



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:41 PM EDT

PDB ID : 1JRZ / pdb_00001jrz
Title : Crystal structure of Arg402Tyr 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

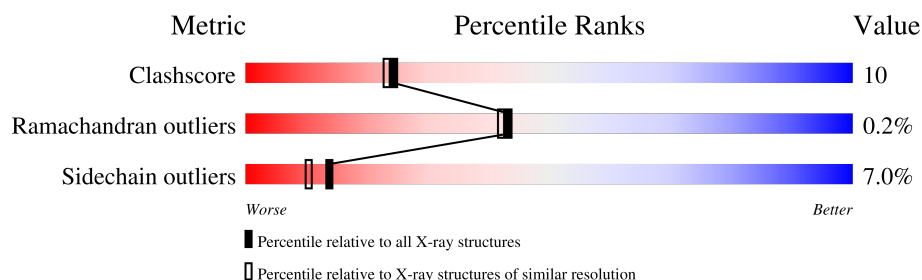
1 Overall quality at a glance

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	-	-	-
4	FAD	B	2805	X	-	-	-
5	FUM	B	2806	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10534 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
			4218	2618	741	834	25			
1	B	568	Total	C	N	O	S	0	0	0
			4218	2618	741	834	25			

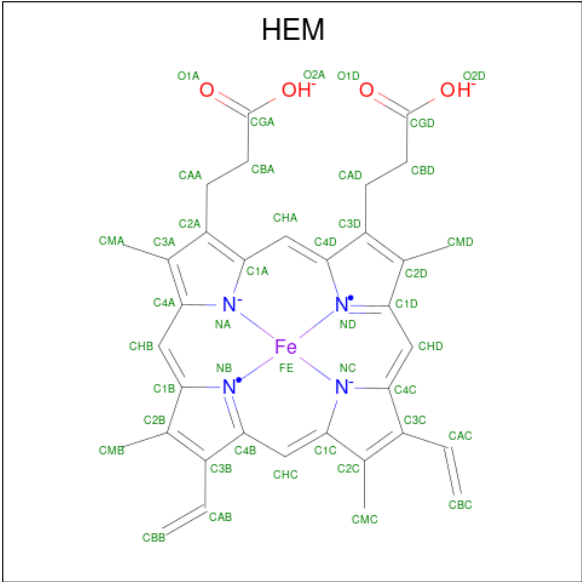
There are 2 discrepancies between the modelled and reference sequences:

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

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

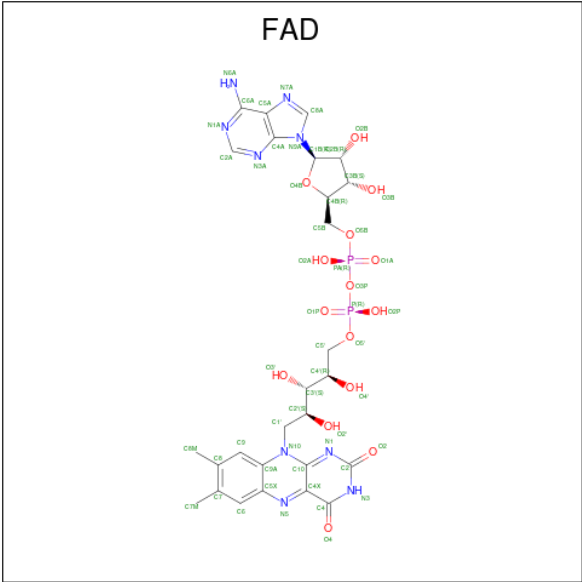
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

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



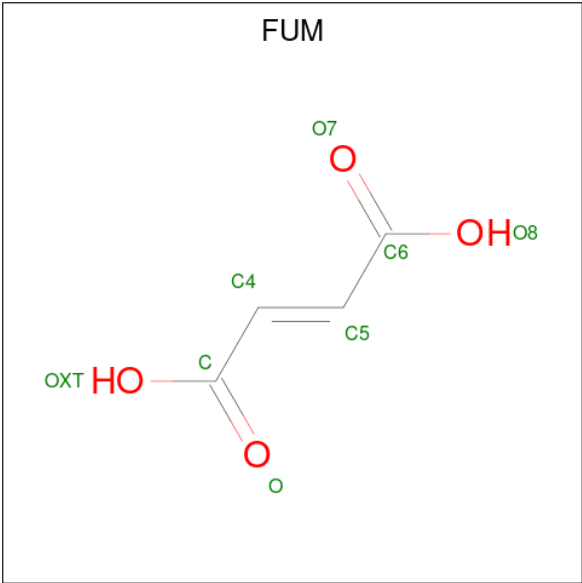
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	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	805	Total 805	O 805	0	0
6	B	825	Total 825	O 825	0	0

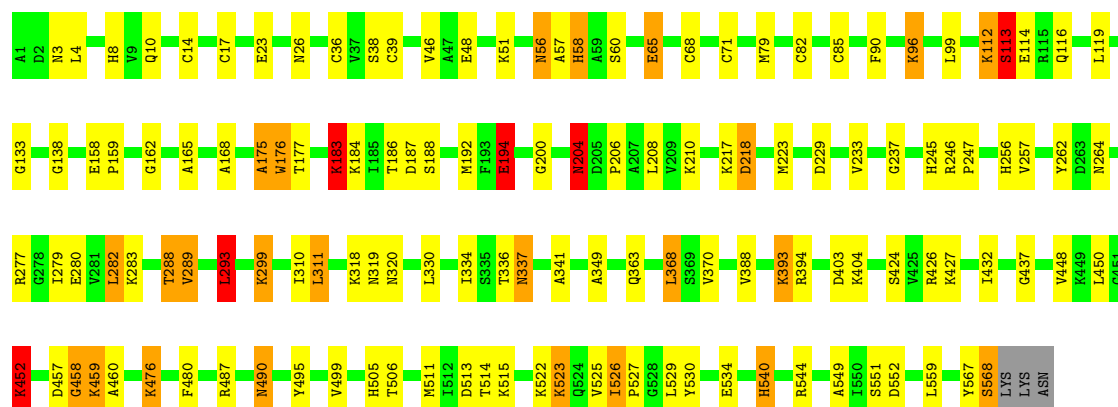
3 Residue-property plots [i](#)

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.

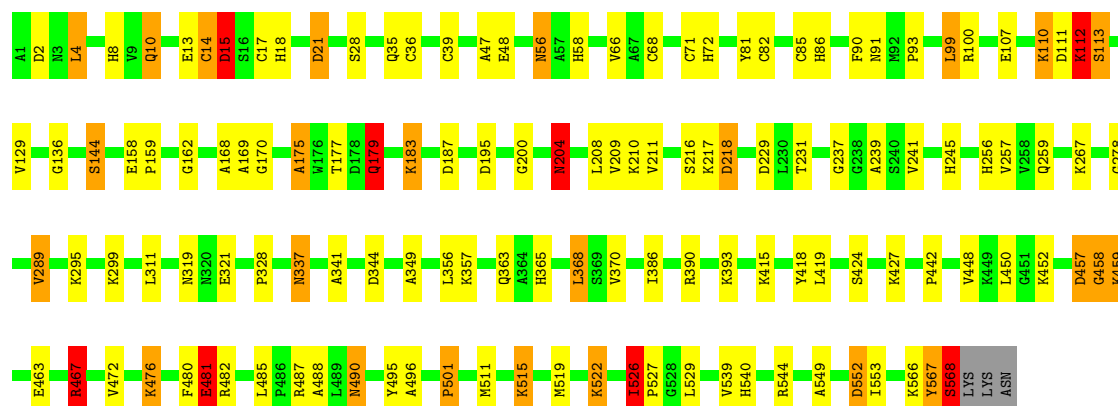
• Molecule 1: FLAVOCYTOCHROME C

Chain A: 



• Molecule 1: FLAVOCYTOCHROME C

Chain B: 



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	78.07Å 87.91Å 90.16Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.4 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10534	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, NA, FAD, HEM

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	0.95	1/4289 (0.0%)	1.90	88/5799 (1.5%)
1	B	0.91	0/4289	1.87	96/5799 (1.7%)
All	All	0.93	1/8578 (0.0%)	1.88	184/11598 (1.6%)

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	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-8.32	1.35	1.46

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	CA-C-N	22.43	164.38	121.54
1	A	175	ALA	C-N-CA	22.43	164.38	121.54
1	B	175	ALA	O-C-N	-15.98	104.72	123.10
1	A	65	GLU	CB-CG-CD	11.13	131.52	112.60
1	A	293	LEU	CA-CB-CG	10.91	154.47	116.30
1	A	567	TYR	CA-C-N	9.26	138.36	121.70
1	A	567	TYR	C-N-CA	9.26	138.36	121.70
1	A	487	ARG	CA-CB-CG	8.97	132.05	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	TYR	CA-C-O	8.97	130.06	120.55
1	A	526	ILE	CB-CA-C	8.92	121.57	111.04
1	A	526	ILE	CA-CB-CG2	8.71	125.30	110.50
1	A	176	TRP	N-CA-CB	8.18	124.31	110.49
1	B	567	TYR	CA-C-O	8.07	129.11	120.55
1	A	112	LYS	CA-C-O	8.05	129.51	120.90
1	B	526	ILE	CB-CA-C	7.98	120.45	111.04
1	B	112	LYS	CA-C-N	7.96	131.86	120.79
1	B	112	LYS	C-N-CA	7.96	131.86	120.79
1	A	217	LYS	CA-C-O	7.90	128.79	120.42
1	A	3	ASN	CA-CB-CG	7.89	120.49	112.60
1	A	480	PHE	CA-CB-CG	-7.86	105.94	113.80
1	A	459	LYS	CA-C-O	-7.84	110.53	119.79
1	B	14	CYS	CA-C-O	7.82	129.27	120.90
1	B	90	PHE	CA-CB-CG	7.65	121.45	113.80
1	A	337	ASN	N-CA-C	7.58	120.31	110.53
1	B	21	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	218	ASP	CA-CB-CG	-7.44	105.16	112.60
1	A	175	ALA	O-C-N	7.41	131.71	123.33
1	A	552	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	112	LYS	CA-C-N	7.24	135.37	121.54
1	A	112	LYS	C-N-CA	7.24	135.37	121.54
1	B	14	CYS	O-C-N	-7.21	114.60	122.09
1	A	58	HIS	CA-CB-CG	-7.12	106.68	113.80
1	A	513	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	35	GLN	CA-C-O	-7.08	112.91	120.42
1	B	390	ARG	NE-CZ-NH2	-7.06	112.84	119.20
1	A	403	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	113	SER	CA-C-N	7.04	135.08	121.63
1	A	113	SER	C-N-CA	7.04	135.08	121.63
1	B	552	ASP	CA-CB-CG	6.97	119.57	112.60
1	B	241	VAL	CA-C-O	-6.88	114.90	121.64
1	B	319	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	336	THR	CA-CB-CG2	6.78	122.02	110.50
1	A	319	ASN	CA-CB-CG	6.59	119.19	112.60
1	B	337	ASN	N-CA-C	6.54	120.08	110.59
1	B	490	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	B	218	ASP	CB-CG-OD1	-6.42	103.63	118.40
1	B	295	LYS	CA-C-N	-6.40	115.36	121.57
1	B	295	LYS	C-N-CA	-6.40	115.36	121.57
1	A	540	HIS	CA-CB-CG	-6.37	107.43	113.80
1	A	505	HIS	CA-C-N	-6.36	113.73	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	HIS	C-N-CA	-6.36	113.73	123.14
1	A	264	ASN	O-C-N	-6.33	114.93	122.15
1	A	175	ALA	N-CA-CB	6.33	123.29	111.52
1	B	170	GLY	N-CA-C	6.32	120.54	112.83
1	B	72	HIS	CA-CB-CG	6.32	120.12	113.80
1	B	418	TYR	CA-C-O	-6.32	113.31	120.32
1	A	437	GLY	CA-C-O	-6.30	114.26	120.75
1	B	129	VAL	CA-C-N	-6.30	115.38	123.19
1	B	129	VAL	C-N-CA	-6.30	115.38	123.19
1	A	162	GLY	N-CA-C	6.28	122.16	114.69
1	B	99	LEU	CA-C-O	-6.22	112.40	119.98
1	A	394	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	B	289	VAL	CA-CB-CG2	6.15	120.85	110.40
1	B	458	GLY	N-CA-C	6.14	119.62	112.50
1	A	457	ASP	CA-C-N	6.13	126.74	119.94
1	A	457	ASP	C-N-CA	6.13	126.74	119.94
1	B	289	VAL	N-CA-CB	6.11	119.65	110.13
1	B	162	GLY	N-CA-C	6.03	121.87	114.69
1	B	488	ALA	CA-C-O	-6.03	114.18	121.05
1	B	487	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	A	114	GLU	N-CA-C	-6.02	107.76	114.62
1	A	237	GLY	CA-C-O	5.99	128.54	121.71
1	A	525	VAL	CA-C-N	-5.99	116.02	122.85
1	A	525	VAL	C-N-CA	-5.99	116.02	122.85
1	B	457	ASP	CA-C-N	5.98	126.58	119.94
1	B	457	ASP	C-N-CA	5.98	126.58	119.94
1	B	480	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	66	VAL	CA-C-O	-5.95	113.75	120.95
1	B	487	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	B	179	GLN	CA-C-N	5.92	128.13	120.44
1	B	179	GLN	C-N-CA	5.92	128.13	120.44
1	A	534	GLU	O-C-N	-5.91	114.70	122.39
1	B	231	THR	N-CA-C	5.91	120.49	113.28
1	A	293	LEU	O-C-N	5.90	129.95	123.22
1	B	487	ARG	CG-CD-NE	-5.89	99.03	112.00
1	B	2	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	187	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	289	VAL	CA-CB-CG2	5.82	120.29	110.40
1	B	289	VAL	CA-C-O	5.80	127.43	121.23
1	B	15	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	100	ARG	CD-NE-CZ	5.79	132.50	124.40
1	B	10	GLN	OE1-CD-NE2	-5.76	116.84	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	GLN	CG-CD-NE2	5.71	124.97	116.40
1	B	169	ALA	CA-C-O	5.71	126.69	119.61
1	B	81	TYR	CA-C-N	5.70	128.70	120.38
1	B	81	TYR	C-N-CA	5.70	128.70	120.38
1	B	356	LEU	CA-C-O	-5.70	114.67	121.56
1	B	568	SER	CA-CB-OG	5.69	122.49	111.10
1	A	293	LEU	CA-C-O	-5.69	114.11	120.54
1	A	277	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	B	187	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	495	TYR	CA-C-O	-5.63	114.53	121.11
1	B	481	GLU	CB-CG-CD	5.61	122.14	112.60
1	B	86	HIS	CA-CB-CG	5.60	119.40	113.80
1	B	424	SER	N-CA-CB	5.60	118.13	110.01
1	B	495	TYR	CA-C-O	-5.60	114.57	121.06
1	A	96	LYS	CG-CD-CE	5.59	124.16	111.30
1	A	388	VAL	N-CA-CB	5.58	122.26	111.93
1	B	217	LYS	CA-C-O	5.56	126.66	120.82
1	B	418	TYR	O-C-N	5.56	129.82	123.31
1	A	393	LYS	N-CA-C	5.53	118.59	109.85
1	A	279	ILE	CB-CA-C	-5.52	106.00	111.30
1	B	93	PRO	O-C-N	-5.48	116.40	123.03
1	A	320	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	B	370	VAL	CA-C-O	5.46	126.63	120.95
1	A	527	PRO	CA-C-O	5.45	127.06	121.23
1	A	499	VAL	CA-C-O	-5.44	115.96	121.67
1	B	56	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	259	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	278	GLY	CA-C-O	-5.42	116.65	121.64
1	A	116	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	A	289	VAL	N-CA-CB	5.40	119.20	110.13
1	B	501	PRO	CA-C-N	5.39	127.96	121.38
1	B	501	PRO	C-N-CA	5.39	127.96	121.38
1	B	448	VAL	O-C-N	-5.36	116.66	121.91
1	A	568	SER	N-CA-C	5.35	125.98	111.00
1	B	204	ASN	CA-CB-CG	5.35	117.95	112.60
1	B	211	VAL	N-CA-C	-5.35	105.28	110.42
1	A	426	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	B	144	SER	CB-CA-C	-5.34	102.43	110.92
1	A	283	LYS	O-C-N	-5.33	116.25	123.19
1	B	18	HIS	N-CA-C	5.32	118.39	110.14
1	A	218	ASP	CB-CG-OD1	-5.32	106.16	118.40
1	A	452	LYS	CA-C-O	-5.32	114.79	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	THR	CA-C-O	-5.30	114.66	120.70
1	A	567	TYR	O-C-N	-5.30	116.50	122.12
1	A	186	THR	CA-C-O	-5.29	114.50	120.32
1	A	551	SER	CA-C-N	5.29	128.15	120.79
1	A	551	SER	C-N-CA	5.29	128.15	120.79
1	B	209	VAL	CA-C-O	5.29	126.18	120.47
1	B	386	ILE	CA-C-O	-5.29	116.06	121.67
1	B	216	SER	N-CA-C	5.28	117.04	111.28
1	A	487	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	458	GLY	N-CA-C	5.27	118.61	112.50
1	B	482	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	330	LEU	CA-C-O	5.26	125.50	119.35
1	B	490	ASN	CB-CG-ND2	5.23	124.25	116.40
1	B	237	GLY	CA-C-O	5.22	126.28	121.58
1	B	349	ALA	O-C-N	-5.22	116.69	122.07
1	B	195	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	28	SER	CA-C-O	5.19	125.75	119.11
1	B	204	ASN	CA-C-O	-5.19	115.44	121.15
1	B	344	ASP	CA-C-N	5.18	125.70	120.00
1	B	344	ASP	C-N-CA	5.18	125.70	120.00
1	B	321	GLU	CB-CG-CD	-5.18	103.79	112.60
1	B	113	SER	N-CA-CB	-5.17	101.96	109.82
1	A	188	SER	N-CA-C	5.16	112.86	108.22
1	A	96	LYS	CB-CG-CD	5.16	123.16	111.30
1	A	490	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	B	539	VAL	CB-CA-C	-5.12	105.38	112.24
1	A	432	ILE	CA-CB-CG1	-5.11	101.72	110.40
1	B	368	LEU	CA-CB-CG	5.10	134.17	116.30
1	B	467	ARG	CD-NE-CZ	5.10	131.54	124.40
1	B	2	ASP	CA-C-N	-5.10	113.51	121.87
1	B	2	ASP	C-N-CA	-5.10	113.51	121.87
1	A	370	VAL	CA-C-O	5.09	126.57	121.17
1	A	183	LYS	CA-C-O	5.09	125.31	119.35
1	B	91	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	183	LYS	CA-C-N	5.05	130.01	122.74
1	B	183	LYS	C-N-CA	5.05	130.01	122.74
1	A	3	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	194	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	526	ILE	CA-C-O	5.04	123.08	119.25
1	A	288	THR	CA-C-N	-5.04	113.74	120.50
1	A	288	THR	C-N-CA	-5.04	113.74	120.50
1	A	404	LYS	CA-C-O	5.03	125.75	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	GLN	O-C-N	-5.03	117.48	123.22
1	A	526	ILE	O-C-N	-5.03	118.20	121.37
1	A	204	ASN	CA-CB-CG	5.03	117.62	112.60
1	B	111	ASP	CA-C-N	5.02	127.00	120.28
1	B	111	ASP	C-N-CA	5.02	127.00	120.28
1	B	368	LEU	CA-C-O	-5.01	115.16	120.92
1	B	239	ALA	O-C-N	-5.01	117.33	123.19
1	B	363	GLN	CA-C-O	5.00	126.67	120.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ALA	Peptide
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	4218	0	4155	85	0
1	B	4218	0	4156	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	27	0
3	B	172	0	120	26	0
4	A	53	0	30	5	0
4	B	53	0	28	4	0
5	A	8	0	1	0	0
5	B	8	0	1	1	0
6	A	805	0	0	17	0
6	B	825	0	0	20	0
All	All	10534	0	8611	174	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 10.

All (174) 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:A:36:CYS:SG	3:A:802:HEM:CAB	2.45	1.04
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.71	1.02
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.48	1.02
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.50	1.00
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.50	0.99
1:B:85:CYS:SG	3:B:804:HEM:CAC	2.53	0.97
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.53	0.96
1:B:71:CYS:SG	3:B:803:HEM:CAC	2.54	0.95
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.54	0.95
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.55	0.95
1:B:17:CYS:SG	3:B:801:HEM:CAC	2.54	0.95
1:B:14:CYS:SG	3:B:801:HEM:CAB	2.55	0.94
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.57	0.93
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.57	0.92
1:B:39:CYS:SG	3:B:802:HEM:CAC	2.60	0.90
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.59	0.90
1:A:229:ASP:H	1:A:256:HIS:HE1	1.18	0.88
1:A:82:CYS:HG	3:A:804:HEM:CAB	1.87	0.87
1:B:229:ASP:H	1:B:256:HIS:HE1	1.20	0.86
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.64	0.85
1:A:282:LEU:HD11	1:A:293:LEU:HD12	1.59	0.85
1:A:204:ASN:HD22	1:A:204:ASN:H	1.22	0.85
1:A:280:GLU:HB3	1:A:293:LEU:HD13	1.56	0.85
1:A:36:CYS:SG	3:A:802:HEM:HAB	2.15	0.85
1:B:204:ASN:H	1:B:204:ASN:HD22	1.25	0.83
1:B:200:GLY:HA3	1:B:204:ASN:HD21	1.43	0.81
1:B:368:LEU:HB2	6:B:1693:HOH:O	1.82	0.80
1:B:229:ASP:H	1:B:256:HIS:CE1	1.99	0.79
1:A:515:LYS:HG3	6:A:2568:HOH:O	1.81	0.79
1:B:299:LYS:HB2	6:B:1879:HOH:O	1.81	0.78
1:B:48:GLU:HG3	6:B:2255:HOH:O	1.84	0.77
1:B:511:MET:HB2	6:B:2646:HOH:O	1.83	0.77
1:B:311:LEU:HD21	1:B:529:LEU:HD11	1.68	0.76
1:A:39:CYS:HG	3:A:802:HEM:CAC	1.99	0.76
1:A:229:ASP:H	1:A:256:HIS:CE1	2.05	0.74
1:B:179:GLN:H	1:B:179:GLN:HE21	1.36	0.72
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.55	0.71
1:A:68:CYS:SG	3:A:803:HEM:HAB	2.29	0.70
1:B:515:LYS:HG3	6:B:2539:HOH:O	1.91	0.70
1:A:65:GLU:HG2	1:A:262:TYR:OH	1.92	0.69
1:B:4:LEU:HD22	1:B:8:HIS:CE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ILE:HG21	6:B:2357:HOH:O	1.93	0.68
1:A:452:LYS:HE2	6:A:2186:HOH:O	1.93	0.67
1:A:368:LEU:HB2	6:A:2108:HOH:O	1.95	0.66
1:B:36:CYS:SG	3:B:802:HEM:HAB	2.35	0.66
1:A:218:ASP:HB3	6:A:2135:HOH:O	1.95	0.66
1:A:544:ARG:HD2	1:A:549:ALA:HB2	1.77	0.66
1:B:4:LEU:HD22	1:B:8:HIS:HE1	1.59	0.66
1:B:179:GLN:H	1:B:179:GLN:NE2	1.94	0.65
1:A:393:LYS:HE2	6:A:2107:HOH:O	1.97	0.64
1:A:427:LYS:HE3	1:B:328:PRO:HB3	1.80	0.64
1:B:68:CYS:SG	3:B:803:HEM:HAB	2.36	0.64
1:A:334:ILE:HB	6:A:2309:HOH:O	1.97	0.63
1:B:71:CYS:SG	3:B:803:HEM:HAC	2.39	0.63
1:B:14:CYS:SG	3:B:801:HEM:HAB	2.39	0.62
1:A:183:LYS:O	1:A:184:LYS:HB2	1.98	0.62
1:B:210:LYS:O	1:B:210:LYS:HD2	1.99	0.61
1:A:368:LEU:HD22	6:A:2309:HOH:O	2.00	0.61
1:A:204:ASN:H	1:A:204:ASN:ND2	1.97	0.61
1:A:282:LEU:CD1	1:A:293:LEU:HD12	2.29	0.60
1:B:17:CYS:SG	3:B:801:HEM:HAC	2.42	0.59
1:A:459:LYS:HD2	1:A:460:ALA:N	2.17	0.59
1:B:481:GLU:HG3	6:B:1075:HOH:O	2.03	0.59
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.42	0.59
1:B:82:CYS:SG	3:B:804:HEM:HAB	2.41	0.59
1:A:39:CYS:SG	3:A:802:HEM:HAC	2.43	0.58
1:A:183:LYS:CE	1:A:233:VAL:H	2.16	0.58
1:B:519:MET:SD	6:B:2657:HOH:O	2.57	0.58
1:B:567:TYR:O	1:B:568:SER:HB3	2.04	0.58
1:B:13:GLU:HB3	1:B:15:ASP:OD1	2.03	0.57
1:B:218:ASP:HB3	6:B:1918:HOH:O	2.05	0.57
1:B:136:GLY:HA3	1:B:553:ILE:HD12	1.85	0.57
1:B:112:LYS:HE3	1:B:112:LYS:HA	1.87	0.57
1:A:299:LYS:HB3	6:A:2596:HOH:O	2.04	0.57
1:A:311:LEU:HD23	1:A:349:ALA:HB2	1.88	0.56
1:B:467:ARG:HD2	6:B:2256:HOH:O	2.05	0.56
1:B:15:ASP:HB3	6:B:1861:HOH:O	2.06	0.56
1:B:168:ALA:HA	4:B:2805:FAD:N5	2.20	0.56
1:A:183:LYS:HE2	1:A:233:VAL:H	1.71	0.56
1:B:311:LEU:HD22	1:B:311:LEU:N	2.23	0.53
1:A:60:SER:HB3	3:A:804:HEM:HMB1	1.90	0.53
1:A:511:MET:HE1	1:A:523:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:N	1:A:476:LYS:HD3	2.24	0.53
1:B:476:LYS:N	1:B:476:LYS:HD3	2.23	0.53
1:B:158:GLU:HB3	1:B:159:PRO:HD2	1.90	0.52
1:A:194:GLU:O	1:A:194:GLU:HG2	2.08	0.52
1:B:85:CYS:SG	3:B:804:HEM:HAC	2.47	0.51
1:A:79:MET:HE1	6:A:1890:HOH:O	2.08	0.51
1:B:177:THR:OG1	1:B:245:HIS:HE1	1.93	0.51
1:B:452:LYS:HD2	1:B:452:LYS:O	2.09	0.51
1:B:511:MET:HG2	6:B:2657:HOH:O	2.10	0.51
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.04	0.51
1:B:522:LYS:HD2	6:B:2380:HOH:O	2.12	0.50
1:B:183:LYS:HE2	6:B:1245:HOH:O	2.10	0.50
1:B:107:GLU:O	1:B:110:LYS:HG2	2.12	0.50
1:A:168:ALA:HA	4:A:1805:FAD:N5	2.27	0.50
1:A:424:SER:HB2	6:A:2301:HOH:O	2.11	0.50
1:B:204:ASN:H	1:B:204:ASN:ND2	1.96	0.50
1:A:85:CYS:SG	3:A:804:HEM:HAC	2.48	0.49
1:B:82:CYS:SG	3:B:804:HEM:C3B	3.00	0.49
1:B:39:CYS:SG	3:B:802:HEM:C3C	3.05	0.49
1:B:540:HIS:HE1	1:B:552:ASP:OD2	1.94	0.49
1:A:458:GLY:HA3	6:A:2459:HOH:O	2.13	0.49
1:A:549:ALA:HB3	4:A:1805:FAD:N1	2.28	0.49
1:B:168:ALA:HA	4:B:2805:FAD:C5X	2.43	0.48
1:A:158:GLU:HB3	1:A:159:PRO:HD2	1.94	0.48
1:A:26:ASN:HA	1:A:299:LYS:HE3	1.96	0.48
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.06	0.48
1:B:476:LYS:HD3	1:B:476:LYS:H	1.77	0.48
1:B:549:ALA:HB3	4:B:2805:FAD:N1	2.28	0.48
1:B:229:ASP:N	1:B:256:HIS:HE1	2.00	0.47
1:A:119:LEU:HD11	1:A:293:LEU:HD11	1.96	0.47
1:A:168:ALA:HA	4:A:1805:FAD:C5X	2.44	0.47
1:B:17:CYS:SG	3:B:801:HEM:C3C	3.07	0.47
1:B:71:CYS:SG	3:B:803:HEM:C3C	3.08	0.47
1:A:82:CYS:SG	3:A:804:HEM:HAB	2.52	0.47
1:A:204:ASN:HD22	1:A:204:ASN:N	2.03	0.47
1:B:56:ASN:HD22	1:B:58:HIS:H	1.63	0.47
1:B:457:ASP:OD1	1:B:459:LYS:HE3	2.15	0.47
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.50	0.46
1:B:419:LEU:O	1:B:496:ALA:HA	2.16	0.46
1:B:458:GLY:HA3	6:B:2671:HOH:O	2.14	0.46
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:HA	6:B:2659:HOH:O	2.15	0.46
1:B:82:CYS:SG	3:B:804:HEM:CBB	3.03	0.46
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.04	0.46
1:B:13:GLU:HG3	6:B:1618:HOH:O	2.16	0.46
1:B:311:LEU:HD21	1:B:529:LEU:CD1	2.43	0.46
1:B:357:LYS:HG2	6:B:2646:HOH:O	2.14	0.46
1:A:459:LYS:HD2	1:A:460:ALA:H	1.79	0.45
1:A:210:LYS:HD3	6:A:1871:HOH:O	2.16	0.45
1:A:56:ASN:HD22	1:A:58:HIS:H	1.64	0.45
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.98	0.45
1:A:168:ALA:HA	4:A:1805:FAD:C6	2.47	0.45
1:B:544:ARG:HD2	1:B:549:ALA:HB2	1.98	0.45
1:B:341:ALA:HA	6:B:1175:HOH:O	2.17	0.45
1:A:310:ILE:HG12	1:A:530:TYR:HB2	1.98	0.44
1:A:17:CYS:SG	3:A:801:HEM:HAC	2.51	0.44
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.11	0.44
1:B:311:LEU:CD2	1:B:529:LEU:HD11	2.44	0.44
1:B:85:CYS:SG	3:B:804:HEM:C3C	3.11	0.44
1:A:56:ASN:HD22	1:A:56:ASN:C	2.24	0.44
1:A:57:ALA:HB2	1:A:90:PHE:CE2	2.53	0.44
1:A:177:THR:OG1	1:A:245:HIS:HE1	2.00	0.44
1:A:82:CYS:SG	3:A:804:HEM:C3B	3.06	0.43
1:B:472:VAL:HG22	1:B:485:LEU:HB3	1.99	0.43
1:A:341:ALA:HA	6:A:1906:HOH:O	2.19	0.43
1:B:210:LYS:HD2	1:B:210:LYS:C	2.43	0.43
1:A:288:THR:HG22	6:A:1878:HOH:O	2.19	0.43
1:B:459:LYS:HE2	6:B:2650:HOH:O	2.17	0.43
1:A:204:ASN:O	1:A:206:PRO:HD3	2.18	0.43
1:A:540:HIS:CD2	1:A:544:ARG:HG3	2.53	0.43
1:B:442:PRO:HD2	1:B:496:ALA:O	2.19	0.42
1:A:192:MET:HG3	6:A:2598:HOH:O	2.18	0.42
1:A:246:ARG:HB2	1:A:247:PRO:HD2	2.01	0.42
3:A:801:HEM:CMC	3:A:801:HEM:HBC2	2.49	0.42
3:B:801:HEM:HHA	3:B:801:HEM:HBD2	2.01	0.42
1:B:47:ALA:HA	1:B:58:HIS:HB2	2.02	0.42
1:B:56:ASN:ND2	1:B:58:HIS:H	2.17	0.42
4:B:2805:FAD:HI'1	4:B:2805:FAD:H9	1.77	0.42
1:A:246:ARG:HB2	1:A:247:PRO:CD	2.50	0.42
1:B:68:CYS:SG	3:B:803:HEM:C3B	3.13	0.42
1:B:365:HIS:O	1:B:501:PRO:HA	2.20	0.42
1:B:36:CYS:SG	3:B:802:HEM:C3B	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HA	4:A:1805:FAD:O4'	2.20	0.41
1:A:223:MET:HE2	1:A:257:VAL:HG13	2.02	0.41
1:B:544:ARG:HH22	5:B:2806:FUM:C6	2.33	0.41
1:B:85:CYS:SG	3:B:804:HEM:CBC	3.05	0.41
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.12	0.41
1:A:514:THR:OG1	1:A:515:LYS:HE2	2.21	0.41
1:B:526:ILE:HA	1:B:527:PRO:HD3	1.89	0.41
1:A:183:LYS:HD3	6:A:2057:HOH:O	2.21	0.40
1:A:133:GLY:O	1:A:138:GLY:HA3	2.21	0.40
1:A:299:LYS:CB	6:A:2596:HOH:O	2.66	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%)	544 (96%)	20 (4%)	2 (0%)	30	27
1	B	566/571 (99%)	546 (96%)	20 (4%)	0	100	100
All	All	1132/1142 (99%)	1090 (96%)	40 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	A	113	SER

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	442/445 (99%)	410 (93%)	32 (7%)	13	10
1	B	442/445 (99%)	412 (93%)	30 (7%)	14	11
All	All	884/890 (99%)	822 (93%)	62 (7%)	14	10

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	38	SER
1	A	48	GLU
1	A	51	LYS
1	A	56	ASN
1	A	96	LYS
1	A	99	LEU
1	A	112	LYS
1	A	113	SER
1	A	183	LYS
1	A	194	GLU
1	A	204	ASN
1	A	208	LEU
1	A	282	LEU
1	A	289	VAL
1	A	293	LEU
1	A	299	LYS
1	A	311	LEU
1	A	318	LYS
1	A	337	ASN
1	A	368	LEU
1	A	448	VAL
1	A	450	LEU
1	A	452	LYS
1	A	476	LYS
1	A	490	ASN
1	A	522	LYS
1	A	523	LYS
1	A	526	ILE
1	A	529	LEU
1	A	559	LEU
1	A	568	SER
1	B	4	LEU

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Mol	Chain	Res	Type
1	B	15	ASP
1	B	21	ASP
1	B	99	LEU
1	B	110	LYS
1	B	112	LYS
1	B	113	SER
1	B	144	SER
1	B	179	GLN
1	B	204	ASN
1	B	208	LEU
1	B	257	VAL
1	B	267	LYS
1	B	289	VAL
1	B	337	ASN
1	B	393	LYS
1	B	415	LYS
1	B	427	LYS
1	B	450	LEU
1	B	459	LYS
1	B	463	GLU
1	B	467	ARG
1	B	476	LYS
1	B	481	GLU
1	B	490	ASN
1	B	515	LYS
1	B	522	LYS
1	B	526	ILE
1	B	566	LYS
1	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	56	ASN
1	A	91	ASN
1	A	116	GLN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	389	ASN
1	A	412	GLN

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Mol	Chain	Res	Type
1	A	490	ASN
1	A	540	HIS
1	B	35	GLN
1	B	56	ASN
1	B	91	ASN
1	B	173	ASN
1	B	179	GLN
1	B	202	ASN
1	B	204	ASN
1	B	245	HIS
1	B	256	HIS
1	B	269	ASN
1	B	540	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 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	B	801	1	50,50,50	1.56	13 (26%)	67,82,82	1.19	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	802	1	50,50,50	1.38	9 (18%)	67,82,82	1.36	12 (17%)
3	HEM	B	804	1	50,50,50	1.42	8 (16%)	67,82,82	1.06	6 (8%)
3	HEM	A	803	1	50,50,50	1.38	9 (18%)	67,82,82	1.08	5 (7%)
5	FUM	A	1806	-	7,7,7	2.09	3 (42%)	8,8,8	1.84	2 (25%)
3	HEM	B	803	1	50,50,50	1.35	10 (20%)	67,82,82	1.06	3 (4%)
3	HEM	A	804	1	50,50,50	1.38	9 (18%)	67,82,82	1.11	4 (5%)
4	FAD	A	1805	-	58,58,58	1.38	8 (13%)	85,89,89	1.87	17 (20%)
3	HEM	A	801	1	50,50,50	1.45	10 (20%)	67,82,82	1.41	10 (14%)
3	HEM	B	802	1	50,50,50	1.30	6 (12%)	67,82,82	1.30	11 (16%)
5	FUM	B	2806	-	7,7,7	2.61	4 (57%)	8,8,8	1.68	2 (25%)
4	FAD	B	2805	-	58,58,58	1.52	10 (17%)	85,89,89	1.79	17 (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	B	801	1	-	4/14/54/54	-
3	HEM	A	802	1	-	4/14/54/54	-
3	HEM	B	804	1	-	2/14/54/54	-
3	HEM	A	803	1	-	3/14/54/54	-
5	FUM	A	1806	-	-	2/5/5/5	-
3	HEM	B	803	1	-	1/14/54/54	-
3	HEM	B	802	1	-	3/14/54/54	-
3	HEM	A	804	1	-	4/14/54/54	-
3	HEM	A	801	1	-	4/14/54/54	-
4	FAD	A	1805	-	2/2/9/9	12/34/50/50	0/6/6/6
5	FUM	B	2806	-	-	2/5/5/5	-
4	FAD	B	2805	-	2/2/9/9	10/34/50/50	0/6/6/6

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2806	FUM	O8-C6	-4.65	1.18	1.30
4	B	2805	FAD	C9-C8	4.10	1.45	1.39
4	B	2805	FAD	C6-C5X	3.86	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1805	FAD	C9-C8	3.53	1.44	1.39
4	B	2805	FAD	C1'-C2'	-3.50	1.47	1.52
5	A	1806	FUM	O7-C6	3.44	1.31	1.23
4	A	1805	FAD	C6-C5X	3.36	1.45	1.40
3	B	801	HEM	CAB-C3B	3.23	1.56	1.47
3	B	801	HEM	FE-ND	3.20	2.04	1.94
3	A	802	HEM	CAC-C3C	3.19	1.55	1.47
3	B	804	HEM	FE-NB	3.19	2.04	1.94
4	A	1805	FAD	C5'-C4'	3.14	1.56	1.51
3	A	801	HEM	CAB-C3B	3.14	1.55	1.47
4	A	1805	FAD	O4-C4	-3.11	1.17	1.23
3	B	801	HEM	CMC-C2C	3.10	1.57	1.50
3	A	804	HEM	FE-NB	3.06	2.04	1.94
4	B	2805	FAD	O4-C4	-3.05	1.17	1.23
3	B	802	HEM	CAC-C3C	3.04	1.55	1.47
3	B	804	HEM	CAC-C3C	3.01	1.55	1.47
3	B	802	HEM	FE-NB	3.00	2.04	1.94
3	A	803	HEM	FE-NC	2.98	2.05	1.95
3	B	803	HEM	CAC-C3C	2.95	1.55	1.47
3	A	804	HEM	CAC-C3C	2.89	1.55	1.47
4	B	2805	FAD	C1'-N10	2.87	1.54	1.47
5	B	2806	FUM	O7-C6	2.86	1.30	1.23
4	B	2805	FAD	C5'-C4'	2.85	1.55	1.51
3	A	803	HEM	CAC-C3C	2.84	1.55	1.47
5	B	2806	FUM	O-C	2.83	1.30	1.23
3	A	801	HEM	CAC-C3C	2.79	1.54	1.47
3	B	804	HEM	FE-ND	2.76	2.03	1.94
3	B	801	HEM	CAA-C2A	2.68	1.58	1.51
4	B	2805	FAD	O2-C2	-2.68	1.19	1.24
3	A	803	HEM	CMB-C2B	2.64	1.56	1.50
4	A	1805	FAD	C1'-N10	2.62	1.54	1.47
3	B	802	HEM	CMD-C2D	2.60	1.56	1.50
5	A	1806	FUM	O8-C6	-2.59	1.23	1.30
3	A	803	HEM	CAB-C3B	2.57	1.54	1.47
3	B	801	HEM	CAC-C3C	2.56	1.54	1.47
3	B	801	HEM	CMA-C3A	2.55	1.56	1.50
3	B	804	HEM	CAB-C3B	2.54	1.54	1.47
3	A	802	HEM	FE-NB	2.53	2.02	1.94
3	A	804	HEM	CAB-C3B	2.52	1.54	1.47
3	A	802	HEM	FE-ND	2.51	2.02	1.94
4	A	1805	FAD	O2-C2	-2.50	1.19	1.24
3	A	802	HEM	CMD-C2D	2.49	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1806	FUM	O-C	2.48	1.29	1.23
3	A	802	HEM	CAB-C3B	2.48	1.54	1.47
3	A	804	HEM	CMB-C2B	2.46	1.55	1.50
3	B	804	HEM	CAA-C2A	2.46	1.57	1.51
4	B	2805	FAD	C9A-N10	-2.45	1.36	1.41
3	B	803	HEM	C2A-C3A	-2.40	1.32	1.38
3	A	801	HEM	C3B-C2B	-2.40	1.32	1.37
3	A	801	HEM	FE-ND	2.40	2.02	1.94
3	B	802	HEM	CMA-C3A	2.39	1.55	1.50
3	A	802	HEM	CMC-C2C	2.39	1.55	1.50
3	A	802	HEM	CMA-C3A	2.39	1.55	1.50
3	A	801	HEM	CAA-C2A	2.38	1.57	1.51
3	A	801	HEM	CMA-C3A	2.38	1.55	1.50
3	A	802	HEM	C1B-NB	-2.37	1.36	1.40
3	B	803	HEM	CAD-C3D	2.37	1.57	1.51
3	B	803	HEM	C3C-C2C	-2.35	1.32	1.37
3	A	803	HEM	FE-NA	2.34	2.02	1.95
3	B	801	HEM	C3B-C2B	-2.32	1.32	1.37
3	A	801	HEM	CMD-C2D	2.32	1.55	1.50
3	A	804	HEM	CAA-C2A	2.31	1.57	1.51
3	B	803	HEM	CAB-C3B	2.30	1.53	1.47
3	B	802	HEM	CAB-C3B	2.25	1.53	1.47
3	B	801	HEM	C3C-C2C	-2.25	1.32	1.37
3	A	803	HEM	CMA-C3A	2.24	1.55	1.50
3	A	803	HEM	CMD-C2D	2.24	1.55	1.50
3	A	803	HEM	CAD-C3D	2.24	1.57	1.51
3	B	803	HEM	CMA-C3A	2.23	1.55	1.50
3	A	804	HEM	FE-NC	2.23	2.02	1.95
3	A	801	HEM	CMC-C2C	2.22	1.55	1.50
4	A	1805	FAD	P-O2P	-2.22	1.45	1.55
3	B	802	HEM	FE-ND	2.21	2.01	1.94
4	B	2805	FAD	P-O2P	-2.20	1.45	1.55
3	B	801	HEM	C2A-C3A	-2.19	1.33	1.38
3	B	801	HEM	CAD-C3D	2.18	1.57	1.51
3	B	803	HEM	CMD-C2D	2.17	1.55	1.50
3	B	804	HEM	C3B-C2B	-2.14	1.32	1.37
3	B	803	HEM	CMB-C2B	2.14	1.55	1.50
3	B	801	HEM	CMB-C2B	2.13	1.55	1.50
3	B	801	HEM	FE-NB	2.13	2.01	1.94
3	B	804	HEM	CMD-C2D	2.12	1.55	1.50
3	A	803	HEM	C2A-C3A	-2.12	1.33	1.38
4	B	2805	FAD	C10-N1	-2.11	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	HEM	FE-NA	2.10	2.02	1.95
3	A	801	HEM	CMB-C2B	2.10	1.55	1.50
5	B	2806	FUM	C5-C6	2.07	1.53	1.48
3	B	801	HEM	CMD-C2D	2.06	1.55	1.50
3	B	803	HEM	FE-ND	2.06	2.01	1.94
4	A	1805	FAD	P-O3P	2.05	1.61	1.59
3	A	804	HEM	FE-ND	2.05	2.01	1.94
3	B	803	HEM	FE-NC	2.05	2.01	1.95
3	A	804	HEM	C3B-C2B	-2.04	1.33	1.37
3	A	801	HEM	FE-NB	2.03	2.01	1.94
3	B	804	HEM	FE-NA	2.02	2.01	1.95
3	A	802	HEM	C2A-C3A	-2.01	1.33	1.38

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1805	FAD	C4'-C3'-C2'	7.47	126.00	113.57
4	B	2805	FAD	C4'-C3'-C2'	5.51	122.74	113.57
4	B	2805	FAD	C5'-C4'-C3'	-5.41	102.01	112.22
4	A	1805	FAD	C5'-C4'-C3'	-5.30	102.22	112.22
4	A	1805	FAD	O3'-C3'-C4'	5.00	120.28	108.93
4	B	2805	FAD	C1'-C2'-C3'	4.95	123.08	109.66
4	B	2805	FAD	O3'-C3'-C4'	4.32	118.74	108.93
4	B	2805	FAD	O4B-C4B-C5B	4.30	123.11	109.33
4	B	2805	FAD	O4-C4-N3	4.26	128.12	120.11
4	A	1805	FAD	O4B-C1B-C2B	-4.14	97.76	106.62
4	A	1805	FAD	C5A-C6A-N6A	3.86	132.84	123.29
3	A	804	HEM	CBD-CAD-C3D	3.48	122.15	112.53
3	B	804	HEM	CMB-C2B-C1B	-3.44	119.66	125.03
3	A	803	HEM	O2A-CGA-O1A	3.42	132.14	123.33
3	A	801	HEM	CMB-C2B-C1B	-3.30	119.88	125.03
3	A	803	HEM	CAD-CBD-CGD	3.10	121.89	113.67
4	B	2805	FAD	O4B-C1B-C2B	-2.93	100.35	106.62
4	B	2805	FAD	O5B-C5B-C4B	2.88	118.79	108.99
4	A	1805	FAD	O5B-C5B-C4B	2.85	118.71	108.99
3	A	802	HEM	C1B-NB-C4B	2.84	108.57	105.21
3	B	802	HEM	O1A-CGA-CBA	-2.80	114.21	123.09
4	B	2805	FAD	O4-C4-C4X	-2.79	119.16	126.53
4	A	1805	FAD	C7M-C7-C6	2.79	124.49	119.57
4	A	1805	FAD	O4B-C4B-C5B	2.79	118.26	109.33
3	A	804	HEM	O1D-CGD-CBD	-2.78	114.29	123.09
5	B	2806	FUM	O7-C6-C5	-2.73	112.70	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C1B-NB-C4B	2.72	108.42	105.21
3	A	802	HEM	O1D-CGD-CBD	-2.71	114.49	123.09
4	A	1805	FAD	C2A-N3A-C4A	-2.71	105.22	111.83
5	A	1806	FUM	O-C-C4	-2.71	112.77	121.06
3	B	801	HEM	O2D-CGD-CBD	2.67	122.43	114.00
3	A	802	HEM	CHC-C1C-NC	-2.66	121.55	124.45
4	A	1805	FAD	C2B-C1B-N9A	-2.64	106.74	113.30
4	B	2805	FAD	O3'-C3'-C2'	2.63	114.90	108.93
3	A	801	HEM	CMD-C2D-C1D	-2.58	121.00	125.03
4	A	1805	FAD	O2-C2-N3	-2.57	113.66	118.58
4	B	2805	FAD	N6A-C6A-N1A	-2.57	112.66	118.38
3	A	803	HEM	C3B-C2B-C1B	2.56	108.33	106.41
3	A	802	HEM	CHA-C4D-C3D	2.53	129.90	125.23
4	A	1805	FAD	O4'-C4'-C3'	-2.53	103.33	109.25
3	A	801	HEM	CHC-C4B-NB	2.51	127.13	124.42
3	A	802	HEM	CAC-C3C-C4C	-2.49	118.88	124.82
4	B	2805	FAD	O4'-C4'-C3'	-2.49	103.43	109.25
4	A	1805	FAD	C3B-C2B-C1B	-2.48	96.78	101.46
3	B	803	HEM	C2A-C1A-NA	-2.47	107.42	110.15
3	A	801	HEM	CBB-CAB-C3B	-2.39	115.58	127.53
4	B	2805	FAD	C7M-C7-C6	2.39	123.78	119.57
3	A	801	HEM	C3B-C4B-NB	-2.39	107.75	109.47
3	B	801	HEM	C1B-NB-C4B	2.38	108.03	105.21
3	B	804	HEM	C3B-C2B-C1B	2.38	108.20	106.41
4	B	2805	FAD	C9-C9A-N10	-2.38	118.66	121.85
3	A	802	HEM	C4A-CHB-C1B	-2.36	120.70	126.25
5	A	1806	FUM	O7-C6-C5	-2.35	113.87	121.06
3	B	802	HEM	C1B-NB-C4B	2.33	107.97	105.21
3	A	804	HEM	C4C-C3C-C2C	2.33	108.83	106.81
3	A	802	HEM	C4D-ND-C1D	2.32	107.95	105.21
3	B	802	HEM	CBA-CAA-C2A	2.32	118.94	112.53
3	A	801	HEM	C2B-C1B-NB	-2.31	107.18	109.84
3	B	804	HEM	C4C-C3C-C2C	2.31	108.81	106.81
3	B	804	HEM	CBC-CAC-C3C	-2.30	116.05	127.53
4	B	2805	FAD	C7M-C7-C8	-2.29	116.08	120.76
3	B	802	HEM	C4A-CHB-C1B	-2.28	120.89	126.25
3	B	802	HEM	C4D-ND-C1D	2.26	107.89	105.21
3	B	801	HEM	CMD-C2D-C3D	2.26	132.26	126.15
3	A	801	HEM	CMD-C2D-C3D	2.26	132.26	126.15
3	B	802	HEM	CAD-CBD-CGD	2.26	119.65	113.67
3	A	802	HEM	O2D-CGD-CBD	2.25	121.12	114.00
3	B	801	HEM	CMD-C2D-C1D	-2.24	121.53	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2805	FAD	C5X-C9A-N10	2.23	119.99	117.97
3	A	801	HEM	O2D-CGD-CBD	2.23	121.03	114.00
3	A	804	HEM	CMB-C2B-C1B	-2.23	121.56	125.03
3	B	804	HEM	O2D-CGD-CBD	2.21	120.97	114.00
3	B	801	HEM	CMC-C2C-C1C	-2.20	120.86	124.73
3	B	804	HEM	O1D-CGD-CBD	-2.17	116.22	123.09
3	A	802	HEM	C4C-C3C-C2C	2.16	108.68	106.81
4	B	2805	FAD	C2B-C1B-N9A	-2.13	108.01	113.30
5	B	2806	FUM	C4-C5-C6	-2.13	116.22	127.05
3	B	802	HEM	C3D-C4D-ND	-2.12	107.84	110.17
3	B	802	HEM	O2A-CGA-O1A	2.11	128.77	123.33
3	B	803	HEM	CAD-CBD-CGD	2.09	119.22	113.67
4	A	1805	FAD	C5A-C4A-N3A	2.09	129.59	126.72
3	B	801	HEM	C2B-C1B-NB	-2.08	107.45	109.84
3	B	801	HEM	CHD-C1D-ND	2.07	126.65	124.42
3	B	802	HEM	CHC-C1C-C2C	2.06	129.78	125.49
4	A	1805	FAD	C9A-C5X-N5	-2.06	120.27	122.45
4	A	1805	FAD	N3A-C4A-N9A	-2.06	123.66	127.17
3	A	803	HEM	CBD-CAD-C3D	-2.06	106.85	112.53
3	A	802	HEM	C3D-C4D-ND	-2.05	107.92	110.17
3	A	802	HEM	CMD-C2D-C1D	-2.05	121.84	125.03
3	A	802	HEM	C3B-C2B-C1B	2.04	107.94	106.41
3	B	801	HEM	C4B-C3B-C2B	2.04	109.16	107.28
3	B	803	HEM	CAA-C2A-C1A	-2.04	120.96	124.94
3	A	803	HEM	C2A-C1A-NA	-2.03	107.90	110.15
3	B	801	HEM	CBD-CAD-C3D	-2.02	106.94	112.53
4	A	1805	FAD	C5A-C6A-N1A	-2.02	112.40	117.51
3	A	801	HEM	O1A-CGA-CBA	-2.01	116.70	123.09
3	B	802	HEM	CAC-C3C-C4C	-2.01	120.03	124.82
3	B	802	HEM	CBD-CAD-C3D	2.00	118.07	112.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1805	FAD	C4'
4	A	1805	FAD	C3'
4	B	2805	FAD	C4'
4	B	2805	FAD	C3'

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1805	FAD	C1'-C2'-C3'-O3'
4	A	1805	FAD	C1'-C2'-C3'-C4'
4	A	1805	FAD	O2'-C2'-C3'-C4'
4	A	1805	FAD	O4'-C4'-C5'-O5'
4	B	2805	FAD	C1'-C2'-C3'-O3'
4	B	2805	FAD	C1'-C2'-C3'-C4'
4	B	2805	FAD	O2'-C2'-C3'-C4'
4	B	2805	FAD	O4'-C4'-C5'-O5'
5	A	1806	FUM	O-C-C4-C5
5	A	1806	FUM	OXT-C-C4-C5
5	B	2806	FUM	OXT-C-C4-C5
5	B	2806	FUM	O-C-C4-C5
4	A	1805	FAD	O2'-C2'-C3'-O3'
3	A	803	HEM	C2A-CAA-CBA-CGA
3	B	802	HEM	C3D-CAD-CBD-CGD
4	A	1805	FAD	C3'-C4'-C5'-O5'
4	B	2805	FAD	C3'-C4'-C5'-O5'
4	B	2805	FAD	P-O3P-PA-O1A
4	A	1805	FAD	C2'-C3'-C4'-C5'
4	B	2805	FAD	PA-O3P-P-O5'
4	B	2805	FAD	N10-C1'-C2'-O2'
4	A	1805	FAD	P-O3P-PA-O1A
4	A	1805	FAD	P-O3P-PA-O2A
4	B	2805	FAD	P-O3P-PA-O2A
4	A	1805	FAD	C2'-C3'-C4'-O4'
3	A	802	HEM	C4B-C3B-CAB-CBB
3	B	803	HEM	C3D-CAD-CBD-CGD
3	A	801	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAA-CBA-CGA-O2A
3	B	804	HEM	CAA-CBA-CGA-O2A
3	B	804	HEM	CAA-CBA-CGA-O1A
3	A	804	HEM	CAA-CBA-CGA-O1A
3	B	802	HEM	CAD-CBD-CGD-O2D
3	B	801	HEM	CAD-CBD-CGD-O1D
4	A	1805	FAD	PA-O3P-P-O5'
4	B	2805	FAD	O2'-C2'-C3'-O3'
3	A	801	HEM	CAD-CBD-CGD-O2D
3	A	802	HEM	CAD-CBD-CGD-O1D
3	A	802	HEM	CAD-CBD-CGD-O2D
3	A	803	HEM	CAA-CBA-CGA-O2A
3	B	802	HEM	CAD-CBD-CGD-O1D
3	A	803	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	C4B-C3B-CAB-CBB

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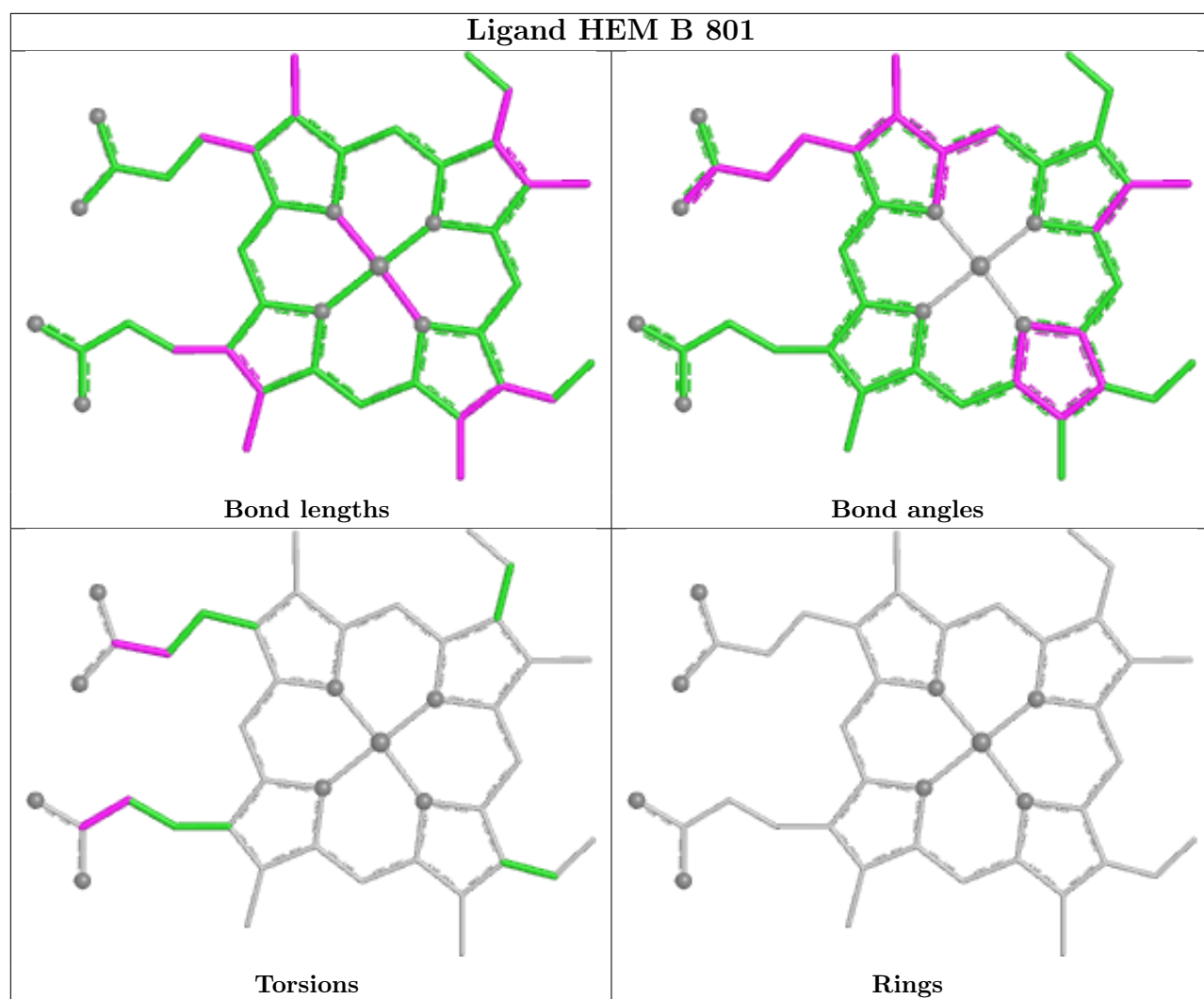
Mol	Chain	Res	Type	Atoms
3	A	801	HEM	C3D-CAD-CBD-CGD
3	A	804	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAD-CBD-CGD-O2D
3	A	802	HEM	C3D-CAD-CBD-CGD
4	A	1805	FAD	O4B-C4B-C5B-O5B
3	B	801	HEM	CAD-CBD-CGD-O2D
3	B	801	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAA-CBA-CGA-O1A

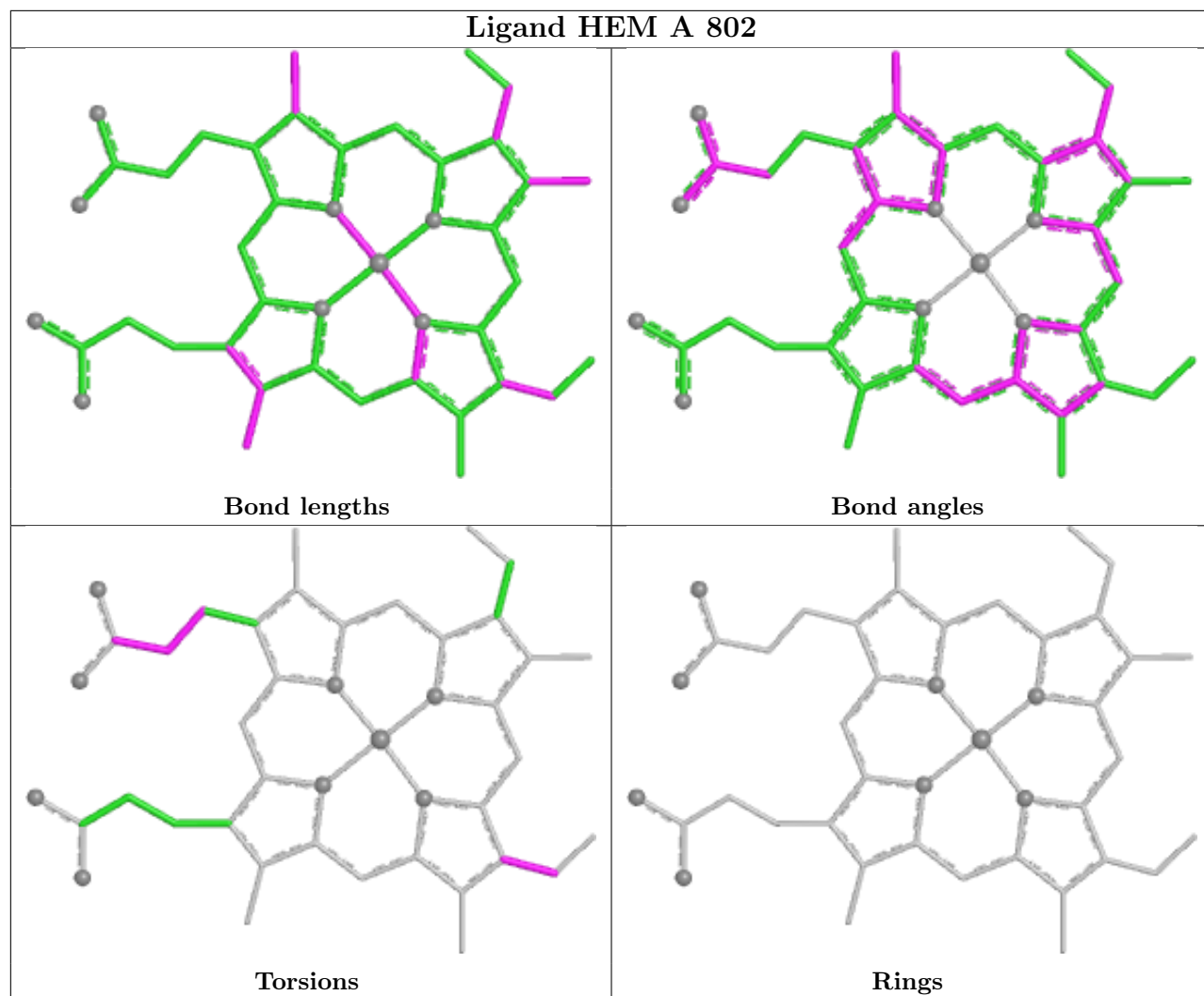
There are no ring outliers.

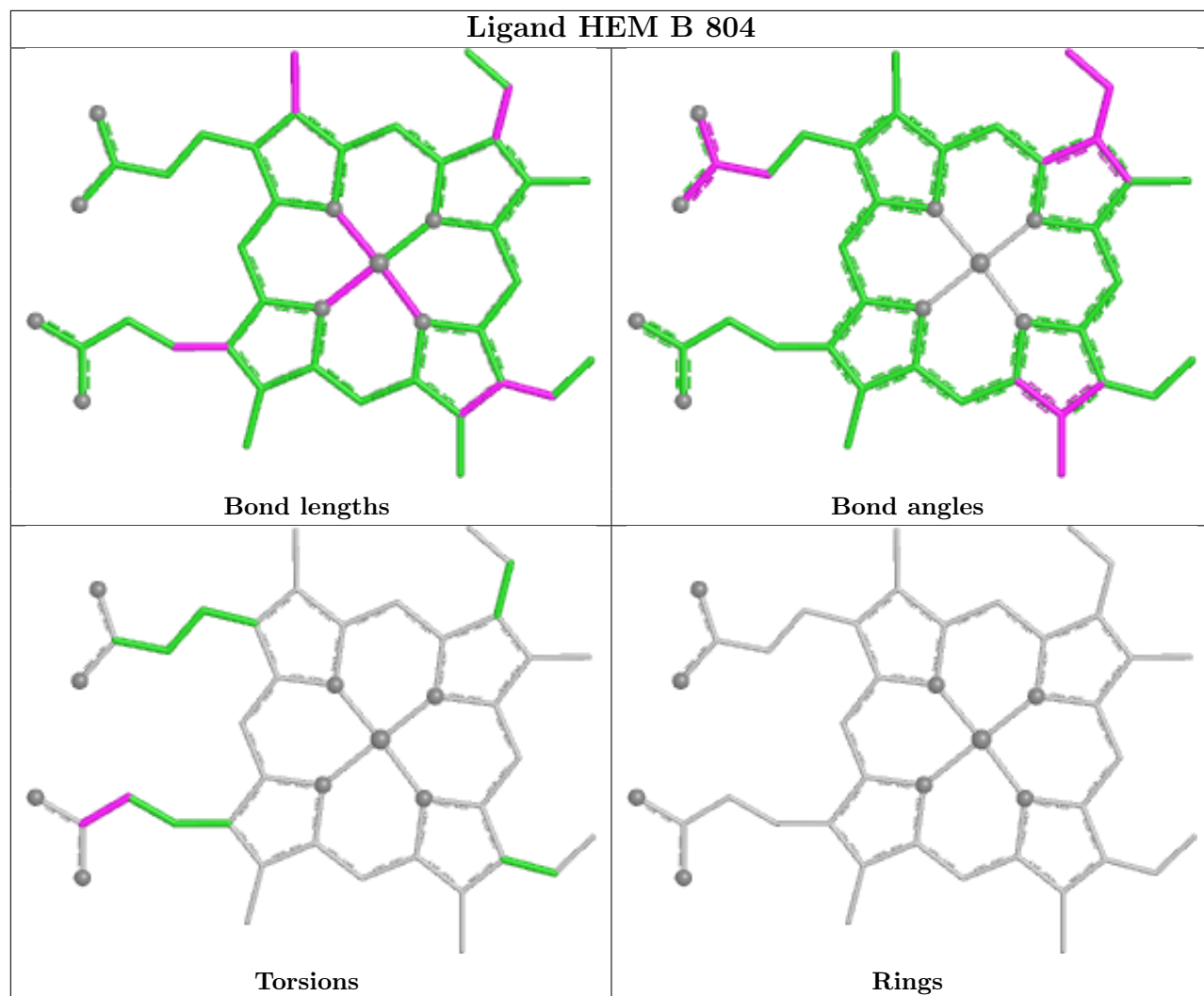
11 monomers are involved in 63 short contacts:

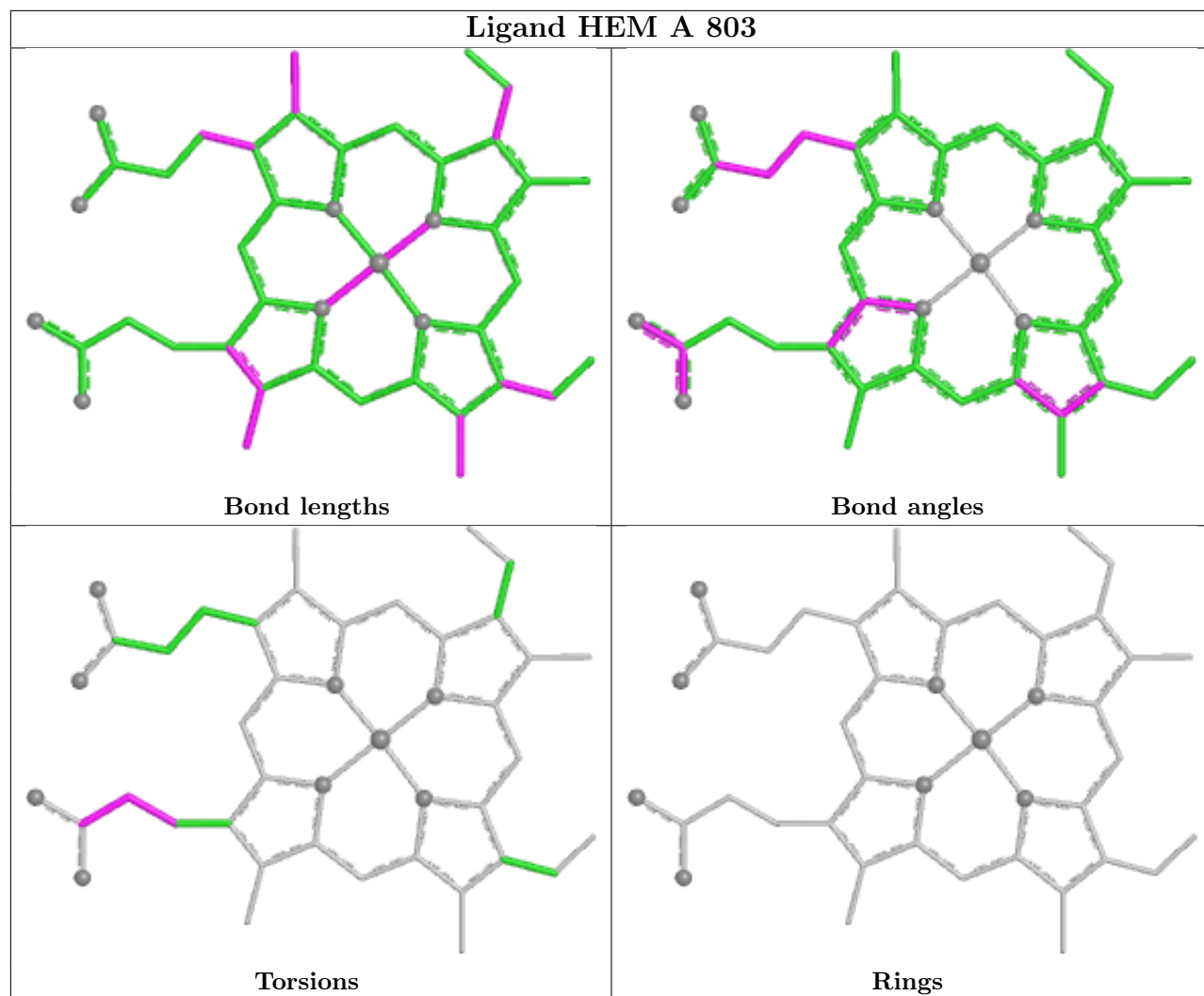
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	HEM	6	0
3	A	802	HEM	6	0
3	B	804	HEM	9	0
3	A	803	HEM	6	0
3	B	803	HEM	6	0
3	A	804	HEM	9	0
4	A	1805	FAD	5	0
3	A	801	HEM	6	0
3	B	802	HEM	5	0
5	B	2806	FUM	1	0
4	B	2805	FAD	4	0

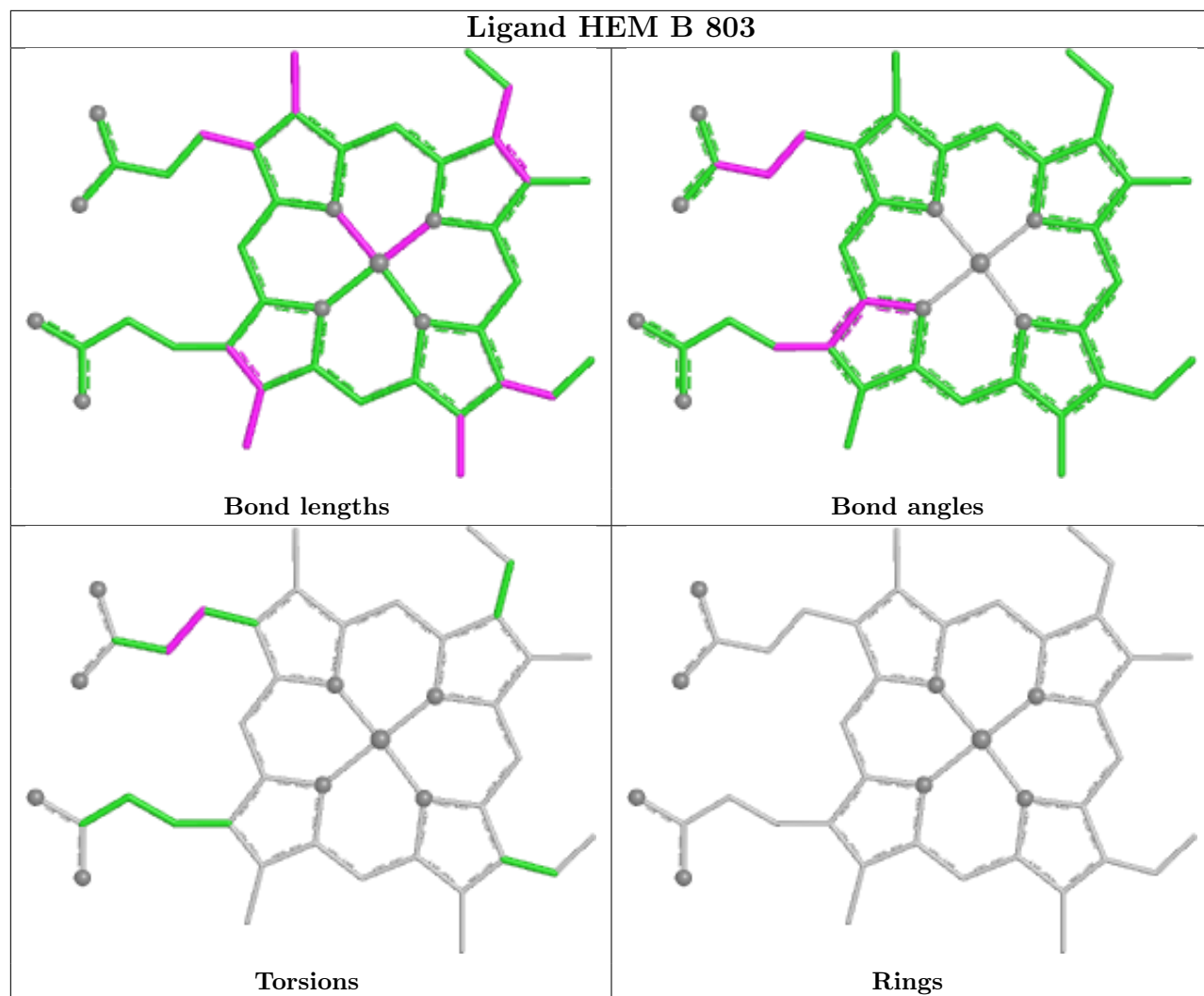
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

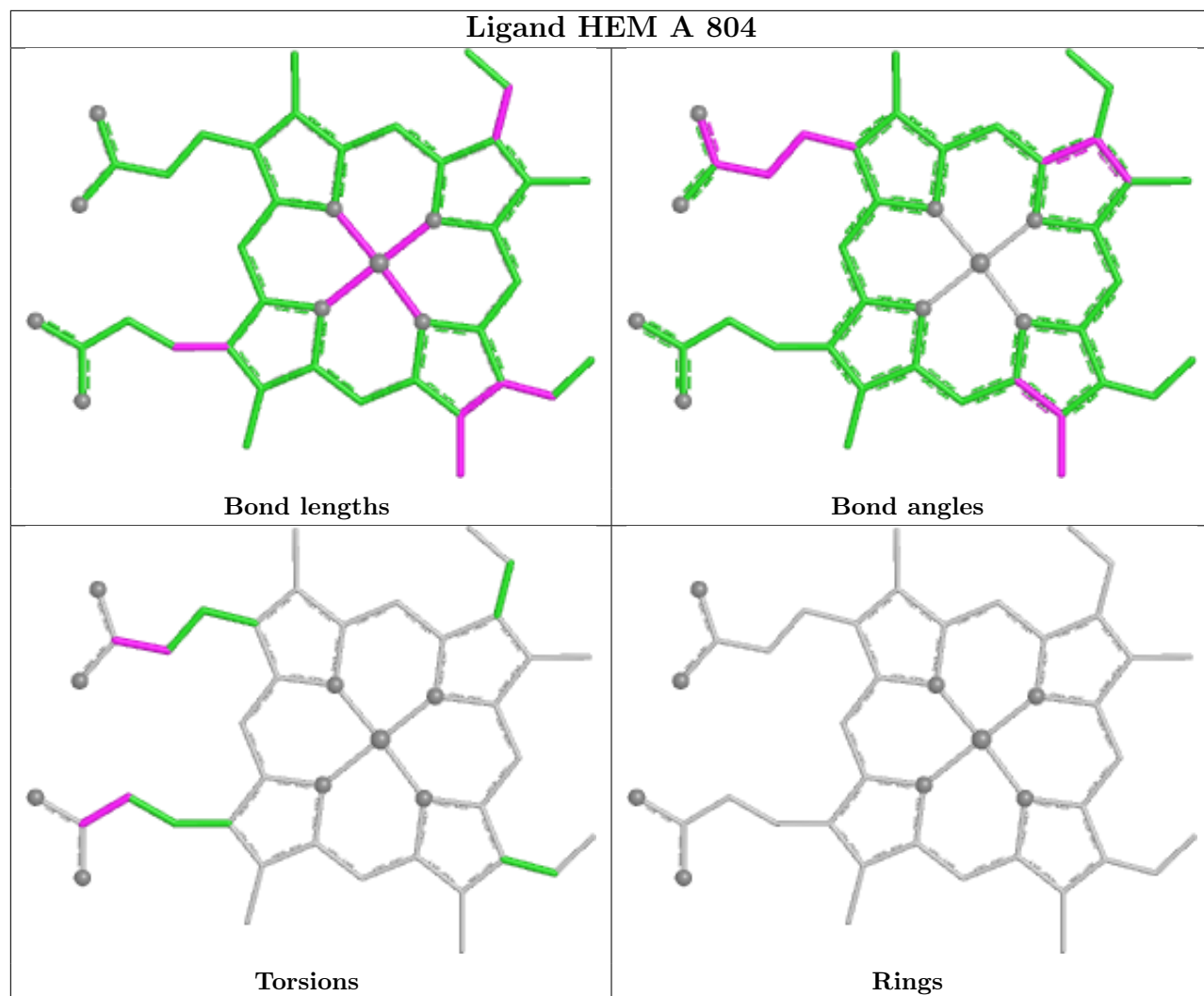


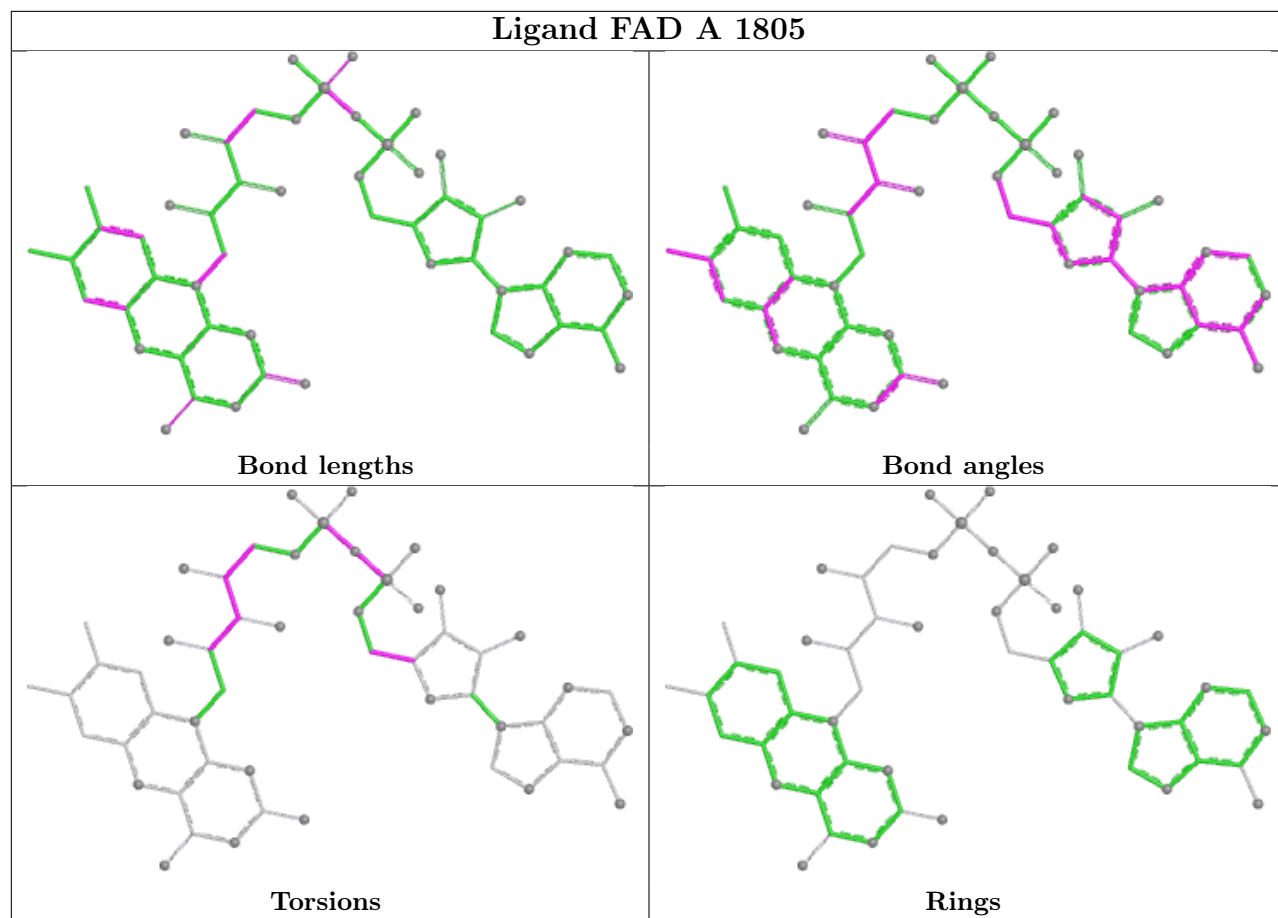


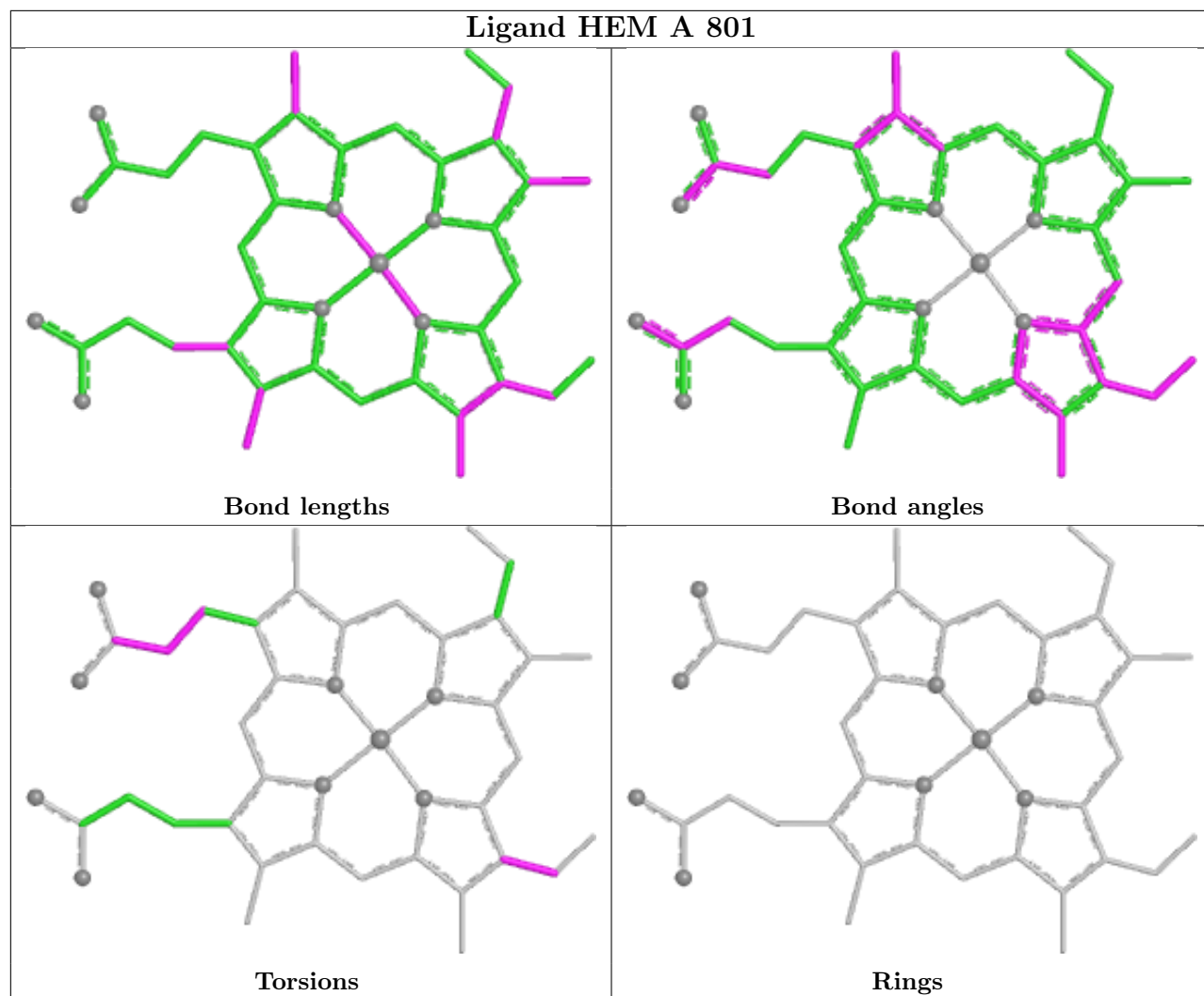


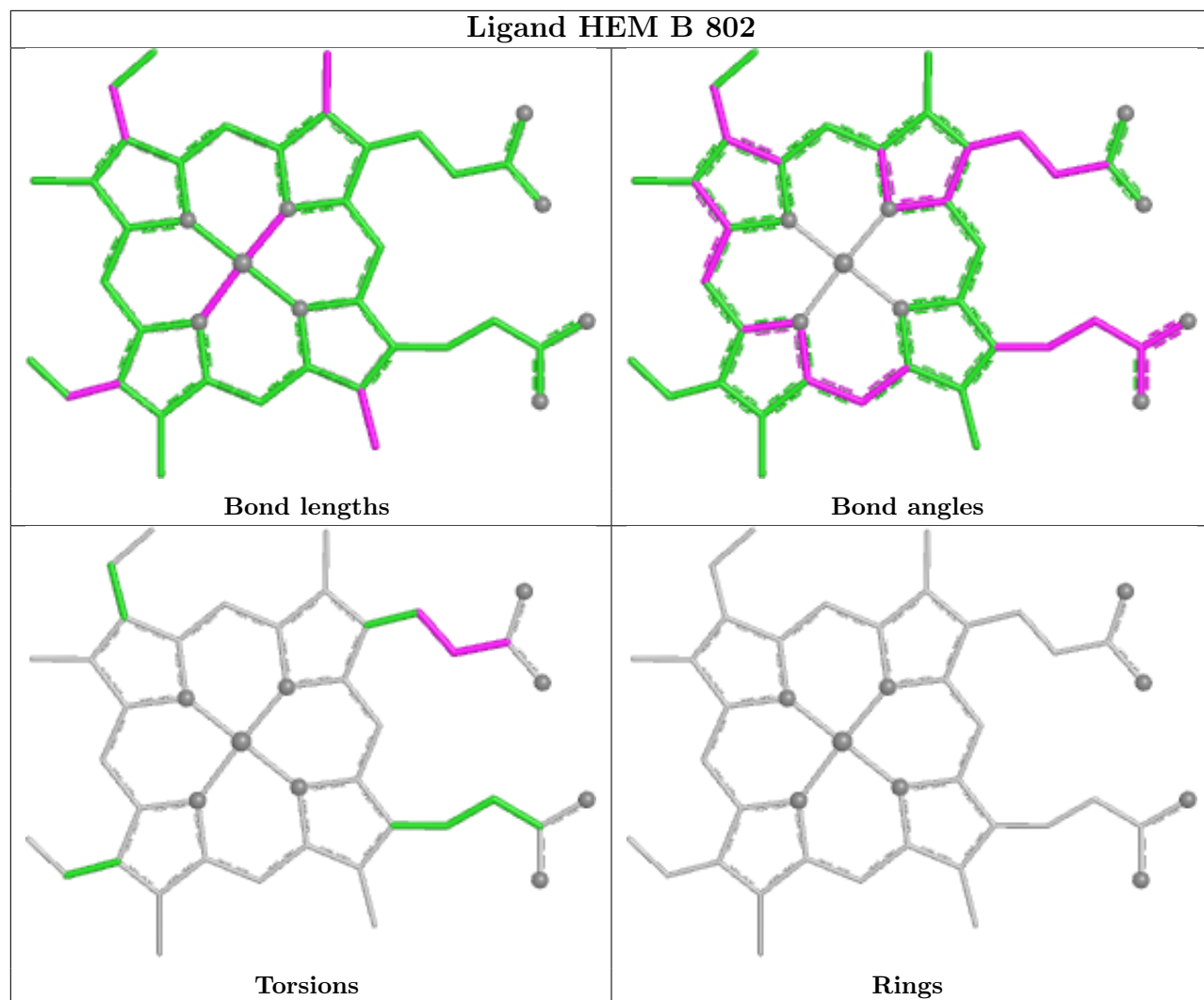


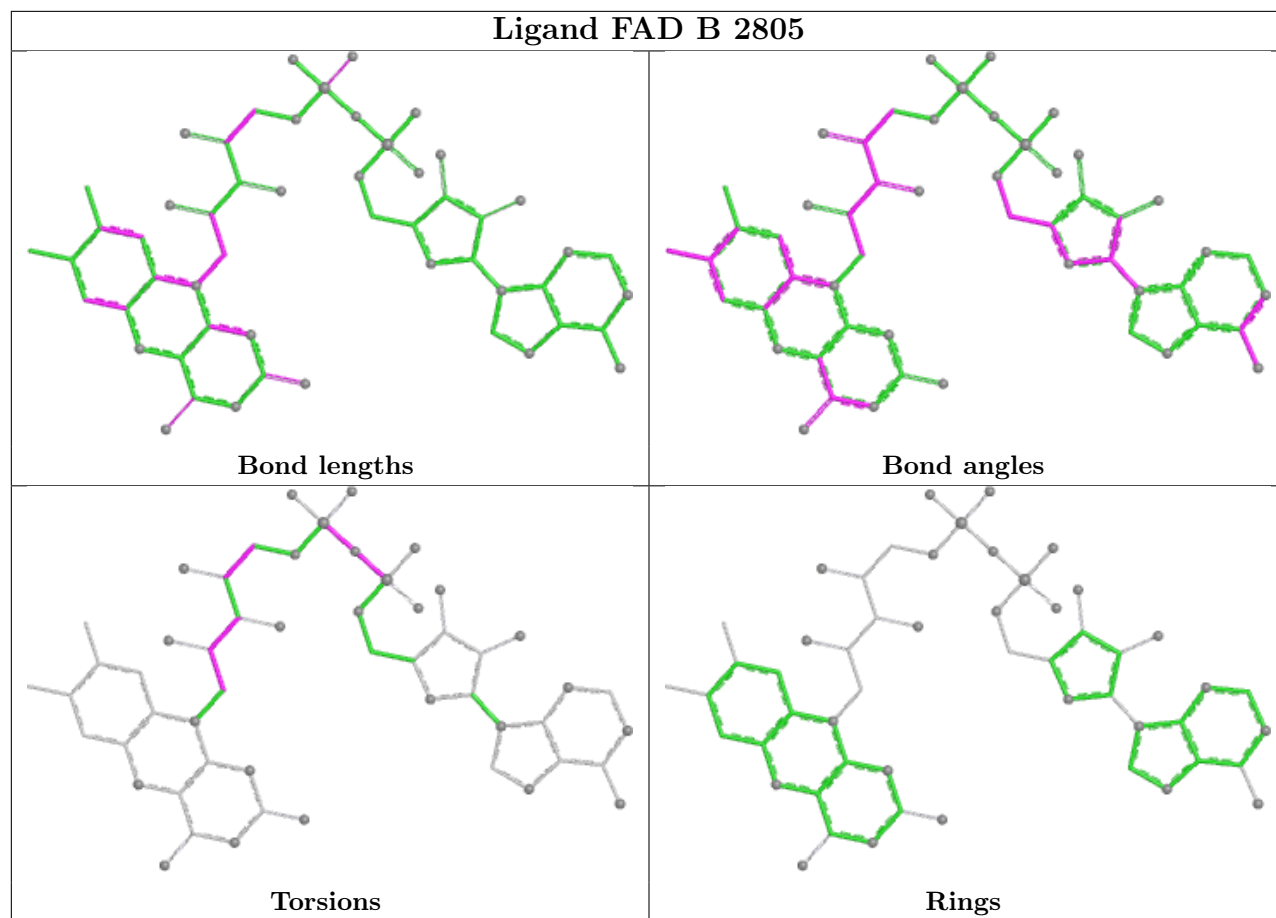












5.7 Other polymers [i](#)

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.