BCL	C15-C16-C17-C18
5	L	1302	BCL	CBD-CGD-O2D-CED
10	M	800	CDL	OB6-CB4-CB6-OB8
5	M	1301	BCL	C11-C12-C13-C14
5	M	1303	BCL	C5-C6-C7-C8
5	L	1304	BCL	C13-C15-C16-C17
5	L	1302	BCL	C11-C12-C13-C15
4	M	702	LDA	C1-C2-C3-C4
10	M	800	CDL	C53-C54-C55-C56
10	M	800	CDL	C40-C41-C42-C43
10	M	800	CDL	OA5-CA3-CA4-OA6
9	M	600	SPN	C9-C10-C11-C12
4	H	701	LDA	C2-C3-C4-C5
10	M	800	CDL	C35-C36-C37-C38
4	H	701	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
5	L	1302	BCL	C13-C15-C16-C17
5	M	1303	BCL	C16-C17-C18-C19
10	M	800	CDL	C36-C37-C38-C39
6	L	401	BPH	C11-C10-C8-C9
6	M	402	BPH	C8-C10-C11-C12
7	L	501	U10	C2-C3-O3-C3M
5	L	1304	BCL	CHA-CBD-CGD-O2D
9	M	600	SPN	CM2-C1-O1-CMA
5	L	1304	BCL	O1D-CGD-O2D-CED
6	M	402	BPH	C13-C15-C16-C17
6	M	402	BPH	C11-C10-C8-C9
6	L	401	BPH	C11-C12-C13-C15
6	M	402	BPH	C11-C12-C13-C15
10	M	800	CDL	OA6-CA4-CA6-OA8
10	M	800	CDL	CB5-C51-C52-C53
5	L	1304	BCL	C16-C17-C18-C19
5	L	1302	BCL	C11-C12-C13-C14
10	M	800	CDL	C75-C76-C77-C78
7	M	502	U10	C34-C36-C37-C38
6	M	402	BPH	C5-C6-C7-C8
4	M	703	LDA	C9-C10-C11-C12
4	M	702	LDA	C4-C5-C6-C7
5	M	1301	BCL	C3-C5-C6-C7
7	M	502	U10	C5-C4-O4-C4M
6	M	402	BPH	C14-C13-C15-C16
10	M	800	CDL	C80-C81-C82-C83
7	L	501	U10	C30-C29-C31-C32
4	H	701	LDA	C3-C4-C5-C6
6	L	401	BPH	C12-C13-C15-C16
6	M	402	BPH	C6-C7-C8-C10
6	M	402	BPH	C11-C10-C8-C7
5	M	1301	BCL	O1A-CGA-O2A-C1
7	L	501	U10	C28-C29-C31-C32
9	M	600	SPN	C2-C3-C4-C5
10	M	800	CDL	OA5-CA3-CA4-CA6
6	M	402	BPH	C2-C1-O2A-CGA
5	M	1301	BCL	CBA-CGA-O2A-C1
7	L	501	U10	C4-C3-O3-C3M
5	L	1302	BCL	C11-C10-C8-C7
5	M	1301	BCL	C12-C13-C15-C16
5	M	1303	BCL	C11-C12-C13-C15
7	L	501	U10	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	M	800	CDL	C32-C31-CA7-OA8
4	H	701	LDA	C7-C8-C9-C10
5	L	1304	BCL	C16-C17-C18-C20
10	M	800	CDL	C72-C71-CB7-OB8
4	H	701	LDA	C11-C10-C9-C8
5	M	1303	BCL	CAA-CBA-CGA-O2A
9	M	600	SPN	C6-C7-C8-C9
5	L	1304	BCL	C12-C13-C15-C16
6	M	402	BPH	O2A-C1-C2-C3
10	M	800	CDL	C72-C71-CB7-OB9
9	M	600	SPN	C18-C19-C20-C21
10	M	800	CDL	C32-C31-CA7-OA9
5	M	1301	BCL	C6-C7-C8-C9
10	M	800	CDL	C19-C20-C21-C22
6	L	401	BPH	C1-C2-C3-C4

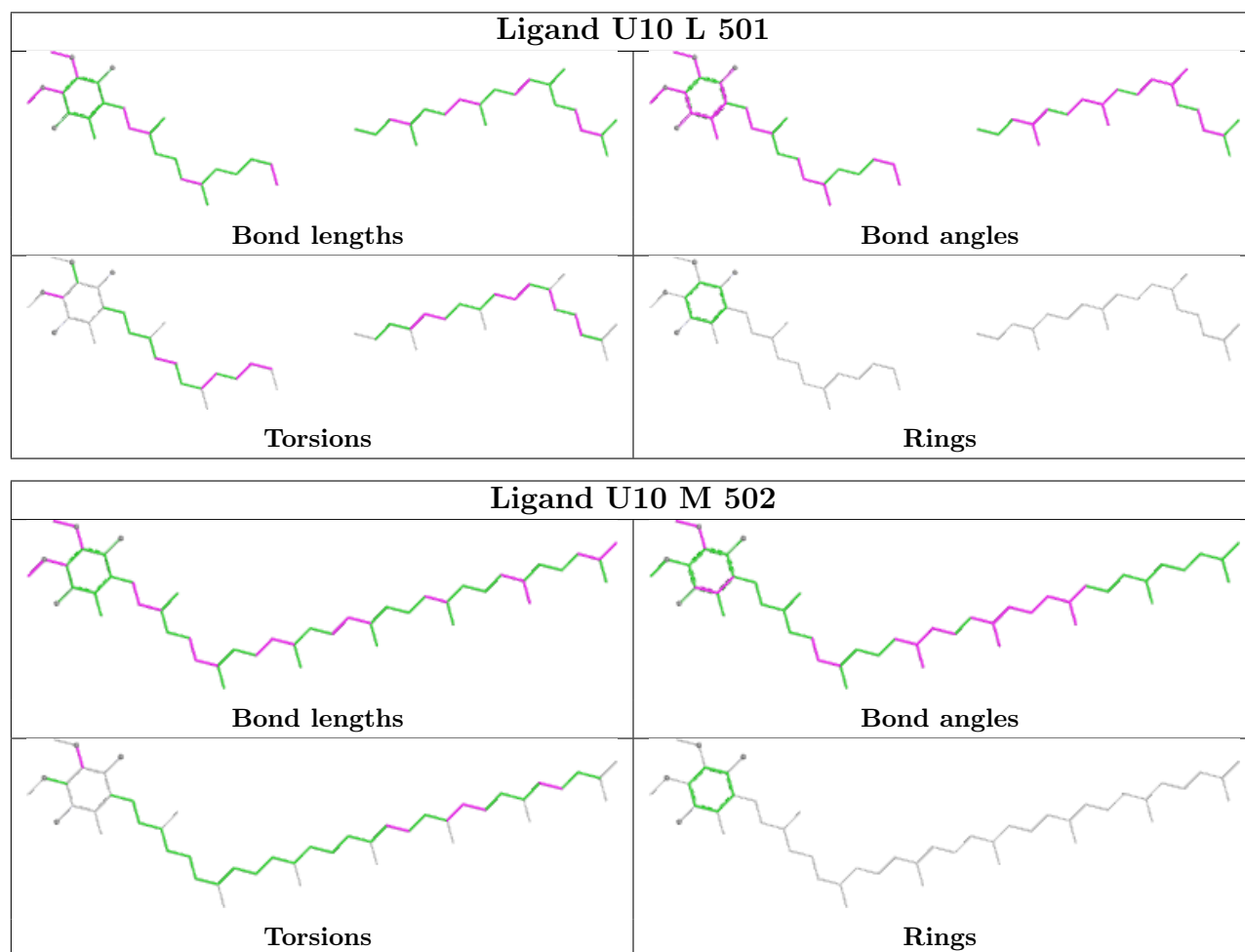
There are no ring outliers.

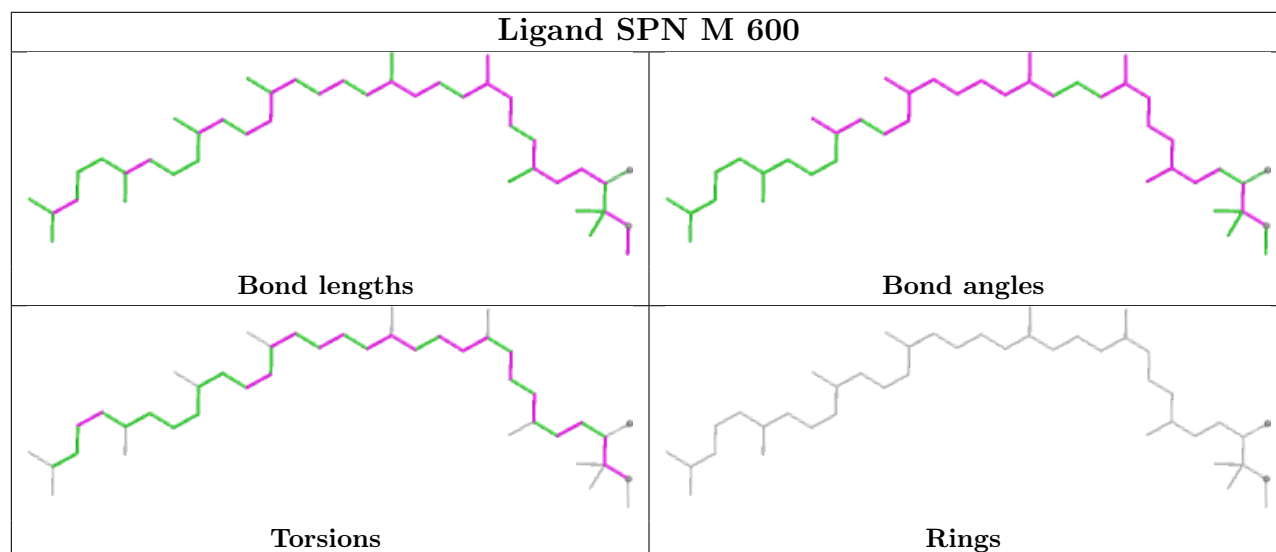
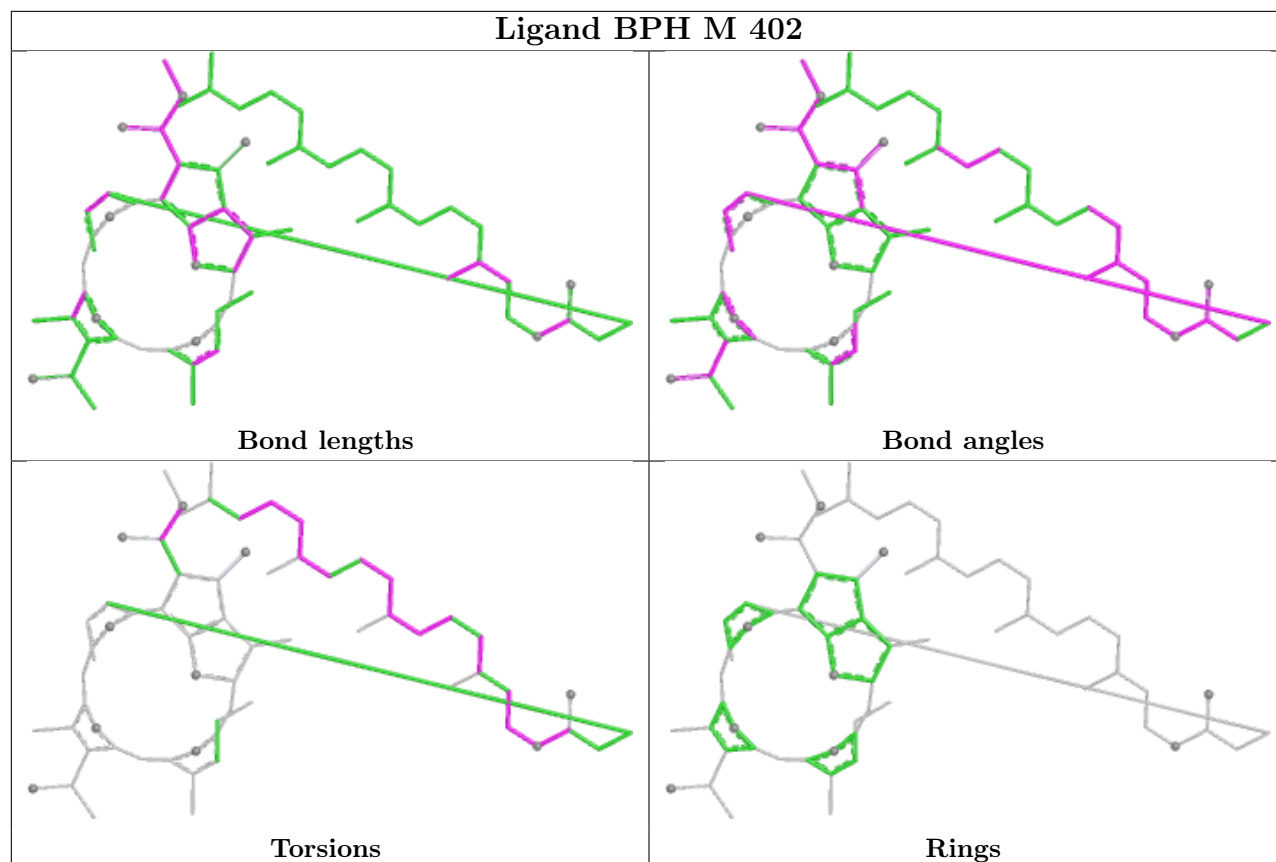
11 monomers are involved in 60 short contacts:

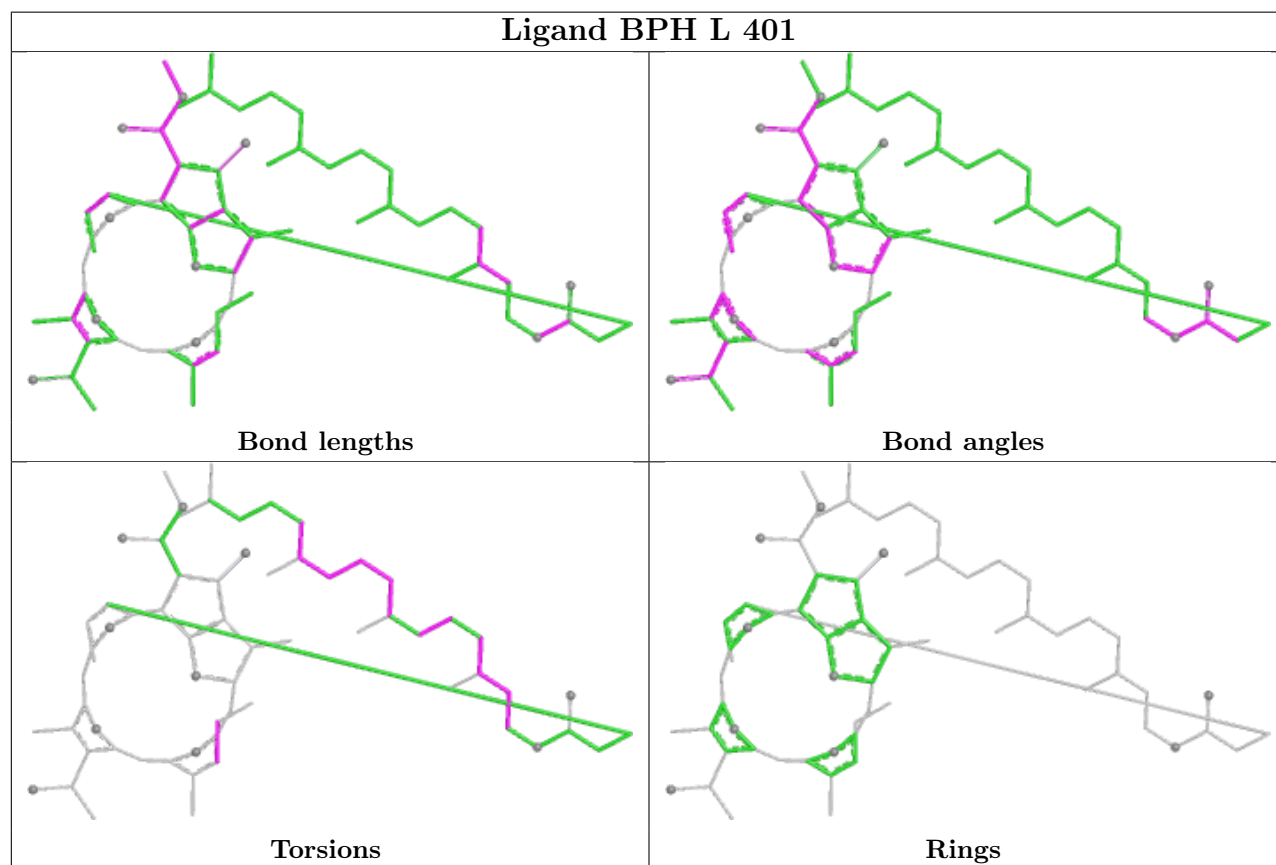
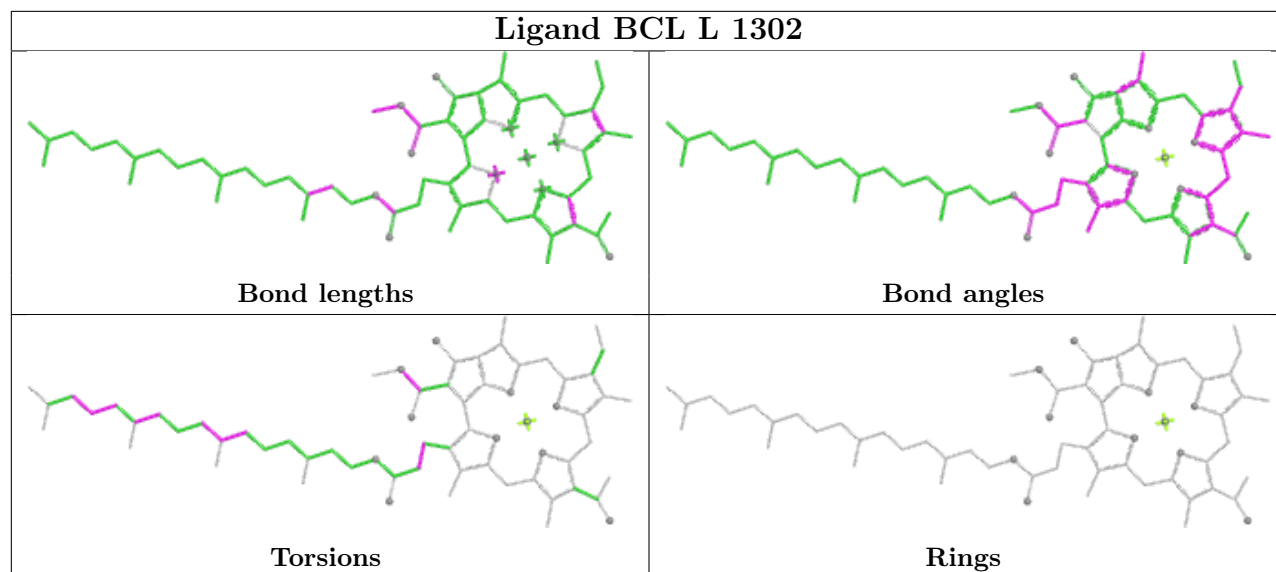
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	703	LDA	2	0
7	L	501	U10	1	0
6	M	402	BPH	5	0
9	M	600	SPN	5	0
5	L	1302	BCL	7	0
6	L	401	BPH	12	0
5	M	1301	BCL	5	0
5	L	1304	BCL	6	0
10	M	800	CDL	16	0
4	M	702	LDA	3	0
5	M	1303	BCL	5	0

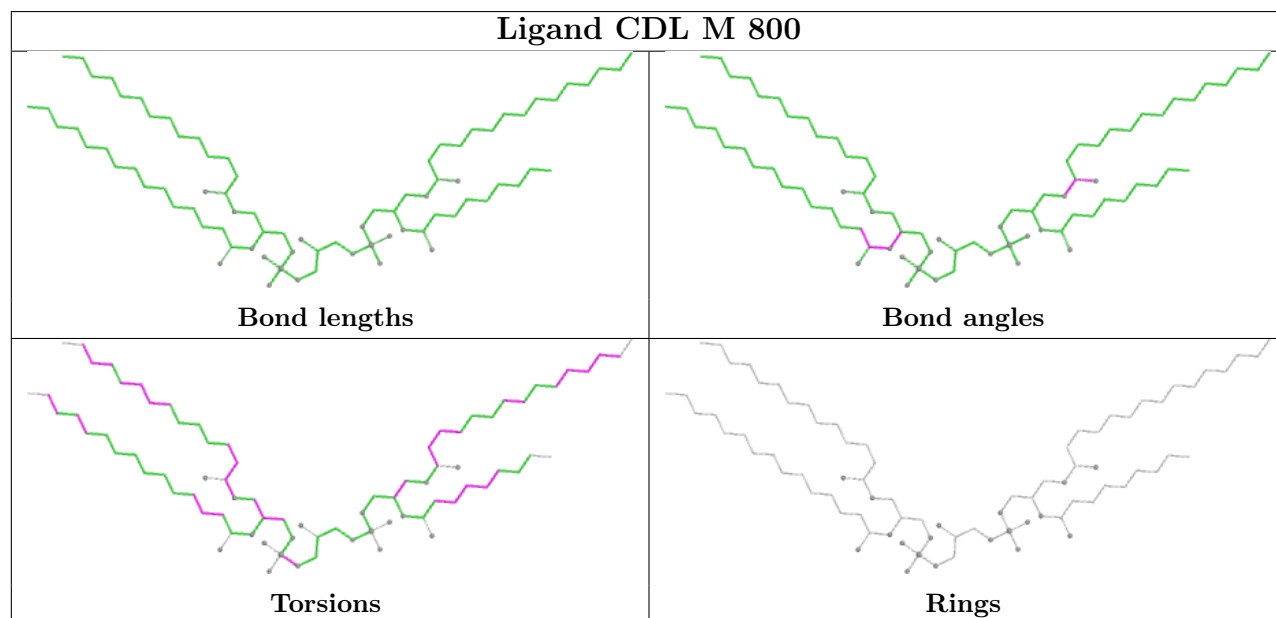
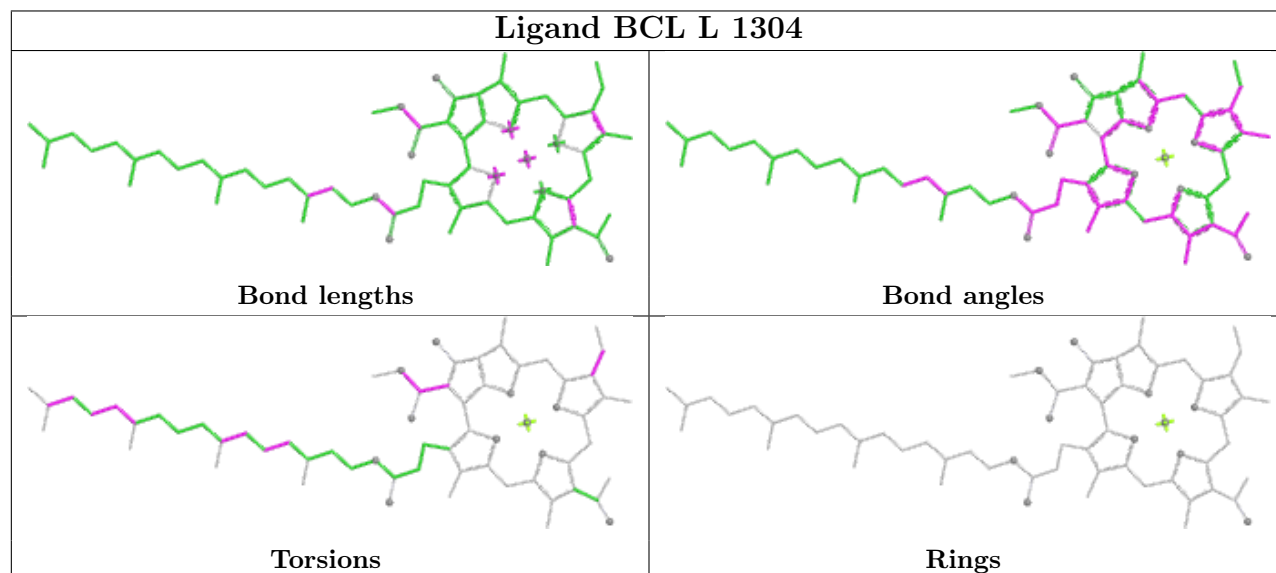
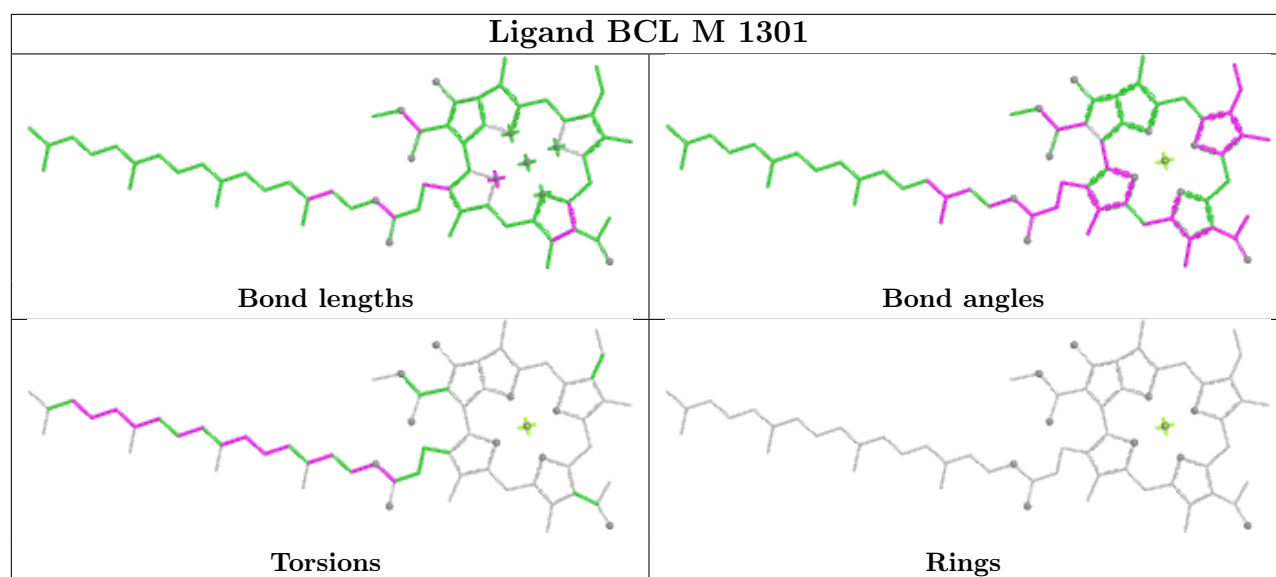
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

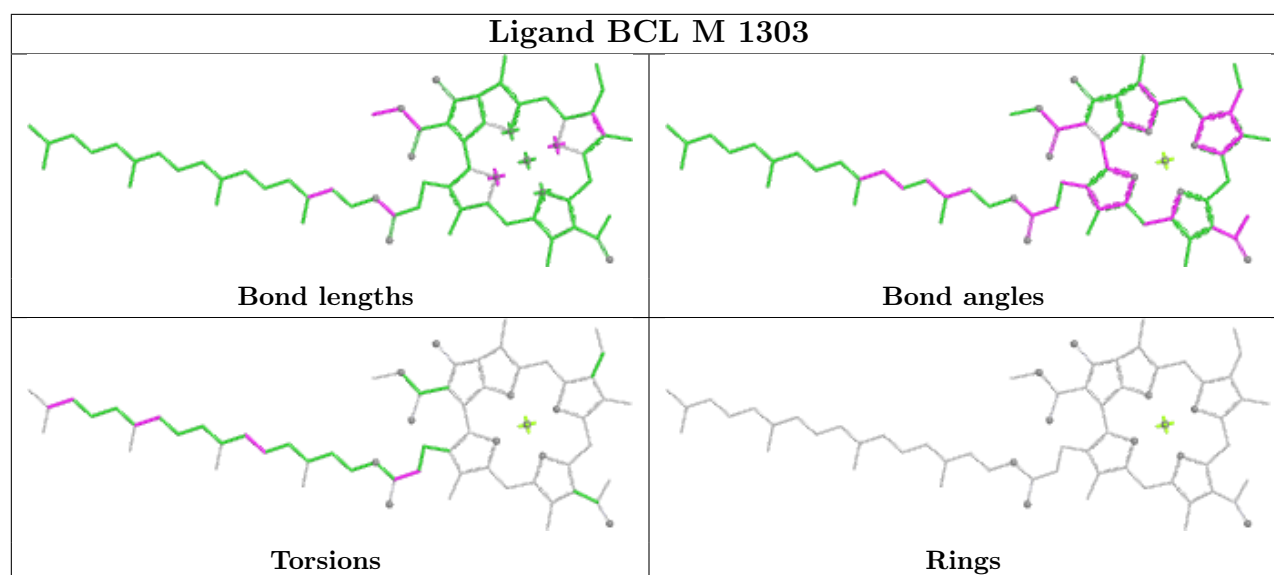
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.