



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:05 PM UTC

PDB ID : 1BFR / pdb_00001bfr
Title : IRON STORAGE AND ELECTRON TRANSPORT
Authors : Dautant, A.; Yariv, J.; Meyer, J.B.; Precigoux, G.; Sweet, R.M.; Frolow, F.; Kalb(Gilboa), A.J.
Deposited on : 1994-12-16
Resolution : 2.94 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

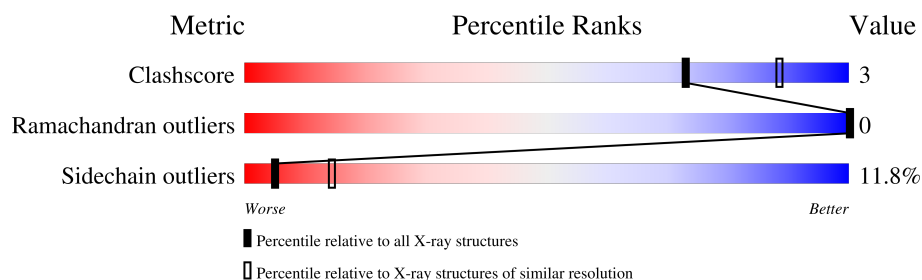
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)

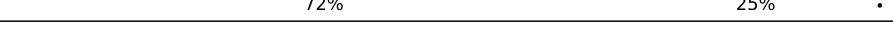
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	A	158	73% 24% .
1	B	158	72% 25% .
1	C	158	70% 27% .
1	D	158	72% 25% .
1	E	158	68% 27% .
1	F	158	77% 20% .
1	G	158	67% 29% .
1	H	158	72% 25% .

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Mol	Chain	Length	Quality of chain
1	I	158	 68% 28% .
1	J	158	 75% 23% .
1	K	158	 68% 28% .
1	L	158	 72% 25% .
1	M	158	 68% 28% .
1	N	158	 72% 25% .
1	O	158	 68% 28% .
1	P	158	 70% 27% .
1	Q	158	 68% 28% .
1	R	158	 72% 25% .
1	S	158	 67% 29% .
1	T	158	 72% 25% .
1	U	158	 67% 29% .
1	V	158	 72% 25% .
1	W	158	 68% 28% .
1	X	158	 73% 24% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31740 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 BACTERIOFERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	B	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	C	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	D	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	E	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	F	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	G	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	H	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	I	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	J	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	K	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	L	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	M	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	N	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	O	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	P	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	R	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	S	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	T	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	U	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	V	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	W	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			
1	X	158	Total	C	N	O	S	0	0	0
			1299	818	222	252	7			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

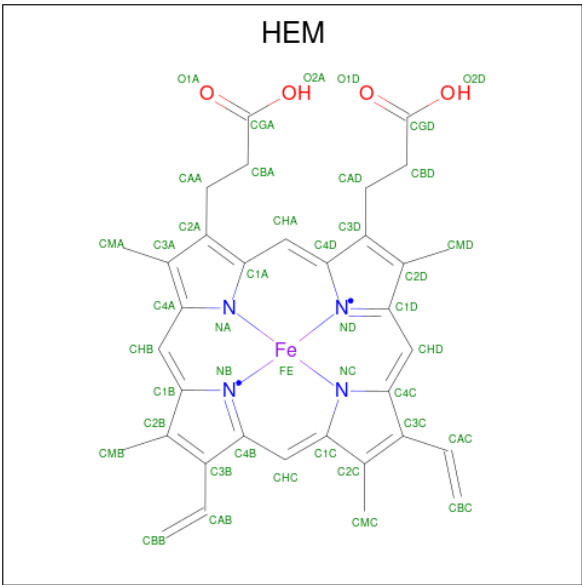
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		
2	G	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	2	Total 2	Mn 2	0	0
2	M	2	Total 2	Mn 2	0	0
2	N	2	Total 2	Mn 2	0	0
2	O	2	Total 2	Mn 2	0	0
2	P	2	Total 2	Mn 2	0	0
2	Q	2	Total 2	Mn 2	0	0
2	R	2	Total 2	Mn 2	0	0
2	S	2	Total 2	Mn 2	0	0
2	T	2	Total 2	Mn 2	0	0
2	U	2	Total 2	Mn 2	0	0
2	V	2	Total 2	Mn 2	0	0
2	W	2	Total 2	Mn 2	0	0
2	X	2	Total 2	Mn 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

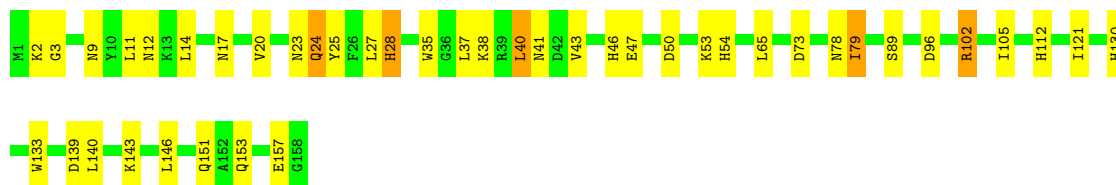
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

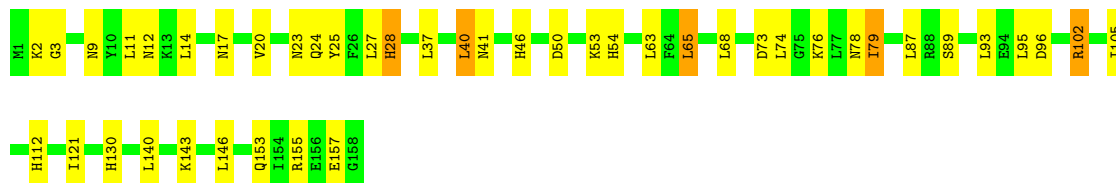
• Molecule 1: BACTERIOFERRITIN

Chain A: 



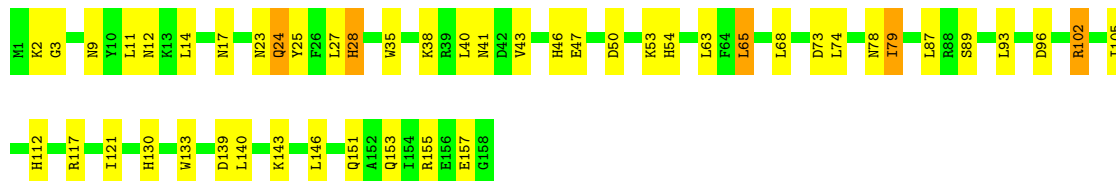
• Molecule 1: BACTERIOFERRITIN

Chain B: 



• Molecule 1: BACTERIOFERRITIN

Chain C: 



• Molecule 1: BACTERIOFERRITIN

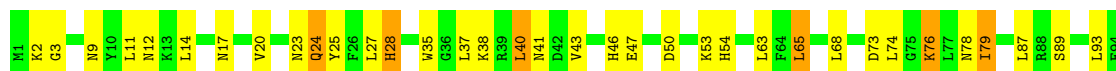
Chain D: 





- Molecule 1: BACTERIOFERRITIN

Chain E: 68% 27% .



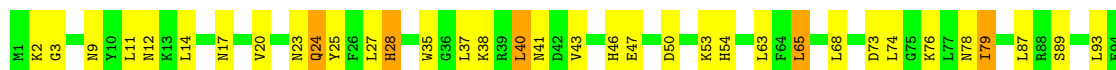
- Molecule 1: BACTERIOFERRITIN

Chain F: 77% 20% .



- Molecule 1: BACTERIOFERRITIN

Chain G: 67% 29% .



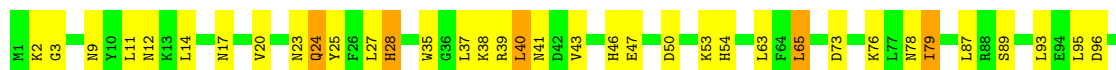
- Molecule 1: BACTERIOFERRITIN

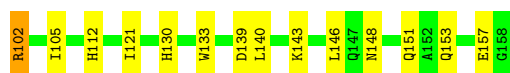
Chain H: 72% 25% .



- Molecule 1: BACTERIOFERRITIN

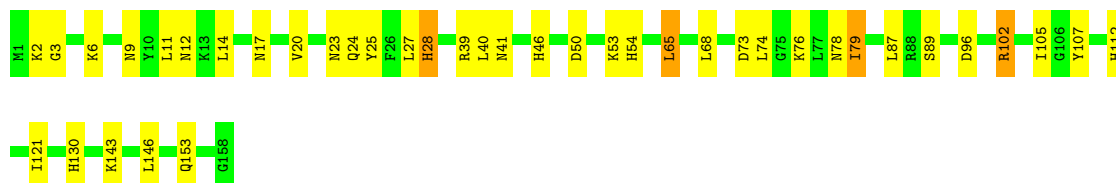
Chain I: 68% 28% .





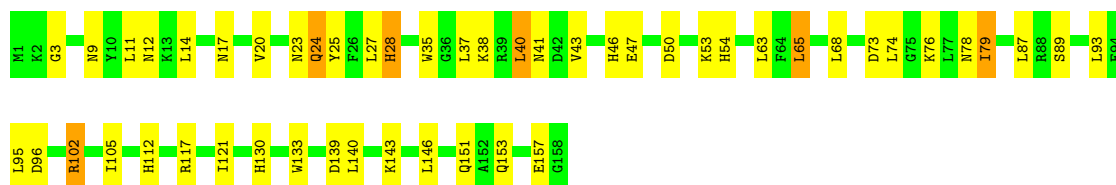
● Molecule 1: BACTERIOFERRITIN

Chain J: 75% 23%



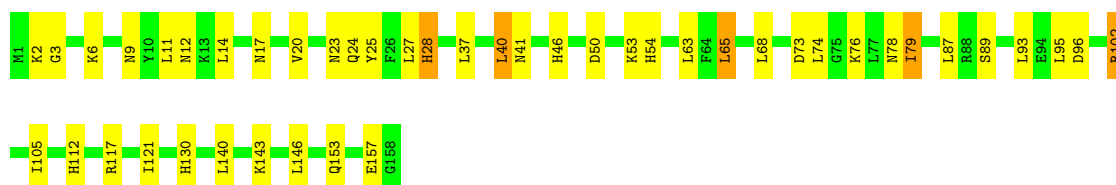
● Molecule 1: BACTERIOFERRITIN

Chain K: 68% 28%



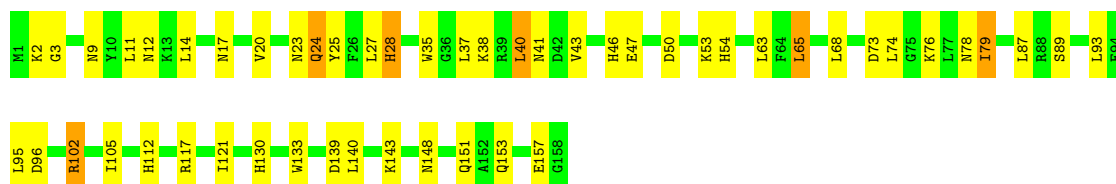
● Molecule 1: BACTERIOFERRITIN

Chain L: 72% 25%



● Molecule 1: BACTERIOFERRITIN

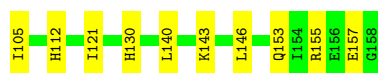
Chain M: 68% 28%



● Molecule 1: BACTERIOFERRITIN

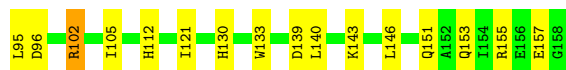
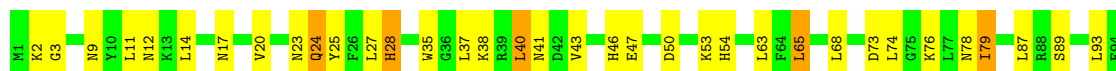
Chain N: 72% 25%





• Molecule 1: BACTERIOFERRITIN

Chain O: 68% 28% .



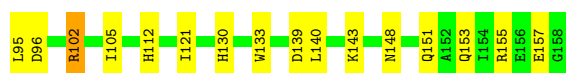
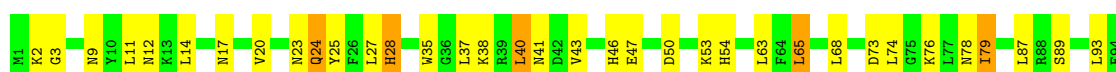
• Molecule 1: BACTERIOFERRITIN

Chain P: 70% 27% .



• Molecule 1: BACTERIOFERRITIN

Chain Q: 68% 28% .



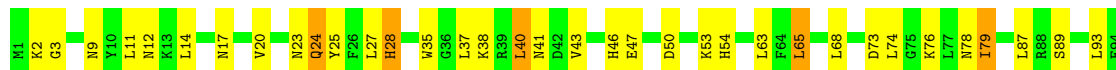
• Molecule 1: BACTERIOFERRITIN

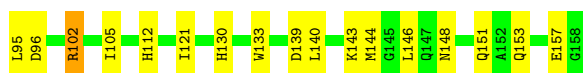
Chain R: 72% 25% .



• Molecule 1: BACTERIOFERRITIN

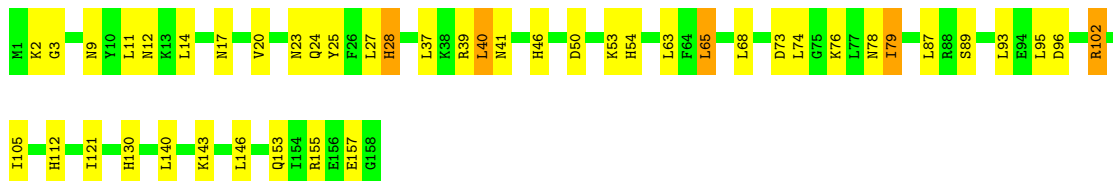
Chain S: 67% 29% .





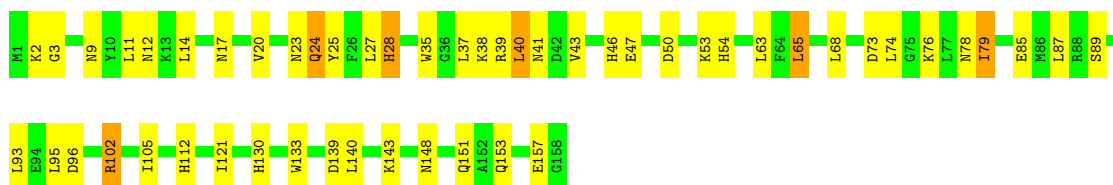
• Molecule 1: BACTERIOFERRITIN

Chain T: 72% 25%



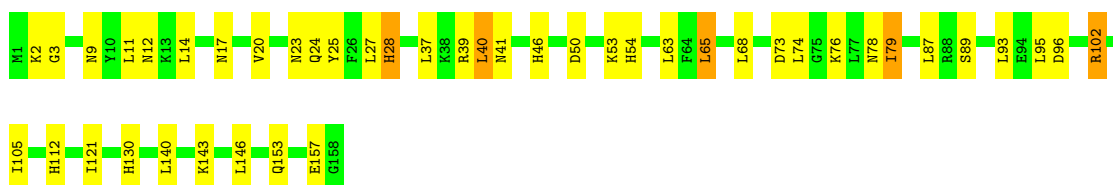
• Molecule 1: BACTERIOFERRITIN

Chain U: 67% 29%



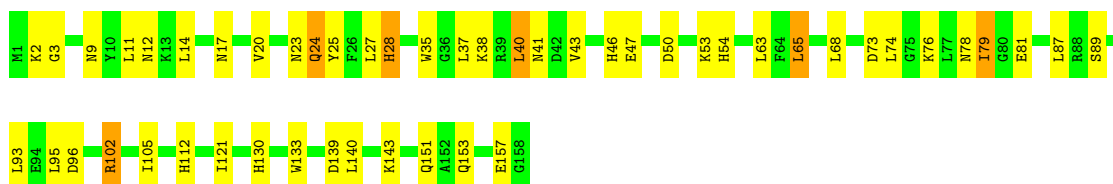
• Molecule 1: BACTERIOFERRITIN

Chain V: 72% 25%



• Molecule 1: BACTERIOFERRITIN

Chain W: 68% 28%



• Molecule 1: BACTERIOFERRITIN

Chain X: 73% 24%



H112	I121	H130	L140	K143	L146	Q153	E157	G158
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.70Å 211.60Å 123.30Å 90.00° 119.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.94	Depositor
% Data completeness (in resolution range)	83.6 (10.00-2.94)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31740	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: HEM, MN

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	A	1.07	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	B	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	C	1.07	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	D	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	E	1.08	5/1318 (0.4%)	1.69	23/1770 (1.3%)
1	F	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	G	1.07	5/1318 (0.4%)	1.69	25/1770 (1.4%)
1	H	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	I	1.08	5/1318 (0.4%)	1.69	25/1770 (1.4%)
1	J	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	K	1.07	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	L	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	M	1.08	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	N	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	O	1.07	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	P	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	Q	1.08	5/1318 (0.4%)	1.68	24/1770 (1.4%)
1	R	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	S	1.07	5/1318 (0.4%)	1.69	25/1770 (1.4%)
1	T	1.07	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	U	1.07	5/1318 (0.4%)	1.69	24/1770 (1.4%)
1	V	1.07	5/1318 (0.4%)	1.68	19/1770 (1.1%)
1	W	1.07	5/1318 (0.4%)	1.69	23/1770 (1.3%)
1	X	1.08	5/1318 (0.4%)	1.68	19/1770 (1.1%)
All	All	1.08	120/31632 (0.4%)	1.68	517/42480 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
All	All	0	48

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	28	HIS	CD2-NE2	-7.32	1.29	1.37
1	K	28	HIS	CD2-NE2	-7.32	1.29	1.37
1	M	28	HIS	CD2-NE2	-7.30	1.29	1.37
1	C	28	HIS	CD2-NE2	-7.30	1.29	1.37
1	I	28	HIS	CD2-NE2	-7.30	1.29	1.37
1	U	28	HIS	CD2-NE2	-7.29	1.29	1.37
1	W	28	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	28	HIS	CD2-NE2	-7.28	1.29	1.37
1	C	54	HIS	CD2-NE2	-7.28	1.29	1.37
1	E	28	HIS	CD2-NE2	-7.26	1.29	1.37
1	Q	28	HIS	CD2-NE2	-7.25	1.29	1.37
1	J	28	HIS	CD2-NE2	-7.21	1.29	1.37
1	O	28	HIS	CD2-NE2	-7.21	1.29	1.37
1	Q	54	HIS	CD2-NE2	-7.21	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	54	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	54	HIS	CD2-NE2	-7.19	1.29	1.37
1	S	54	HIS	CD2-NE2	-7.19	1.29	1.37
1	O	54	HIS	CD2-NE2	-7.18	1.29	1.37
1	I	54	HIS	CD2-NE2	-7.18	1.29	1.37
1	S	28	HIS	CD2-NE2	-7.18	1.29	1.37
1	M	54	HIS	CD2-NE2	-7.18	1.29	1.37
1	E	54	HIS	CD2-NE2	-7.18	1.29	1.37
1	U	54	HIS	CD2-NE2	-7.17	1.29	1.37
1	D	28	HIS	CD2-NE2	-7.17	1.29	1.37
1	H	28	HIS	CD2-NE2	-7.17	1.29	1.37
1	X	28	HIS	CD2-NE2	-7.16	1.29	1.37
1	B	28	HIS	CD2-NE2	-7.14	1.29	1.37
1	N	28	HIS	CD2-NE2	-7.13	1.30	1.37
1	P	28	HIS	CD2-NE2	-7.13	1.30	1.37
1	K	54	HIS	CD2-NE2	-7.13	1.30	1.37
1	R	28	HIS	CD2-NE2	-7.12	1.30	1.37
1	G	54	HIS	CD2-NE2	-7.12	1.30	1.37
1	V	28	HIS	CD2-NE2	-7.12	1.30	1.37
1	T	28	HIS	CD2-NE2	-7.11	1.30	1.37
1	F	28	HIS	CD2-NE2	-7.11	1.30	1.37
1	L	28	HIS	CD2-NE2	-7.10	1.30	1.37
1	E	112	HIS	CD2-NE2	-6.70	1.30	1.37
1	I	112	HIS	CD2-NE2	-6.66	1.30	1.37
1	J	54	HIS	CD2-NE2	-6.66	1.30	1.37
1	S	112	HIS	CD2-NE2	-6.66	1.30	1.37
1	X	54	HIS	CD2-NE2	-6.66	1.30	1.37
1	V	54	HIS	CD2-NE2	-6.65	1.30	1.37
1	P	54	HIS	CD2-NE2	-6.65	1.30	1.37
1	L	54	HIS	CD2-NE2	-6.65	1.30	1.37
1	H	54	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	54	HIS	CD2-NE2	-6.64	1.30	1.37
1	T	54	HIS	CD2-NE2	-6.63	1.30	1.37
1	R	54	HIS	CD2-NE2	-6.63	1.30	1.37
1	Q	112	HIS	CD2-NE2	-6.63	1.30	1.37
1	M	112	HIS	CD2-NE2	-6.62	1.30	1.37
1	G	112	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	112	HIS	CD2-NE2	-6.62	1.30	1.37
1	N	54	HIS	CD2-NE2	-6.61	1.30	1.37
1	C	112	HIS	CD2-NE2	-6.60	1.30	1.37
1	F	54	HIS	CD2-NE2	-6.60	1.30	1.37
1	D	54	HIS	CD2-NE2	-6.60	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	112	HIS	CD2-NE2	-6.59	1.30	1.37
1	O	112	HIS	CD2-NE2	-6.58	1.30	1.37
1	U	112	HIS	CD2-NE2	-6.58	1.30	1.37
1	W	112	HIS	CD2-NE2	-6.55	1.30	1.37
1	W	130	HIS	CD2-NE2	-6.51	1.30	1.37
1	G	130	HIS	CD2-NE2	-6.46	1.30	1.37
1	E	130	HIS	CD2-NE2	-6.45	1.30	1.37
1	T	130	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	130	HIS	CD2-NE2	-6.43	1.30	1.37
1	Q	130	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	130	HIS	CD2-NE2	-6.42	1.30	1.37
1	J	112	HIS	CD2-NE2	-6.42	1.30	1.37
1	H	130	HIS	CD2-NE2	-6.41	1.30	1.37
1	O	130	HIS	CD2-NE2	-6.41	1.30	1.37
1	S	130	HIS	CD2-NE2	-6.41	1.30	1.37
1	U	130	HIS	CD2-NE2	-6.41	1.30	1.37
1	K	130	HIS	CD2-NE2	-6.40	1.30	1.37
1	I	130	HIS	CD2-NE2	-6.40	1.30	1.37
1	M	130	HIS	CD2-NE2	-6.40	1.30	1.37
1	F	112	HIS	CD2-NE2	-6.38	1.30	1.37
1	L	130	HIS	CD2-NE2	-6.37	1.30	1.37
1	J	130	HIS	CD2-NE2	-6.37	1.30	1.37
1	R	112	HIS	CD2-NE2	-6.37	1.30	1.37
1	X	130	HIS	CD2-NE2	-6.37	1.30	1.37
1	N	112	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	130	HIS	CD2-NE2	-6.36	1.30	1.37
1	P	112	HIS	CD2-NE2	-6.36	1.30	1.37
1	R	130	HIS	CD2-NE2	-6.36	1.30	1.37
1	T	112	HIS	CD2-NE2	-6.35	1.30	1.37
1	N	130	HIS	CD2-NE2	-6.35	1.30	1.37
1	B	112	HIS	CD2-NE2	-6.35	1.30	1.37
1	V	112	HIS	CD2-NE2	-6.35	1.30	1.37
1	X	112	HIS	CD2-NE2	-6.34	1.30	1.37
1	F	130	HIS	CD2-NE2	-6.34	1.30	1.37
1	L	112	HIS	CD2-NE2	-6.33	1.30	1.37
1	D	130	HIS	CD2-NE2	-6.33	1.30	1.37
1	P	130	HIS	CD2-NE2	-6.32	1.30	1.37
1	D	112	HIS	CD2-NE2	-6.30	1.30	1.37
1	H	112	HIS	CD2-NE2	-6.30	1.30	1.37
1	V	130	HIS	CD2-NE2	-6.30	1.30	1.37
1	M	46	HIS	CD2-NE2	-5.50	1.31	1.37
1	G	46	HIS	CD2-NE2	-5.44	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	46	HIS	CD2-NE2	-5.44	1.31	1.37
1	C	46	HIS	CD2-NE2	-5.42	1.31	1.37
1	V	46	HIS	CD2-NE2	-5.42	1.31	1.37
1	P	46	HIS	CD2-NE2	-5.41	1.31	1.37
1	I	46	HIS	CD2-NE2	-5.40	1.31	1.37
1	S	46	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	46	HIS	CD2-NE2	-5.40	1.31	1.37
1	L	46	HIS	CD2-NE2	-5.39	1.31	1.37
1	U	46	HIS	CD2-NE2	-5.38	1.31	1.37
1	E	46	HIS	CD2-NE2	-5.38	1.31	1.37
1	H	46	HIS	CD2-NE2	-5.38	1.31	1.37
1	O	46	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	46	HIS	CD2-NE2	-5.35	1.31	1.37
1	Q	46	HIS	CD2-NE2	-5.35	1.31	1.37
1	X	46	HIS	CD2-NE2	-5.35	1.31	1.37
1	T	46	HIS	CD2-NE2	-5.34	1.31	1.37
1	R	46	HIS	CD2-NE2	-5.33	1.31	1.37
1	W	46	HIS	CD2-NE2	-5.33	1.31	1.37
1	N	46	HIS	CD2-NE2	-5.33	1.31	1.37
1	F	46	HIS	CD2-NE2	-5.32	1.32	1.37
1	J	46	HIS	CD2-NE2	-5.31	1.32	1.37
1	D	46	HIS	CD2-NE2	-5.29	1.32	1.37

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	28	HIS	CB-CG-CD2	-8.73	119.85	131.20
1	E	28	HIS	CB-CG-CD2	-8.72	119.86	131.20
1	U	28	HIS	CB-CG-CD2	-8.70	119.89	131.20
1	O	28	HIS	CB-CG-CD2	-8.70	119.89	131.20
1	A	28	HIS	CB-CG-CD2	-8.69	119.90	131.20
1	I	28	HIS	CB-CG-CD2	-8.69	119.91	131.20
1	K	28	HIS	CB-CG-CD2	-8.69	119.91	131.20
1	M	28	HIS	CB-CG-CD2	-8.69	119.91	131.20
1	C	28	HIS	CB-CG-CD2	-8.68	119.91	131.20
1	W	28	HIS	CB-CG-CD2	-8.68	119.91	131.20
1	S	28	HIS	CB-CG-CD2	-8.68	119.92	131.20
1	G	28	HIS	CB-CG-CD2	-8.67	119.93	131.20
1	P	28	HIS	CB-CG-CD2	-8.56	120.07	131.20
1	R	28	HIS	CB-CG-CD2	-8.55	120.09	131.20
1	F	28	HIS	CB-CG-CD2	-8.54	120.09	131.20
1	H	28	HIS	CB-CG-CD2	-8.54	120.10	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	L	28	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	B	28	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	N	28	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	J	28	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	X	28	HIS	CB-CG-CD2	-8.53	120.11	131.20
1	T	28	HIS	CB-CG-CD2	-8.52	120.12	131.20
1	V	28	HIS	CB-CG-CD2	-8.52	120.13	131.20
1	M	9	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	U	9	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	W	9	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	C	9	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	S	9	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	G	9	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	A	9	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	Q	9	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	I	9	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	E	9	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	O	9	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	K	9	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	F	41	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	T	41	ASN	OD1-CG-ND2	-7.50	115.09	122.60
1	R	41	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	D	41	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	J	41	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	X	41	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	B	41	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	H	41	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	L	41	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	V	41	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	P	41	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	N	41	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	M	41	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	I	41	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	O	41	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	E	41	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	W	41	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	41	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	S	41	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	G	41	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	K	41	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	C	41	ASN	OD1-CG-ND2	-7.33	115.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	41	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	M	28	HIS	CB-CG-ND1	7.32	133.68	122.70
1	Q	28	HIS	CB-CG-ND1	7.32	133.68	122.70
1	Q	41	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	U	28	HIS	CB-CG-ND1	7.31	133.66	122.70
1	E	28	HIS	CB-CG-ND1	7.30	133.66	122.70
1	O	28	HIS	CB-CG-ND1	7.30	133.66	122.70
1	N	9	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	W	28	HIS	CB-CG-ND1	7.30	133.65	122.70
1	K	28	HIS	CB-CG-ND1	7.30	133.65	122.70
1	A	28	HIS	CB-CG-ND1	7.29	133.64	122.70
1	C	28	HIS	CB-CG-ND1	7.29	133.64	122.70
1	S	28	HIS	CB-CG-ND1	7.29	133.63	122.70
1	D	9	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	G	28	HIS	CB-CG-ND1	7.28	133.63	122.70
1	I	28	HIS	CB-CG-ND1	7.27	133.61	122.70
1	V	9	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	H	9	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	R	9	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	F	89	SER	CB-CA-C	-7.26	98.74	110.79
1	J	9	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	T	9	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	N	89	SER	CB-CA-C	-7.25	98.76	110.79
1	D	89	SER	CB-CA-C	-7.24	98.76	110.79
1	F	9	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	L	89	SER	CB-CA-C	-7.24	98.77	110.79
1	R	89	SER	CB-CA-C	-7.24	98.78	110.79
1	H	89	SER	CB-CA-C	-7.23	98.78	110.79
1	L	9	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	X	89	SER	CB-CA-C	-7.23	98.79	110.79
1	B	9	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	B	89	SER	CB-CA-C	-7.23	98.79	110.79
1	V	89	SER	CB-CA-C	-7.23	98.79	110.79
1	P	9	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	P	89	SER	CB-CA-C	-7.22	98.80	110.79
1	J	89	SER	CB-CA-C	-7.21	98.81	110.79
1	T	89	SER	CB-CA-C	-7.21	98.82	110.79
1	S	89	SER	CB-CA-C	-7.21	98.82	110.79
1	C	89	SER	CB-CA-C	-7.19	98.85	110.79
1	I	89	SER	CB-CA-C	-7.19	98.85	110.79
1	O	89	SER	CB-CA-C	-7.19	98.86	110.79
1	X	9	ASN	OD1-CG-ND2	-7.18	115.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	89	SER	CB-CA-C	-7.18	98.87	110.79
1	A	89	SER	CB-CA-C	-7.17	98.88	110.79
1	E	89	SER	CB-CA-C	-7.17	98.88	110.79
1	M	89	SER	CB-CA-C	-7.17	98.88	110.79
1	U	89	SER	CB-CA-C	-7.17	98.89	110.79
1	W	89	SER	CB-CA-C	-7.17	98.89	110.79
1	K	89	SER	CB-CA-C	-7.17	98.89	110.79
1	Q	89	SER	CB-CA-C	-7.17	98.89	110.79
1	H	28	HIS	CB-CG-ND1	7.09	133.34	122.70
1	D	28	HIS	CB-CG-ND1	7.09	133.33	122.70
1	L	28	HIS	CB-CG-ND1	7.08	133.33	122.70
1	P	28	HIS	CB-CG-ND1	7.08	133.33	122.70
1	N	28	HIS	CB-CG-ND1	7.08	133.32	122.70
1	J	28	HIS	CB-CG-ND1	7.08	133.32	122.70
1	T	28	HIS	CB-CG-ND1	7.08	133.32	122.70
1	F	28	HIS	CB-CG-ND1	7.08	133.32	122.70
1	B	28	HIS	CB-CG-ND1	7.07	133.31	122.70
1	R	28	HIS	CB-CG-ND1	7.07	133.31	122.70
1	X	28	HIS	CB-CG-ND1	7.05	133.28	122.70
1	V	28	HIS	CB-CG-ND1	7.04	133.27	122.70
1	G	50	ASP	CA-CB-CG	6.99	119.59	112.60
1	K	50	ASP	CA-CB-CG	6.98	119.58	112.60
1	E	50	ASP	CA-CB-CG	6.98	119.58	112.60
1	W	50	ASP	CA-CB-CG	6.97	119.57	112.60
1	U	50	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	50	ASP	CA-CB-CG	6.96	119.56	112.60
1	S	50	ASP	CA-CB-CG	6.96	119.56	112.60
1	Q	50	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	50	ASP	CA-CB-CG	6.95	119.55	112.60
1	O	50	ASP	CA-CB-CG	6.94	119.54	112.60
1	M	50	ASP	CA-CB-CG	6.94	119.54	112.60
1	I	50	ASP	CA-CB-CG	6.93	119.53	112.60
1	T	23	ASN	OD1-CG-ND2	-6.51	116.08	122.60
1	L	23	ASN	OD1-CG-ND2	-6.50	116.11	122.60
1	M	23	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	N	23	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	S	17	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	R	23	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	M	17	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	U	17	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	S	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	C	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	17	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	W	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	F	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	J	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	X	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	23	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	E	23	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	C	17	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	Q	17	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	U	23	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	D	23	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	O	17	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	W	17	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	A	17	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	P	23	ASN	OD1-CG-ND2	-6.45	116.16	122.60
1	A	23	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	G	17	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	H	23	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	K	23	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	O	23	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	K	17	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	U	79	ILE	N-CA-C	6.43	116.58	110.53
1	E	17	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	C	79	ILE	N-CA-C	6.41	116.56	110.53
1	S	79	ILE	N-CA-C	6.41	116.56	110.53
1	V	23	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	O	79	ILE	N-CA-C	6.41	116.55	110.53
1	I	23	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	Q	23	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	79	ILE	N-CA-C	6.40	116.54	110.53
1	W	79	ILE	N-CA-C	6.40	116.54	110.53
1	K	79	ILE	N-CA-C	6.39	116.53	110.53
1	G	79	ILE	N-CA-C	6.39	116.53	110.53
1	G	23	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	I	79	ILE	N-CA-C	6.38	116.53	110.53
1	P	73	ASP	N-CA-C	6.38	118.68	108.41
1	J	73	ASP	N-CA-C	6.38	118.68	108.41
1	H	143	LYS	N-CA-C	6.38	118.03	111.14
1	C	12	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	M	79	ILE	N-CA-C	6.38	116.52	110.53
1	F	73	ASP	N-CA-C	6.36	118.65	108.41
1	B	73	ASP	N-CA-C	6.36	118.65	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	143	LYS	N-CA-C	6.36	118.01	111.14
1	N	73	ASP	N-CA-C	6.36	118.65	108.41
1	X	73	ASP	N-CA-C	6.36	118.65	108.41
1	S	12	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	D	73	ASP	N-CA-C	6.36	118.64	108.41
1	F	143	LYS	N-CA-C	6.36	118.00	111.14
1	L	143	LYS	N-CA-C	6.36	118.00	111.14
1	K	12	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	R	73	ASP	N-CA-C	6.35	118.63	108.41
1	M	12	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	Q	79	ILE	N-CA-C	6.35	116.50	110.53
1	E	12	ASN	OD1-CG-ND2	-6.34	116.25	122.60
1	E	79	ILE	N-CA-C	6.34	116.49	110.53
1	L	73	ASP	N-CA-C	6.34	118.61	108.41
1	H	73	ASP	N-CA-C	6.34	118.61	108.41
1	N	143	LYS	N-CA-C	6.34	117.98	111.14
1	V	73	ASP	N-CA-C	6.34	118.61	108.41
1	G	73	ASP	N-CA-C	6.33	118.61	108.41
1	L	17	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	R	17	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	T	73	ASP	N-CA-C	6.33	118.61	108.41
1	V	96	ASP	N-CA-C	6.33	118.19	111.28
1	G	12	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	V	17	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	143	LYS	N-CA-C	6.33	117.98	111.14
1	J	143	LYS	N-CA-C	6.33	117.97	111.14
1	X	143	LYS	N-CA-C	6.32	117.97	111.14
1	I	12	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	T	96	ASP	N-CA-C	6.32	118.17	111.28
1	H	96	ASP	N-CA-C	6.32	118.17	111.28
1	K	73	ASP	N-CA-C	6.32	118.58	108.41
1	J	96	ASP	N-CA-C	6.32	118.17	111.28
1	R	143	LYS	N-CA-C	6.32	117.96	111.14
1	F	17	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	W	73	ASP	N-CA-C	6.32	118.58	108.41
1	P	143	LYS	N-CA-C	6.31	117.96	111.14
1	C	73	ASP	N-CA-C	6.31	118.57	108.41
1	O	73	ASP	N-CA-C	6.31	118.57	108.41
1	W	12	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	D	143	LYS	N-CA-C	6.31	117.95	111.14
1	A	12	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	Q	12	ASN	OD1-CG-ND2	-6.30	116.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	N-CA-C	6.30	118.55	108.41
1	J	17	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	L	96	ASP	N-CA-C	6.30	118.15	111.28
1	T	17	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	U	12	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	17	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	96	ASP	N-CA-C	6.29	118.14	111.28
1	M	73	ASP	N-CA-C	6.29	118.55	108.41
1	N	96	ASP	N-CA-C	6.29	118.14	111.28
1	E	73	ASP	N-CA-C	6.29	118.53	108.41
1	Q	73	ASP	N-CA-C	6.29	118.54	108.41
1	S	73	ASP	N-CA-C	6.29	118.54	108.41
1	U	73	ASP	N-CA-C	6.29	118.53	108.41
1	V	143	LYS	N-CA-C	6.29	117.93	111.14
1	H	17	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	I	73	ASP	N-CA-C	6.29	118.53	108.41
1	P	17	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	O	12	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	D	96	ASP	N-CA-C	6.28	118.12	111.28
1	P	96	ASP	N-CA-C	6.27	118.12	111.28
1	W	9	ASN	CB-CG-ND2	6.27	125.81	116.40
1	D	17	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	S	9	ASN	CB-CG-ND2	6.26	125.80	116.40
1	H	79	ILE	N-CA-C	6.26	116.42	110.53
1	F	96	ASP	N-CA-C	6.26	118.11	111.28
1	O	9	ASN	CB-CG-ND2	6.26	125.79	116.40
1	R	96	ASP	N-CA-C	6.26	118.10	111.28
1	X	96	ASP	N-CA-C	6.26	118.10	111.28
1	L	79	ILE	N-CA-C	6.26	116.41	110.53
1	N	17	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	U	9	ASN	CB-CG-ND2	6.25	125.78	116.40
1	X	17	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	Q	9	ASN	CB-CG-ND2	6.25	125.77	116.40
1	M	9	ASN	CB-CG-ND2	6.24	125.77	116.40
1	A	9	ASN	CB-CG-ND2	6.24	125.76	116.40
1	I	9	ASN	CB-CG-ND2	6.24	125.76	116.40
1	F	79	ILE	N-CA-C	6.24	116.39	110.53
1	E	9	ASN	CB-CG-ND2	6.23	125.75	116.40
1	C	9	ASN	CB-CG-ND2	6.23	125.75	116.40
1	P	79	ILE	N-CA-C	6.23	116.39	110.53
1	T	79	ILE	N-CA-C	6.23	116.39	110.53
1	X	79	ILE	N-CA-C	6.22	116.38	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ILE	N-CA-C	6.22	116.38	110.53
1	G	9	ASN	CB-CG-ND2	6.22	125.73	116.40
1	J	79	ILE	N-CA-C	6.22	116.37	110.53
1	K	9	ASN	CB-CG-ND2	6.21	125.72	116.40
1	V	79	ILE	N-CA-C	6.21	116.37	110.53
1	N	79	ILE	N-CA-C	6.21	116.36	110.53
1	R	79	ILE	N-CA-C	6.20	116.36	110.53
1	S	96	ASP	N-CA-C	6.19	117.69	111.07
1	D	79	ILE	N-CA-C	6.19	116.35	110.53
1	O	96	ASP	N-CA-C	6.18	117.68	111.07
1	I	96	ASP	N-CA-C	6.18	117.68	111.07
1	G	96	ASP	N-CA-C	6.16	117.67	111.07
1	W	96	ASP	N-CA-C	6.16	117.67	111.07
1	A	96	ASP	N-CA-C	6.16	117.66	111.07
1	K	96	ASP	N-CA-C	6.15	117.65	111.07
1	E	96	ASP	N-CA-C	6.15	117.65	111.07
1	U	96	ASP	N-CA-C	6.14	117.64	111.07
1	C	96	ASP	N-CA-C	6.13	117.63	111.07
1	Q	96	ASP	N-CA-C	6.13	117.62	111.07
1	M	96	ASP	N-CA-C	6.12	117.62	111.07
1	S	143	LYS	N-CA-C	6.07	117.70	111.14
1	O	12	ASN	N-CA-C	6.07	117.90	111.28
1	M	143	LYS	N-CA-C	6.07	117.69	111.14
1	C	12	ASN	N-CA-C	6.07	117.89	111.28
1	Q	143	LYS	N-CA-C	6.07	117.69	111.14
1	O	143	LYS	N-CA-C	6.06	117.69	111.14
1	K	143	LYS	N-CA-C	6.06	117.68	111.14
1	U	143	LYS	N-CA-C	6.05	117.68	111.14
1	I	143	LYS	N-CA-C	6.05	117.67	111.14
1	U	12	ASN	N-CA-C	6.05	117.87	111.28
1	A	143	LYS	N-CA-C	6.05	117.67	111.14
1	A	12	ASN	N-CA-C	6.04	117.87	111.28
1	G	143	LYS	N-CA-C	6.04	117.67	111.14
1	W	12	ASN	N-CA-C	6.04	117.87	111.28
1	C	143	LYS	N-CA-C	6.04	117.66	111.14
1	E	12	ASN	N-CA-C	6.04	117.86	111.28
1	K	12	ASN	N-CA-C	6.04	117.86	111.28
1	W	143	LYS	N-CA-C	6.04	117.66	111.14
1	G	12	ASN	N-CA-C	6.03	117.86	111.28
1	S	12	ASN	N-CA-C	6.03	117.86	111.28
1	D	12	ASN	N-CA-C	6.03	117.85	111.28
1	E	143	LYS	N-CA-C	6.02	117.64	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	12	ASN	N-CA-C	6.01	117.83	111.28
1	M	12	ASN	N-CA-C	6.00	117.82	111.28
1	I	12	ASN	N-CA-C	6.00	117.82	111.28
1	R	12	ASN	N-CA-C	6.00	117.82	111.28
1	V	12	ASN	N-CA-C	6.00	117.82	111.28
1	H	12	ASN	N-CA-C	6.00	117.82	111.28
1	L	12	ASN	N-CA-C	5.99	117.81	111.28
1	P	12	ASN	N-CA-C	5.98	117.80	111.28
1	J	12	ASN	N-CA-C	5.97	117.79	111.28
1	B	12	ASN	N-CA-C	5.97	117.79	111.28
1	N	12	ASN	N-CA-C	5.97	117.78	111.28
1	T	12	ASN	N-CA-C	5.96	117.78	111.28
1	X	12	ASN	N-CA-C	5.95	117.76	111.28
1	F	12	ASN	N-CA-C	5.93	117.75	111.28
1	T	50	ASP	CA-CB-CG	5.91	118.50	112.60
1	H	50	ASP	CA-CB-CG	5.89	118.49	112.60
1	V	50	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	50	ASP	CA-CB-CG	5.88	118.48	112.60
1	F	50	ASP	CA-CB-CG	5.88	118.48	112.60
1	X	50	ASP	CA-CB-CG	5.87	118.47	112.60
1	R	50	ASP	CA-CB-CG	5.87	118.47	112.60
1	L	50	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	50	ASP	CA-CB-CG	5.86	118.46	112.60
1	N	50	ASP	CA-CB-CG	5.86	118.46	112.60
1	J	50	ASP	CA-CB-CG	5.86	118.46	112.60
1	P	50	ASP	CA-CB-CG	5.84	118.44	112.60
1	V	12	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	L	12	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	F	12	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	B	12	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	D	12	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	T	12	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	X	12	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	H	12	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	N	12	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	P	12	ASN	OD1-CG-ND2	-5.78	116.83	122.60
1	J	12	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	R	12	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	N	9	ASN	CB-CG-ND2	5.66	124.89	116.40
1	V	9	ASN	CB-CG-ND2	5.66	124.89	116.40
1	F	9	ASN	CB-CG-ND2	5.65	124.88	116.40
1	H	9	ASN	CB-CG-ND2	5.64	124.87	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	9	ASN	CB-CG-ND2	5.64	124.86	116.40
1	B	9	ASN	CB-CG-ND2	5.64	124.86	116.40
1	L	9	ASN	CB-CG-ND2	5.64	124.86	116.40
1	D	9	ASN	CB-CG-ND2	5.63	124.84	116.40
1	J	9	ASN	CB-CG-ND2	5.62	124.84	116.40
1	T	9	ASN	CB-CG-ND2	5.62	124.83	116.40
1	R	9	ASN	CB-CG-ND2	5.62	124.83	116.40
1	X	9	ASN	CB-CG-ND2	5.61	124.81	116.40
1	O	24	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	S	53	LYS	CB-CG-CD	-5.58	98.45	111.30
1	C	53	LYS	CB-CG-CD	-5.58	98.47	111.30
1	U	53	LYS	CB-CG-CD	-5.58	98.48	111.30
1	M	53	LYS	CB-CG-CD	-5.57	98.48	111.30
1	G	24	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	U	24	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	E	24	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	I	24	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	K	53	LYS	CB-CG-CD	-5.57	98.49	111.30
1	O	53	LYS	CB-CG-CD	-5.57	98.50	111.30
1	I	53	LYS	CB-CG-CD	-5.57	98.50	111.30
1	A	53	LYS	CB-CG-CD	-5.56	98.50	111.30
1	W	53	LYS	CB-CG-CD	-5.56	98.50	111.30
1	G	53	LYS	CB-CG-CD	-5.56	98.51	111.30
1	E	53	LYS	CB-CG-CD	-5.56	98.52	111.30
1	Q	53	LYS	CB-CG-CD	-5.56	98.51	111.30
1	W	24	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	24	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	M	24	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	C	24	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	S	24	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	K	24	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	F	53	LYS	CB-CG-CD	-5.50	98.64	111.30
1	D	53	LYS	CB-CG-CD	-5.49	98.67	111.30
1	T	53	LYS	CB-CG-CD	-5.49	98.67	111.30
1	B	53	LYS	CB-CG-CD	-5.49	98.68	111.30
1	Q	24	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	J	53	LYS	CB-CG-CD	-5.49	98.68	111.30
1	H	53	LYS	CB-CG-CD	-5.48	98.69	111.30
1	L	53	LYS	CB-CG-CD	-5.48	98.69	111.30
1	P	53	LYS	CB-CG-CD	-5.48	98.69	111.30
1	N	53	LYS	CB-CG-CD	-5.48	98.69	111.30
1	V	53	LYS	CB-CG-CD	-5.48	98.70	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	53	LYS	CB-CG-CD	-5.48	98.71	111.30
1	X	53	LYS	CB-CG-CD	-5.47	98.71	111.30
1	K	47	GLU	CA-CB-CG	-5.46	103.18	114.10
1	U	47	GLU	CA-CB-CG	-5.46	103.18	114.10
1	G	47	GLU	CA-CB-CG	-5.46	103.19	114.10
1	M	47	GLU	CA-CB-CG	-5.46	103.19	114.10
1	W	47	GLU	CA-CB-CG	-5.45	103.21	114.10
1	I	47	GLU	CA-CB-CG	-5.45	103.21	114.10
1	O	47	GLU	CA-CB-CG	-5.45	103.21	114.10
1	A	47	GLU	CA-CB-CG	-5.44	103.22	114.10
1	E	47	GLU	CA-CB-CG	-5.44	103.23	114.10
1	S	47	GLU	CA-CB-CG	-5.43	103.23	114.10
1	Q	47	GLU	CA-CB-CG	-5.43	103.24	114.10
1	C	47	GLU	CA-CB-CG	-5.42	103.26	114.10
1	M	102	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	W	102	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	K	102	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	K	46	HIS	CA-CB-CG	-5.34	108.46	113.80
1	W	46	HIS	CA-CB-CG	-5.33	108.47	113.80
1	E	46	HIS	CA-CB-CG	-5.33	108.47	113.80
1	S	46	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	46	HIS	CA-CB-CG	-5.31	108.49	113.80
1	O	102	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	U	46	HIS	CA-CB-CG	-5.31	108.49	113.80
1	C	46	HIS	CA-CB-CG	-5.31	108.49	113.80
1	C	102	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	G	46	HIS	CA-CB-CG	-5.30	108.50	113.80
1	A	102	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	I	46	HIS	CA-CB-CG	-5.30	108.50	113.80
1	S	102	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	F	46	HIS	CA-CB-CG	-5.29	108.51	113.80
1	V	46	HIS	CA-CB-CG	-5.29	108.51	113.80
1	O	46	HIS	CA-CB-CG	-5.29	108.51	113.80
1	G	102	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	Q	46	HIS	CA-CB-CG	-5.29	108.51	113.80
1	N	46	HIS	CA-CB-CG	-5.29	108.51	113.80
1	U	102	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	M	46	HIS	CA-CB-CG	-5.28	108.52	113.80
1	I	102	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	Q	102	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	E	102	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	D	46	HIS	CA-CB-CG	-5.26	108.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	46	HIS	CA-CB-CG	-5.25	108.55	113.80
1	J	46	HIS	CA-CB-CG	-5.25	108.55	113.80
1	R	46	HIS	CA-CB-CG	-5.24	108.56	113.80
1	B	46	HIS	CA-CB-CG	-5.24	108.56	113.80
1	H	46	HIS	CA-CB-CG	-5.22	108.58	113.80
1	T	46	HIS	CA-CB-CG	-5.22	108.58	113.80
1	P	46	HIS	CA-CB-CG	-5.22	108.58	113.80
1	X	46	HIS	CA-CB-CG	-5.19	108.61	113.80
1	J	146	LEU	N-CA-C	5.18	116.61	111.07
1	O	35	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	N	146	LEU	N-CA-C	5.16	116.59	111.07
1	D	146	LEU	N-CA-C	5.16	116.59	111.07
1	R	146	LEU	N-CA-C	5.15	116.58	111.07
1	I	35	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	C	38	LYS	N-CA-C	5.14	117.28	111.11
1	L	146	LEU	N-CA-C	5.13	116.56	111.07
1	Q	35	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	B	146	LEU	N-CA-C	5.13	116.56	111.07
1	G	38	LYS	N-CA-C	5.13	117.26	111.11
1	X	146	LEU	N-CA-C	5.13	116.56	111.07
1	S	35	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	W	38	LYS	N-CA-C	5.13	117.26	111.11
1	K	35	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	K	38	LYS	N-CA-C	5.12	117.26	111.11
1	T	146	LEU	N-CA-C	5.12	116.55	111.07
1	I	151	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	Q	38	LYS	N-CA-C	5.12	117.25	111.11
1	E	35	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	M	38	LYS	N-CA-C	5.12	117.25	111.11
1	P	146	LEU	N-CA-C	5.12	116.55	111.07
1	H	146	LEU	N-CA-C	5.12	116.55	111.07
1	O	38	LYS	N-CA-C	5.12	117.25	111.11
1	A	35	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	U	35	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	C	151	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	I	38	LYS	N-CA-C	5.11	117.24	111.11
1	F	146	LEU	N-CA-C	5.11	116.53	111.07
1	V	146	LEU	N-CA-C	5.11	116.53	111.07
1	A	38	LYS	N-CA-C	5.11	117.24	111.11
1	G	35	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	M	35	TRP	CG-CD2-CE3	5.11	139.00	133.90
1	E	151	GLN	OE1-CD-NE2	-5.10	117.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	35	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	C	35	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	E	38	LYS	N-CA-C	5.09	117.22	111.11
1	S	38	LYS	N-CA-C	5.09	117.22	111.11
1	U	38	LYS	N-CA-C	5.09	117.22	111.11
1	W	151	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	G	151	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	R	102	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	A	151	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	L	102	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	M	151	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	U	151	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	K	151	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	J	102	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	U	148	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	K	146	LEU	N-CA-C	5.06	116.48	111.07
1	B	102	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	I	146	LEU	N-CA-C	5.06	116.48	111.07
1	Q	151	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	H	102	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	N	102	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	C	146	LEU	N-CA-C	5.05	116.47	111.07
1	O	151	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	M	148	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	O	146	LEU	N-CA-C	5.05	116.47	111.07
1	P	102	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	I	148	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	T	102	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	S	151	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	F	102	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	G	146	LEU	N-CA-C	5.03	116.45	111.07
1	X	102	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	146	LEU	N-CA-C	5.02	116.44	111.07
1	S	146	LEU	N-CA-C	5.02	116.44	111.07
1	V	102	ARG	NE-CZ-NH2	-5.02	114.69	119.20
1	D	102	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	Q	148	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	G	148	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	S	148	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	25	TYR	Sidechain
1	B	102	ARG	Sidechain
1	B	25	TYR	Sidechain
1	C	102	ARG	Sidechain
1	C	25	TYR	Sidechain
1	D	102	ARG	Sidechain
1	D	25	TYR	Sidechain
1	E	102	ARG	Sidechain
1	E	25	TYR	Sidechain
1	F	102	ARG	Sidechain
1	F	25	TYR	Sidechain
1	G	102	ARG	Sidechain
1	G	25	TYR	Sidechain
1	H	102	ARG	Sidechain
1	H	25	TYR	Sidechain
1	I	102	ARG	Sidechain
1	I	25	TYR	Sidechain
1	J	102	ARG	Sidechain
1	J	25	TYR	Sidechain
1	K	102	ARG	Sidechain
1	K	25	TYR	Sidechain
1	L	102	ARG	Sidechain
1	L	25	TYR	Sidechain
1	M	102	ARG	Sidechain
1	M	25	TYR	Sidechain
1	N	102	ARG	Sidechain
1	N	25	TYR	Sidechain
1	O	102	ARG	Sidechain
1	O	25	TYR	Sidechain
1	P	102	ARG	Sidechain
1	P	25	TYR	Sidechain
1	Q	102	ARG	Sidechain
1	Q	25	TYR	Sidechain
1	R	102	ARG	Sidechain
1	R	25	TYR	Sidechain
1	S	102	ARG	Sidechain
1	S	25	TYR	Sidechain
1	T	102	ARG	Sidechain
1	T	25	TYR	Sidechain
1	U	102	ARG	Sidechain
1	U	25	TYR	Sidechain
1	V	102	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	V	25	TYR	Sidechain
1	W	102	ARG	Sidechain
1	W	25	TYR	Sidechain
1	X	102	ARG	Sidechain
1	X	25	TYR	Sidechain

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	A	1299	0	1280	8	0
1	B	1299	0	1280	8	0
1	C	1299	0	1280	10	0
1	D	1299	0	1280	8	0
1	E	1299	0	1280	9	5
1	F	1299	0	1280	7	0
1	G	1299	0	1280	9	0
1	H	1299	0	1280	8	0
1	I	1299	0	1280	9	0
1	J	1299	0	1280	9	0
1	K	1299	0	1280	9	0
1	L	1299	0	1280	8	1
1	M	1299	0	1280	9	0
1	N	1299	0	1280	9	5
1	O	1299	0	1280	9	0
1	P	1299	0	1280	10	1
1	Q	1299	0	1280	9	0
1	R	1299	0	1280	8	0
1	S	1299	0	1280	9	0
1	T	1299	0	1280	9	0
1	U	1299	0	1280	9	1
1	V	1299	0	1280	8	0
1	W	1299	0	1280	8	1
1	X	1299	0	1280	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
3	B	43	0	30	0	0
3	D	43	0	30	0	0
3	F	43	0	30	0	0
3	H	43	0	30	0	0
3	J	43	0	30	0	0
3	L	43	0	30	0	0
3	N	43	0	30	0	0
3	P	43	0	30	0	0
3	R	43	0	30	0	0
3	T	43	0	30	0	0
3	V	43	0	30	0	0
3	X	43	0	30	0	0
All	All	31740	0	31080	198	7

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 3.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:HIS:HE1	1:G:79:ILE:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:28:HIS:HE1	1:W:79:ILE:O	1.91	0.54
1:C:28:HIS:HE1	1:C:79:ILE:O	1.91	0.54
1:I:28:HIS:HE1	1:I:79:ILE:O	1.91	0.54
1:K:28:HIS:HE1	1:K:79:ILE:O	1.91	0.54
1:A:28:HIS:HE1	1:A:79:ILE:O	1.91	0.53
1:M:28:HIS:HE1	1:M:79:ILE:O	1.91	0.53
1:S:28:HIS:HE1	1:S:79:ILE:O	1.91	0.53
1:U:28:HIS:HE1	1:U:79:ILE:O	1.91	0.53
1:O:28:HIS:HE1	1:O:79:ILE:O	1.91	0.53
1:Q:28:HIS:HE1	1:Q:79:ILE:O	1.91	0.53
1:H:28:HIS:HE1	1:H:79:ILE:O	1.92	0.53
1:E:28:HIS:HE1	1:E:79:ILE:O	1.91	0.53
1:B:28:HIS:HE1	1:B:79:ILE:O	1.92	0.53
1:F:28:HIS:HE1	1:F:79:ILE:O	1.92	0.52
1:X:28:HIS:HE1	1:X:79:ILE:O	1.92	0.52
1:J:28:HIS:HE1	1:J:79:ILE:O	1.92	0.52
1:R:28:HIS:HE1	1:R:79:ILE:O	1.92	0.52
1:D:28:HIS:HE1	1:D:79:ILE:O	1.92	0.52
1:P:28:HIS:HE1	1:P:79:ILE:O	1.92	0.52
1:T:28:HIS:HE1	1:T:79:ILE:O	1.92	0.52
1:L:28:HIS:HE1	1:L:79:ILE:O	1.92	0.52
1:V:28:HIS:HE1	1:V:79:ILE:O	1.92	0.52
1:N:28:HIS:HE1	1:N:79:ILE:O	1.92	0.52
1:L:3:GLY:HA3	1:L:65:LEU:HG	1.93	0.51
1:V:3:GLY:HA3	1:V:65:LEU:HG	1.93	0.50
1:T:3:GLY:HA3	1:T:65:LEU:HG	1.93	0.50
1:L:27:LEU:HD23	1:L:79:ILE:HD12	1.94	0.50
1:R:27:LEU:HD23	1:R:79:ILE:HD12	1.94	0.50
1:U:3:GLY:HA3	1:U:65:LEU:HG	1.94	0.50
1:C:3:GLY:HA3	1:C:65:LEU:HG	1.94	0.50
1:F:3:GLY:HA3	1:F:65:LEU:HG	1.93	0.50
1:O:3:GLY:HA3	1:O:65:LEU:HG	1.94	0.50
1:K:3:GLY:HA3	1:K:65:LEU:HG	1.94	0.50
1:N:3:GLY:HA3	1:N:65:LEU:HG	1.93	0.50
1:D:27:LEU:HD23	1:D:79:ILE:HD12	1.94	0.50
1:H:27:LEU:HD23	1:H:79:ILE:HD12	1.94	0.50
1:A:3:GLY:HA3	1:A:65:LEU:HG	1.94	0.50
1:E:3:GLY:HA3	1:E:65:LEU:HG	1.94	0.50
1:H:3:GLY:HA3	1:H:65:LEU:HG	1.93	0.49
1:R:3:GLY:HA3	1:R:65:LEU:HG	1.93	0.49
1:B:3:GLY:HA3	1:B:65:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:3:GLY:HA3	1:Q:65:LEU:HG	1.94	0.49
1:W:3:GLY:HA3	1:W:65:LEU:HG	1.94	0.49
1:J:3:GLY:HA3	1:J:65:LEU:HG	1.93	0.49
1:X:3:GLY:HA3	1:X:65:LEU:HG	1.93	0.49
1:T:27:LEU:HD23	1:T:79:ILE:HD12	1.94	0.49
1:V:27:LEU:HD23	1:V:79:ILE:HD12	1.94	0.49
1:F:27:LEU:HD23	1:F:79:ILE:HD12	1.94	0.49
1:P:3:GLY:HA3	1:P:65:LEU:HG	1.93	0.49
1:I:3:GLY:HA3	1:I:65:LEU:HG	1.94	0.49
1:J:27:LEU:HD23	1:J:79:ILE:HD12	1.94	0.49
1:D:3:GLY:HA3	1:D:65:LEU:HG	1.93	0.49
1:G:3:GLY:HA3	1:G:65:LEU:HG	1.94	0.49
1:M:3:GLY:HA3	1:M:65:LEU:HG	1.94	0.48
1:P:27:LEU:HD23	1:P:79:ILE:HD12	1.94	0.48
1:S:3:GLY:HA3	1:S:65:LEU:HG	1.94	0.48
1:B:27:LEU:HD23	1:B:79:ILE:HD12	1.94	0.48
1:I:40:LEU:HD22	1:I:153:GLN:HG3	1.96	0.48
1:M:40:LEU:HD22	1:M:153:GLN:HG3	1.96	0.48
1:N:40:LEU:HD22	1:N:153:GLN:HG3	1.96	0.48
1:Q:40:LEU:HD22	1:Q:153:GLN:HG3	1.96	0.48
1:B:40:LEU:HD22	1:B:153:GLN:HG3	1.96	0.48
1:L:40:LEU:HD22	1:L:153:GLN:HG3	1.96	0.48
1:J:40:LEU:HD22	1:J:153:GLN:HG3	1.96	0.48
1:O:40:LEU:HD22	1:O:153:GLN:HG3	1.96	0.48
1:V:40:LEU:HD22	1:V:153:GLN:HG3	1.96	0.48
1:S:40:LEU:HD22	1:S:153:GLN:HG3	1.96	0.48
1:X:40:LEU:HD22	1:X:153:GLN:HG3	1.96	0.48
1:A:40:LEU:HD22	1:A:153:GLN:HG3	1.96	0.48
1:X:27:LEU:HD23	1:X:79:ILE:HD12	1.94	0.48
1:E:40:LEU:HD22	1:E:153:GLN:HG3	1.96	0.48
1:N:27:LEU:HD23	1:N:79:ILE:HD12	1.94	0.47
1:S:28:HIS:CE1	1:S:79:ILE:O	2.68	0.47
1:D:40:LEU:HD22	1:D:153:GLN:HG3	1.96	0.47
1:K:40:LEU:HD22	1:K:153:GLN:HG3	1.96	0.47
1:O:28:HIS:CE1	1:O:79:ILE:O	2.68	0.47
1:R:40:LEU:HD22	1:R:153:GLN:HG3	1.96	0.47
1:W:40:LEU:HD22	1:W:153:GLN:HG3	1.96	0.47
1:K:28:HIS:CE1	1:K:79:ILE:O	2.68	0.47
1:P:40:LEU:HD22	1:P:153:GLN:HG3	1.96	0.47
1:U:28:HIS:CE1	1:U:79:ILE:O	2.68	0.47
1:E:28:HIS:CE1	1:E:79:ILE:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:LEU:HD22	1:F:153:GLN:HG3	1.96	0.47
1:T:40:LEU:HD22	1:T:153:GLN:HG3	1.96	0.47
1:G:28:HIS:CE1	1:G:79:ILE:O	2.68	0.47
1:G:40:LEU:HD22	1:G:153:GLN:HG3	1.96	0.47
1:A:28:HIS:CE1	1:A:79:ILE:O	2.68	0.47
1:C:40:LEU:HD22	1:C:153:GLN:HG3	1.96	0.46
1:U:40:LEU:HD22	1:U:153:GLN:HG3	1.96	0.46
1:I:28:HIS:CE1	1:I:79:ILE:O	2.68	0.46
1:A:27:LEU:HD23	1:A:79:ILE:HD12	1.98	0.46
1:C:28:HIS:CE1	1:C:79:ILE:O	2.68	0.46
1:E:27:LEU:HD23	1:E:79:ILE:HD12	1.98	0.46
1:M:28:HIS:CE1	1:M:79:ILE:O	2.68	0.46
1:W:28:HIS:CE1	1:W:79:ILE:O	2.68	0.46
1:Q:28:HIS:CE1	1:Q:79:ILE:O	2.68	0.46
1:U:27:LEU:HD23	1:U:79:ILE:HD12	1.98	0.46
1:Q:155:ARG:NH2	1:V:39:ARG:HD2	2.30	0.46
1:H:40:LEU:HD22	1:H:153:GLN:HG3	1.96	0.46
1:G:24:GLN:NE2	1:G:78:ASN:H	2.14	0.46
1:Q:27:LEU:HD23	1:Q:79:ILE:HD12	1.98	0.46
1:U:24:GLN:NE2	1:U:78:ASN:H	2.14	0.46
1:E:155:ARG:NH2	1:J:39:ARG:HD2	2.31	0.45
1:G:27:LEU:HD23	1:G:79:ILE:HD12	1.98	0.45
1:I:27:LEU:HD23	1:I:79:ILE:HD12	1.98	0.45
1:O:27:LEU:HD23	1:O:79:ILE:HD12	1.98	0.45
1:C:155:ARG:NH2	1:U:39:ARG:HD2	2.32	0.45
1:K:24:GLN:NE2	1:K:78:ASN:H	2.14	0.45
1:H:28:HIS:CE1	1:H:79:ILE:O	2.70	0.45
1:D:28:HIS:CE1	1:D:79:ILE:O	2.70	0.45
1:M:24:GLN:NE2	1:M:78:ASN:H	2.15	0.45
1:S:27:LEU:HD23	1:S:79:ILE:HD12	1.98	0.45
1:A:24:GLN:NE2	1:A:78:ASN:H	2.14	0.45
1:C:24:GLN:NE2	1:C:78:ASN:H	2.14	0.45
1:L:28:HIS:CE1	1:L:79:ILE:O	2.70	0.45
1:W:24:GLN:NE2	1:W:78:ASN:H	2.14	0.45
1:M:27:LEU:HD23	1:M:79:ILE:HD12	1.98	0.45
1:W:27:LEU:HD23	1:W:79:ILE:HD12	1.98	0.45
1:S:24:GLN:NE2	1:S:78:ASN:H	2.14	0.45
1:P:28:HIS:CE1	1:P:79:ILE:O	2.70	0.45
1:X:28:HIS:CE1	1:X:79:ILE:O	2.70	0.45
1:E:24:GLN:NE2	1:E:78:ASN:H	2.14	0.45
1:K:27:LEU:HD23	1:K:79:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:24:GLN:NE2	1:O:78:ASN:H	2.14	0.44
1:C:27:LEU:HD23	1:C:79:ILE:HD12	1.98	0.44
1:Q:24:GLN:NE2	1:Q:78:ASN:H	2.14	0.44
1:B:28:HIS:CE1	1:B:79:ILE:O	2.70	0.44
1:T:28:HIS:CE1	1:T:79:ILE:O	2.70	0.44
1:F:28:HIS:CE1	1:F:79:ILE:O	2.70	0.44
1:R:28:HIS:CE1	1:R:79:ILE:O	2.70	0.44
1:I:24:GLN:NE2	1:I:78:ASN:H	2.15	0.44
1:J:28:HIS:CE1	1:J:79:ILE:O	2.70	0.44
1:V:28:HIS:CE1	1:V:79:ILE:O	2.70	0.44
1:N:155:ARG:NH2	1:T:39:ARG:HD2	2.33	0.43
1:G:117:ARG:HH11	1:G:117:ARG:HD2	1.70	0.43
1:J:105:ILE:HD13	1:J:121:ILE:HG12	2.01	0.43
1:N:105:ILE:HD13	1:N:121:ILE:HG12	2.01	0.43
1:D:105:ILE:HD13	1:D:121:ILE:HG12	2.01	0.43
1:M:117:ARG:HH11	1:M:117:ARG:HD2	1.70	0.43
1:V:105:ILE:HD13	1:V:121:ILE:HG12	2.01	0.43
1:I:39:ARG:HD2	1:O:155:ARG:NH2	2.34	0.43
1:N:28:HIS:CE1	1:N:79:ILE:O	2.70	0.43
1:R:105:ILE:HD13	1:R:121:ILE:HG12	2.01	0.42
1:P:117:ARG:HH11	1:P:117:ARG:HD2	1.71	0.42
1:H:24:GLN:NE2	1:H:78:ASN:H	2.18	0.42
1:J:24:GLN:NE2	1:J:78:ASN:H	2.18	0.42
1:L:105:ILE:HD13	1:L:121:ILE:HG12	2.01	0.42
1:P:24:GLN:NE2	1:P:78:ASN:H	2.18	0.42
1:T:105:ILE:HD13	1:T:121:ILE:HG12	2.01	0.42
1:A:105:ILE:HD13	1:A:121:ILE:HG12	2.02	0.42
1:X:105:ILE:HD13	1:X:121:ILE:HG12	2.01	0.42
1:B:105:ILE:HD13	1:B:121:ILE:HG12	2.01	0.42
1:D:24:GLN:NE2	1:D:78:ASN:H	2.18	0.42
1:G:105:ILE:HD13	1:G:121:ILE:HG12	2.02	0.42
1:R:39:ARG:HD2	1:T:155:ARG:NH2	2.35	0.42
1:V:24:GLN:NE2	1:V:78:ASN:H	2.18	0.42
1:E:105:ILE:HD13	1:E:121:ILE:HG12	2.02	0.42
1:F:105:ILE:HD13	1:F:121:ILE:HG12	2.01	0.42
1:S:105:ILE:HD13	1:S:121:ILE:HG12	2.02	0.42
1:H:105:ILE:HD13	1:H:121:ILE:HG12	2.01	0.42
1:W:105:ILE:HD13	1:W:121:ILE:HG12	2.02	0.42
1:X:24:GLN:NE2	1:X:78:ASN:H	2.18	0.41
1:C:105:ILE:HD13	1:C:121:ILE:HG12	2.02	0.41
1:I:43:VAL:HG11	1:I:133:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:ILE:HD13	1:I:121:ILE:HG12	2.02	0.41
1:N:24:GLN:NE2	1:N:78:ASN:H	2.18	0.41
1:W:43:VAL:HG11	1:W:133:TRP:CE2	2.56	0.41
1:G:43:VAL:HG11	1:G:133:TRP:CE2	2.56	0.41
1:K:117:ARG:HH11	1:K:117:ARG:HD2	1.70	0.41
1:O:43:VAL:HG11	1:O:133:TRP:CE2	2.56	0.41
1:R:24:GLN:NE2	1:R:78:ASN:H	2.18	0.41
1:B:24:GLN:NE2	1:B:78:ASN:H	2.18	0.41
1:F:24:GLN:NE2	1:F:78:ASN:H	2.18	0.41
1:P:105:ILE:HD13	1:P:121:ILE:HG12	2.01	0.41
1:S:43:VAL:HG11	1:S:133:TRP:CE2	2.56	0.41
1:E:43:VAL:HG11	1:E:133:TRP:CE2	2.56	0.41
1:Q:43:VAL:HG11	1:Q:133:TRP:CE2	2.56	0.41
1:T:24:GLN:NE2	1:T:78:ASN:H	2.18	0.41
1:L:24:GLN:NE2	1:L:78:ASN:H	2.18	0.41
1:N:39:ARG:HD2	1:P:155:ARG:NH2	2.35	0.41
1:A:43:VAL:HG11	1:A:133:TRP:CE2	2.56	0.41
1:B:155:ARG:NH2	1:H:39:ARG:HD2	2.36	0.41
1:K:43:VAL:HG11	1:K:133:TRP:CE2	2.56	0.41
1:O:105:ILE:HD13	1:O:121:ILE:HG12	2.02	0.41
1:U:105:ILE:HD13	1:U:121:ILE:HG12	2.02	0.41
1:L:117:ARG:HH11	1:L:117:ARG:HD2	1.71	0.41
1:M:43:VAL:HG11	1:M:133:TRP:CE2	2.56	0.41
1:M:105:ILE:HD13	1:M:121:ILE:HG12	2.02	0.41
1:K:105:ILE:HD13	1:K:121:ILE:HG12	2.02	0.41
1:C:43:VAL:HG11	1:C:133:TRP:CE2	2.56	0.40
1:Q:105:ILE:HD13	1:Q:121:ILE:HG12	2.02	0.40
1:S:144:MET:HE2	1:S:144:MET:HB3	1.96	0.40
1:C:117:ARG:HH11	1:C:117:ARG:HD2	1.70	0.40
1:D:6:LYS:HB3	1:D:107:TYR:CE2	2.57	0.40
1:J:6:LYS:HB3	1:J:107:TYR:CE2	2.57	0.40
1:P:6:LYS:HB3	1:P:107:TYR:CE2	2.57	0.40
1:U:43:VAL:HG11	1:U:133:TRP:CE2	2.56	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:LYS:CE	1:N:68:LEU:CD1[1_454]	1.67	0.53
1:E:76:LYS:CG	1:N:68:LEU:CD1[1_454]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:LYS:NZ	1:W:81:GLU:OE1[2_656]	1.93	0.27
1:E:76:LYS:CD	1:N:68:LEU:CD1[1_454]	2.04	0.16
1:E:76:LYS:CE	1:N:68:LEU:CB[1_454]	2.10	0.10
1:P:6:LYS:CE	1:U:85:GLU:OE1[2_645]	2.10	0.10
1:E:76:LYS:NZ	1:N:68:LEU:CD1[1_454]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	C	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	D	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	G	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	H	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	I	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	J	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	K	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	L	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	M	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	N	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	O	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	P	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	Q	156/158 (99%)	155 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	S	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	T	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	U	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	V	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	W	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	X	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	3744/3792 (99%)	3720 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	95/139 (68%)	86 (90%)	9 (10%)	8	21
1	B	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	C	86/139 (62%)	74 (86%)	12 (14%)	3	9
1	D	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	E	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	F	96/139 (69%)	88 (92%)	8 (8%)	10	26
1	G	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	H	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	I	126/139 (91%)	111 (88%)	15 (12%)	5	14
1	J	47/139 (34%)	38 (81%)	9 (19%)	1	3
1	K	134/139 (96%)	118 (88%)	16 (12%)	5	14
1	L	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	M	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	N	139/139 (100%)	123 (88%)	16 (12%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	P	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	Q	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	R	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	S	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	T	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	U	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	V	139/139 (100%)	123 (88%)	16 (12%)	5	15
1	W	139/139 (100%)	122 (88%)	17 (12%)	5	13
1	X	139/139 (100%)	123 (88%)	16 (12%)	5	15
All	All	3086/3336 (92%)	2721 (88%)	365 (12%)	5	14

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	11	LEU
1	A	14	LEU
1	A	20	VAL
1	A	37	LEU
1	A	40	LEU
1	A	139	ASP
1	A	140	LEU
1	A	157	GLU
1	B	2	LYS
1	B	11	LEU
1	B	14	LEU
1	B	20	VAL
1	B	37	LEU
1	B	40	LEU
1	B	63	LEU
1	B	65	LEU
1	B	68	LEU
1	B	74	LEU
1	B	76	LYS
1	B	87	LEU
1	B	93	LEU
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	140	LEU
1	B	157	GLU
1	C	2	LYS
1	C	11	LEU
1	C	14	LEU
1	C	63	LEU
1	C	65	LEU
1	C	68	LEU
1	C	74	LEU
1	C	87	LEU
1	C	93	LEU
1	C	139	ASP
1	C	140	LEU
1	C	157	GLU
1	D	2	LYS
1	D	11	LEU
1	D	14	LEU
1	D	20	VAL
1	D	37	LEU
1	D	40	LEU
1	D	63	LEU
1	D	65	LEU
1	D	68	LEU
1	D	74	LEU
1	D	76	LYS
1	D	87	LEU
1	D	93	LEU
1	D	95	LEU
1	D	140	LEU
1	D	157	GLU
1	E	2	LYS
1	E	11	LEU
1	E	14	LEU
1	E	20	VAL
1	E	37	LEU
1	E	40	LEU
1	E	63	LEU
1	E	65	LEU
1	E	68	LEU
1	E	74	LEU
1	E	76	LYS
1	E	87	LEU

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Mol	Chain	Res	Type
1	E	93	LEU
1	E	95	LEU
1	E	139	ASP
1	E	140	LEU
1	E	157	GLU
1	F	2	LYS
1	F	11	LEU
1	F	14	LEU
1	F	20	VAL
1	F	37	LEU
1	F	40	LEU
1	F	140	LEU
1	F	157	GLU
1	G	2	LYS
1	G	11	LEU
1	G	14	LEU
1	G	20	VAL
1	G	37	LEU
1	G	40	LEU
1	G	63	LEU
1	G	65	LEU
1	G	68	LEU
1	G	74	LEU
1	G	76	LYS
1	G	87	LEU
1	G	93	LEU
1	G	95	LEU
1	G	139	ASP
1	G	140	LEU
1	G	157	GLU
1	H	2	LYS
1	H	11	LEU
1	H	14	LEU
1	H	20	VAL
1	H	37	LEU
1	H	40	LEU
1	H	63	LEU
1	H	65	LEU
1	H	68	LEU
1	H	74	LEU
1	H	76	LYS
1	H	87	LEU

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Mol	Chain	Res	Type
1	H	93	LEU
1	H	95	LEU
1	H	140	LEU
1	H	157	GLU
1	I	2	LYS
1	I	11	LEU
1	I	14	LEU
1	I	20	VAL
1	I	37	LEU
1	I	40	LEU
1	I	63	LEU
1	I	65	LEU
1	I	76	LYS
1	I	87	LEU
1	I	93	LEU
1	I	95	LEU
1	I	139	ASP
1	I	140	LEU
1	I	157	GLU
1	J	2	LYS
1	J	11	LEU
1	J	14	LEU
1	J	20	VAL
1	J	65	LEU
1	J	68	LEU
1	J	74	LEU
1	J	76	LYS
1	J	87	LEU
1	K	11	LEU
1	K	14	LEU
1	K	20	VAL
1	K	37	LEU
1	K	40	LEU
1	K	63	LEU
1	K	65	LEU
1	K	68	LEU
1	K	74	LEU
1	K	76	LYS
1	K	87	LEU
1	K	93	LEU
1	K	95	LEU
1	K	139	ASP

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Mol	Chain	Res	Type
1	K	140	LEU
1	K	157	GLU
1	L	2	LYS
1	L	11	LEU
1	L	14	LEU
1	L	20	VAL
1	L	37	LEU
1	L	40	LEU
1	L	63	LEU
1	L	65	LEU
1	L	68	LEU
1	L	74	LEU
1	L	76	LYS
1	L	87	LEU
1	L	93	LEU
1	L	95	LEU
1	L	140	LEU
1	L	157	GLU
1	M	2	LYS
1	M	11	LEU
1	M	14	LEU
1	M	20	VAL
1	M	37	LEU
1	M	40	LEU
1	M	63	LEU
1	M	65	LEU
1	M	68	LEU
1	M	74	LEU
1	M	76	LYS
1	M	87	LEU
1	M	93	LEU
1	M	95	LEU
1	M	139	ASP
1	M	140	LEU
1	M	157	GLU
1	N	2	LYS
1	N	11	LEU
1	N	14	LEU
1	N	20	VAL
1	N	37	LEU
1	N	40	LEU
1	N	63	LEU

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Mol	Chain	Res	Type
1	N	65	LEU
1	N	68	LEU
1	N	74	LEU
1	N	76	LYS
1	N	87	LEU
1	N	93	LEU
1	N	95	LEU
1	N	140	LEU
1	N	157	GLU
1	O	2	LYS
1	O	11	LEU
1	O	14	LEU
1	O	20	VAL
1	O	37	LEU
1	O	40	LEU
1	O	63	LEU
1	O	65	LEU
1	O	68	LEU
1	O	74	LEU
1	O	76	LYS
1	O	87	LEU
1	O	93	LEU
1	O	95	LEU
1	O	139	ASP
1	O	140	LEU
1	O	157	GLU
1	P	2	LYS
1	P	11	LEU
1	P	14	LEU
1	P	20	VAL
1	P	37	LEU
1	P	40	LEU
1	P	63	LEU
1	P	65	LEU
1	P	68	LEU
1	P	74	LEU
1	P	76	LYS
1	P	87	LEU
1	P	93	LEU
1	P	95	LEU
1	P	140	LEU
1	P	157	GLU

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Mol	Chain	Res	Type
1	Q	2	LYS
1	Q	11	LEU
1	Q	14	LEU
1	Q	20	VAL
1	Q	37	LEU
1	Q	40	LEU
1	Q	63	LEU
1	Q	65	LEU
1	Q	68	LEU
1	Q	74	LEU
1	Q	76	LYS
1	Q	87	LEU
1	Q	93	LEU
1	Q	95	LEU
1	Q	139	ASP
1	Q	140	LEU
1	Q	157	GLU
1	R	2	LYS
1	R	11	LEU
1	R	14	LEU
1	R	20	VAL
1	R	37	LEU
1	R	40	LEU
1	R	63	LEU
1	R	65	LEU
1	R	68	LEU
1	R	74	LEU
1	R	76	LYS
1	R	87	LEU
1	R	93	LEU
1	R	95	LEU
1	R	140	LEU
1	R	157	GLU
1	S	2	LYS
1	S	11	LEU
1	S	14	LEU
1	S	20	VAL
1	S	37	LEU
1	S	40	LEU
1	S	63	LEU
1	S	65	LEU
1	S	68	LEU

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Mol	Chain	Res	Type
1	S	74	LEU
1	S	76	LYS
1	S	87	LEU
1	S	93	LEU
1	S	95	LEU
1	S	139	ASP
1	S	140	LEU
1	S	157	GLU
1	T	2	LYS
1	T	11	LEU
1	T	14	LEU
1	T	20	VAL
1	T	37	LEU
1	T	40	LEU
1	T	63	LEU
1	T	65	LEU
1	T	68	LEU
1	T	74	LEU
1	T	76	LYS
1	T	87	LEU
1	T	93	LEU
1	T	95	LEU
1	T	140	LEU
1	T	157	GLU
1	U	2	LYS
1	U	11	LEU
1	U	14	LEU
1	U	20	VAL
1	U	37	LEU
1	U	40	LEU
1	U	63	LEU
1	U	65	LEU
1	U	68	LEU
1	U	74	LEU
1	U	76	LYS
1	U	87	LEU
1	U	93	LEU
1	U	95	LEU
1	U	139	ASP
1	U	140	LEU
1	U	157	GLU
1	V	2	LYS

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Mol	Chain	Res	Type
1	V	11	LEU
1	V	14	LEU
1	V	20	VAL
1	V	37	LEU
1	V	40	LEU
1	V	63	LEU
1	V	65	LEU
1	V	68	LEU
1	V	74	LEU
1	V	76	LYS
1	V	87	LEU
1	V	93	LEU
1	V	95	LEU
1	V	140	LEU
1	V	157	GLU
1	W	2	LYS
1	W	11	LEU
1	W	14	LEU
1	W	20	VAL
1	W	37	LEU
1	W	40	LEU
1	W	63	LEU
1	W	65	LEU
1	W	68	LEU
1	W	74	LEU
1	W	76	LYS
1	W	87	LEU
1	W	93	LEU
1	W	95	LEU
1	W	139	ASP
1	W	140	LEU
1	W	157	GLU
1	X	2	LYS
1	X	11	LEU
1	X	14	LEU
1	X	20	VAL
1	X	37	LEU
1	X	40	LEU
1	X	63	LEU
1	X	65	LEU
1	X	68	LEU
1	X	74	LEU

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Mol	Chain	Res	Type
1	X	76	LYS
1	X	87	LEU
1	X	93	LEU
1	X	95	LEU
1	X	140	LEU
1	X	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	HIS
1	B	24	GLN
1	B	28	HIS
1	B	78	ASN
1	B	100	ASN
1	B	112	HIS
1	C	112	HIS
1	D	24	GLN
1	D	28	HIS
1	D	78	ASN
1	D	100	ASN
1	D	112	HIS
1	E	24	GLN
1	E	28	HIS
1	E	78	ASN
1	E	112	HIS
1	F	24	GLN
1	F	28	HIS
1	F	112	HIS
1	G	24	GLN
1	G	28	HIS
1	G	78	ASN
1	G	112	HIS
1	H	24	GLN
1	H	28	HIS
1	H	78	ASN
1	H	112	HIS
1	I	24	GLN
1	I	28	HIS
1	I	78	ASN
1	I	112	HIS

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Mol	Chain	Res	Type
1	J	24	GLN
1	J	28	HIS
1	J	78	ASN
1	K	24	GLN
1	K	28	HIS
1	K	78	ASN
1	K	112	HIS
1	L	24	GLN
1	L	28	HIS
1	L	78	ASN
1	L	100	ASN
1	L	112	HIS
1	M	24	GLN
1	M	28	HIS
1	M	78	ASN
1	M	112	HIS
1	N	24	GLN
1	N	28	HIS
1	N	78	ASN
1	N	112	HIS
1	O	24	GLN
1	O	28	HIS
1	O	78	ASN
1	O	112	HIS
1	P	24	GLN
1	P	28	HIS
1	P	78	ASN
1	P	112	HIS
1	Q	24	GLN
1	Q	28	HIS
1	Q	78	ASN
1	Q	112	HIS
1	R	24	GLN
1	R	28	HIS
1	R	78	ASN
1	R	100	ASN
1	R	112	HIS
1	S	24	GLN
1	S	28	HIS
1	S	78	ASN
1	S	112	HIS
1	T	24	GLN

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Mol	Chain	Res	Type
1	T	28	HIS
1	T	78	ASN
1	T	112	HIS
1	U	24	GLN
1	U	28	HIS
1	U	78	ASN
1	U	112	HIS
1	V	24	GLN
1	V	28	HIS
1	V	78	ASN
1	V	112	HIS
1	W	24	GLN
1	W	28	HIS
1	W	78	ASN
1	W	112	HIS
1	X	24	GLN
1	X	28	HIS
1	X	78	ASN
1	X	112	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 48 are monoatomic - leaving 12 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	$\# Z > 2$
3	HEM	H	200	1	50,50,50	1.28	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	V	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	N	200	1	50,50,50	1.28	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	J	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	L	200	1	50,50,50	1.29	6 (12%)	67,82,82	1.31	7 (10%)
3	HEM	D	200	1	50,50,50	1.29	6 (12%)	67,82,82	1.31	7 (10%)
3	HEM	R	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	B	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	T	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	X	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	P	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)
3	HEM	F	200	1	50,50,50	1.29	5 (10%)	67,82,82	1.31	7 (10%)

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
3	HEM	H	200	1	-	8/14/54/54	-
3	HEM	V	200	1	-	8/14/54/54	-
3	HEM	N	200	1	-	8/14/54/54	-
3	HEM	J	200	1	-	8/14/54/54	-
3	HEM	L	200	1	-	8/14/54/54	-
3	HEM	D	200	1	-	8/14/54/54	-
3	HEM	R	200	1	-	8/14/54/54	-
3	HEM	B	200	1	-	8/14/54/54	-
3	HEM	T	200	1	-	8/14/54/54	-
3	HEM	X	200	1	-	8/14/54/54	-
3	HEM	P	200	1	-	8/14/54/54	-
3	HEM	F	200	1	-	8/14/54/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	200	HEM	CAB-C3B	-3.98	1.36	1.47
3	T	200	HEM	CAB-C3B	-3.97	1.36	1.47
3	P	200	HEM	CAB-C3B	-3.96	1.36	1.47
3	V	200	HEM	CAB-C3B	-3.96	1.36	1.47
3	J	200	HEM	CAB-C3B	-3.96	1.36	1.47
3	B	200	HEM	CAB-C3B	-3.95	1.36	1.47
3	F	200	HEM	CAB-C3B	-3.95	1.36	1.47
3	D	200	HEM	CAB-C3B	-3.95	1.36	1.47
3	H	200	HEM	CAB-C3B	-3.94	1.36	1.47
3	X	200	HEM	CAB-C3B	-3.94	1.36	1.47
3	R	200	HEM	CAB-C3B	-3.93	1.36	1.47
3	N	200	HEM	CAB-C3B	-3.93	1.36	1.47
3	L	200	HEM	CAC-C3C	-3.76	1.37	1.47
3	D	200	HEM	CAC-C3C	-3.75	1.37	1.47
3	B	200	HEM	CAC-C3C	-3.75	1.37	1.47
3	V	200	HEM	CAC-C3C	-3.75	1.37	1.47
3	X	200	HEM	CAC-C3C	-3.74	1.37	1.47
3	N	200	HEM	CAC-C3C	-3.74	1.37	1.47
3	P	200	HEM	CAC-C3C	-3.74	1.37	1.47
3	F	200	HEM	CAC-C3C	-3.74	1.37	1.47
3	T	200	HEM	CAC-C3C	-3.74	1.37	1.47
3	R	200	HEM	CAC-C3C	-3.73	1.37	1.47
3	H	200	HEM	CAC-C3C	-3.73	1.37	1.47
3	J	200	HEM	CAC-C3C	-3.72	1.37	1.47
3	J	200	HEM	CBB-CAB	2.78	1.43	1.30
3	V	200	HEM	CBB-CAB	2.78	1.43	1.30
3	L	200	HEM	CBB-CAB	2.77	1.43	1.30
3	B	200	HEM	CBB-CAB	2.76	1.43	1.30
3	H	200	HEM	CBB-CAB	2.76	1.43	1.30
3	N	200	HEM	CBB-CAB	2.76	1.43	1.30
3	P	200	HEM	CBB-CAB	2.76	1.43	1.30
3	T	200	HEM	CBB-CAB	2.76	1.43	1.30
3	D	200	HEM	CBB-CAB	2.75	1.43	1.30
3	R	200	HEM	CBB-CAB	2.75	1.43	1.30
3	X	200	HEM	CBB-CAB	2.75	1.43	1.30
3	F	200	HEM	CBB-CAB	2.75	1.43	1.30
3	R	200	HEM	CBC-CAC	2.39	1.41	1.30
3	H	200	HEM	CBC-CAC	2.38	1.41	1.30
3	D	200	HEM	CBC-CAC	2.38	1.41	1.30
3	F	200	HEM	CBC-CAC	2.38	1.41	1.30
3	B	200	HEM	CBC-CAC	2.38	1.41	1.30
3	V	200	HEM	CBC-CAC	2.37	1.41	1.30
3	L	200	HEM	CBC-CAC	2.37	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	200	HEM	CBC-CAC	2.37	1.41	1.30
3	J	200	HEM	CBC-CAC	2.37	1.41	1.30
3	N	200	HEM	CBC-CAC	2.37	1.41	1.30
3	T	200	HEM	CBC-CAC	2.36	1.41	1.30
3	P	200	HEM	CBC-CAC	2.36	1.41	1.30
3	X	200	HEM	C3C-C2C	-2.30	1.32	1.37
3	R	200	HEM	C3C-C2C	-2.28	1.32	1.37
3	N	200	HEM	C3C-C2C	-2.28	1.32	1.37
3	F	200	HEM	C3C-C2C	-2.28	1.32	1.37
3	J	200	HEM	C3C-C2C	-2.27	1.32	1.37
3	B	200	HEM	C3C-C2C	-2.26	1.32	1.37
3	P	200	HEM	C3C-C2C	-2.26	1.32	1.37
3	H	200	HEM	C3C-C2C	-2.26	1.32	1.37
3	D	200	HEM	C3C-C2C	-2.26	1.32	1.37
3	T	200	HEM	C3C-C2C	-2.26	1.32	1.37
3	L	200	HEM	C3C-C2C	-2.25	1.32	1.37
3	V	200	HEM	C3C-C2C	-2.23	1.32	1.37
3	D	200	HEM	O2D-CGD	-2.02	1.24	1.30
3	L	200	HEM	O2D-CGD	-2.00	1.24	1.30

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	200	HEM	CMC-C2C-C1C	4.15	132.04	124.73
3	H	200	HEM	CMC-C2C-C1C	4.13	132.01	124.73
3	P	200	HEM	CMC-C2C-C1C	4.12	131.99	124.73
3	T	200	HEM	CMC-C2C-C1C	4.12	131.99	124.73
3	F	200	HEM	CMC-C2C-C1C	4.12	131.98	124.73
3	B	200	HEM	CMC-C2C-C1C	4.12	131.98	124.73
3	J	200	HEM	CMC-C2C-C1C	4.12	131.98	124.73
3	X	200	HEM	CMC-C2C-C1C	4.12	131.97	124.73
3	L	200	HEM	CMC-C2C-C1C	4.11	131.97	124.73
3	N	200	HEM	CMC-C2C-C1C	4.11	131.96	124.73
3	D	200	HEM	CMC-C2C-C1C	4.11	131.96	124.73
3	R	200	HEM	CMC-C2C-C1C	4.10	131.95	124.73
3	J	200	HEM	C3B-C2B-C1B	-3.14	104.05	106.41
3	X	200	HEM	C3B-C2B-C1B	-3.13	104.06	106.41
3	H	200	HEM	C3B-C2B-C1B	-3.12	104.06	106.41
3	B	200	HEM	C3B-C2B-C1B	-3.10	104.08	106.41
3	F	200	HEM	C3B-C2B-C1B	-3.10	104.08	106.41
3	N	200	HEM	C3B-C2B-C1B	-3.10	104.08	106.41
3	T	200	HEM	C3B-C2B-C1B	-3.10	104.08	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	200	HEM	C3B-C2B-C1B	-3.09	104.09	106.41
3	D	200	HEM	C3B-C2B-C1B	-3.08	104.09	106.41
3	P	200	HEM	C3B-C2B-C1B	-3.08	104.10	106.41
3	L	200	HEM	C3B-C2B-C1B	-3.06	104.11	106.41
3	V	200	HEM	C3B-C2B-C1B	-3.06	104.12	106.41
3	H	200	HEM	C2B-C1B-NB	2.82	113.08	109.84
3	T	200	HEM	C2B-C1B-NB	2.82	113.08	109.84
3	D	200	HEM	C2B-C1B-NB	2.81	113.07	109.84
3	F	200	HEM	C2B-C1B-NB	2.81	113.07	109.84
3	N	200	HEM	C2B-C1B-NB	2.81	113.07	109.84
3	J	200	HEM	C2B-C1B-NB	2.81	113.07	109.84
3	B	200	HEM	C2B-C1B-NB	2.81	113.07	109.84
3	R	200	HEM	C2B-C1B-NB	2.80	113.06	109.84
3	X	200	HEM	C2B-C1B-NB	2.80	113.06	109.84
3	P	200	HEM	C2B-C1B-NB	2.80	113.06	109.84
3	L	200	HEM	C2B-C1B-NB	2.78	113.03	109.84
3	V	200	HEM	C2B-C1B-NB	2.77	113.03	109.84
3	H	200	HEM	CMB-C2B-C1B	2.71	129.27	125.03
3	T	200	HEM	CMB-C2B-C1B	2.71	129.27	125.03
3	F	200	HEM	CMB-C2B-C1B	2.71	129.27	125.03
3	D	200	HEM	CMB-C2B-C1B	2.70	129.25	125.03
3	N	200	HEM	CMB-C2B-C1B	2.69	129.24	125.03
3	V	200	HEM	CMB-C2B-C1B	2.69	129.24	125.03
3	B	200	HEM	CMB-C2B-C1B	2.69	129.24	125.03
3	J	200	HEM	CMB-C2B-C1B	2.69	129.23	125.03
3	L	200	HEM	CMC-C2C-C3C	-2.68	121.94	128.43
3	P	200	HEM	CMB-C2B-C1B	2.68	129.22	125.03
3	V	200	HEM	CMC-C2C-C3C	-2.68	121.94	128.43
3	L	200	HEM	CMB-C2B-C1B	2.67	129.21	125.03
3	X	200	HEM	CMB-C2B-C1B	2.67	129.21	125.03
3	R	200	HEM	CMB-C2B-C1B	2.67	129.20	125.03
3	F	200	HEM	CMC-C2C-C3C	-2.66	121.98	128.43
3	X	200	HEM	CMC-C2C-C3C	-2.66	121.98	128.43
3	B	200	HEM	CMC-C2C-C3C	-2.66	121.99	128.43
3	D	200	HEM	CMC-C2C-C3C	-2.66	121.99	128.43
3	H	200	HEM	CMC-C2C-C3C	-2.66	122.00	128.43
3	N	200	HEM	CMC-C2C-C3C	-2.66	122.00	128.43
3	J	200	HEM	CMC-C2C-C3C	-2.65	122.00	128.43
3	P	200	HEM	CMC-C2C-C3C	-2.65	122.00	128.43
3	T	200	HEM	CMC-C2C-C3C	-2.65	122.02	128.43
3	R	200	HEM	CMC-C2C-C3C	-2.64	122.04	128.43
3	R	200	HEM	CAC-C3C-C2C	-2.08	121.66	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	200	HEM	CAC-C3C-C2C	-2.08	121.67	128.43
3	J	200	HEM	CAC-C3C-C2C	-2.08	121.67	128.43
3	T	200	HEM	CAC-C3C-C2C	-2.08	121.68	128.43
3	H	200	HEM	CAC-C3C-C4C	2.08	129.78	124.82
3	V	200	HEM	CAC-C3C-C4C	2.07	129.77	124.82
3	P	200	HEM	CAC-C3C-C2C	-2.07	121.69	128.43
3	B	200	HEM	CAC-C3C-C2C	-2.07	121.69	128.43
3	B	200	HEM	CAC-C3C-C4C	2.07	129.77	124.82
3	N	200	HEM	CAC-C3C-C2C	-2.07	121.70	128.43
3	J	200	HEM	CAC-C3C-C4C	2.07	129.76	124.82
3	R	200	HEM	CAC-C3C-C4C	2.07	129.76	124.82
3	D	200	HEM	CAC-C3C-C2C	-2.07	121.70	128.43
3	F	200	HEM	CAC-C3C-C2C	-2.07	121.70	128.43
3	V	200	HEM	CAC-C3C-C2C	-2.07	121.70	128.43
3	L	200	HEM	CAC-C3C-C4C	2.07	129.76	124.82
3	D	200	HEM	CAC-C3C-C4C	2.07	129.75	124.82
3	X	200	HEM	CAC-C3C-C2C	-2.06	121.73	128.43
3	F	200	HEM	CAC-C3C-C4C	2.06	129.74	124.82
3	T	200	HEM	CAC-C3C-C4C	2.06	129.74	124.82
3	L	200	HEM	CAC-C3C-C2C	-2.06	121.74	128.43
3	P	200	HEM	CAC-C3C-C4C	2.06	129.74	124.82
3	X	200	HEM	CAC-C3C-C4C	2.06	129.73	124.82
3	N	200	HEM	CAC-C3C-C4C	2.05	129.71	124.82

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	200	HEM	C2C-C3C-CAC-CBC
3	D	200	HEM	C2C-C3C-CAC-CBC
3	F	200	HEM	C2C-C3C-CAC-CBC
3	H	200	HEM	C2C-C3C-CAC-CBC
3	J	200	HEM	C2C-C3C-CAC-CBC
3	L	200	HEM	C2C-C3C-CAC-CBC
3	N	200	HEM	C2C-C3C-CAC-CBC
3	P	200	HEM	C2C-C3C-CAC-CBC
3	R	200	HEM	C2C-C3C-CAC-CBC
3	T	200	HEM	C2C-C3C-CAC-CBC
3	V	200	HEM	C2C-C3C-CAC-CBC
3	X	200	HEM	C2C-C3C-CAC-CBC
3	B	200	HEM	C2B-C3B-CAB-CBB
3	D	200	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	F	200	HEM	C2B-C3B-CAB-CBB
3	H	200	HEM	C2B-C3B-CAB-CBB
3	J	200	HEM	C2B-C3B-CAB-CBB
3	L	200	HEM	C2B-C3B-CAB-CBB
3	N	200	HEM	C2B-C3B-CAB-CBB
3	P	200	HEM	C2B-C3B-CAB-CBB
3	R	200	HEM	C2B-C3B-CAB-CBB
3	T	200	HEM	C2B-C3B-CAB-CBB
3	V	200	HEM	C2B-C3B-CAB-CBB
3	X	200	HEM	C2B-C3B-CAB-CBB
3	B	200	HEM	C4C-C3C-CAC-CBC
3	D	200	HEM	C4C-C3C-CAC-CBC
3	F	200	HEM	C4C-C3C-CAC-CBC
3	H	200	HEM	C4C-C3C-CAC-CBC
3	J	200	HEM	C4C-C3C-CAC-CBC
3	L	200	HEM	C4C-C3C-CAC-CBC
3	N	200	HEM	C4C-C3C-CAC-CBC
3	P	200	HEM	C4C-C3C-CAC-CBC
3	R	200	HEM	C4C-C3C-CAC-CBC
3	T	200	HEM	C4C-C3C-CAC-CBC
3	V	200	HEM	C4C-C3C-CAC-CBC
3	X	200	HEM	C4C-C3C-CAC-CBC
3	B	200	HEM	CAA-CBA-CGA-O2A
3	F	200	HEM	CAA-CBA-CGA-O2A
3	J	200	HEM	CAA-CBA-CGA-O2A
3	L	200	HEM	CAA-CBA-CGA-O2A
3	N	200	HEM	CAA-CBA-CGA-O2A
3	P	200	HEM	CAA-CBA-CGA-O2A
3	R	200	HEM	CAA-CBA-CGA-O2A
3	T	200	HEM	CAA-CBA-CGA-O2A
3	V	200	HEM	CAA-CBA-CGA-O2A
3	X	200	HEM	CAA-CBA-CGA-O2A
3	D	200	HEM	CAA-CBA-CGA-O2A
3	H	200	HEM	CAA-CBA-CGA-O2A
3	B	200	HEM	CAA-CBA-CGA-O1A
3	D	200	HEM	CAA-CBA-CGA-O1A
3	F	200	HEM	CAA-CBA-CGA-O1A
3	J	200	HEM	CAA-CBA-CGA-O1A
3	L	200	HEM	CAA-CBA-CGA-O1A
3	N	200	HEM	CAA-CBA-CGA-O1A
3	P	200	HEM	CAA-CBA-CGA-O1A
3	T	200	HEM	CAA-CBA-CGA-O1A

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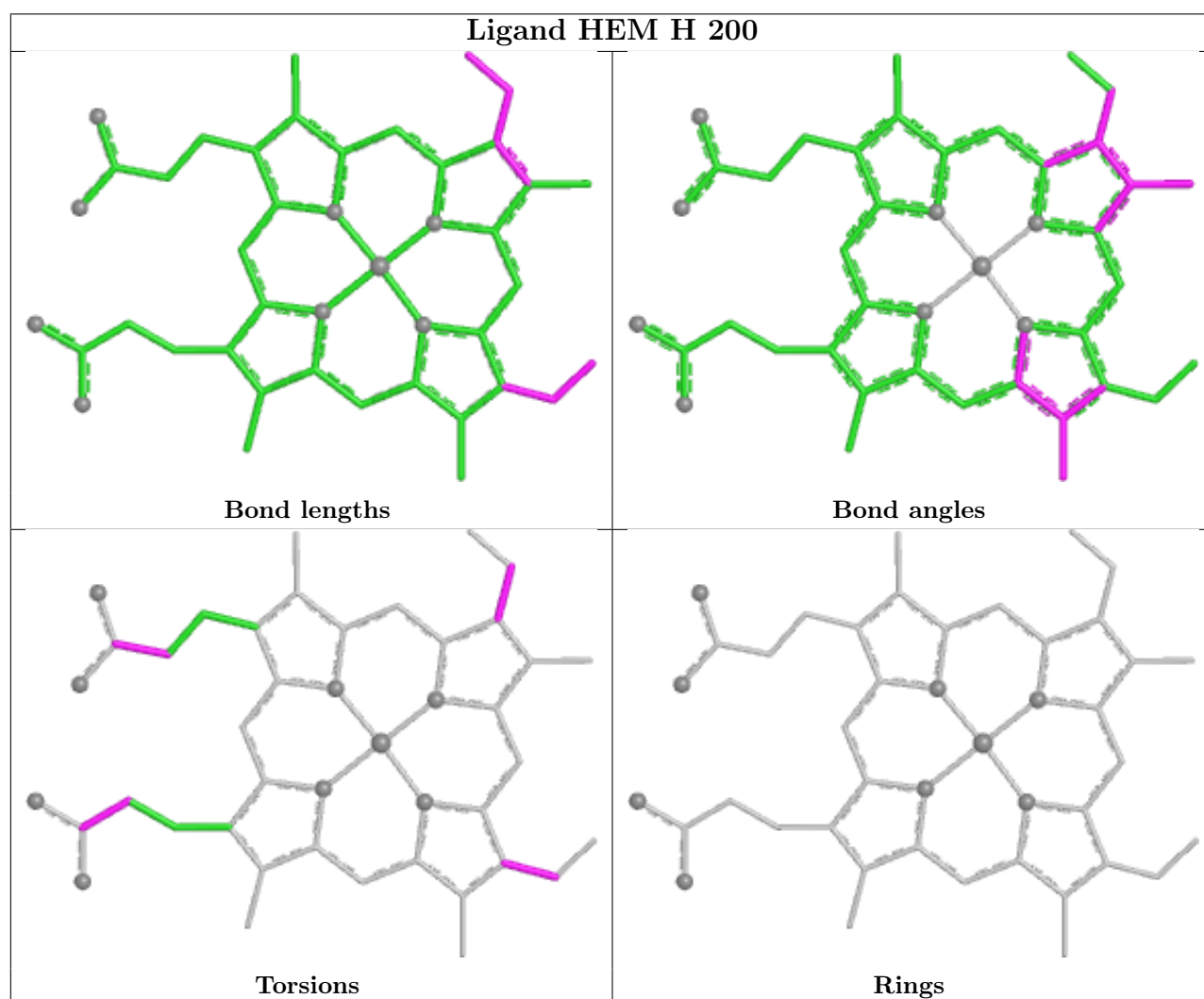
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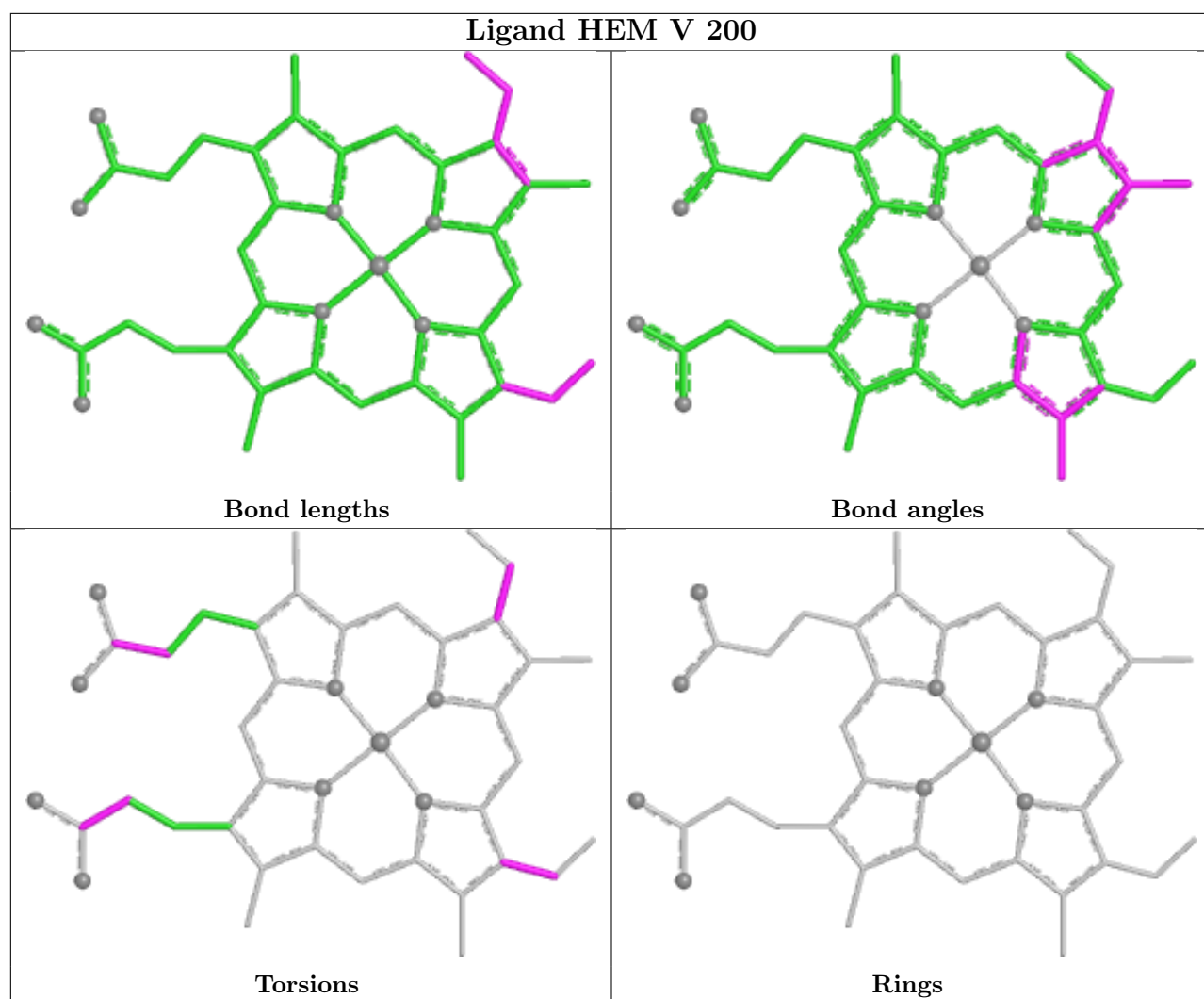
Mol	Chain	Res	Type	Atoms
3	V	200	HEM	CAA-CBA-CGA-O1A
3	X	200	HEM	CAA-CBA-CGA-O1A
3	H	200	HEM	CAA-CBA-CGA-O1A
3	R	200	HEM	CAA-CBA-CGA-O1A
3	B	200	HEM	C4B-C3B-CAB-CBB
3	D	200	HEM	C4B-C3B-CAB-CBB
3	F	200	HEM	C4B-C3B-CAB-CBB
3	H	200	HEM	C4B-C3B-CAB-CBB
3	J	200	HEM	C4B-C3B-CAB-CBB
3	L	200	HEM	C4B-C3B-CAB-CBB
3	N	200	HEM	C4B-C3B-CAB-CBB
3	P	200	HEM	C4B-C3B-CAB-CBB
3	R	200	HEM	C4B-C3B-CAB-CBB
3	T	200	HEM	C4B-C3B-CAB-CBB
3	V	200	HEM	C4B-C3B-CAB-CBB
3	X	200	HEM	C4B-C3B-CAB-CBB
3	B	200	HEM	CAD-CBD-CGD-O1D
3	F	200	HEM	CAD-CBD-CGD-O1D
3	H	200	HEM	CAD-CBD-CGD-O1D
3	J	200	HEM	CAD-CBD-CGD-O1D
3	L	200	HEM	CAD-CBD-CGD-O1D
3	P	200	HEM	CAD-CBD-CGD-O1D
3	R	200	HEM	CAD-CBD-CGD-O1D
3	X	200	HEM	CAD-CBD-CGD-O1D
3	B	200	HEM	CAD-CBD-CGD-O2D
3	D	200	HEM	CAD-CBD-CGD-O1D
3	D	200	HEM	CAD-CBD-CGD-O2D
3	F	200	HEM	CAD-CBD-CGD-O2D
3	H	200	HEM	CAD-CBD-CGD-O2D
3	J	200	HEM	CAD-CBD-CGD-O2D
3	L	200	HEM	CAD-CBD-CGD-O2D
3	N	200	HEM	CAD-CBD-CGD-O1D
3	N	200	HEM	CAD-CBD-CGD-O2D
3	R	200	HEM	CAD-CBD-CGD-O2D
3	T	200	HEM	CAD-CBD-CGD-O1D
3	V	200	HEM	CAD-CBD-CGD-O1D
3	P	200	HEM	CAD-CBD-CGD-O2D
3	T	200	HEM	CAD-CBD-CGD-O2D
3	V	200	HEM	CAD-CBD-CGD-O2D
3	X	200	HEM	CAD-CBD-CGD-O2D

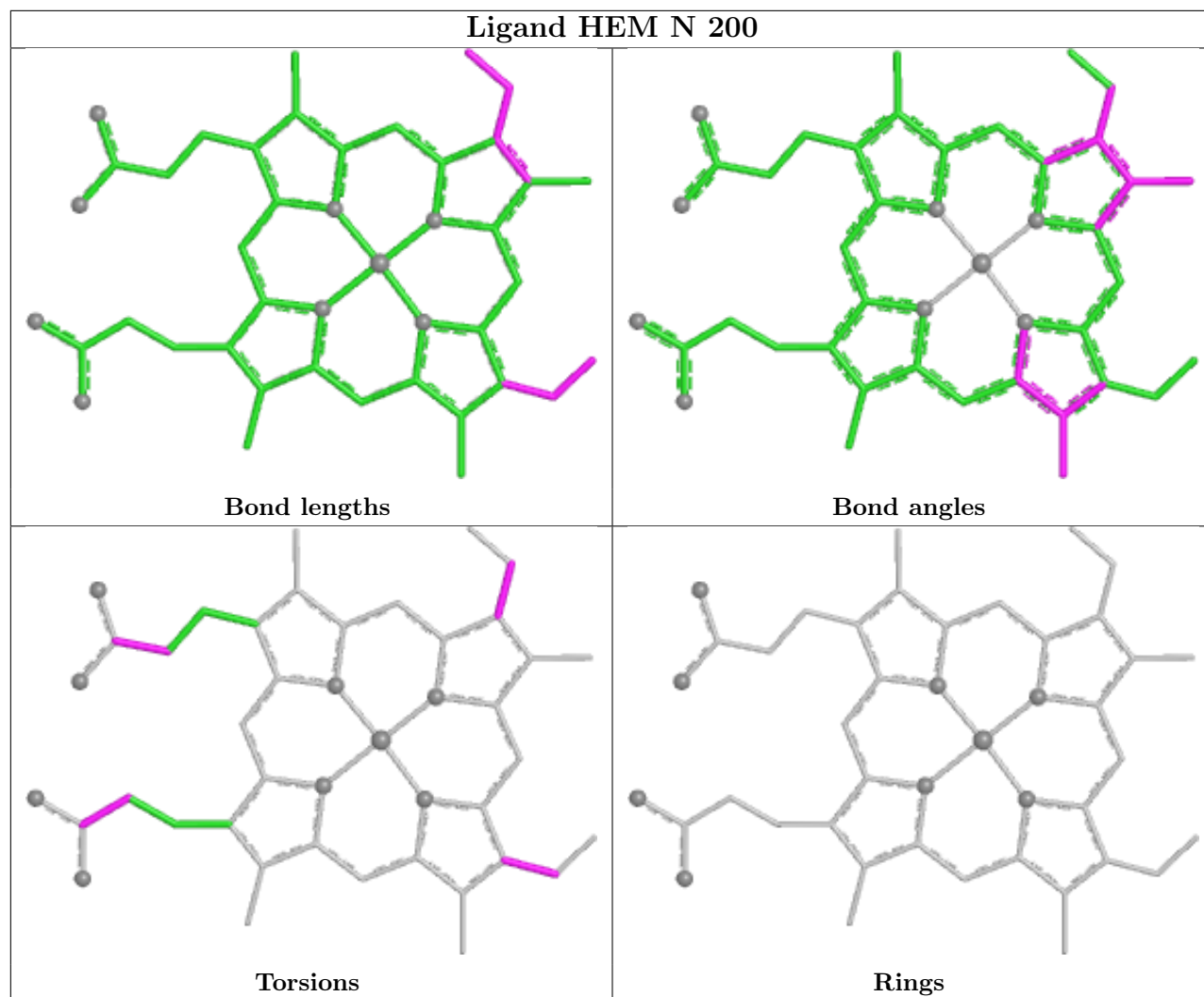
There are no ring outliers.

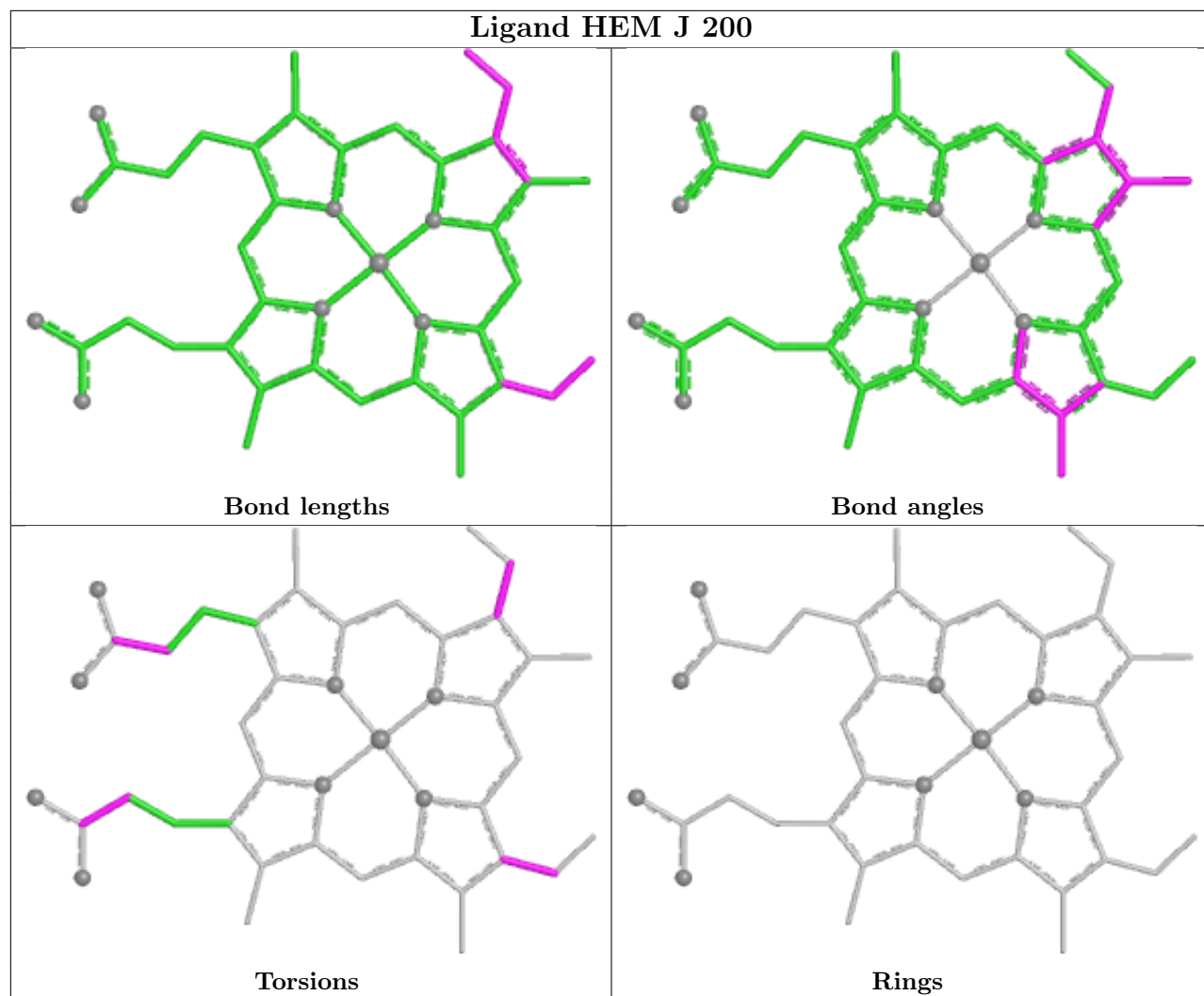
No monomer is involved in short contacts.

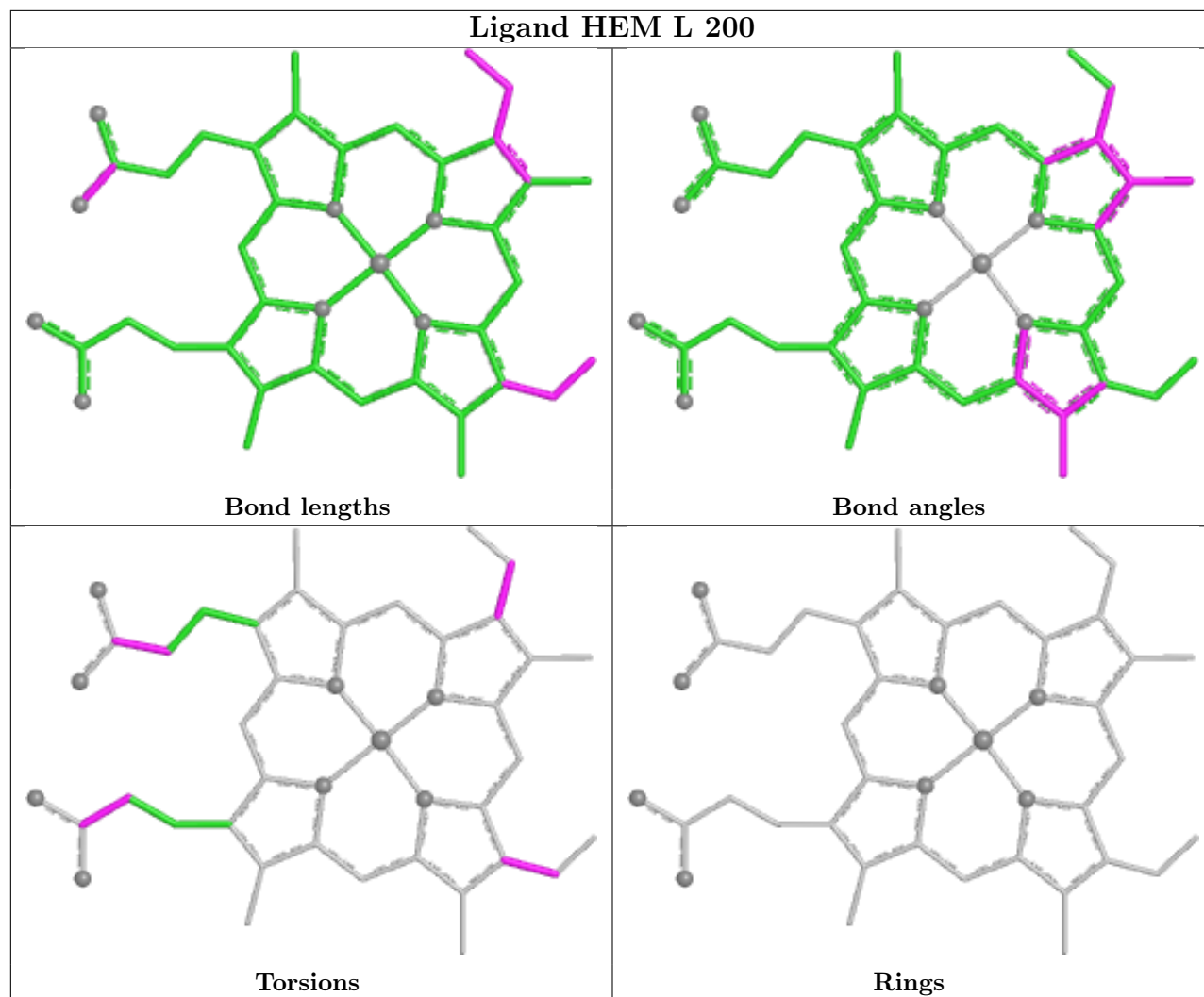
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

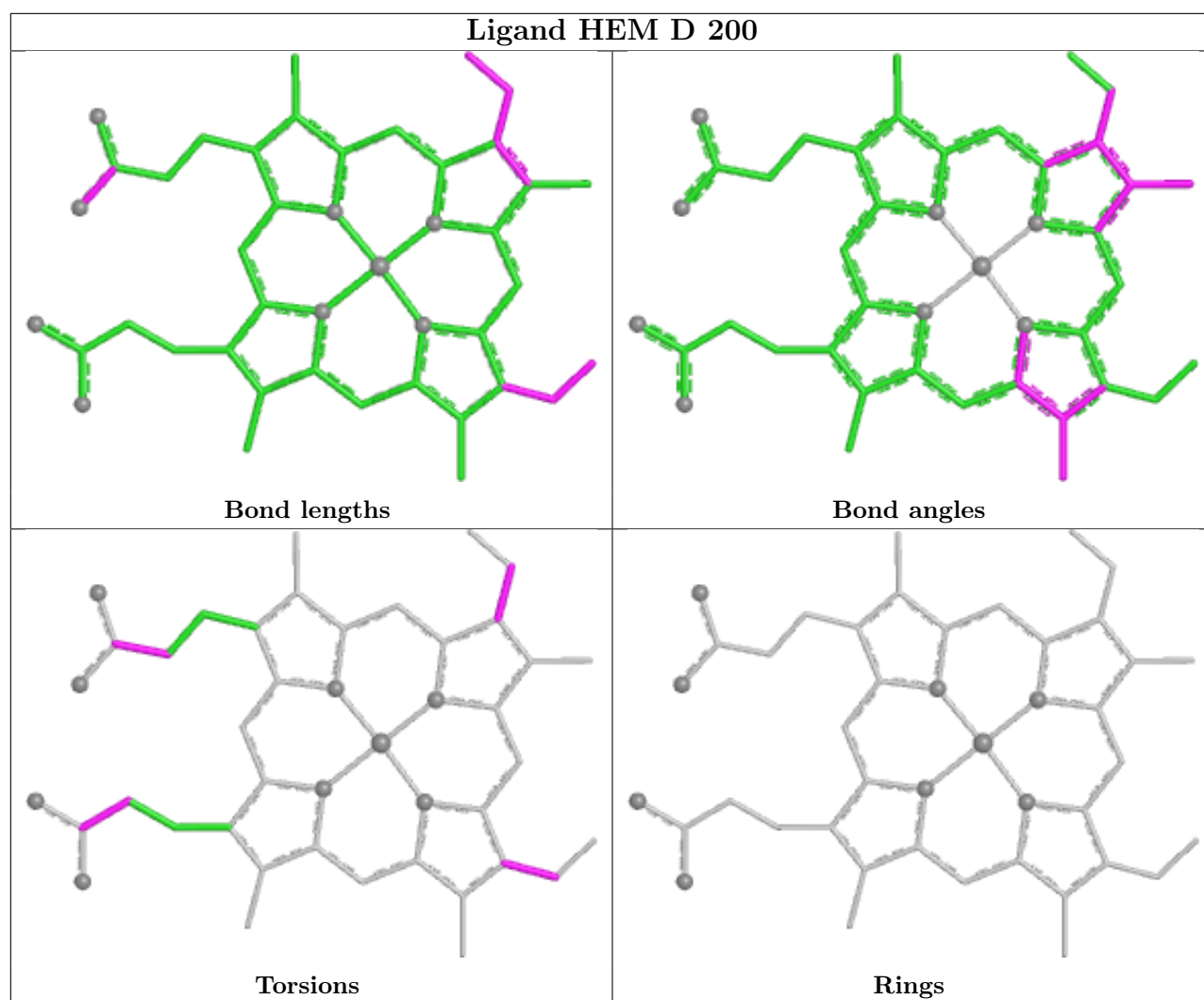


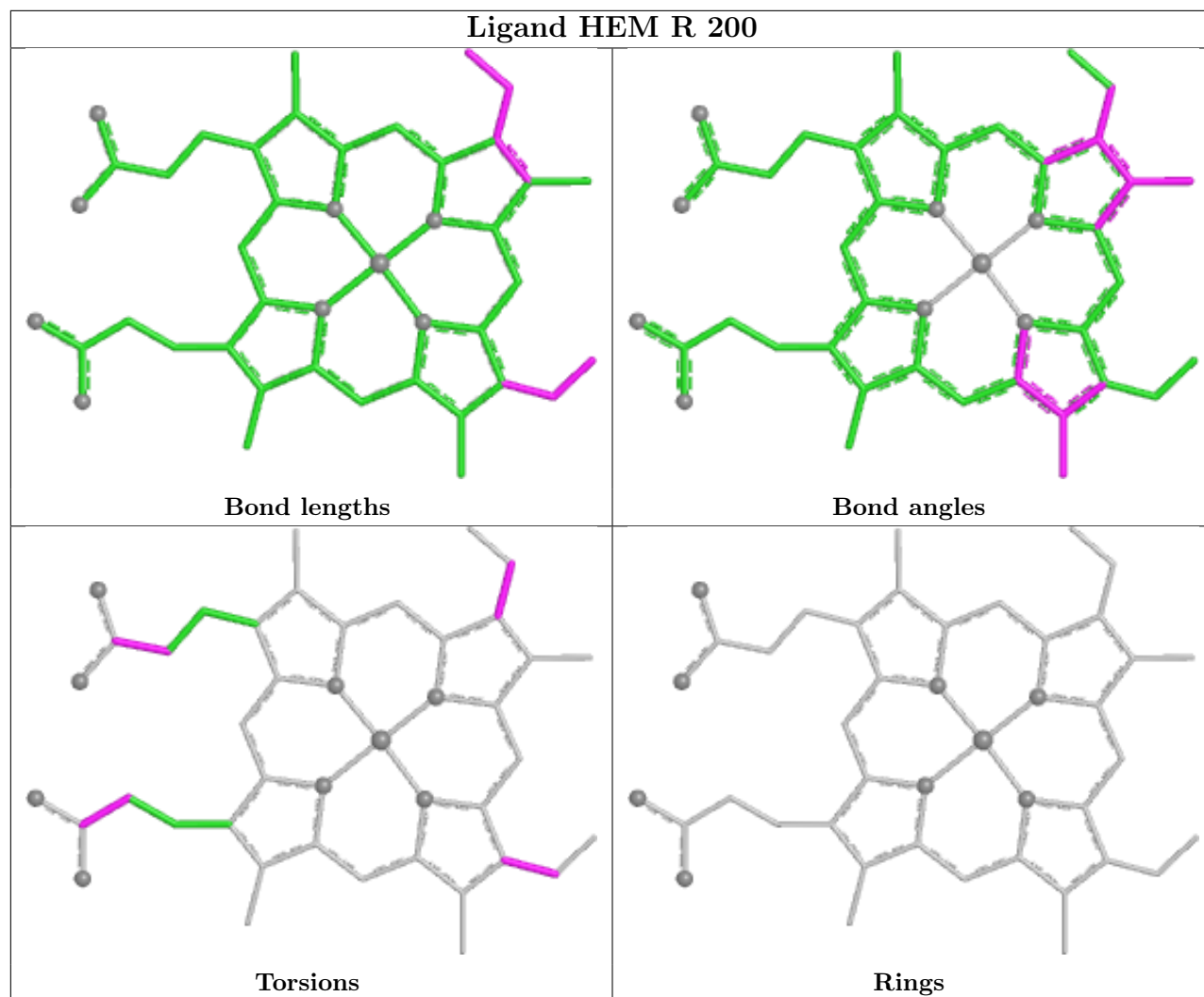


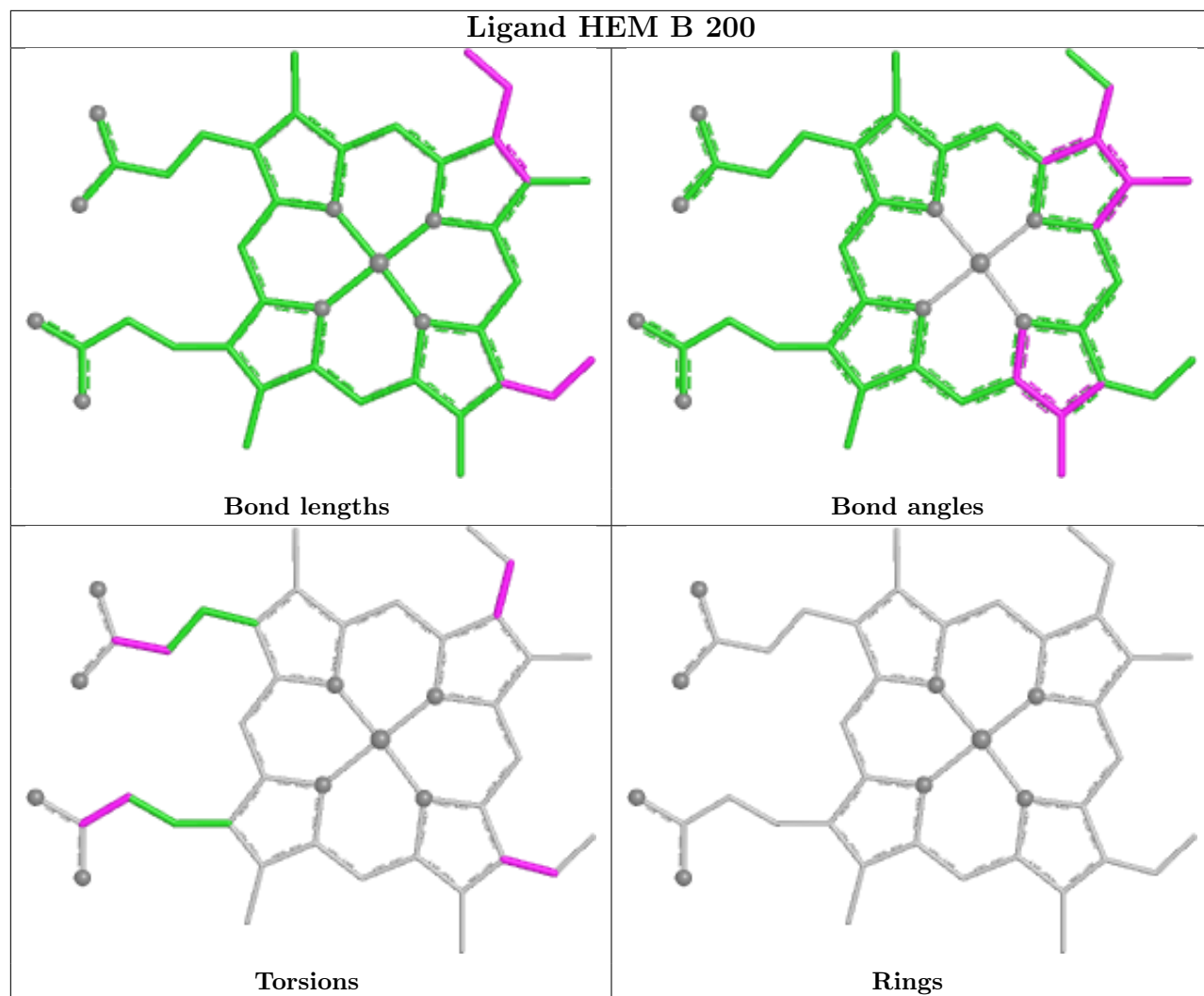


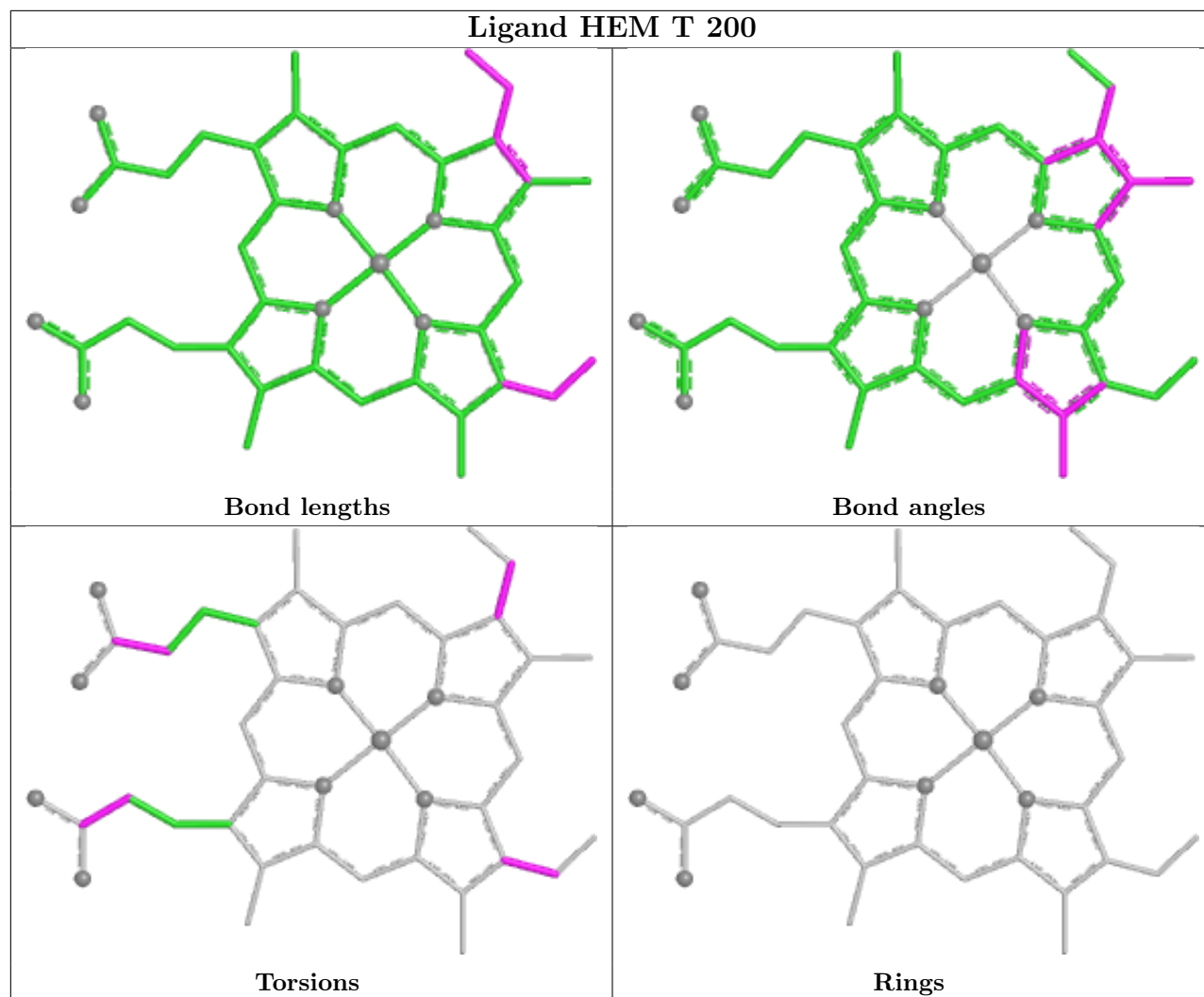


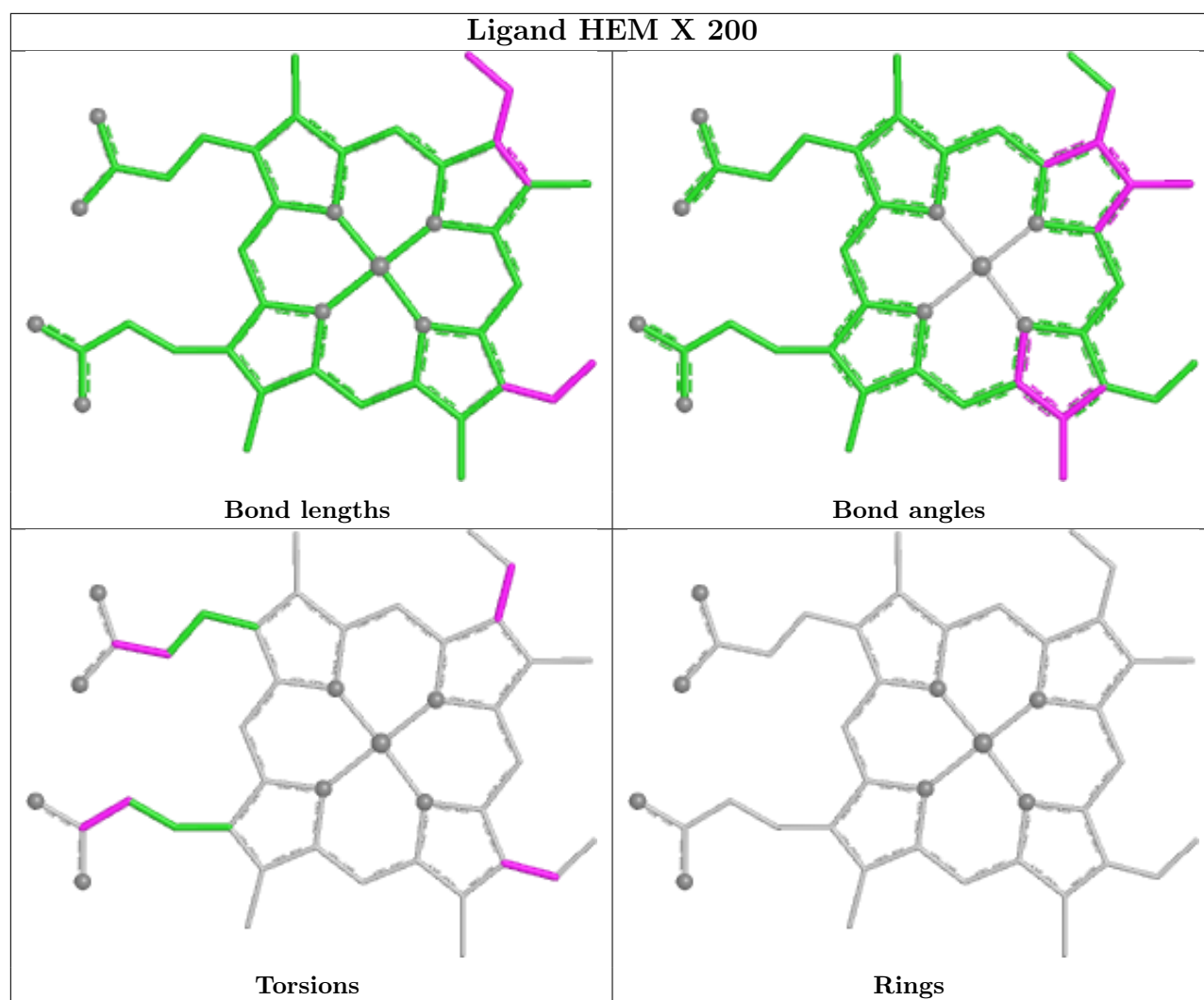


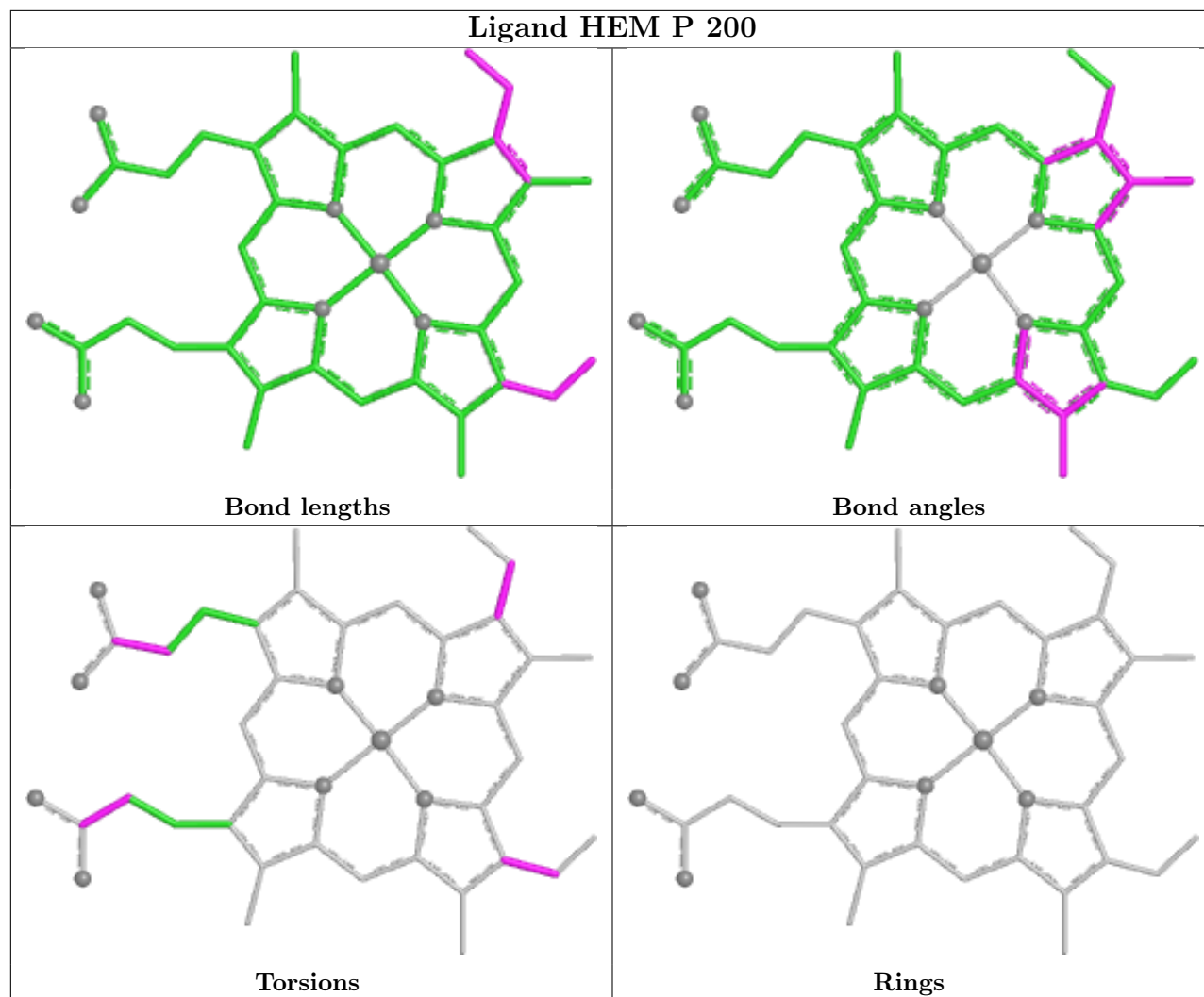


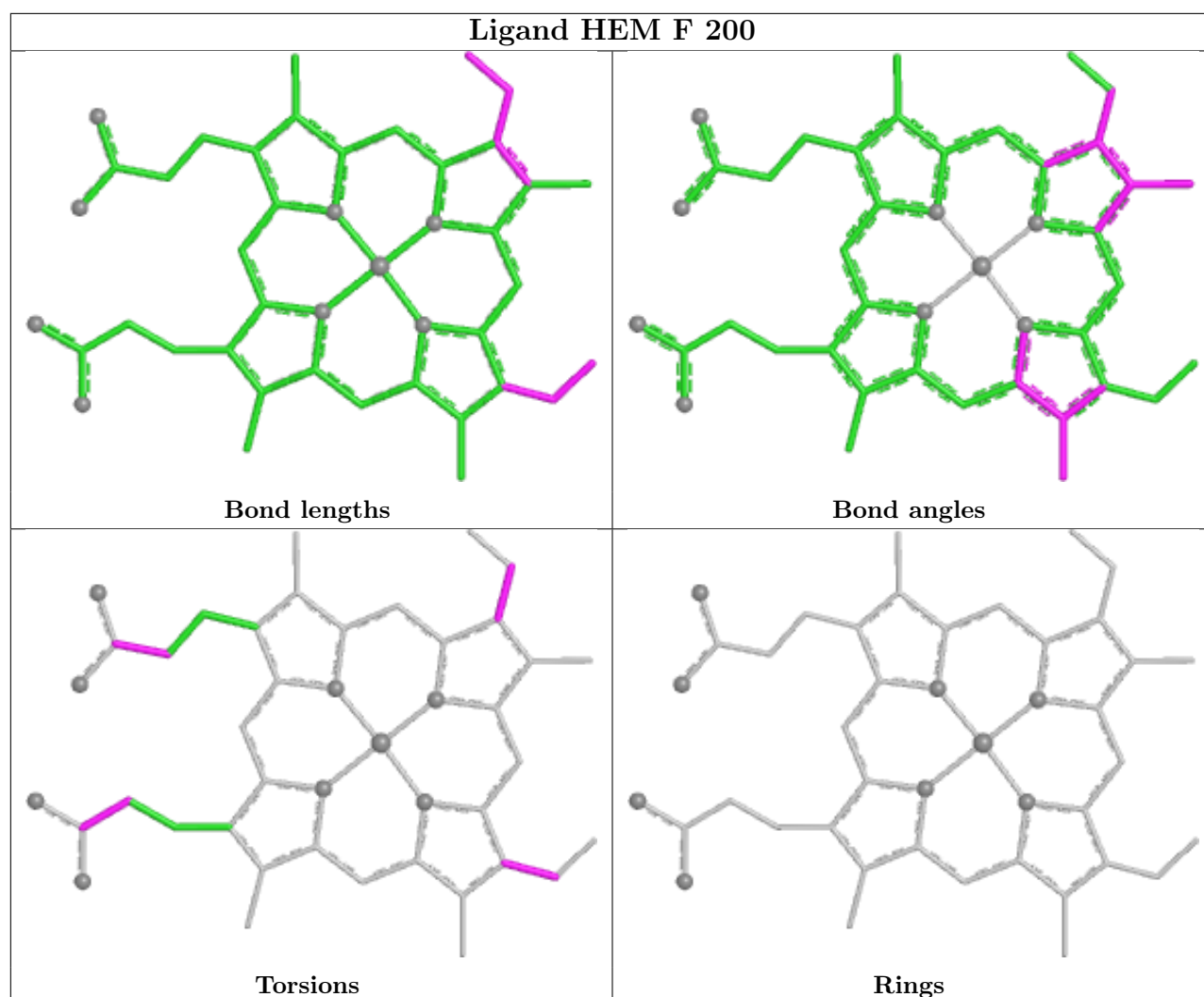












5.7 Other polymers [i](#)

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.