



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:31 AM EDT

PDB ID : 1JRX / pdb_00001jrx
Title : Crystal structure of Arg402Ala mutant flavocytochrome c3 from *Shewanella frigidimarina*
Authors : Mowat, C.G.; Moysey, R.; Miles, C.S.; Leys, D.; Doherty, M.K.; Taylor, P.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2001-08-15
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

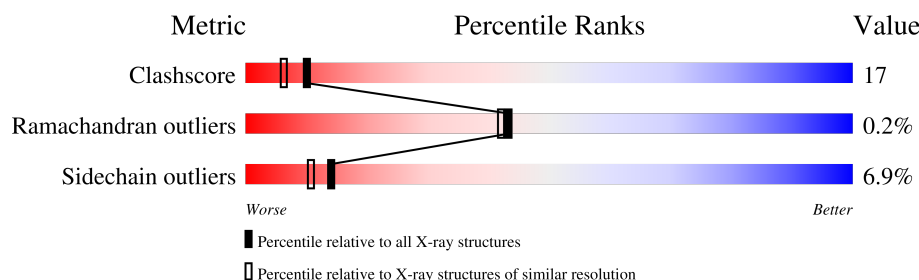
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FAD	A	1805	X	-	-	-
5	FUM	A	1806	-	X	-	-
5	FUM	B	2806	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10555 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 FLAVOCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4207	2609	740	833	25			
1	B	568	Total	C	N	O	S	0	0	0
			4204	2609	741	829	25			

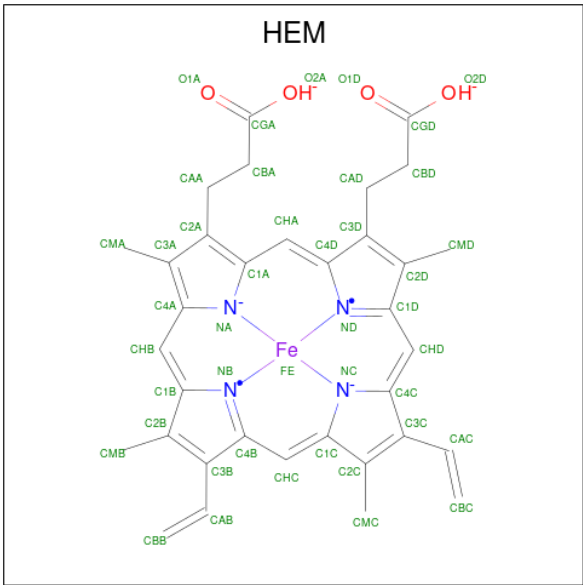
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	ALA	ARG	engineered mutation	UNP Q02469
B	402	ALA	ARG	engineered mutation	UNP Q02469

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



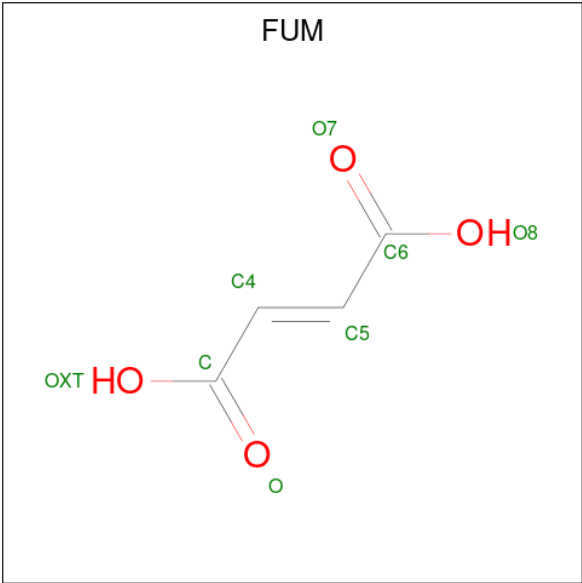
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

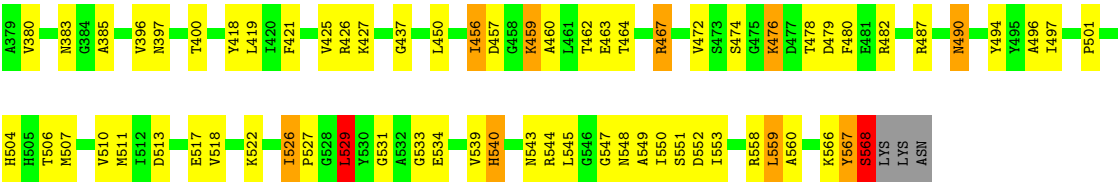
- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	822	Total 822	O 822	0	0
6	B	854	Total 854	O 854	0	0



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	75.97Å 85.93Å 88.32Å 90.00° 104.74° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.4 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10555	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: FUM, HEM, FAD, NA

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	0.94	1/4277 (0.0%)	2.10	128/5784 (2.2%)
1	B	0.96	3/4274 (0.1%)	2.02	123/5779 (2.1%)
All	All	0.95	4/8551 (0.0%)	2.06	251/11563 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	TRP	N-CA	-6.91	1.37	1.46
1	A	176	TRP	N-CA	-6.27	1.34	1.46
1	B	175	ALA	C-O	-5.99	1.17	1.23
1	B	176	TRP	CA-CB	-5.57	1.44	1.53

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	CA-C-N	30.45	176.52	121.70
1	A	175	ALA	C-N-CA	30.45	176.52	121.70
1	B	487	ARG	CD-NE-CZ	28.82	164.75	124.40
1	B	175	ALA	CA-C-N	16.93	153.88	121.54
1	B	175	ALA	C-N-CA	16.93	153.88	121.54
1	B	176	TRP	N-CA-CB	15.28	136.31	110.49
1	A	567	TYR	CA-C-N	14.16	147.20	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	TYR	C-N-CA	14.16	147.20	121.70
1	A	112	LYS	CA-CB-CG	12.99	140.07	114.10
1	A	33	ASN	CA-CB-CG	-10.37	102.23	112.60
1	A	487	ARG	CD-NE-CZ	9.98	138.38	124.40
1	A	320	ASN	CA-CB-CG	-9.89	102.71	112.60
1	A	567	TYR	CA-C-O	9.79	131.17	120.10
1	B	463	GLU	CB-CG-CD	9.45	128.67	112.60
1	A	202	ASN	CA-CB-CG	-9.39	103.20	112.60
1	B	164	ASN	OD1-CG-ND2	9.34	131.94	122.60
1	A	565	ALA	CA-C-N	8.92	132.03	120.44
1	A	565	ALA	C-N-CA	8.92	132.03	120.44
1	A	567	TYR	O-C-N	-8.46	112.33	122.22
1	B	273	ARG	NE-CZ-NH1	-8.32	113.18	121.50
1	A	264	ASN	CA-CB-CG	-8.21	104.39	112.60
1	A	338	GLN	OE1-CD-NE2	-8.07	114.53	122.60
1	A	176	TRP	N-CA-CB	8.05	124.18	110.50
1	A	286	LYS	CA-CB-CG	7.91	129.93	114.10
1	A	216	SER	CA-C-O	-7.86	112.21	120.55
1	B	540	HIS	CA-CB-CG	-7.86	105.94	113.80
1	A	277	ARG	NE-CZ-NH2	-7.83	112.16	119.20
1	B	202	ASN	CA-CB-CG	-7.82	104.78	112.60
1	B	293	LEU	CA-CB-CG	7.81	143.63	116.30
1	A	506	THR	CA-C-O	-7.69	112.54	120.54
1	A	566	LYS	CA-CB-CG	7.66	129.42	114.10
1	B	71	CYS	CA-C-N	-7.51	113.08	122.84
1	B	71	CYS	C-N-CA	-7.51	113.08	122.84
1	B	289	VAL	N-CA-CB	7.50	121.84	110.13
1	A	112	LYS	CA-C-N	7.46	135.78	121.54
1	A	112	LYS	C-N-CA	7.46	135.78	121.54
1	B	456	ILE	CA-C-O	-7.41	112.62	120.48
1	B	204	ASN	CA-CB-CG	7.37	119.97	112.60
1	A	164	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	A	540	HIS	CA-CB-CG	-7.24	106.56	113.80
1	A	480	PHE	CA-CB-CG	-7.23	106.57	113.80
1	B	5	ALA	CA-C-O	7.21	128.57	121.00
1	B	178	ASP	CA-CB-CG	-7.20	105.40	112.60
1	A	316	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	531	GLY	CA-C-O	-7.16	115.35	120.94
1	B	286	LYS	N-CA-CB	7.14	121.80	110.73
1	A	16	SER	N-CA-C	-7.14	103.54	111.82
1	A	216	SER	O-C-N	7.08	129.63	122.12
1	B	276	THR	CA-C-N	-7.08	112.95	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	THR	C-N-CA	-7.08	112.95	122.72
1	B	18	HIS	CA-CB-CG	-7.07	106.73	113.80
1	B	462	THR	CA-C-O	-7.04	113.08	120.55
1	A	298	TYR	CA-C-O	-7.04	111.44	118.97
1	B	337	ASN	N-CA-C	7.03	120.04	110.55
1	A	526	ILE	CB-CA-C	7.02	119.33	111.04
1	B	338	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	254	GLY	N-CA-C	6.93	120.88	112.49
1	B	531	GLY	O-C-N	6.90	129.01	123.49
1	A	221	ASP	CA-C-O	6.87	127.83	120.55
1	A	40	HIS	CA-CB-CG	-6.86	106.94	113.80
1	A	293	LEU	CA-CB-CG	6.85	140.26	116.30
1	A	426	ARG	CA-C-O	6.84	128.22	120.90
1	A	333	PHE	CA-CB-CG	6.83	120.62	113.80
1	A	115	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	B	294	VAL	O-C-N	6.76	130.44	123.00
1	B	497	ILE	CA-C-O	-6.76	113.68	120.31
1	A	177	THR	CA-C-O	6.74	129.67	121.72
1	A	513	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	8	HIS	CA-CB-CG	-6.61	107.19	113.80
1	A	112	LYS	CB-CG-CD	6.61	126.50	111.30
1	B	264	ASN	CA-CB-CG	-6.60	106.00	112.60
1	A	511	MET	CA-CB-CG	6.58	127.26	114.10
1	B	175	ALA	CB-CA-C	-6.58	98.62	109.80
1	A	65	GLU	CB-CG-CD	6.54	123.72	112.60
1	A	296	GLY	N-CA-C	-6.49	100.14	111.62
1	A	334	ILE	N-CA-C	-6.45	103.02	110.05
1	A	175	ALA	N-CA-CB	6.45	122.67	111.13
1	A	143	ILE	CA-C-N	6.43	129.22	120.54
1	A	143	ILE	C-N-CA	6.43	129.22	120.54
1	B	464	THR	CA-CB-OG1	-6.43	99.96	109.60
1	B	112	LYS	CA-CB-CG	6.41	126.92	114.10
1	B	296	GLY	N-CA-C	-6.35	101.67	111.64
1	B	283	LYS	CB-CG-CD	6.33	125.86	111.30
1	A	543	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	A	147	ASP	CA-CB-CG	-6.29	106.31	112.60
1	B	294	VAL	CA-C-O	-6.27	115.27	121.67
1	B	383	ASN	CA-CB-CG	-6.26	106.34	112.60
1	A	412	GLN	CG-CD-NE2	6.26	125.78	116.40
1	B	265	ALA	CA-C-O	6.22	127.35	120.82
1	B	176	TRP	N-CA-C	-6.21	97.58	110.80
1	A	52	HIS	N-CA-C	-6.20	99.70	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	A	293	LEU	O-C-N	6.18	130.33	123.16
1	A	501	PRO	N-CA-CB	6.17	108.80	103.31
1	A	293	LEU	N-CA-CB	6.16	120.21	110.23
1	A	322	ARG	CA-C-O	6.14	126.93	120.42
1	A	170	GLY	N-CA-C	6.14	121.28	113.24
1	A	295	LYS	CA-C-N	-6.12	115.63	121.57
1	A	295	LYS	C-N-CA	-6.12	115.63	121.57
1	A	11	ASN	OD1-CG-ND2	6.11	128.71	122.60
1	A	170	GLY	CA-C-N	-6.09	112.17	121.62
1	A	170	GLY	C-N-CA	-6.09	112.17	121.62
1	A	130	VAL	N-CA-CB	6.08	119.12	111.46
1	B	164	ASN	CA-CB-CG	-6.07	106.53	112.60
1	B	175	ALA	CA-C-O	6.05	128.37	120.21
1	A	536	THR	CA-C-O	-6.03	114.60	121.72
1	B	289	VAL	CA-CB-CG2	6.03	120.65	110.40
1	B	534	GLU	CA-C-O	-6.02	112.20	119.49
1	A	397	ASN	N-CA-C	-6.02	100.48	109.15
1	B	175	ALA	N-CA-CB	6.00	120.67	110.71
1	B	153	ILE	N-CA-CB	5.98	119.38	111.25
1	B	3	ASN	CA-C-O	5.96	127.66	121.10
1	B	346	LEU	CB-CA-C	-5.92	99.31	110.67
1	B	568	SER	CA-C-O	-5.89	110.78	120.80
1	B	376	VAL	N-CA-C	-5.88	99.94	108.17
1	B	319	ASN	OD1-CG-ND2	5.88	128.47	122.60
1	B	504	HIS	N-CA-CB	-5.87	100.58	110.49
1	A	515	LYS	N-CA-C	-5.86	105.32	112.88
1	B	482	ARG	N-CA-C	-5.85	100.89	109.50
1	B	243	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	B	293	LEU	N-CA-CB	5.84	119.69	110.23
1	A	175	ALA	CA-C-O	5.82	127.58	120.60
1	B	567	TYR	CA-C-O	5.82	126.93	120.82
1	A	476	LYS	CA-C-O	5.79	127.40	120.28
1	B	61	HIS	CA-CB-CG	-5.78	108.02	113.80
1	B	205	ASP	CA-C-N	5.78	125.46	119.05
1	B	205	ASP	C-N-CA	5.78	125.46	119.05
1	A	18	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	342	VAL	N-CA-C	5.77	117.65	112.17
1	A	128	ASP	CA-CB-CG	-5.77	106.83	112.60
1	B	277	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	B	540	HIS	N-CA-CB	-5.74	102.00	110.49
1	B	109	ALA	CA-C-N	5.72	129.76	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ALA	C-N-CA	5.72	129.76	120.60
1	A	412	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	B	548	ASN	OD1-CG-ND2	5.69	128.29	122.60
1	A	269	ASN	OD1-CG-ND2	5.66	128.26	122.60
1	B	480	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	241	VAL	CA-C-O	-5.66	115.78	121.49
1	B	217	LYS	CA-C-O	5.66	126.42	120.42
1	A	280	GLU	O-C-N	5.65	129.87	123.42
1	A	36	CYS	O-C-N	5.63	128.09	122.12
1	A	311	LEU	O-C-N	-5.63	116.10	123.02
1	B	286	LYS	CA-CB-CG	5.61	125.31	114.10
1	A	424	SER	N-CA-CB	5.59	118.43	110.16
1	A	75	HIS	CA-CB-CG	-5.57	108.23	113.80
1	B	367	THR	N-CA-C	5.57	116.40	108.54
1	B	130	VAL	N-CA-C	-5.57	100.37	108.17
1	A	419	LEU	N-CA-C	-5.57	101.41	110.20
1	A	127	VAL	CA-C-O	-5.57	115.60	121.44
1	A	560	ALA	CB-CA-C	-5.56	101.56	110.79
1	A	457	ASP	CA-C-O	-5.56	114.31	120.70
1	A	439	GLY	N-CA-C	-5.56	107.59	115.43
1	B	132	VAL	CA-C-O	-5.56	114.16	120.66
1	B	90	PHE	CA-C-N	-5.55	114.88	122.87
1	B	90	PHE	C-N-CA	-5.55	114.88	122.87
1	A	337	ASN	OD1-CG-ND2	5.54	128.14	122.60
1	A	247	PRO	CA-C-O	5.54	127.98	121.56
1	B	529	LEU	CA-C-O	5.53	126.40	120.32
1	B	115	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	B	558	ARG	CA-C-O	5.50	126.60	120.82
1	B	551	SER	CA-C-N	5.49	127.58	120.44
1	B	551	SER	C-N-CA	5.49	127.58	120.44
1	A	51	LYS	CA-C-O	5.49	127.23	121.19
1	B	203	ILE	N-CA-C	-5.49	104.61	112.35
1	B	175	ALA	O-C-N	-5.49	116.69	123.44
1	B	286	LYS	CD-CE-NZ	5.48	129.44	111.90
1	B	36	CYS	N-CA-CB	5.48	118.17	110.12
1	B	427	LYS	CD-CE-NZ	5.47	129.40	111.90
1	A	46	VAL	O-C-N	-5.46	116.57	121.87
1	A	322	ARG	NH1-CZ-NH2	5.46	126.40	119.30
1	A	390	ARG	CA-CB-CG	-5.45	103.19	114.10
1	B	128	ASP	CA-C-O	5.45	127.12	120.31
1	A	46	VAL	CA-C-N	5.45	127.84	120.38
1	A	46	VAL	C-N-CA	5.45	127.84	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	CA-C-O	-5.45	115.60	120.56
1	B	193	PHE	CA-C-N	5.44	127.57	120.28
1	B	193	PHE	C-N-CA	5.44	127.57	120.28
1	B	72	HIS	CA-C-O	-5.43	114.89	120.54
1	B	365	HIS	N-CA-C	-5.41	102.96	109.83
1	A	8	HIS	N-CA-C	5.41	117.93	111.71
1	B	193	PHE	CA-C-O	5.41	126.50	120.82
1	B	273	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	80	VAL	N-CA-CB	5.41	117.16	111.00
1	B	377	THR	CA-C-N	5.41	128.06	120.28
1	B	377	THR	C-N-CA	5.41	128.06	120.28
1	A	226	MET	CA-C-O	5.40	126.02	119.11
1	A	525	VAL	CA-C-N	-5.37	116.73	122.85
1	A	525	VAL	C-N-CA	-5.37	116.73	122.85
1	B	96	LYS	N-CA-C	-5.36	100.92	109.23
1	A	501	PRO	CA-C-O	5.36	127.45	121.34
1	A	378	GLU	N-CA-CB	-5.35	101.98	110.22
1	B	28	SER	CA-C-O	5.34	125.94	119.11
1	B	222	TRP	CA-C-O	5.34	126.42	120.82
1	A	522	LYS	CA-C-N	5.33	129.69	122.07
1	A	522	LYS	C-N-CA	5.33	129.69	122.07
1	A	519	MET	CA-CB-CG	-5.33	103.44	114.10
1	A	218	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	12	GLN	CA-C-O	-5.29	114.92	121.06
1	B	160	VAL	CA-C-O	-5.29	115.14	121.28
1	A	456	ILE	CA-C-O	-5.28	114.88	120.48
1	A	398	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	551	SER	CA-C-O	5.25	126.52	120.90
1	A	360	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	B	129	VAL	CA-C-N	-5.25	116.68	123.19
1	B	129	VAL	C-N-CA	-5.25	116.68	123.19
1	B	545	LEU	CA-C-O	-5.23	115.09	121.05
1	A	383	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	27	ASP	CA-C-O	-5.22	112.95	119.38
1	B	337	ASN	CA-C-O	5.22	127.97	121.81
1	B	75	HIS	N-CA-C	5.20	118.65	112.72
1	A	240	SER	CA-C-N	-5.19	116.06	123.17
1	A	240	SER	C-N-CA	-5.19	116.06	123.17
1	B	111	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	85	CYS	O-C-N	5.19	127.60	122.10
1	A	513	ASP	N-CA-C	-5.18	102.34	110.17
1	B	460	ALA	CA-C-O	5.18	126.25	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	HIS	CE1-NE2-CD2	5.16	114.16	109.00
1	A	498	GLU	CA-CB-CG	-5.16	103.79	114.10
1	B	426	ARG	O-C-N	-5.16	116.73	122.09
1	B	437	GLY	N-CA-C	-5.12	106.52	113.37
1	B	396	VAL	CB-CA-C	-5.11	106.94	111.74
1	A	551	SER	O-C-N	-5.10	116.78	122.09
1	B	472	VAL	N-CA-C	-5.10	105.52	110.42
1	B	285	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	410	LEU	CA-C-O	-5.09	113.12	119.38
1	A	340	GLY	O-C-N	-5.08	116.47	122.27
1	B	52	HIS	N-CA-C	-5.07	101.66	109.52
1	A	104	THR	N-CA-C	-5.06	104.00	110.53
1	B	39	CYS	N-CA-C	5.06	119.53	112.90
1	B	277	ARG	CB-CG-CD	-5.06	99.66	111.30
1	A	532	ALA	O-C-N	5.05	129.32	123.41
1	A	547	GLY	CA-C-O	5.05	124.67	119.27
1	B	347	ASP	N-CA-C	-5.04	105.86	111.36
1	B	522	LYS	CA-C-N	5.04	129.30	122.19
1	B	522	LYS	C-N-CA	5.04	129.30	122.19
1	B	39	CYS	CA-CB-SG	-5.04	102.82	114.40
1	A	339	PRO	N-CA-C	5.03	120.44	113.65
1	B	494	TYR	CA-C-N	-5.03	114.77	122.62
1	B	494	TYR	C-N-CA	-5.03	114.77	122.62
1	A	154	LEU	CA-C-N	-5.03	115.14	122.68
1	A	154	LEU	C-N-CA	-5.03	115.14	122.68
1	B	560	ALA	CA-C-O	-5.03	115.22	120.55
1	A	76	GLU	CA-C-O	-5.02	115.90	121.33
1	A	317	ALA	CA-C-O	-5.02	114.20	119.97
1	B	323	VAL	O-C-N	5.02	126.74	121.87
1	B	232	ASP	CA-CB-CG	-5.02	107.58	112.60
1	B	113	SER	N-CA-C	-5.01	102.22	109.59
1	A	365	HIS	N-CA-C	-5.01	103.34	109.65
1	B	539	VAL	N-CA-C	5.00	115.67	110.82
1	B	135	GLY	N-CA-C	-5.00	105.44	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	GLU	Mainchain
1	B	175	ALA	Peptide,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	A	4207	0	4140	152	0
1	B	4204	0	4145	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	43	0
3	B	172	0	120	31	0
4	A	53	0	31	5	0
4	B	53	0	31	7	0
5	A	8	0	1	0	0
5	B	8	0	1	1	0
6	A	822	0	0	20	0
6	B	854	0	0	23	0
All	All	10555	0	8589	302	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 17.

All (302) 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:B:165:ALA:HA	6:B:3035:HOH:O	1.57	1.04
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.46	1.03
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.47	1.03
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.49	1.01
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.48	1.01
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.50	0.99
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.51	0.99
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.51	0.99
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.50	0.98
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.54	0.96
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.53	0.96
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.56	0.93
1:B:279:ILE:HB	1:B:293:LEU:HD13	1.47	0.93
1:B:204:ASN:H	1:B:204:ASN:HD22	1.15	0.92
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.59	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.59	0.90
1:B:79:MET:HE3	1:B:96:LYS:HE3	1.52	0.90
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.60	0.90
1:A:280:GLU:HB3	1:A:293:LEU:HD11	1.53	0.90
1:B:229:ASP:H	1:B:256:HIS:HE1	1.22	0.87
1:B:183:LYS:HD3	6:B:1812:HOH:O	1.73	0.86
1:A:280:GLU:HB3	1:A:293:LEU:CD1	2.07	0.84
1:B:293:LEU:HB2	6:B:1852:HOH:O	1.78	0.83
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.68	0.82
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.67	0.82
1:A:14:CYS:HG	3:A:801:HEM:CAB	1.91	0.81
1:B:1:ALA:HB1	1:B:6:GLU:HB3	1.61	0.81
1:A:431:LYS:HA	1:A:434:LYS:HD3	1.63	0.81
1:A:229:ASP:H	1:A:256:HIS:HE1	1.30	0.79
1:B:14:CYS:HG	3:B:801:HEM:CAB	1.95	0.79
1:A:39:CYS:HG	3:A:802:HEM:CAC	1.95	0.79
1:A:279:ILE:HB	1:A:293:LEU:HD13	1.66	0.78
1:B:229:ASP:H	1:B:256:HIS:CE1	2.03	0.77
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.50	0.76
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.26	0.75
1:A:204:ASN:HD22	1:A:204:ASN:H	1.36	0.74
1:B:286:LYS:HE3	6:B:3107:HOH:O	1.85	0.74
1:A:229:ASP:H	1:A:256:HIS:CE1	2.05	0.74
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.27	0.73
4:B:2805:FAD:C9A	4:B:2805:FAD:O2'	2.36	0.72
1:B:279:ILE:HB	1:B:293:LEU:CD1	2.18	0.72
1:A:157:LYS:HZ1	1:A:340:GLY:HA3	1.55	0.71
1:A:357:LYS:HD2	1:A:511:MET:HE3	1.71	0.70
1:A:82:CYS:HG	3:A:804:HEM:CAB	2.03	0.69
1:B:180:GLN:HB3	1:B:185:ILE:HB	1.74	0.69
1:A:311:LEU:HD23	1:A:349:ALA:HB2	1.74	0.69
1:A:427:LYS:HG3	1:B:328:PRO:HB2	1.74	0.68
1:A:218:ASP:HB3	6:A:2029:HOH:O	1.94	0.66
4:B:2805:FAD:O2'	6:B:3035:HOH:O	2.11	0.66
1:B:204:ASN:H	1:B:204:ASN:ND2	1.91	0.65
1:B:21:ASP:OD1	1:B:23:GLU:HB3	1.97	0.65
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.61	0.65
1:A:71:CYS:HG	3:A:803:HEM:CAC	2.07	0.65
1:A:174:ALA:HA	1:A:216:SER:HB2	1.77	0.64
1:B:280:GLU:HB3	1:B:293:LEU:CD1	2.28	0.64
1:B:568:SER:HA	6:B:1293:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HB3	1:A:261:LEU:HB3	1.80	0.64
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.79	0.63
1:A:565:ALA:O	1:A:568:SER:HA	1.98	0.63
1:B:567:TYR:O	1:B:568:SER:HB2	1.98	0.63
1:A:427:LYS:HG3	1:B:328:PRO:CB	2.28	0.63
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.39	0.62
3:A:801:HEM:HBC2	3:A:801:HEM:HMC2	1.83	0.61
1:B:507:MET:HE3	1:B:543:ASN:HA	1.81	0.61
1:A:431:LYS:HD3	1:A:434:LYS:HD3	1.83	0.60
1:B:168:ALA:HA	4:B:2805:FAD:N5	2.17	0.60
1:A:39:CYS:SG	3:A:802:HEM:C3C	2.95	0.59
1:A:168:ALA:HA	4:A:1805:FAD:N5	2.17	0.59
1:A:204:ASN:H	1:A:204:ASN:ND2	2.00	0.59
1:B:286:LYS:HD3	6:B:3421:HOH:O	2.02	0.59
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.41	0.58
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.43	0.58
1:A:183:LYS:HD3	6:A:2375:HOH:O	2.03	0.57
1:B:174:ALA:HA	1:B:216:SER:HB2	1.85	0.57
1:B:418:TYR:CG	1:B:456:ILE:HD11	2.39	0.57
1:A:60:SER:HB3	3:A:804:HEM:HBB2	1.86	0.57
1:A:17:CYS:SG	3:A:801:HEM:CBC	2.92	0.57
1:A:140:SER:O	1:A:144:SER:HB2	2.05	0.57
1:A:230:LEU:HB3	1:A:245:HIS:HB3	1.86	0.57
1:A:293:LEU:HB2	6:A:2201:HOH:O	2.04	0.57
1:A:427:LYS:CG	1:B:328:PRO:HB2	2.34	0.57
1:B:36:CYS:SG	3:B:802:HEM:C3B	2.97	0.57
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.87	0.57
1:B:8:HIS:O	1:B:12:GLN:HG2	2.04	0.57
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.40	0.57
1:A:533:GLY:HA2	1:A:553:ILE:HG22	1.86	0.57
1:A:133:GLY:O	1:A:138:GLY:HA3	2.05	0.57
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.44	0.57
1:A:144:SER:HB3	1:A:561:GLY:HA3	1.87	0.56
1:A:302:TYR:HA	6:A:2308:HOH:O	2.06	0.56
1:B:17:CYS:SG	3:B:801:HEM:CBC	2.94	0.56
1:B:71:CYS:SG	3:B:803:HEM:C3C	2.98	0.56
1:B:112:LYS:HE2	6:B:3268:HOH:O	2.05	0.56
1:A:17:CYS:SG	3:A:801:HEM:C3C	2.98	0.56
1:B:158:GLU:HB3	1:B:159:PRO:HD2	1.88	0.56
1:B:311:LEU:HD22	1:B:529:LEU:HD21	1.87	0.56
1:A:463:GLU:HG2	6:A:2070:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:O	1:B:110:LYS:HB2	2.06	0.55
1:A:177:THR:OG1	1:A:245:HIS:HE1	1.88	0.55
1:B:17:CYS:SG	3:B:801:HEM:C3C	2.98	0.55
1:B:280:GLU:N	1:B:293:LEU:HD12	2.22	0.55
1:B:223:MET:HE2	1:B:257:VAL:HG13	1.88	0.55
1:A:79:MET:HE3	1:A:96:LYS:HE3	1.88	0.55
1:B:157:LYS:NZ	1:B:340:GLY:HA3	2.21	0.55
1:B:180:GLN:HG2	1:B:233:VAL:HG11	1.88	0.54
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.47	0.54
1:B:194:GLU:HG2	6:B:1685:HOH:O	2.06	0.54
1:B:112:LYS:HA	1:B:112:LYS:HE3	1.90	0.54
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.01	0.54
1:A:157:LYS:HZ1	1:A:340:GLY:CA	2.20	0.54
1:A:112:LYS:HE3	6:A:2573:HOH:O	2.07	0.54
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.00	0.53
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.91	0.53
1:A:431:LYS:HZ2	1:A:434:LYS:HE2	1.72	0.53
3:A:801:HEM:HBC2	3:A:801:HEM:CMC	2.38	0.53
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.01	0.53
1:B:419:LEU:O	1:B:496:ALA:HA	2.07	0.53
1:A:280:GLU:CB	1:A:293:LEU:HD11	2.33	0.53
1:B:457:ASP:OD1	1:B:459:LYS:HG3	2.08	0.53
1:A:91:ASN:HB2	6:A:2321:HOH:O	2.08	0.53
1:B:139:PHE:HB3	1:B:261:LEU:HB3	1.90	0.53
3:A:803:HEM:HBC2	3:A:803:HEM:HMC1	1.90	0.52
1:A:168:ALA:HA	4:A:1805:FAD:C5X	2.39	0.52
1:B:107:GLU:HB3	6:B:1540:HOH:O	2.09	0.52
1:A:85:CYS:SG	3:A:804:HEM:HAC	2.47	0.52
1:B:365:HIS:O	1:B:501:PRO:HA	2.09	0.52
1:B:191:LEU:HD21	1:B:240:SER:HB2	1.92	0.52
1:B:337:ASN:N	1:B:337:ASN:HD22	2.08	0.52
1:A:415:LYS:HD3	6:A:2560:HOH:O	2.08	0.52
1:A:68:CYS:SG	3:A:803:HEM:C3B	3.03	0.52
1:B:47:ALA:HA	1:B:58:HIS:HB2	1.93	0.51
1:B:559:LEU:HD13	1:B:559:LEU:C	2.36	0.51
1:B:85:CYS:SG	3:B:804:HEM:CBC	2.97	0.51
1:B:157:LYS:HZ1	1:B:340:GLY:HA3	1.74	0.51
1:B:490:ASN:C	1:B:490:ASN:HD22	2.19	0.51
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.04	0.51
1:A:237:GLY:N	1:A:378:GLU:OE2	2.32	0.51
1:B:540:HIS:CD2	1:B:544:ARG:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLY:O	1:B:138:GLY:HA3	2.10	0.51
1:B:297:MET:HE1	6:B:1434:HOH:O	2.10	0.51
1:A:157:LYS:NZ	1:A:340:GLY:HA3	2.24	0.51
1:B:183:LYS:O	1:B:184:LYS:HB2	2.11	0.51
1:A:280:GLU:HB3	1:A:293:LEU:HD12	1.91	0.50
1:B:550:ILE:HD11	6:B:3035:HOH:O	2.10	0.50
1:B:113:SER:O	1:B:114:GLU:CB	2.59	0.50
1:B:313:THR:OG1	1:B:345:GLY:HA3	2.11	0.50
1:A:293:LEU:CB	6:A:2201:HOH:O	2.60	0.50
1:B:11:ASN:HB2	6:B:3063:HOH:O	2.12	0.50
1:B:85:CYS:SG	3:B:804:HEM:HAC	2.44	0.50
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.48	0.49
1:B:236:MET:HB3	1:B:378:GLU:OE2	2.12	0.49
1:A:481:GLU:HG3	6:A:2061:HOH:O	2.11	0.49
1:A:393:LYS:HD3	6:A:2231:HOH:O	2.11	0.49
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.48	0.49
1:B:210:LYS:HD3	6:B:1521:HOH:O	2.11	0.49
1:A:365:HIS:O	1:A:501:PRO:HA	2.12	0.49
1:B:68:CYS:SG	3:B:803:HEM:C3B	3.05	0.49
1:A:112:LYS:O	1:A:116:GLN:HB2	2.12	0.49
1:A:313:THR:OG1	1:A:345:GLY:HA3	2.13	0.49
1:B:198:LYS:HG2	6:B:1728:HOH:O	2.13	0.49
1:B:204:ASN:HD22	1:B:204:ASN:N	1.94	0.49
1:B:136:GLY:HA3	1:B:553:ILE:HD12	1.94	0.48
1:A:457:ASP:OD1	1:A:459:LYS:HG3	2.13	0.48
1:A:39:CYS:SG	3:A:802:HEM:CBC	3.01	0.48
1:A:558:ARG:O	1:A:562:GLU:HG3	2.13	0.48
1:B:56:ASN:HD22	1:B:58:HIS:H	1.61	0.48
1:B:380:VAL:HG12	1:B:385:ALA:HB2	1.94	0.48
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.06	0.48
1:B:513:ASP:OD2	1:B:517:GLU:OE1	2.32	0.48
1:B:540:HIS:HD2	6:B:1162:HOH:O	1.96	0.48
1:A:44:ALA:O	1:A:47:ALA:HB3	2.14	0.48
1:A:65:GLU:HG3	1:A:262:TYR:CE2	2.49	0.48
1:A:368:LEU:HB3	1:A:500:THR:O	2.13	0.48
1:A:418:TYR:CG	1:A:456:ILE:HD11	2.49	0.48
1:B:476:LYS:HG2	1:B:478:THR:HG23	1.96	0.48
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.07	0.47
1:B:25:SER:O	1:B:26:ASN:HB3	2.14	0.47
1:B:226:MET:HB3	1:B:264:ASN:ND2	2.29	0.47
1:A:164:ASN:HB2	4:A:1805:FAD:H4'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.00	0.47
1:B:511:MET:HB2	1:B:511:MET:HE3	1.72	0.47
1:A:183:LYS:HD2	6:A:1944:HOH:O	2.15	0.47
1:A:517:GLU:HB3	1:A:525:VAL:HG13	1.96	0.47
1:B:46:VAL:HG21	3:B:803:HEM:HMB3	1.97	0.47
1:B:280:GLU:HB3	1:B:293:LEU:HD12	1.96	0.47
1:B:380:VAL:HG12	1:B:385:ALA:CB	2.44	0.47
1:B:50:THR:HG21	1:B:58:HIS:CE1	2.49	0.46
1:B:19:THR:HB	1:B:20:PRO:HD2	1.98	0.46
1:A:47:ALA:HA	1:A:58:HIS:HB2	1.97	0.46
1:A:519:MET:HE2	1:A:523:LYS:O	2.16	0.46
1:A:297:MET:HE1	6:A:2116:HOH:O	2.14	0.46
1:A:318:LYS:HE3	1:A:339:PRO:HA	1.97	0.46
1:A:429:LEU:HD23	1:A:432:ILE:HG13	1.98	0.46
1:A:24:LEU:HG	3:A:801:HEM:HBA1	1.98	0.46
1:A:39:CYS:HG	3:A:802:HEM:CBC	2.28	0.46
1:A:431:LYS:HA	1:A:434:LYS:CD	2.41	0.46
1:A:86:HIS:CD2	3:A:804:HEM:NB	2.84	0.46
1:B:280:GLU:HB3	1:B:293:LEU:HD11	1.97	0.45
1:A:165:ALA:HB2	4:A:1805:FAD:O4'	2.16	0.45
1:B:229:ASP:N	1:B:256:HIS:HE1	2.02	0.45
1:A:60:SER:CB	3:A:804:HEM:HBB2	2.46	0.45
4:B:2805:FAD:C2	5:B:2806:FUM:O7	2.64	0.45
1:A:431:LYS:NZ	1:A:434:LYS:HE2	2.30	0.45
1:A:6:GLU:HA	1:A:9:VAL:HG22	1.99	0.45
1:B:218:ASP:HB2	6:B:1321:HOH:O	2.17	0.45
1:A:42:THR:O	1:A:46:VAL:HG23	2.16	0.45
1:A:229:ASP:N	1:A:256:HIS:HE1	2.08	0.45
1:A:520:ASN:HB2	6:A:1871:HOH:O	2.16	0.45
1:B:14:CYS:SG	3:B:801:HEM:C3B	3.10	0.45
1:A:174:ALA:HA	1:A:216:SER:CB	2.47	0.45
4:B:2805:FAD:O2'	4:B:2805:FAD:C9	2.65	0.45
4:B:2805:FAD:H1'1	6:B:1141:HOH:O	2.16	0.45
1:A:490:ASN:HD22	1:A:490:ASN:C	2.23	0.45
1:B:48:GLU:HG3	6:B:1998:HOH:O	2.15	0.44
1:B:518:VAL:HG21	1:B:529:LEU:HD13	1.99	0.44
1:B:526:ILE:HD13	1:B:529:LEU:HD12	1.99	0.44
1:A:396:VAL:HG22	1:A:397:ASN:N	2.32	0.44
1:B:60:SER:HB3	3:B:804:HEM:HMB1	1.99	0.44
1:A:199:GLY:HA3	1:A:545:LEU:HD21	2.00	0.44
1:A:252:GLY:H	1:A:434:LYS:NZ	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ALA:HB1	6:B:1913:HOH:O	2.15	0.44
1:A:82:CYS:SG	3:A:804:HEM:CBB	3.03	0.44
1:B:544:ARG:CZ	1:B:549:ALA:HB2	2.46	0.44
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.98	0.44
1:A:367:THR:HA	1:A:499:VAL:HB	2.00	0.44
1:A:64:GLY:HA2	1:A:262:TYR:CD2	2.53	0.43
1:B:99:LEU:HD12	6:B:1879:HOH:O	2.16	0.43
1:B:199:GLY:O	1:B:543:ASN:HB3	2.18	0.43
1:B:237:GLY:N	1:B:378:GLU:OE2	2.33	0.43
1:A:79:MET:HE1	1:A:99:LEU:O	2.19	0.43
3:B:803:HEM:HBC1	3:B:804:HEM:HBB1	1.99	0.43
1:A:60:SER:HB3	3:A:804:HEM:CMB	2.47	0.43
1:A:183:LYS:HB3	1:A:183:LYS:HE2	1.78	0.43
1:A:526:ILE:CD1	1:A:529:LEU:HD12	2.47	0.43
1:B:510:VAL:CG1	1:B:518:VAL:HG13	2.49	0.43
3:A:803:HEM:HBB2	3:A:803:HEM:CMB	2.48	0.43
1:B:4:LEU:HD21	3:B:802:HEM:HMB3	2.00	0.43
1:B:112:LYS:HA	1:B:112:LYS:CE	2.49	0.43
1:A:127:VAL:HG11	1:A:153:ILE:HG13	2.00	0.43
1:A:513:ASP:OD2	1:A:517:GLU:OE1	2.37	0.43
1:B:125:ASP:HB2	1:B:304:VAL:HG13	2.00	0.43
1:B:316:PHE:CE2	1:B:506:THR:HB	2.53	0.43
1:A:371:LYS:HE2	6:A:2408:HOH:O	2.18	0.43
1:A:14:CYS:SG	3:A:801:HEM:C3B	3.10	0.43
1:A:55:TYR:OH	1:A:89:ASP:HB3	2.19	0.43
1:A:194:GLU:HB2	6:A:2458:HOH:O	2.18	0.43
1:A:380:VAL:HG22	1:A:432:ILE:HG12	2.01	0.43
1:B:321:GLU:O	1:B:325:LYS:HG3	2.19	0.43
1:B:293:LEU:CB	6:B:1852:HOH:O	2.54	0.43
1:A:341:ALA:HA	6:A:1831:HOH:O	2.19	0.43
3:A:804:HEM:HMB1	3:A:804:HEM:HBB2	1.99	0.43
1:B:68:CYS:SG	3:B:803:HEM:CBB	3.06	0.43
1:A:284:ASP:HA	1:A:290:LYS:HD3	2.01	0.42
1:A:487:ARG:HD3	6:A:2316:HOH:O	2.19	0.42
1:B:397:ASN:O	1:B:400:THR:HG22	2.20	0.42
1:A:434:LYS:HG3	6:A:2259:HOH:O	2.19	0.42
1:A:68:CYS:SG	3:A:803:HEM:CBB	3.06	0.42
1:A:283:LYS:NZ	1:A:352:ALA:O	2.44	0.42
1:A:540:HIS:CG	1:A:544:ARG:HG3	2.54	0.42
1:B:141:ALA:HB1	1:B:310:ILE:HD13	2.01	0.42
1:B:288:THR:HB	1:B:527:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HB3	1:A:337:ASN:OD1	2.20	0.42
1:B:280:GLU:H	1:B:293:LEU:HD12	1.84	0.42
1:B:102:GLU:OE2	1:B:157:LYS:HE2	2.19	0.42
1:B:467:ARG:NE	1:B:479:ASP:OD2	2.53	0.42
1:A:129:VAL:O	1:A:152:VAL:HA	2.19	0.42
1:A:137:ALA:HA	1:A:553:ILE:O	2.19	0.42
1:A:552:ASP:OD1	1:A:552:ASP:C	2.62	0.42
1:A:559:LEU:C	1:A:559:LEU:HD13	2.44	0.42
1:B:168:ALA:HA	4:B:2805:FAD:C5X	2.49	0.42
1:A:36:CYS:SG	3:A:802:HEM:CBB	3.06	0.42
1:B:421:PHE:HB2	1:B:425:VAL:HB	2.01	0.41
1:B:113:SER:O	1:B:114:GLU:HB2	2.21	0.41
1:B:223:MET:HE1	1:B:261:LEU:HG	2.01	0.41
1:B:69:THR:HA	1:B:72:HIS:O	2.20	0.41
1:A:512:ILE:HA	1:A:517:GLU:O	2.20	0.41
1:A:247:PRO:O	1:A:248:THR:C	2.63	0.41
1:A:184:LYS:HA	1:A:184:LYS:HD2	1.87	0.41
1:A:346:LEU:HD21	1:A:509:GLY:HA2	2.02	0.41
1:A:357:LYS:HB3	1:A:511:MET:HE3	2.03	0.41
1:A:544:ARG:HD2	1:A:549:ALA:HB2	2.03	0.41
1:B:52:HIS:HB2	1:B:55:TYR:O	2.20	0.41
1:B:474:SER:OG	1:B:476:LYS:NZ	2.37	0.41
1:B:533:GLY:HA2	1:B:553:ILE:HG22	2.02	0.41
1:A:279:ILE:HB	1:A:293:LEU:CD1	2.44	0.41
1:A:431:LYS:O	1:A:434:LYS:HB2	2.20	0.41
1:A:550:ILE:HG12	4:A:1805:FAD:C2	2.51	0.41
1:B:10:GLN:HG3	6:B:1489:HOH:O	2.20	0.41
1:B:127:VAL:HG11	1:B:153:ILE:HG13	2.03	0.41
1:B:286:LYS:HE2	1:B:286:LYS:HB2	1.28	0.41
1:A:43:LEU:HD23	6:A:2300:HOH:O	2.21	0.40
1:A:505:HIS:CG	1:A:544:ARG:HE	2.39	0.40
1:A:289:VAL:HG21	1:A:309:VAL:HG23	2.03	0.40
1:A:337:ASN:HD22	1:A:337:ASN:N	2.18	0.40
1:B:171:GLY:O	1:B:547:GLY:HA2	2.21	0.40
1:A:173:ASN:HA	1:A:243:ARG:O	2.20	0.40
1:B:4:LEU:CD2	3:B:802:HEM:HMB3	2.52	0.40
1:B:376:VAL:HG11	1:B:419:LEU:CD1	2.52	0.40
1:A:128:ASP:HB2	1:A:150:ALA:HB1	2.03	0.40
1:A:250:GLY:HA3	1:A:429:LEU:HD12	2.03	0.40
1:A:490:ASN:C	1:A:490:ASN:ND2	2.80	0.40
1:B:275:ASN:HB3	1:B:297:MET:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/571 (99%)	543 (96%)	23 (4%)	0	100	100
1	B	566/571 (99%)	544 (96%)	20 (4%)	2 (0%)	30	27
All	All	1132/1142 (99%)	1087 (96%)	43 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	GLU
1	B	176	TRP

5.3.2 Protein sidechains [i](#)

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	440/444 (99%)	412 (94%)	28 (6%)	16	12
1	B	439/444 (99%)	406 (92%)	33 (8%)	12	9
All	All	879/888 (99%)	818 (93%)	61 (7%)	14	11

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN

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Mol	Chain	Res	Type
1	A	23	GLU
1	A	112	LYS
1	A	183	LYS
1	A	184	LYS
1	A	198	LYS
1	A	204	ASN
1	A	282	LEU
1	A	289	VAL
1	A	293	LEU
1	A	311	LEU
1	A	318	LYS
1	A	434	LYS
1	A	450	LEU
1	A	452	LYS
1	A	459	LYS
1	A	467	ARG
1	A	481	GLU
1	A	490	ASN
1	A	515	LYS
1	A	523	LYS
1	A	526	ILE
1	A	529	LEU
1	A	552	ASP
1	A	555	THR
1	A	559	LEU
1	A	566	LYS
1	A	568	SER
1	B	6	GLU
1	B	56	ASN
1	B	110	LYS
1	B	112	LYS
1	B	113	SER
1	B	119	LEU
1	B	157	LYS
1	B	183	LYS
1	B	198	LYS
1	B	204	ASN
1	B	208	LEU
1	B	210	LYS
1	B	218	ASP
1	B	267	LYS
1	B	282	LEU

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Mol	Chain	Res	Type
1	B	286	LYS
1	B	288	THR
1	B	289	VAL
1	B	293	LEU
1	B	299	LYS
1	B	311	LEU
1	B	321	GLU
1	B	337	ASN
1	B	450	LEU
1	B	459	LYS
1	B	467	ARG
1	B	476	LYS
1	B	490	ASN
1	B	526	ILE
1	B	529	LEU
1	B	559	LEU
1	B	566	LYS
1	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	35	GLN
1	A	56	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	490	ASN
1	A	540	HIS
1	B	35	GLN
1	B	56	ASN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	363	GLN
1	B	490	ASN
1	B	540	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 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	A	801	1	50,50,50	1.45	6 (12%)	67,82,82	1.46	13 (19%)
3	HEM	B	801	1	50,50,50	1.46	9 (18%)	67,82,82	1.52	11 (16%)
3	HEM	A	802	1	50,50,50	1.30	7 (14%)	67,82,82	1.27	9 (13%)
4	FAD	B	2805	-	58,58,58	1.67	12 (20%)	85,89,89	2.19	29 (34%)
5	FUM	A	1806	-	7,7,7	2.55	4 (57%)	8,8,8	1.75	2 (25%)
3	HEM	A	804	1	50,50,50	1.41	7 (14%)	67,82,82	1.27	6 (8%)
5	FUM	B	2806	-	7,7,7	2.43	4 (57%)	8,8,8	1.98	3 (37%)
3	HEM	B	802	1	50,50,50	1.33	6 (12%)	67,82,82	1.48	8 (11%)
3	HEM	B	804	1	50,50,50	1.41	7 (14%)	67,82,82	1.19	7 (10%)
3	HEM	A	803	1	50,50,50	1.43	7 (14%)	67,82,82	1.58	10 (14%)
4	FAD	A	1805	-	58,58,58	1.50	8 (13%)	85,89,89	2.22	30 (35%)
3	HEM	B	803	1	50,50,50	1.43	8 (16%)	67,82,82	1.48	14 (20%)

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	A	801	1	-	3/14/54/54	-
3	HEM	B	801	1	-	7/14/54/54	-
3	HEM	A	802	1	-	3/14/54/54	-
4	FAD	B	2805	-	-	10/34/50/50	0/6/6/6
5	FUM	A	1806	-	-	2/5/5/5	-
3	HEM	A	804	1	-	5/14/54/54	-
5	FUM	B	2806	-	-	2/5/5/5	-
3	HEM	B	802	1	-	4/14/54/54	-
3	HEM	B	804	1	-	5/14/54/54	-
3	HEM	A	803	1	-	4/14/54/54	-
4	FAD	A	1805	-	1/1/9/9	12/34/50/50	0/6/6/6
3	HEM	B	803	1	-	2/14/54/54	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2805	FAD	C9-C8	4.90	1.46	1.39
4	A	1805	FAD	C9-C8	4.46	1.45	1.39
4	A	1805	FAD	C5'-C4'	4.44	1.57	1.51
4	B	2805	FAD	C2'-C3'	4.29	1.60	1.53
5	B	2806	FUM	O-C	4.18	1.33	1.23
4	A	1805	FAD	O4-C4	-3.96	1.16	1.23
5	A	1806	FUM	O-C	3.62	1.31	1.23
5	A	1806	FUM	O8-C6	-3.62	1.21	1.30
3	A	801	HEM	CAC-C3C	3.52	1.56	1.47
4	B	2805	FAD	C1'-N10	3.44	1.56	1.47
4	B	2805	FAD	C6-C5X	3.41	1.45	1.40
3	A	804	HEM	CAB-C3B	3.37	1.56	1.47
4	B	2805	FAD	O4-C4	-3.36	1.17	1.23
4	B	2805	FAD	C2A-N3A	3.36	1.39	1.33
4	A	1805	FAD	C2'-C3'	3.25	1.59	1.53
3	A	803	HEM	CAB-C3B	3.24	1.56	1.47
5	B	2806	FUM	O8-C6	-3.16	1.22	1.30
3	B	803	HEM	CAB-C3B	3.13	1.55	1.47
3	B	804	HEM	CAB-C3B	3.11	1.55	1.47
3	A	801	HEM	CMA-C3A	3.06	1.57	1.50
5	A	1806	FUM	OXT-C	-3.05	1.22	1.30
5	A	1806	FUM	O7-C6	3.03	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HEM	CAC-C3C	3.02	1.55	1.47
3	A	801	HEM	FE-NB	3.00	2.04	1.94
3	A	801	HEM	CAB-C3B	2.99	1.55	1.47
3	B	801	HEM	FE-NB	2.98	2.04	1.94
4	A	1805	FAD	C6-C5X	2.93	1.44	1.40
3	B	804	HEM	CAC-C3C	2.90	1.55	1.47
3	B	802	HEM	CAC-C3C	2.88	1.55	1.47
3	A	804	HEM	CAC-C3C	2.87	1.55	1.47
5	B	2806	FUM	OXT-C	-2.81	1.23	1.30
4	B	2805	FAD	C1'-C2'	-2.79	1.48	1.52
3	B	801	HEM	CMA-C3A	2.78	1.56	1.50
3	B	801	HEM	CAC-C3C	2.74	1.54	1.47
3	A	802	HEM	CMA-C3A	2.73	1.56	1.50
3	B	801	HEM	CAB-C3B	2.73	1.54	1.47
4	A	1805	FAD	C9A-N10	-2.71	1.36	1.41
3	B	804	HEM	C2A-C3A	-2.70	1.31	1.38
3	B	802	HEM	CMD-C2D	2.69	1.56	1.50
3	A	803	HEM	FE-NA	2.60	2.03	1.95
3	A	804	HEM	FE-ND	2.59	2.02	1.94
3	A	804	HEM	FE-NB	2.56	2.02	1.94
3	B	801	HEM	C4D-ND	-2.56	1.35	1.40
3	A	803	HEM	C2A-C3A	-2.56	1.32	1.38
3	B	804	HEM	C3B-C2B	-2.56	1.32	1.37
3	B	803	HEM	CAC-C3C	2.56	1.54	1.47
4	B	2805	FAD	C4'-C3'	2.54	1.57	1.53
3	A	803	HEM	C3B-C2B	-2.54	1.32	1.37
3	A	803	HEM	CAC-C3C	2.54	1.54	1.47
3	B	802	HEM	CAB-C3B	2.53	1.54	1.47
3	B	804	HEM	FE-NB	2.53	2.02	1.94
3	A	802	HEM	CMB-C2B	2.49	1.55	1.50
3	B	803	HEM	CMD-C2D	2.49	1.55	1.50
4	B	2805	FAD	O4B-C4B	-2.48	1.39	1.45
3	A	802	HEM	C2A-C3A	-2.42	1.32	1.38
3	B	803	HEM	C3B-C2B	-2.38	1.32	1.37
3	B	801	HEM	C2A-C3A	-2.38	1.32	1.38
3	A	803	HEM	CMB-C2B	2.32	1.55	1.50
3	A	802	HEM	CMD-C2D	2.31	1.55	1.50
3	A	802	HEM	CAB-C3B	2.25	1.53	1.47
3	A	803	HEM	CMD-C2D	2.23	1.55	1.50
4	B	2805	FAD	C2-N1	2.23	1.41	1.36
3	A	802	HEM	FE-NB	2.22	2.01	1.94
3	B	804	HEM	CMD-C2D	2.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	HEM	FE-NB	2.19	2.01	1.94
3	B	803	HEM	C1C-NC	-2.19	1.35	1.39
3	A	801	HEM	C2A-C3A	-2.18	1.33	1.38
5	B	2806	FUM	O7-C6	2.16	1.28	1.23
3	A	804	HEM	C3B-C2B	-2.15	1.32	1.37
3	B	803	HEM	FE-NA	2.14	2.02	1.95
4	A	1805	FAD	C2A-N3A	2.12	1.37	1.33
3	B	801	HEM	C1B-NB	-2.12	1.36	1.40
3	B	803	HEM	C2A-C3A	-2.11	1.33	1.38
3	B	802	HEM	C3C-C2C	-2.10	1.32	1.37
3	A	801	HEM	CMC-C2C	2.09	1.55	1.50
3	B	801	HEM	O2A-CGA	-2.08	1.23	1.30
4	B	2805	FAD	P-O2P	-2.08	1.45	1.55
4	B	2805	FAD	PA-O1A	-2.08	1.43	1.50
3	B	804	HEM	CAA-C2A	2.06	1.56	1.51
3	A	804	HEM	CMB-C2B	2.05	1.55	1.50
3	A	804	HEM	CMD-C2D	2.04	1.55	1.50
3	B	801	HEM	FE-ND	2.03	2.01	1.94
4	A	1805	FAD	C5X-N5	-2.01	1.35	1.39
3	B	802	HEM	FE-ND	2.01	2.01	1.94
3	B	803	HEM	FE-NB	2.01	2.01	1.94

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C4'-C3'-C2'	6.52	124.41	113.57
4	A	1805	FAD	C4-C4X-N5	6.19	126.75	118.21
4	A	1805	FAD	O4-C4-N3	-6.06	108.72	120.11
4	B	2805	FAD	O5B-C5B-C4B	5.60	128.06	108.99
4	B	2805	FAD	O5'-C5'-C4'	-5.54	94.57	109.36
3	A	803	HEM	O2A-CGA-O1A	5.42	137.27	123.33
4	B	2805	FAD	O2-C2-N1	-5.31	112.97	121.80
4	B	2805	FAD	O4B-C1B-C2B	-5.31	95.24	106.62
4	A	1805	FAD	C5X-N5-C4X	4.78	125.81	118.09
4	B	2805	FAD	O4-C4-N3	-4.48	111.68	120.11
4	A	1805	FAD	O5B-C5B-C4B	4.31	123.68	108.99
4	B	2805	FAD	O4B-C4B-C5B	4.31	123.13	109.33
4	A	1805	FAD	O4B-C1B-C2B	-4.30	97.41	106.62
4	B	2805	FAD	O4'-C4'-C3'	-4.16	99.50	109.25
4	A	1805	FAD	O2'-C2'-C3'	-4.16	99.51	109.25
3	B	803	HEM	CHA-C1A-NA	3.97	131.06	123.86
4	B	2805	FAD	C2A-N1A-C6A	3.77	124.92	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	HEM	O1A-CGA-CBA	-3.72	111.30	123.09
3	A	804	HEM	O1D-CGD-CBD	-3.70	111.35	123.09
4	A	1805	FAD	C7M-C7-C6	3.69	126.08	119.57
3	B	802	HEM	C3B-C4B-NB	-3.67	106.83	109.47
4	B	2805	FAD	C5A-C4A-N3A	3.52	131.56	126.72
4	A	1805	FAD	C10-C4X-N5	-3.47	117.72	124.81
4	A	1805	FAD	C9A-C5X-N5	-3.46	118.78	122.45
3	A	803	HEM	O1A-CGA-CBA	-3.41	112.27	123.09
4	A	1805	FAD	C5'-C4'-C3'	-3.38	105.85	112.22
3	B	801	HEM	C4A-CHB-C1B	-3.31	118.47	126.25
4	B	2805	FAD	C8M-C8-C9	-3.29	113.78	119.57
4	B	2805	FAD	C4-C4X-N5	3.29	122.75	118.21
3	A	801	HEM	CHD-C4C-NC	-3.28	120.88	124.45
4	A	1805	FAD	C8M-C8-C9	-3.26	113.82	119.57
3	B	803	HEM	CAA-C2A-C1A	-3.26	118.57	124.94
4	B	2805	FAD	C4A-N9A-C8A	3.17	109.07	105.74
3	A	803	HEM	CHA-C1A-NA	3.16	129.59	123.86
4	B	2805	FAD	O4B-C1B-N9A	-3.11	102.11	108.09
5	A	1806	FUM	O7-C6-C5	-3.09	111.58	121.06
3	A	802	HEM	C1B-NB-C4B	3.07	108.84	105.21
3	B	802	HEM	C1B-NB-C4B	3.05	108.82	105.21
4	A	1805	FAD	O4-C4-C4X	3.05	134.59	126.53
4	B	2805	FAD	O3B-C3B-C2B	3.04	121.57	111.82
3	B	801	HEM	C4D-ND-C1D	3.03	108.80	105.21
3	A	803	HEM	CAA-C2A-C1A	-3.02	119.04	124.94
3	B	803	HEM	C1A-CHA-C4D	-2.98	119.24	126.25
3	B	801	HEM	CHB-C1B-NB	2.97	128.04	124.37
4	B	2805	FAD	O3'-C3'-C4'	-2.94	102.25	108.93
3	B	801	HEM	O2D-CGD-O1D	-2.89	115.89	123.33
3	A	801	HEM	CMB-C2B-C1B	-2.89	120.52	125.03
5	B	2806	FUM	OXT-C-O	-2.88	116.83	122.70
3	A	803	HEM	C2A-C1A-NA	-2.88	106.96	110.15
3	A	804	HEM	CMA-C3A-C4A	-2.88	121.03	125.42
3	B	802	HEM	CMC-C2C-C1C	-2.86	119.70	124.73
3	B	804	HEM	O1D-CGD-CBD	-2.84	114.08	123.09
3	B	801	HEM	CHD-C4C-NC	-2.84	121.37	124.45
4	A	1805	FAD	O4B-C1B-N9A	-2.82	102.67	108.09
3	A	803	HEM	CBB-CAB-C3B	-2.81	113.49	127.53
4	A	1805	FAD	C4-N3-C2	-2.80	120.67	125.64
3	B	802	HEM	O1D-CGD-CBD	-2.77	114.30	123.09
3	B	803	HEM	CAA-CBA-CGA	-2.76	106.35	113.67
4	A	1805	FAD	C5X-C9A-N10	-2.74	115.49	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C6-C5X-N5	2.74	122.99	118.44
3	A	801	HEM	CMA-C3A-C4A	2.74	129.59	125.42
3	A	801	HEM	CHD-C4C-C3C	2.72	129.79	125.21
3	A	804	HEM	CMA-C3A-C2A	2.72	131.39	125.62
4	B	2805	FAD	C4A-N9A-C1B	-2.68	120.37	126.63
3	B	803	HEM	CBA-CAA-C2A	2.68	119.93	112.53
4	B	2805	FAD	C4'-C3'-C2'	2.67	118.02	113.57
5	B	2806	FUM	OXT-C-C4	2.67	125.97	116.16
3	A	802	HEM	C3D-C4D-ND	-2.66	107.25	110.17
3	A	801	HEM	CHB-C1B-NB	2.64	127.63	124.37
3	B	803	HEM	C4C-C3C-C2C	2.62	109.08	106.81
4	B	2805	FAD	C5B-C4B-C3B	-2.62	105.80	115.21
3	A	802	HEM	CAD-CBD-CGD	2.60	120.55	113.67
3	A	801	HEM	O2D-CGD-CBD	2.59	122.18	114.00
3	B	803	HEM	CAA-C2A-C3A	2.56	132.81	127.07
3	B	801	HEM	O2A-CGA-O1A	2.55	129.88	123.33
3	A	804	HEM	C4C-C3C-C2C	2.54	109.02	106.81
3	B	804	HEM	CMA-C3A-C2A	2.54	131.01	125.62
3	A	802	HEM	C3B-C4B-NB	-2.51	107.67	109.47
3	A	804	HEM	CMB-C2B-C1B	-2.49	121.15	125.03
3	B	804	HEM	CMA-C3A-C4A	-2.46	121.67	125.42
3	B	801	HEM	C3D-C4D-ND	-2.44	107.50	110.17
4	B	2805	FAD	O2-C2-N3	2.44	123.26	118.58
4	A	1805	FAD	O5'-C5'-C4'	-2.43	102.86	109.36
4	A	1805	FAD	C5B-C4B-C3B	-2.43	106.48	115.21
4	A	1805	FAD	O2A-PA-O1A	2.42	123.69	112.44
4	A	1805	FAD	O3B-C3B-C4B	-2.41	104.16	111.08
3	B	804	HEM	C4C-C3C-C2C	2.40	108.89	106.81
4	B	2805	FAD	C4-N3-C2	-2.36	121.45	125.64
3	B	803	HEM	CBD-CAD-C3D	-2.35	106.02	112.53
4	B	2805	FAD	O4-C4-C4X	2.33	132.69	126.53
3	B	802	HEM	CHC-C4B-C3B	2.31	129.69	125.07
3	A	803	HEM	CBD-CAD-C3D	-2.31	106.15	112.53
4	A	1805	FAD	O2-C2-N1	-2.31	117.97	121.80
3	B	802	HEM	C1A-CHA-C4D	-2.28	120.88	126.25
3	A	802	HEM	C3B-C2B-C1B	2.28	108.12	106.41
3	A	803	HEM	C3B-C4B-NB	-2.28	107.83	109.47
3	A	801	HEM	O2D-CGD-O1D	-2.28	117.48	123.33
5	B	2806	FUM	O7-C6-C5	-2.27	114.10	121.06
3	B	801	HEM	CHD-C4C-C3C	2.27	129.03	125.21
3	B	803	HEM	C2A-C1A-NA	-2.27	107.64	110.15
3	B	801	HEM	C1B-NB-C4B	2.26	107.88	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C5A-C4A-N3A	2.25	129.82	126.72
4	A	1805	FAD	O4B-C4B-C5B	2.25	116.55	109.33
3	B	802	HEM	O2D-CGD-CBD	2.23	121.05	114.00
4	A	1805	FAD	C9A-N10-C10	2.23	124.15	120.75
4	B	2805	FAD	O3'-C3'-C2'	-2.23	103.87	108.93
4	A	1805	FAD	C2B-C1B-N9A	-2.22	107.79	113.30
3	B	802	HEM	CMB-C2B-C1B	-2.22	121.57	125.03
4	B	2805	FAD	PA-O5B-C5B	2.21	134.00	121.35
4	B	2805	FAD	C6-C7-C8	-2.20	116.46	119.69
3	A	801	HEM	CBA-CAA-C2A	-2.20	106.45	112.53
4	B	2805	FAD	O2'-C2'-C1'	-2.19	101.18	110.20
3	B	803	HEM	O1A-CGA-CBA	-2.19	116.14	123.09
3	B	804	HEM	CMB-C2B-C1B	-2.19	121.61	125.03
3	A	802	HEM	C4D-ND-C1D	2.19	107.80	105.21
3	A	801	HEM	CAD-CBD-CGD	2.18	119.45	113.67
3	A	802	HEM	C2B-C1B-NB	-2.18	107.33	109.84
3	B	803	HEM	CMD-C2D-C1D	-2.18	121.63	125.03
3	B	804	HEM	CHB-C4A-NA	2.17	127.80	123.86
3	A	804	HEM	O2D-CGD-CBD	2.17	120.86	114.00
4	B	2805	FAD	N3A-C2A-N1A	-2.17	125.30	128.58
3	A	802	HEM	CMB-C2B-C1B	-2.15	121.67	125.03
4	B	2805	FAD	N9A-C8A-N7A	-2.14	110.90	113.94
3	B	803	HEM	CBC-CAC-C3C	-2.12	116.94	127.53
3	A	803	HEM	CMB-C2B-C1B	-2.10	121.76	125.03
3	A	801	HEM	CHA-C1A-NA	2.09	127.65	123.86
4	A	1805	FAD	C7M-C7-C8	-2.08	116.50	120.76
3	B	801	HEM	CMD-C2D-C3D	2.08	131.78	126.15
3	B	803	HEM	O2A-CGA-O1A	2.08	128.68	123.33
3	A	801	HEM	O2A-CGA-O1A	2.07	128.66	123.33
4	A	1805	FAD	O3'-C3'-C2'	-2.05	104.27	108.93
4	A	1805	FAD	O2A-PA-O5B	-2.05	98.28	107.57
3	A	801	HEM	C3D-C4D-ND	-2.05	107.92	110.17
4	B	2805	FAD	C2A-N3A-C4A	-2.04	106.84	111.83
3	A	802	HEM	O2D-CGD-CBD	2.03	120.42	114.00
4	B	2805	FAD	N3A-C4A-N9A	-2.02	123.73	127.17
3	B	803	HEM	CBB-CAB-C3B	-2.02	117.46	127.53
3	A	803	HEM	C4B-C3B-C2B	2.01	109.13	107.28
3	B	804	HEM	CBD-CAD-C3D	2.01	118.08	112.53
3	A	801	HEM	CBB-CAB-C3B	-2.00	117.52	127.53
4	A	1805	FAD	C2A-N1A-C6A	2.00	122.02	118.73
5	A	1806	FUM	O-C-C4	-2.00	114.93	121.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1805	FAD	C4'

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	HEM	C2A-CAA-CBA-CGA
4	A	1805	FAD	N10-C1'-C2'-O2'
4	A	1805	FAD	N10-C1'-C2'-C3'
4	A	1805	FAD	C2'-C3'-C4'-O4'
4	A	1805	FAD	O3'-C3'-C4'-O4'
4	A	1805	FAD	O3'-C3'-C4'-C5'
4	A	1805	FAD	O4'-C4'-C5'-O5'
4	A	1805	FAD	PA-O3P-P-O5'
4	B	2805	FAD	N10-C1'-C2'-O2'
4	B	2805	FAD	N10-C1'-C2'-C3'
4	B	2805	FAD	C2'-C3'-C4'-O4'
4	B	2805	FAD	C2'-C3'-C4'-C5'
4	B	2805	FAD	O3'-C3'-C4'-O4'
4	B	2805	FAD	O3'-C3'-C4'-C5'
4	B	2805	FAD	PA-O3P-P-O5'
5	A	1806	FUM	OXT-C-C4-C5
5	A	1806	FUM	O-C-C4-C5
5	B	2806	FUM	OXT-C-C4-C5
5	B	2806	FUM	O-C-C4-C5
4	A	1805	FAD	C2'-C3'-C4'-C5'
3	A	802	HEM	C3D-CAD-CBD-CGD
3	B	801	HEM	C3D-CAD-CBD-CGD
4	A	1805	FAD	C3'-C4'-C5'-O5'
4	A	1805	FAD	P-O3P-PA-O1A
3	A	801	HEM	C3D-CAD-CBD-CGD
3	B	804	HEM	C2A-CAA-CBA-CGA
4	A	1805	FAD	P-O3P-PA-O2A
4	B	2805	FAD	P-O3P-PA-O1A
4	B	2805	FAD	P-O3P-PA-O2A
3	B	801	HEM	C4B-C3B-CAB-CBB
3	A	804	HEM	CAA-CBA-CGA-O2A
3	A	803	HEM	C3D-CAD-CBD-CGD
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	802	HEM	CAD-CBD-CGD-O1D
3	B	801	HEM	CAD-CBD-CGD-O1D
3	B	803	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAD-CBD-CGD-O1D
3	B	803	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	802	HEM	CAD-CBD-CGD-O2D
3	B	804	HEM	CAA-CBA-CGA-O1A
3	B	804	HEM	CAA-CBA-CGA-O2A
3	A	804	HEM	C2A-CAA-CBA-CGA
3	A	801	HEM	CAD-CBD-CGD-O2D
3	A	803	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAD-CBD-CGD-O2D
3	A	803	HEM	CAA-CBA-CGA-O1A
3	B	802	HEM	CAD-CBD-CGD-O1D
3	B	804	HEM	CAD-CBD-CGD-O1D
3	B	802	HEM	CAD-CBD-CGD-O2D
4	B	2805	FAD	C2B-C1B-N9A-C8A
3	A	804	HEM	CAD-CBD-CGD-O2D
4	A	1805	FAD	C2B-C1B-N9A-C8A
3	B	801	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAA-CBA-CGA-O1A
3	B	804	HEM	CAD-CBD-CGD-O2D
3	A	804	HEM	CAD-CBD-CGD-O1D
3	B	801	HEM	C2B-C3B-CAB-CBB
3	B	802	HEM	C3D-CAD-CBD-CGD
3	B	802	HEM	CAA-CBA-CGA-O2A

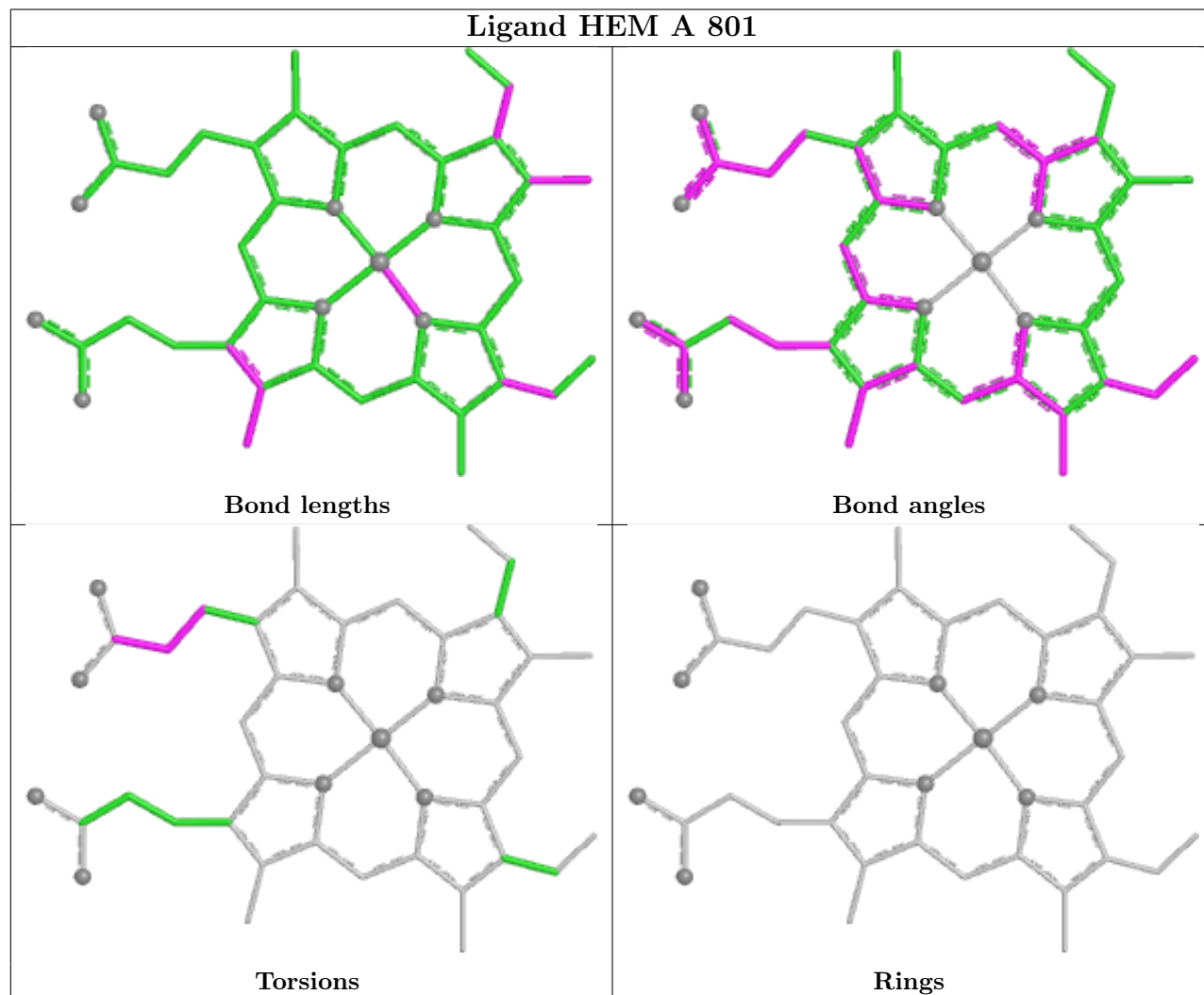
There are no ring outliers.

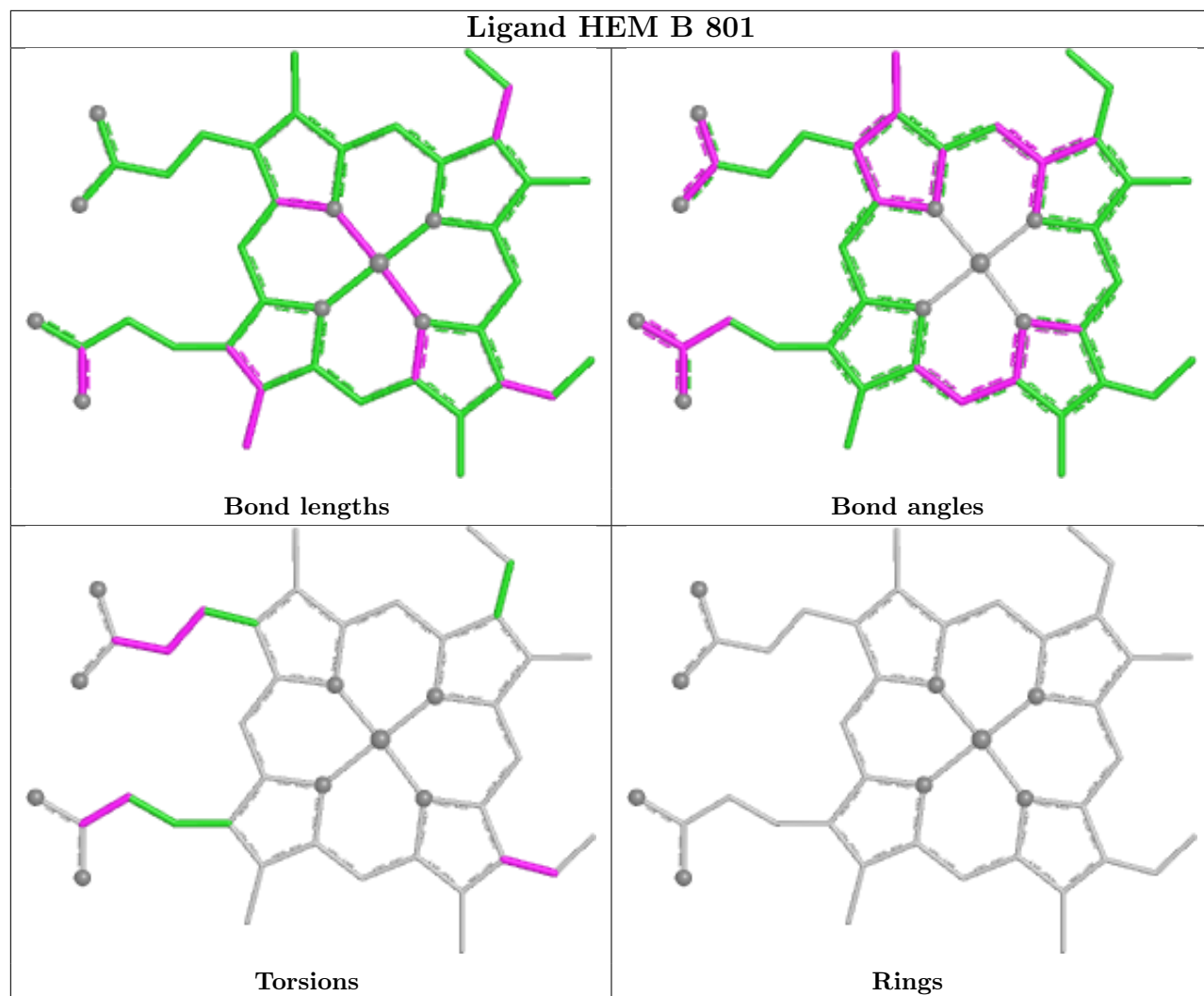
11 monomers are involved in 86 short contacts:

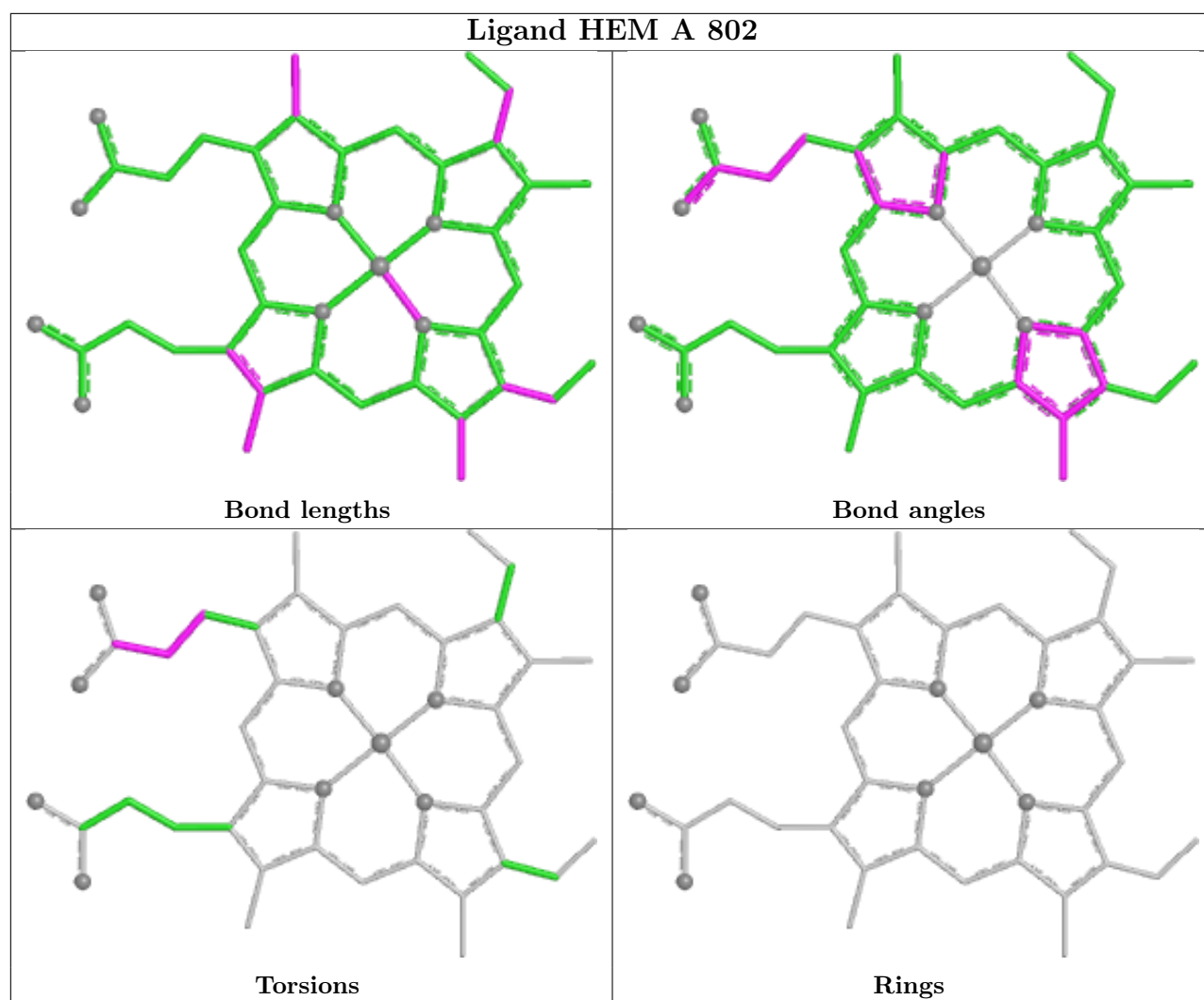
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	HEM	10	0
3	B	801	HEM	7	0
3	A	802	HEM	8	0
4	B	2805	FAD	7	0
3	A	804	HEM	14	0
5	B	2806	FUM	1	0
3	B	802	HEM	7	0
3	B	804	HEM	9	0
3	A	803	HEM	11	0
4	A	1805	FAD	5	0
3	B	803	HEM	9	0

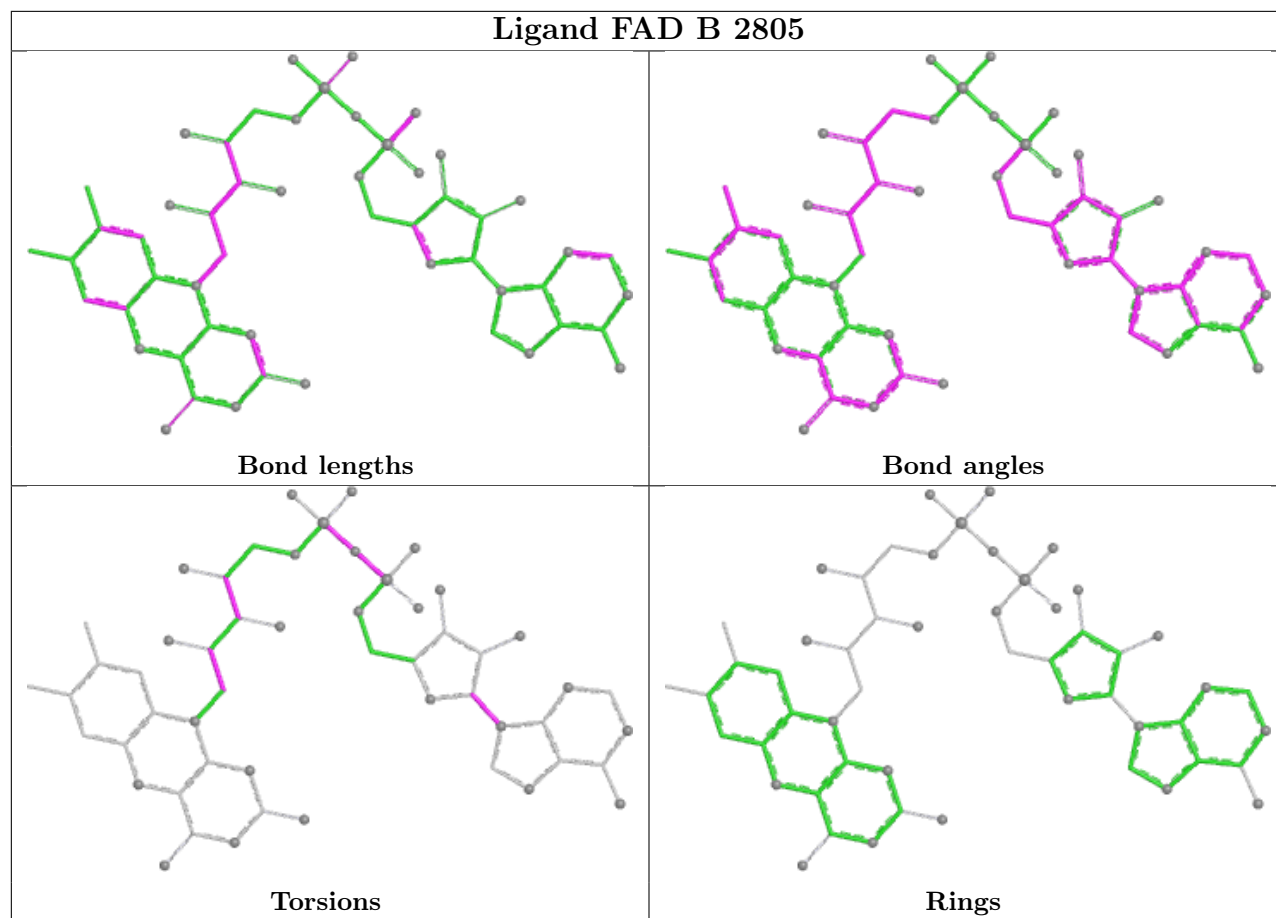
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

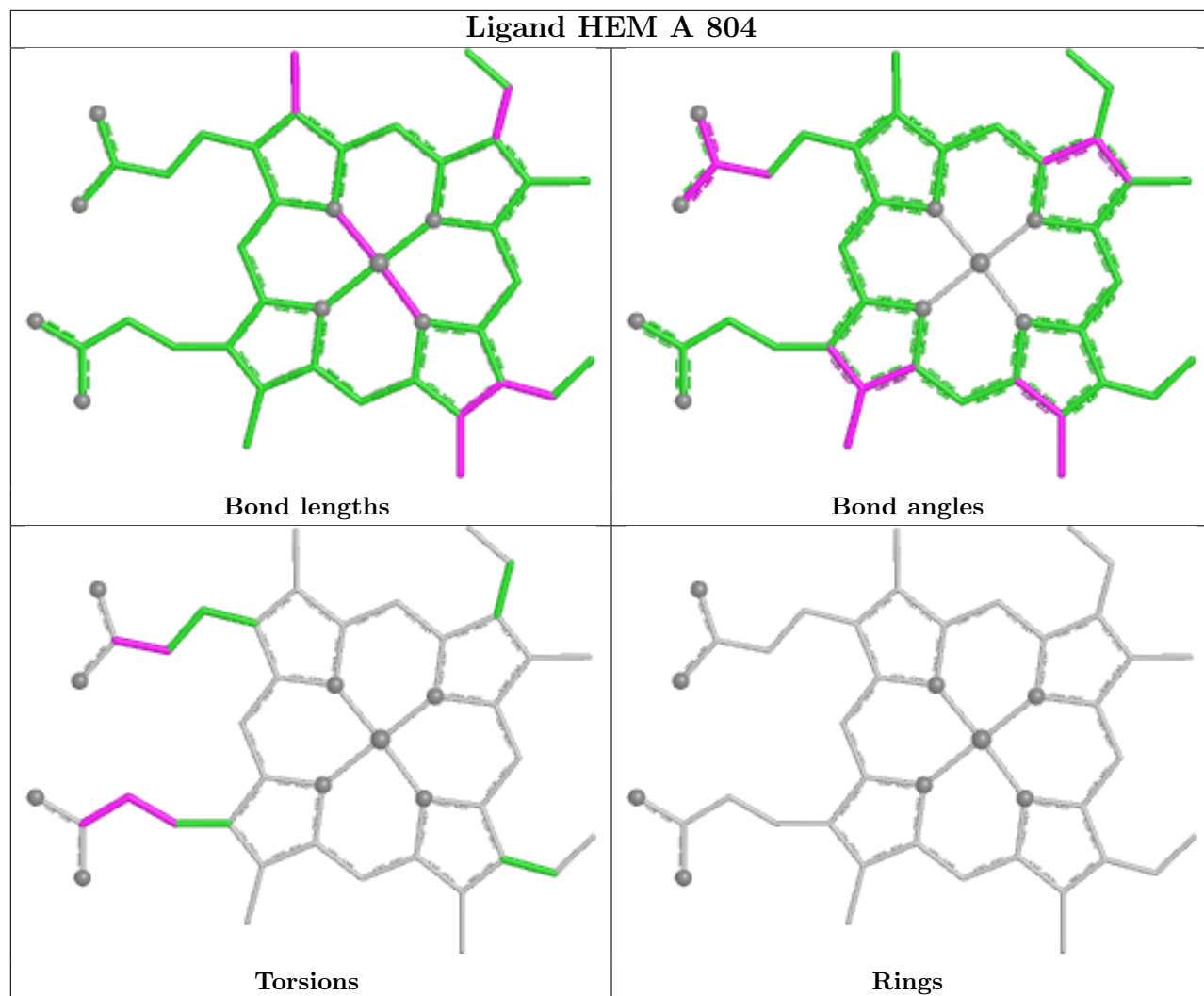
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

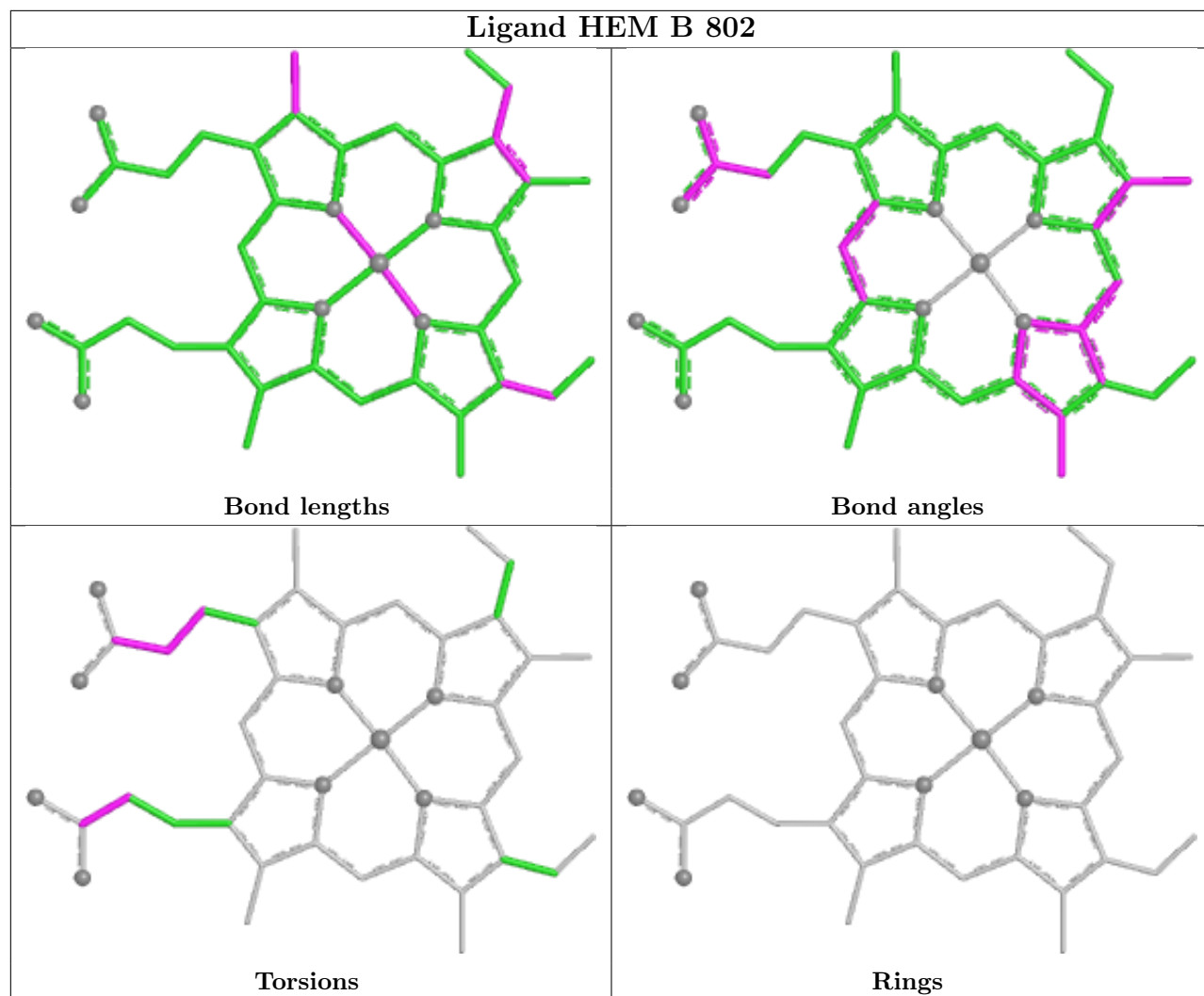


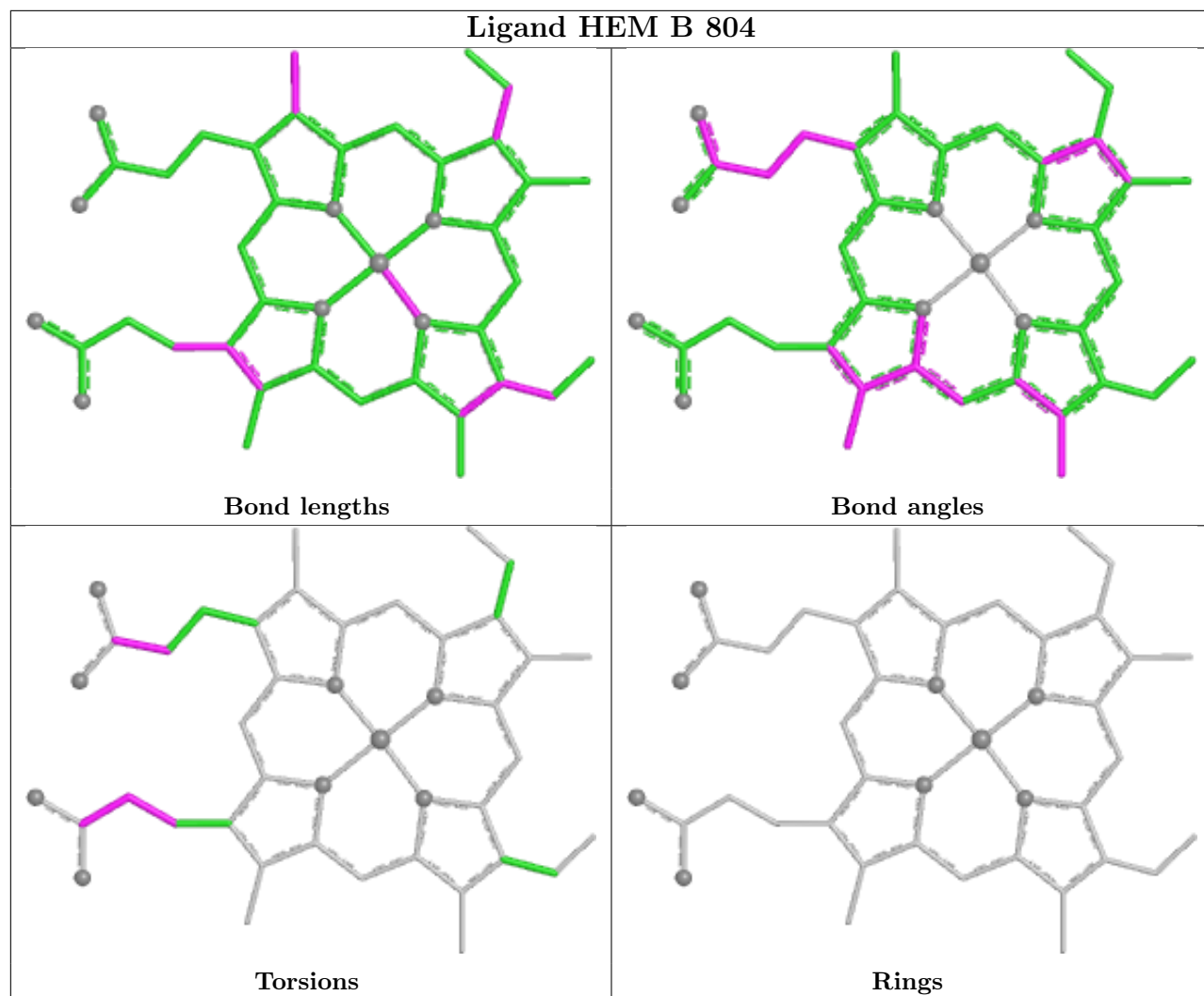


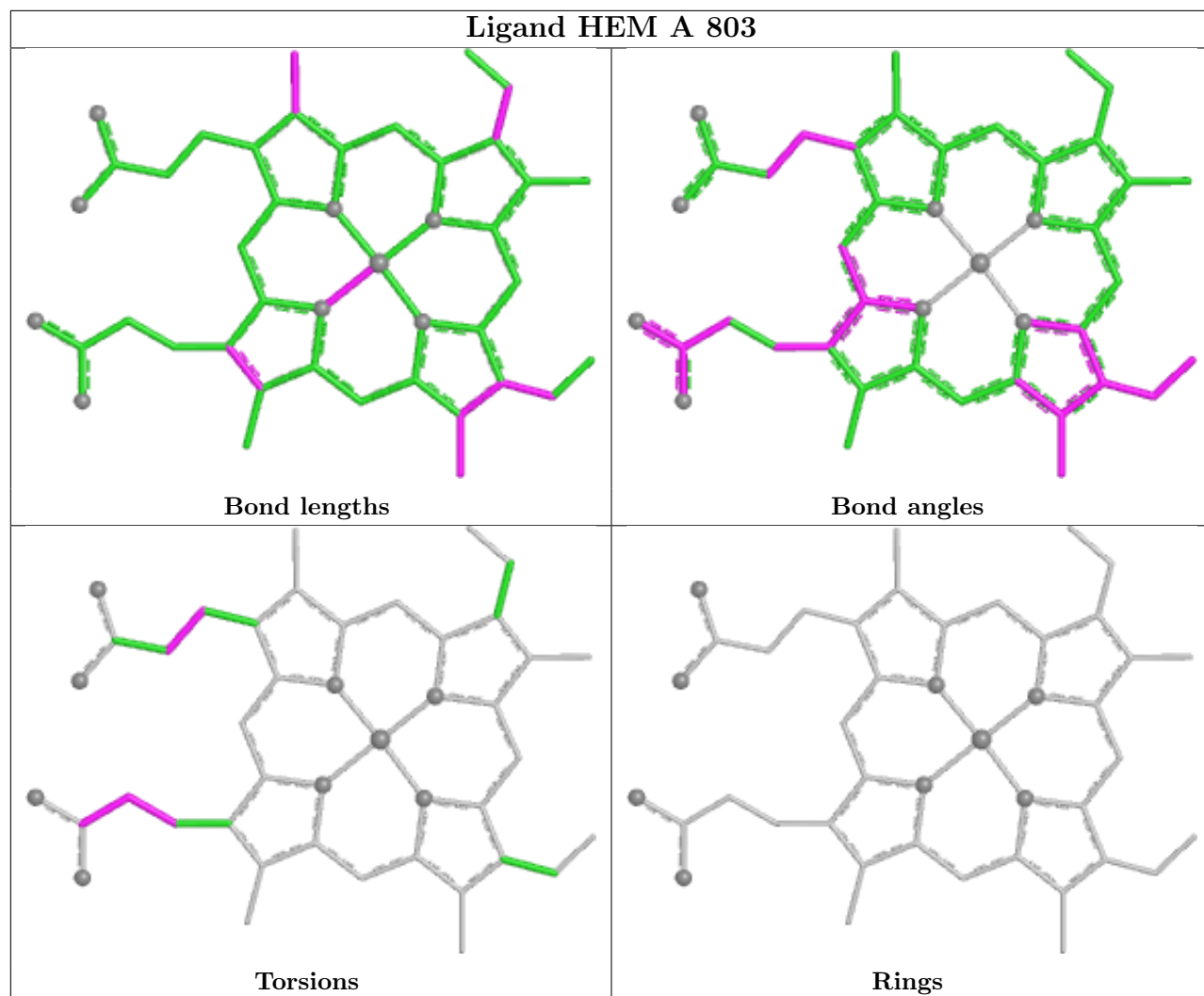


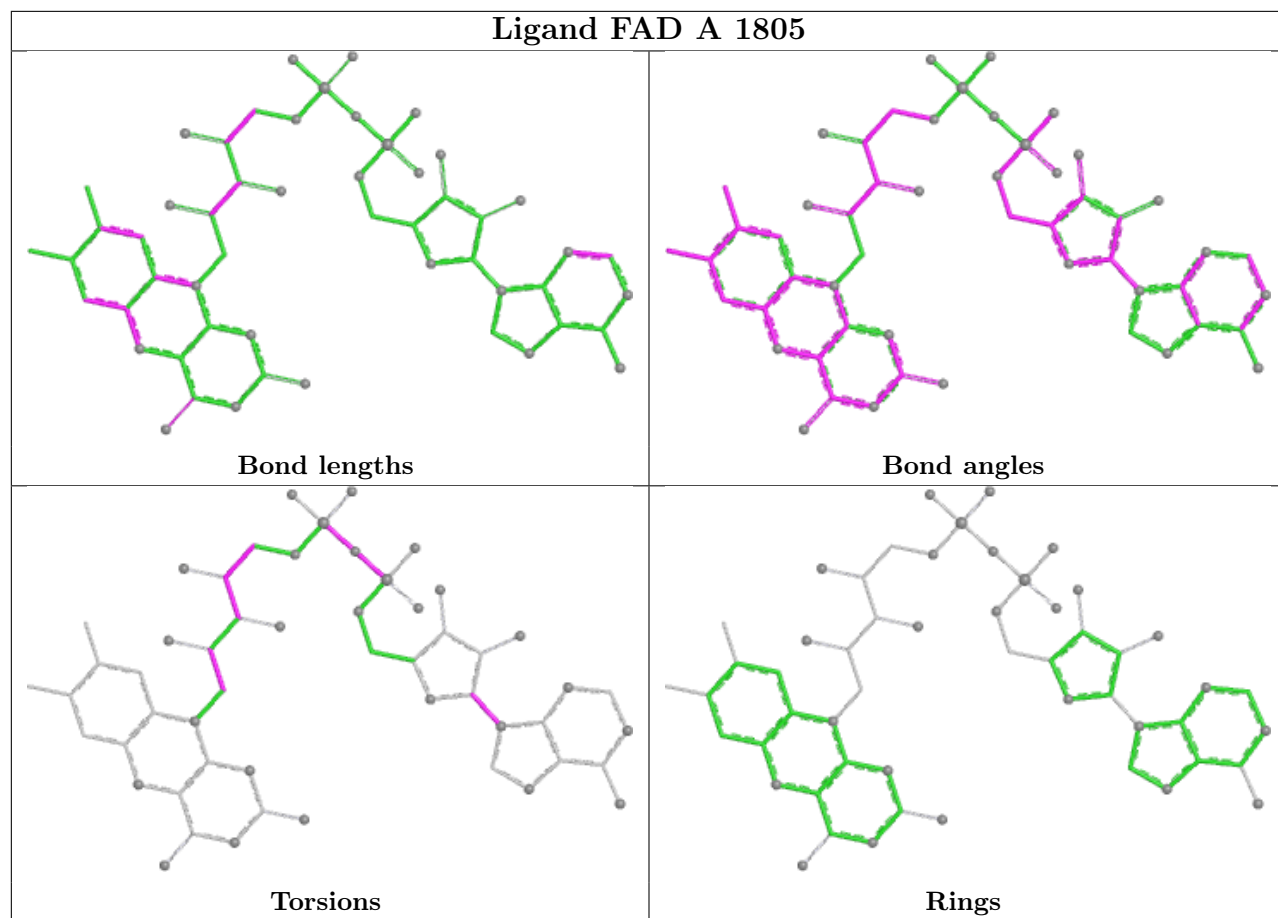


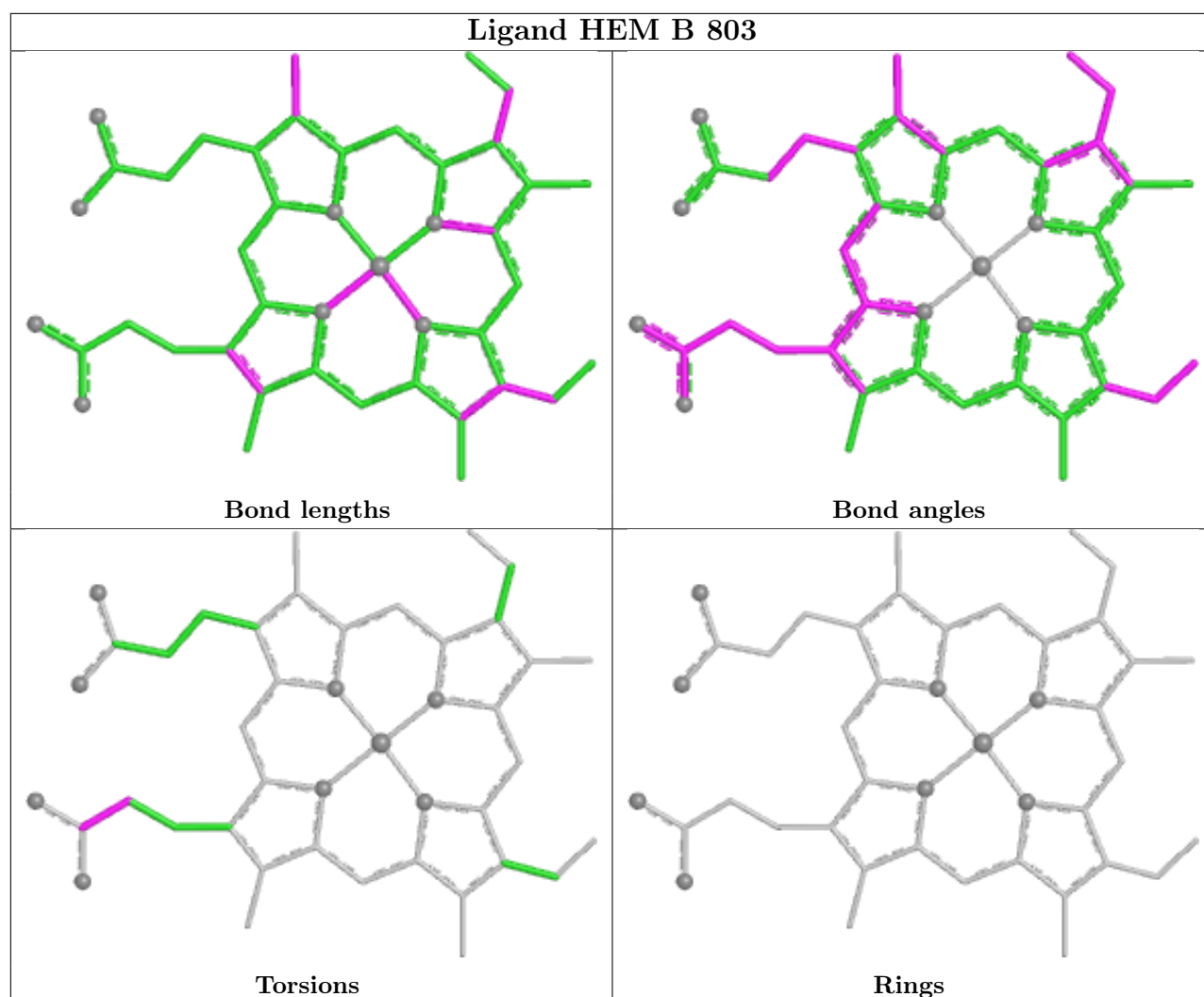












5.7 Other polymers [i](#)

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.