



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:30 AM EDT

PDB ID : 1P2H / pdb_00001p2h
Title : H61M mutant of flavocytochrome c3
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Deposited on : 2003-04-15
Resolution : 2.10 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

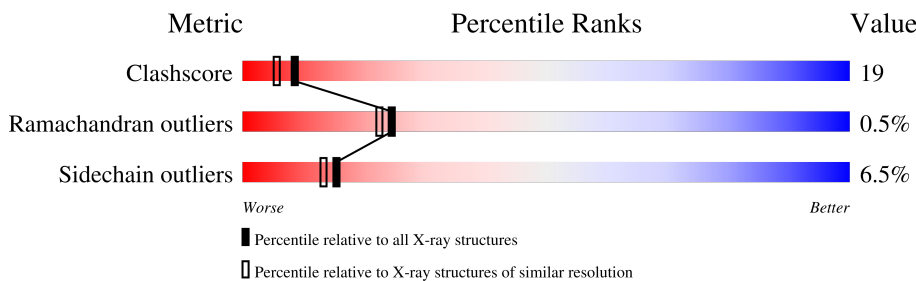
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	47% 38% 12% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TEO	A	806	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4994 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 c3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4178	2592	733	827	26			

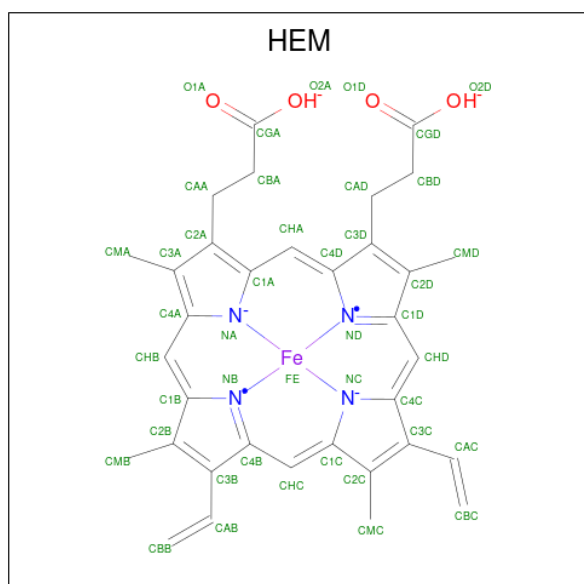
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	HIS	engineered mutation	UNP Q02469

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

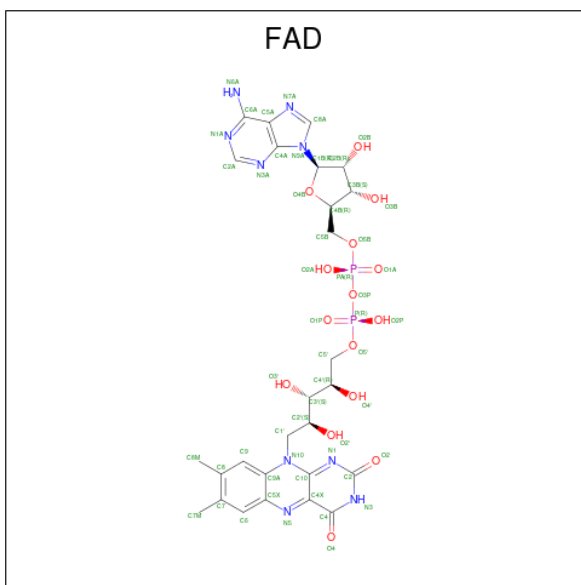
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

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



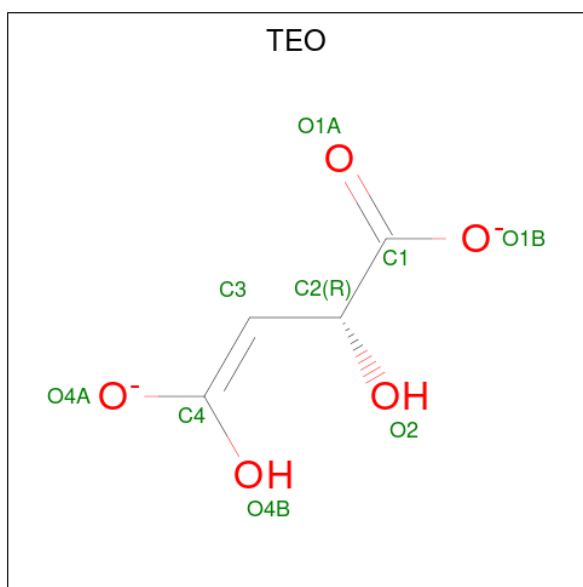
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is MALATE LIKE INTERMEDIATE (CCD ID: TEO) (formula: $C_4H_4O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is water.

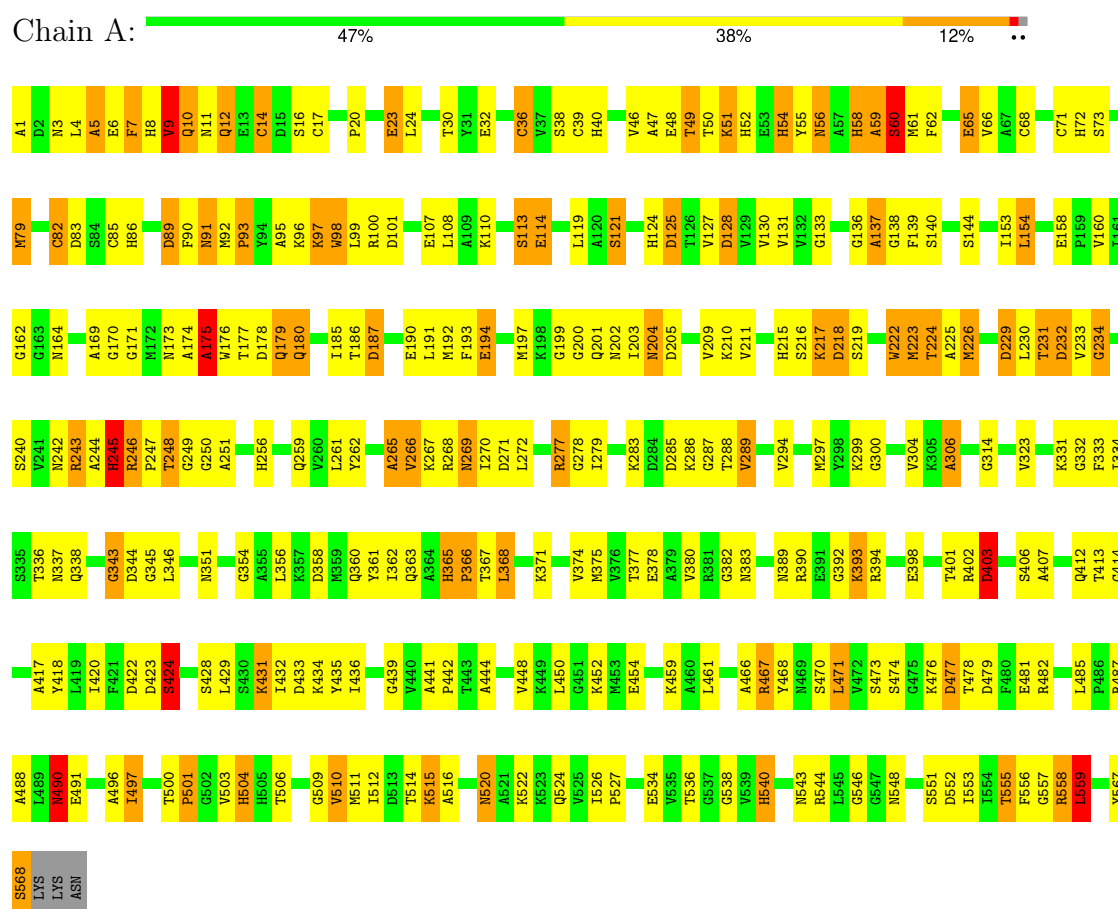
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	581	Total	O	0	0
			581	581		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: flavocytochrome c3



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	44.69Å 87.29Å 76.99Å 90.00° 104.35° 90.00°	Depositor
Resolution (Å)	17.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4994	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: FAD, HEM, TEO, 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	1.21	3/4247 (0.1%)	2.53	293/5750 (5.1%)

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	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-5.23	1.36	1.46
1	A	365	HIS	CG-ND1	-5.17	1.32	1.38
1	A	175	ALA	C-N	-5.05	1.26	1.33

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	CA-C-N	27.84	171.81	121.70
1	A	175	ALA	C-N-CA	27.84	171.81	121.70
1	A	467	ARG	CD-NE-CZ	14.27	144.38	124.40
1	A	434	LYS	CA-C-O	-10.96	108.93	120.55
1	A	360	GLN	OE1-CD-NE2	-10.87	111.73	122.60
1	A	12	GLN	CA-CB-CG	10.65	135.40	114.10
1	A	510	VAL	CB-CA-C	-10.60	95.14	111.26
1	A	510	VAL	N-CA-CB	10.47	126.47	110.13
1	A	93	PRO	CA-C-N	9.98	138.74	123.47
1	A	93	PRO	C-N-CA	9.98	138.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PRO	CB-CA-C	9.84	124.15	111.46
1	A	390	ARG	NE-CZ-NH2	-9.70	110.47	119.20
1	A	176	TRP	N-CA-CB	9.65	126.90	110.50
1	A	390	ARG	NE-CZ-NH1	9.52	131.02	121.50
1	A	179	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	A	171	GLY	N-CA-C	9.30	123.21	110.56
1	A	125	ASP	CA-C-O	-9.29	110.81	121.58
1	A	377	THR	CA-C-N	9.23	133.57	120.28
1	A	377	THR	C-N-CA	9.23	133.57	120.28
1	A	371	LYS	CA-C-O	-8.90	111.66	121.00
1	A	175	ALA	CA-C-O	8.84	131.21	120.60
1	A	54	HIS	CA-CB-CG	-8.69	105.11	113.80
1	A	38	SER	O-C-N	-8.68	112.06	122.22
1	A	420	ILE	CA-C-O	-8.48	111.48	120.39
1	A	7	PHE	CA-C-O	-8.46	111.76	121.07
1	A	175	ALA	N-CA-CB	8.46	126.27	111.13
1	A	242	ASN	CA-CB-CG	8.46	121.06	112.60
1	A	351	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	A	223	MET	CA-C-O	8.31	129.36	120.55
1	A	51	LYS	CA-C-O	8.30	132.38	120.51
1	A	60	SER	N-CA-C	8.11	128.07	110.80
1	A	130	VAL	O-C-N	8.09	131.68	123.18
1	A	231	THR	CA-CB-OG1	8.09	121.73	109.60
1	A	226	MET	N-CA-C	7.96	122.99	113.28
1	A	509	GLY	CA-C-O	-7.88	115.47	120.91
1	A	490	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	A	501	PRO	CA-C-N	7.87	128.94	121.46
1	A	501	PRO	C-N-CA	7.87	128.94	121.46
1	A	36	CYS	O-C-N	7.79	130.20	122.09
1	A	520	ASN	CA-C-N	7.68	131.59	120.38
1	A	520	ASN	C-N-CA	7.68	131.59	120.38
1	A	96	LYS	N-CA-CB	7.66	125.76	111.52
1	A	277	ARG	NE-CZ-NH1	-7.64	113.86	121.50
1	A	234	GLY	CA-C-O	-7.56	113.08	121.77
1	A	224	THR	N-CA-C	-7.53	103.02	111.07
1	A	51	LYS	CA-C-N	7.51	135.15	121.94
1	A	51	LYS	C-N-CA	7.51	135.15	121.94
1	A	279	ILE	CB-CA-C	-7.50	104.32	111.44
1	A	229	ASP	CA-C-O	-7.50	112.16	120.70
1	A	435	TYR	CA-C-O	7.46	128.55	119.97
1	A	377	THR	CA-C-O	7.45	129.35	121.15
1	A	331	LYS	CA-C-O	-7.44	112.43	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ALA	CA-C-N	7.43	135.72	121.54
1	A	59	ALA	C-N-CA	7.43	135.72	121.54
1	A	512	ILE	N-CA-CB	7.34	122.07	112.60
1	A	555	THR	CA-C-O	-7.34	113.14	120.70
1	A	488	ALA	O-C-N	-7.32	114.22	122.86
1	A	60	SER	CA-C-O	7.31	130.97	120.51
1	A	262	TYR	CA-C-O	-7.31	113.33	121.00
1	A	3	ASN	CA-C-O	-7.22	113.51	121.23
1	A	394	ARG	CD-NE-CZ	7.22	134.50	124.40
1	A	218	ASP	CA-C-N	-7.21	111.06	120.44
1	A	218	ASP	C-N-CA	-7.21	111.06	120.44
1	A	130	VAL	CA-C-O	-7.20	112.85	120.48
1	A	128	ASP	CA-C-O	-7.18	111.24	120.00
1	A	439	GLY	CA-C-N	-7.15	112.12	122.28
1	A	439	GLY	C-N-CA	-7.15	112.12	122.28
1	A	175	ALA	O-C-N	-7.15	114.68	123.33
1	A	466	ALA	CA-C-O	-7.14	111.76	119.97
1	A	323	VAL	O-C-N	-7.14	114.92	121.91
1	A	79	MET	N-CA-C	7.07	121.55	110.17
1	A	500	THR	O-C-N	-7.00	116.37	121.83
1	A	500	THR	CA-C-N	7.00	126.99	119.78
1	A	500	THR	C-N-CA	7.00	126.99	119.78
1	A	394	ARG	CA-C-O	-6.98	113.77	121.87
1	A	289	VAL	CA-C-O	6.98	128.70	121.23
1	A	536	THR	CA-CB-OG1	6.92	119.99	109.60
1	A	287	GLY	O-C-N	-6.92	114.42	122.31
1	A	164	ASN	CA-CB-CG	-6.91	105.69	112.60
1	A	567	TYR	CA-C-N	6.84	134.01	121.70
1	A	567	TYR	C-N-CA	6.84	134.01	121.70
1	A	306	ALA	CA-C-O	-6.84	114.13	121.38
1	A	224	THR	CA-C-N	-6.78	110.47	120.38
1	A	224	THR	C-N-CA	-6.78	110.47	120.38
1	A	12	GLN	CG-CD-NE2	6.78	126.57	116.40
1	A	354	GLY	CA-C-O	-6.71	115.54	121.58
1	A	271	ASP	CA-C-O	6.71	128.18	120.60
1	A	540	HIS	CA-CB-CG	-6.66	107.14	113.80
1	A	202	ASN	CA-CB-CG	-6.65	105.95	112.60
1	A	559	LEU	N-CA-CB	6.63	120.56	110.28
1	A	180	GLN	CB-CG-CD	-6.63	101.33	112.60
1	A	100	ARG	CD-NE-CZ	6.61	133.65	124.40
1	A	568	SER	CA-C-O	-6.60	109.58	120.80
1	A	534	GLU	O-C-N	-6.60	113.59	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	548	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	180	GLN	CG-CD-NE2	6.48	126.13	116.40
1	A	179	GLN	CB-CG-CD	6.47	123.60	112.60
1	A	180	GLN	CG-CD-OE1	-6.46	107.87	120.80
1	A	314	GLY	CA-C-O	-6.45	113.82	122.33
1	A	433	ASP	CA-C-O	6.43	127.36	120.55
1	A	277	ARG	O-C-N	6.41	130.51	123.27
1	A	32	GLU	CA-C-O	-6.39	112.88	120.10
1	A	506	THR	CA-C-O	-6.39	113.90	120.54
1	A	551	SER	N-CA-C	-6.38	104.40	111.36
1	A	382	GLY	O-C-N	-6.36	116.00	122.17
1	A	403	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	358	ASP	CA-C-N	6.33	129.40	120.28
1	A	358	ASP	C-N-CA	6.33	129.40	120.28
1	A	333	PHE	N-CA-CB	-6.33	100.66	109.97
1	A	169	ALA	CA-C-N	6.33	127.00	119.98
1	A	169	ALA	C-N-CA	6.33	127.00	119.98
1	A	285	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	218	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	12	GLN	CB-CA-C	6.30	122.34	110.62
1	A	205	ASP	CA-C-O	6.29	124.30	119.46
1	A	90	PHE	CA-C-N	-6.28	114.53	123.20
1	A	90	PHE	C-N-CA	-6.28	114.53	123.20
1	A	337	ASN	CA-C-O	-6.28	114.31	121.72
1	A	265	ALA	CA-C-N	6.28	128.47	120.56
1	A	265	ALA	C-N-CA	6.28	128.47	120.56
1	A	283	LYS	CA-C-O	6.28	128.45	121.11
1	A	98	TRP	O-C-N	-6.26	116.10	123.11
1	A	72	HIS	CA-C-O	-6.24	113.90	120.58
1	A	548	ASN	N-CA-C	6.24	120.15	112.54
1	A	367	THR	N-CA-C	6.23	119.55	107.71
1	A	332	GLY	O-C-N	-6.23	114.80	122.46
1	A	5	ALA	N-CA-C	-6.19	104.45	111.14
1	A	361	TYR	CA-C-N	-6.19	115.03	123.14
1	A	361	TYR	C-N-CA	-6.19	115.03	123.14
1	A	503	VAL	CA-C-O	-6.16	114.02	121.04
1	A	65	GLU	CA-C-N	6.15	130.58	122.95
1	A	65	GLU	C-N-CA	6.15	130.58	122.95
1	A	452	LYS	CA-C-O	-6.13	113.92	120.42
1	A	137	ALA	CA-C-O	-6.12	113.93	120.42
1	A	51	LYS	O-C-N	-6.12	114.45	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	GLY	CA-C-O	6.12	125.63	119.27
1	A	403	ASP	CA-C-N	6.11	128.47	120.28
1	A	403	ASP	C-N-CA	6.11	128.47	120.28
1	A	504	HIS	CA-CB-CG	6.10	119.90	113.80
1	A	428	SER	CA-C-O	-6.09	111.31	119.11
1	A	178	ASP	N-CA-C	-6.07	104.58	112.23
1	A	119	LEU	O-C-N	6.06	129.73	122.27
1	A	362	ILE	CA-C-O	-6.06	114.03	120.39
1	A	16	SER	N-CA-C	-6.05	104.60	112.23
1	A	294	VAL	CA-C-O	-6.05	115.50	121.67
1	A	95	ALA	CA-C-N	6.04	132.55	121.85
1	A	95	ALA	C-N-CA	6.04	132.55	121.85
1	A	487	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	A	511	MET	CB-CA-C	6.02	120.16	110.29
1	A	124	HIS	O-C-N	-6.02	115.29	122.15
1	A	378	GLU	CA-C-O	-6.01	113.31	120.10
1	A	30	THR	N-CA-C	6.00	117.49	111.07
1	A	243	ARG	CD-NE-CZ	5.99	132.79	124.40
1	A	548	ASN	CA-C-O	-5.98	112.02	119.38
1	A	121	SER	CA-C-O	5.97	128.81	121.94
1	A	153	ILE	CA-C-N	-5.97	114.69	123.05
1	A	153	ILE	C-N-CA	-5.97	114.69	123.05
1	A	248	THR	CB-CA-C	5.95	122.27	110.42
1	A	3	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	345	GLY	CA-C-O	-5.95	114.97	120.80
1	A	470	SER	N-CA-C	-5.92	104.41	111.69
1	A	30	THR	CA-C-O	5.92	127.03	120.82
1	A	300	GLY	O-C-N	-5.91	116.42	122.98
1	A	477	ASP	CA-CB-CG	5.89	118.50	112.60
1	A	73	SER	N-CA-C	-5.88	102.07	110.59
1	A	187	ASP	N-CA-CB	-5.86	101.87	111.66
1	A	215	HIS	N-CA-C	5.86	120.42	113.28
1	A	222	TRP	CA-C-N	5.84	128.11	120.28
1	A	222	TRP	C-N-CA	5.84	128.11	120.28
1	A	79	MET	N-CA-CB	-5.83	101.12	110.63
1	A	97	LYS	N-CA-CB	-5.83	101.16	109.85
1	A	558	ARG	CA-C-O	-5.82	114.71	120.82
1	A	179	GLN	O-C-N	-5.82	115.95	122.12
1	A	269	ASN	OD1-CG-ND2	5.82	128.42	122.60
1	A	14	CYS	CB-CA-C	-5.81	98.85	110.42
1	A	412	GLN	O-C-N	5.81	129.45	122.94
1	A	304	VAL	CA-C-O	-5.80	114.30	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LYS	CB-CA-C	-5.78	102.14	111.28
1	A	424	SER	CB-CA-C	5.77	120.04	110.81
1	A	246	ARG	N-CA-CB	5.76	117.22	111.29
1	A	407	ALA	CA-C-O	5.74	126.84	120.82
1	A	454	GLU	N-CA-C	5.71	120.24	113.16
1	A	380	VAL	N-CA-C	-5.70	104.80	110.62
1	A	140	SER	O-C-N	5.70	128.16	122.12
1	A	96	LYS	O-C-N	5.70	129.77	123.33
1	A	433	ASP	CB-CA-C	5.69	120.24	110.79
1	A	436	ILE	N-CA-C	-5.69	104.96	110.42
1	A	130	VAL	CA-C-N	-5.69	115.72	123.12
1	A	130	VAL	C-N-CA	-5.69	115.72	123.12
1	A	435	TYR	CA-C-N	5.69	127.73	120.56
1	A	435	TYR	C-N-CA	5.69	127.73	120.56
1	A	551	SER	CA-CB-OG	5.69	122.48	111.10
1	A	243	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	86	HIS	CG-CD2-NE2	5.66	112.86	107.20
1	A	304	VAL	O-C-N	5.65	129.36	123.26
1	A	412	GLN	N-CA-C	-5.64	102.17	110.52
1	A	23	GLU	CA-C-N	5.63	128.76	120.82
1	A	23	GLU	C-N-CA	5.63	128.76	120.82
1	A	403	ASP	CB-CG-OD1	5.63	131.34	118.40
1	A	336	THR	CA-C-O	-5.62	112.49	119.18
1	A	9	VAL	N-CA-CB	5.61	117.11	110.55
1	A	300	GLY	CA-C-N	5.59	129.42	121.42
1	A	300	GLY	C-N-CA	5.59	129.42	121.42
1	A	5	ALA	CA-C-O	-5.59	114.95	120.70
1	A	137	ALA	N-CA-C	-5.58	105.27	111.36
1	A	439	GLY	O-C-N	5.58	129.02	122.38
1	A	556	PHE	CA-C-N	5.58	126.02	119.94
1	A	556	PHE	C-N-CA	5.58	126.02	119.94
1	A	89	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	398	GLU	CA-C-O	-5.55	112.55	119.38
1	A	246	ARG	N-CA-C	-5.55	103.13	108.07
1	A	176	TRP	CB-CA-C	5.53	120.60	110.10
1	A	245	HIS	CB-CG-CD2	5.51	138.37	131.20
1	A	173	ASN	OD1-CG-ND2	5.50	128.09	122.60
1	A	154	LEU	CA-C-O	-5.49	114.28	120.32
1	A	114	GLU	CA-CB-CG	5.49	125.08	114.10
1	A	187	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	20	PRO	CB-CA-C	5.44	121.59	112.62
1	A	289	VAL	N-CA-CB	5.43	118.60	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	338	GLN	CA-C-N	5.41	125.03	119.56
1	A	338	GLN	C-N-CA	5.41	125.03	119.56
1	A	363	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	240	SER	CA-CB-OG	-5.41	100.28	111.10
1	A	414	GLY	CA-C-N	5.41	131.54	123.05
1	A	414	GLY	C-N-CA	5.41	131.54	123.05
1	A	36	CYS	CA-C-O	-5.41	115.12	120.90
1	A	66	VAL	CA-C-O	-5.40	114.54	120.97
1	A	406	SER	CA-C-O	5.40	126.49	120.82
1	A	232	ASP	CB-CA-C	-5.40	102.47	110.67
1	A	497	ILE	CA-C-O	-5.39	115.03	120.31
1	A	444	ALA	CA-C-O	-5.39	115.67	121.38
1	A	448	VAL	O-C-N	-5.39	116.30	121.90
1	A	389	ASN	CB-CG-ND2	-5.38	108.33	116.40
1	A	392	GLY	CA-C-O	5.37	126.42	119.44
1	A	393	LYS	CG-CD-CE	5.36	123.63	111.30
1	A	510	VAL	CG1-CB-CG2	5.36	122.60	110.80
1	A	366	PRO	CB-CA-C	-5.35	103.79	112.62
1	A	431	LYS	N-CA-CB	-5.35	101.68	110.14
1	A	131	VAL	CA-C-O	-5.35	114.81	120.53
1	A	551	SER	CB-CA-C	5.34	119.93	110.85
1	A	378	GLU	CB-CA-C	-5.33	100.76	110.63
1	A	179	GLN	CG-CD-OE1	5.31	131.41	120.80
1	A	406	SER	O-C-N	-5.28	116.63	122.07
1	A	461	LEU	O-C-N	5.28	127.72	122.12
1	A	506	THR	CB-CA-C	5.28	119.22	110.78
1	A	368	LEU	CA-C-O	-5.28	115.40	121.47
1	A	526	ILE	CA-C-O	5.26	125.63	119.89
1	A	540	HIS	CA-C-N	5.26	128.53	120.07
1	A	540	HIS	C-N-CA	5.26	128.53	120.07
1	A	444	ALA	O-C-N	5.24	128.76	123.26
1	A	557	GLY	CA-C-O	5.23	126.76	120.90
1	A	96	LYS	CA-C-O	-5.23	115.13	120.99
1	A	504	HIS	N-CA-CB	-5.23	101.65	110.49
1	A	246	ARG	O-C-N	5.23	126.73	121.56
1	A	144	SER	CA-C-O	-5.22	115.01	120.55
1	A	162	GLY	CA-C-O	-5.22	113.68	119.27
1	A	334	ILE	O-C-N	-5.22	116.99	122.57
1	A	452	LYS	N-CA-CB	5.22	117.88	110.16
1	A	383	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	286	LYS	N-CA-CB	5.20	119.51	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLY	N-CA-C	5.20	122.79	115.30
1	A	546	GLY	CA-C-N	-5.20	115.14	123.31
1	A	546	GLY	C-N-CA	-5.20	115.14	123.31
1	A	278	GLY	CA-C-N	5.20	128.33	123.08
1	A	278	GLY	C-N-CA	5.20	128.33	123.08
1	A	113	SER	CB-CA-C	5.19	119.10	110.90
1	A	223	MET	N-CA-C	5.19	116.94	111.28
1	A	40	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	194	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	413	THR	CA-C-O	5.17	126.39	120.80
1	A	211	VAL	CA-CB-CG1	5.17	119.19	110.40
1	A	351	ASN	CB-CG-ND2	5.17	124.15	116.40
1	A	337	ASN	N-CA-C	5.14	118.13	110.52
1	A	441	ALA	CA-C-N	5.14	126.26	119.84
1	A	441	ALA	C-N-CA	5.14	126.26	119.84
1	A	343	GLY	O-C-N	5.13	128.45	122.45
1	A	91	ASN	CA-C-N	-5.12	111.21	120.94
1	A	91	ASN	C-N-CA	-5.12	111.21	120.94
1	A	259	GLN	CA-C-O	-5.12	114.08	119.97
1	A	36	CYS	CB-CA-C	-5.12	102.63	110.81
1	A	536	THR	N-CA-C	5.11	118.04	110.48
1	A	244	ALA	CA-C-O	-5.10	115.13	120.58
1	A	160	VAL	CA-C-O	-5.08	114.61	121.32
1	A	246	ARG	CB-CA-C	-5.08	104.57	110.76
1	A	14	CYS	CA-CB-SG	-5.07	102.75	114.40
1	A	170	GLY	CA-C-O	-5.06	115.54	120.75
1	A	377	THR	O-C-N	-5.04	116.82	122.97
1	A	471	LEU	CA-C-N	5.04	127.00	120.70
1	A	471	LEU	C-N-CA	5.04	127.00	120.70
1	A	7	PHE	N-CA-C	-5.03	104.89	111.02
1	A	487	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ASP	Mainchain
1	A	158	GLU	Mainchain
1	A	175	ALA	Peptide
1	A	192	MET	Mainchain
1	A	266	VAL	Mainchain
1	A	417	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	9	VAL	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	4178	0	4072	156	0
2	A	1	0	0	0	0
3	A	172	0	120	37	0
4	A	53	0	31	1	0
5	A	9	0	2	2	0
6	A	581	0	0	30	0
All	All	4994	0	4225	163	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 19.

All (163) 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:204:ASN:HD22	1:A:204:ASN:H	1.01	0.98
1:A:71:CYS:SG	3:A:803:HEM:CAC	2.53	0.96
1:A:85:CYS:SG	3:A:804:HEM:CAC	2.59	0.91
1:A:229:ASP:H	1:A:256:HIS:HE1	1.13	0.87
1:A:82:CYS:SG	3:A:804:HEM:CAB	2.64	0.85
3:A:804:HEM:HMB1	3:A:804:HEM:HBB2	1.57	0.85
1:A:68:CYS:SG	3:A:803:HEM:CAB	2.65	0.85
3:A:801:HEM:HMC3	6:A:1124:HOH:O	1.76	0.84
1:A:14:CYS:SG	3:A:801:HEM:CAB	2.66	0.83
1:A:48:GLU:HG3	6:A:967:HOH:O	1.78	0.82
1:A:229:ASP:H	1:A:256:HIS:CE1	2.00	0.80
1:A:17:CYS:SG	3:A:801:HEM:CAC	2.71	0.79
1:A:418:TYR:HB3	6:A:1368:HOH:O	1.81	0.79
1:A:204:ASN:H	1:A:204:ASN:ND2	1.82	0.77
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.75	0.75
1:A:204:ASN:HD22	1:A:204:ASN:N	1.80	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:HA3	1:A:204:ASN:HD21	1.53	0.72
1:A:39:CYS:HG	3:A:802:HEM:CAC	2.04	0.70
1:A:55:TYR:OH	1:A:89:ASP:HB3	1.91	0.70
1:A:422:ASP:OD2	1:A:424:SER:HB3	1.92	0.69
1:A:71:CYS:SG	3:A:803:HEM:HAC	2.32	0.69
1:A:39:CYS:SG	3:A:802:HEM:CAC	2.83	0.67
1:A:218:ASP:HB3	6:A:1338:HOH:O	1.95	0.66
1:A:516:ALA:HB2	1:A:559:LEU:HD21	1.78	0.65
3:A:802:HEM:HMB1	3:A:802:HEM:HBB2	1.77	0.65
1:A:180:GLN:HB3	1:A:185:ILE:HB	1.76	0.65
1:A:108:LEU:HD23	6:A:1378:HOH:O	1.98	0.64
1:A:219:SER:OG	1:A:555:THR:OG1	2.14	0.64
1:A:114:GLU:HB2	6:A:1074:HOH:O	1.97	0.63
1:A:82:CYS:HG	3:A:804:HEM:CAB	2.11	0.63
1:A:101:ASP:HB3	6:A:1097:HOH:O	1.99	0.63
1:A:12:GLN:HB2	6:A:991:HOH:O	1.98	0.62
1:A:266:VAL:O	1:A:267:LYS:C	2.41	0.62
1:A:61:MET:HG2	6:A:909:HOH:O	2.00	0.62
1:A:230:LEU:O	1:A:245:HIS:HB3	2.00	0.62
1:A:393:LYS:HE3	6:A:993:HOH:O	1.99	0.62
1:A:442:PRO:HD2	1:A:496:ALA:O	2.01	0.61
1:A:246:ARG:HB2	1:A:247:PRO:CD	2.31	0.61
1:A:366:PRO:HD3	1:A:402:ARG:HG2	1.82	0.61
1:A:154:LEU:HD23	1:A:272:LEU:HD13	1.81	0.61
1:A:232:ASP:HB3	1:A:246:ARG:HG2	1.82	0.61
1:A:62:PHE:HZ	3:A:804:HEM:HMC3	1.66	0.61
1:A:190:GLU:O	1:A:194:GLU:HG2	2.01	0.61
1:A:9:VAL:O	1:A:11:ASN:N	2.34	0.60
1:A:200:GLY:O	1:A:201:GLN:HB2	2.00	0.60
1:A:268:ARG:O	1:A:269:ASN:HB2	2.01	0.60
1:A:246:ARG:HB2	1:A:247:PRO:HD2	1.83	0.59
1:A:402:ARG:HH22	5:A:806:TEO:C3	2.15	0.59
1:A:365:HIS:O	1:A:501:PRO:HA	2.02	0.59
1:A:92:MET:HG3	3:A:803:HEM:C3D	2.38	0.58
1:A:265:ALA:HA	1:A:270:ILE:HD12	1.85	0.58
1:A:520:ASN:HD21	1:A:524:GLN:HB2	1.67	0.58
1:A:52:HIS:HB2	1:A:55:TYR:O	2.04	0.58
1:A:490:ASN:HD22	1:A:490:ASN:C	2.11	0.58
1:A:79:MET:HE3	1:A:98:TRP:CE3	2.38	0.58
1:A:476:LYS:HD2	1:A:478:THR:HG22	1.85	0.58
1:A:127:VAL:O	1:A:306:ALA:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:HA	1:A:216:SER:HB2	1.86	0.57
1:A:193:PHE:O	1:A:197:MET:HG2	2.06	0.56
1:A:197:MET:SD	1:A:209:VAL:HG21	2.46	0.56
1:A:14:CYS:SG	3:A:801:HEM:HAB	2.45	0.55
1:A:467:ARG:HD2	1:A:479:ASP:OD2	2.06	0.55
1:A:139:PHE:HB3	1:A:261:LEU:HB3	1.88	0.55
1:A:516:ALA:HB2	1:A:559:LEU:CD2	2.35	0.55
1:A:54:HIS:HB2	6:A:1357:HOH:O	2.06	0.55
1:A:175:ALA:O	1:A:217:LYS:HG2	2.06	0.55
1:A:191:LEU:HA	1:A:194:GLU:HG2	1.88	0.54
1:A:515:LYS:O	1:A:516:ALA:HB3	2.05	0.54
3:A:803:HEM:CMB	3:A:803:HEM:HBB2	2.36	0.54
1:A:180:GLN:NE2	1:A:187:ASP:OD2	2.40	0.54
1:A:14:CYS:HG	3:A:801:HEM:CAB	2.18	0.54
1:A:496:ALA:HB1	6:A:1368:HOH:O	2.07	0.54
1:A:82:CYS:SG	3:A:804:HEM:CBB	2.96	0.54
1:A:217:LYS:HD3	6:A:865:HOH:O	2.07	0.54
1:A:520:ASN:ND2	1:A:524:GLN:HB2	2.22	0.54
1:A:61:MET:HE3	6:A:929:HOH:O	2.08	0.53
1:A:234:GLY:HA3	1:A:246:ARG:NH2	2.22	0.53
1:A:46:VAL:HG21	3:A:803:HEM:HMB3	1.90	0.53
1:A:56:ASN:HB3	1:A:59:ALA:HB2	1.92	0.52
1:A:468:TYR:O	1:A:471:LEU:HB2	2.09	0.52
1:A:482:ARG:HG2	1:A:485:LEU:HD23	1.91	0.52
1:A:1:ALA:HB3	6:A:1203:HOH:O	2.08	0.52
1:A:24:LEU:HD11	3:A:801:HEM:HBA1	1.91	0.52
1:A:229:ASP:N	1:A:256:HIS:HE1	1.95	0.51
1:A:11:ASN:O	1:A:12:GLN:HB3	2.09	0.51
1:A:224:THR:O	1:A:225:ALA:C	2.50	0.51
3:A:804:HEM:HBB2	3:A:804:HEM:CMB	2.35	0.51
1:A:431:LYS:NZ	3:A:804:HEM:O1D	2.38	0.50
1:A:4:LEU:HD21	3:A:802:HEM:HMB2	1.94	0.50
1:A:559:LEU:C	1:A:559:LEU:HD23	2.37	0.50
1:A:179:GLN:HA	6:A:1230:HOH:O	2.11	0.50
1:A:375:MET:HE2	5:A:806:TEO:O2	2.11	0.50
1:A:4:LEU:O	1:A:8:HIS:ND1	2.32	0.49
1:A:199:GLY:O	1:A:543:ASN:HB3	2.13	0.49
1:A:6:GLU:O	1:A:7:PHE:C	2.54	0.49
1:A:540:HIS:HB3	1:A:544:ARG:HB2	1.94	0.48
1:A:9:VAL:O	1:A:10:GLN:C	2.55	0.48
1:A:217:LYS:HE2	6:A:861:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:O	1:A:98:TRP:C	2.55	0.48
1:A:299:LYS:HB2	6:A:1058:HOH:O	2.13	0.48
1:A:423:ASP:O	1:A:424:SER:C	2.54	0.48
1:A:226:MET:HG3	6:A:1277:HOH:O	2.13	0.48
1:A:366:PRO:CD	1:A:402:ARG:HG2	2.44	0.48
1:A:17:CYS:SG	3:A:801:HEM:C3C	3.07	0.47
1:A:9:VAL:O	1:A:12:GLN:N	2.39	0.47
1:A:85:CYS:SG	3:A:804:HEM:CBC	3.02	0.47
1:A:514:THR:CB	6:A:902:HOH:O	2.62	0.47
1:A:137:ALA:HB2	1:A:553:ILE:HB	1.96	0.47
1:A:222:TRP:CE3	1:A:558:ARG:HD2	2.50	0.47
1:A:55:TYR:HH	1:A:89:ASP:HB3	1.80	0.47
1:A:490:ASN:HD22	1:A:491:GLU:N	2.12	0.47
1:A:5:ALA:O	1:A:9:VAL:N	2.46	0.46
1:A:490:ASN:C	1:A:490:ASN:ND2	2.73	0.46
1:A:17:CYS:SG	3:A:801:HEM:CBC	3.03	0.46
1:A:46:VAL:O	1:A:49:THR:HG23	2.16	0.46
1:A:107:GLU:HB3	6:A:973:HOH:O	2.17	0.45
1:A:4:LEU:HD21	3:A:802:HEM:CMB	2.46	0.45
1:A:128:ASP:HB3	1:A:568:SER:O	2.16	0.45
1:A:346:LEU:HD22	1:A:356:LEU:HD22	1.99	0.45
1:A:497:ILE:N	6:A:1368:HOH:O	2.50	0.45
1:A:193:PHE:CE1	1:A:197:MET:HG3	2.52	0.45
1:A:429:LEU:HD23	1:A:432:ILE:HG13	1.98	0.45
1:A:110:LYS:NZ	6:A:1378:HOH:O	2.50	0.44
1:A:210:LYS:O	1:A:210:LYS:HG2	2.17	0.44
1:A:85:CYS:SG	3:A:804:HEM:C3C	3.10	0.44
1:A:343:GLY:O	1:A:346:LEU:HB2	2.17	0.44
1:A:177:THR:OG1	1:A:245:HIS:HE1	2.00	0.44
1:A:180:GLN:HG2	1:A:233:VAL:HG11	1.99	0.44
1:A:83:ASP:HB2	1:A:98:TRP:HB2	1.99	0.44
1:A:114:GLU:HG2	6:A:1066:HOH:O	2.18	0.44
1:A:191:LEU:HA	1:A:194:GLU:CG	2.48	0.44
1:A:243:ARG:O	1:A:245:HIS:HD2	2.01	0.43
3:A:801:HEM:HMC1	3:A:801:HEM:HBC2	1.99	0.43
1:A:231:THR:OG1	1:A:248:THR:OG1	2.34	0.43
1:A:39:CYS:SG	3:A:802:HEM:C3C	3.12	0.43
1:A:297:MET:HE1	6:A:1065:HOH:O	2.19	0.43
1:A:47:ALA:HA	1:A:50:THR:OG1	2.18	0.43
1:A:477:ASP:O	1:A:481:GLU:HA	2.18	0.43
1:A:514:THR:HB	6:A:902:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:HE22	3:A:802:HEM:CBC	2.32	0.43
1:A:82:CYS:HG	3:A:804:HEM:CBB	2.30	0.42
1:A:6:GLU:HA	1:A:9:VAL:HG22	2.00	0.42
4:A:805:FAD:H1'1	6:A:854:HOH:O	2.19	0.42
1:A:209:VAL:O	1:A:210:LYS:C	2.60	0.42
1:A:223:MET:HE1	1:A:261:LEU:HG	2.01	0.42
1:A:401:THR:OG1	1:A:403:ASP:OD1	2.35	0.42
1:A:231:THR:O	1:A:233:VAL:HG23	2.20	0.42
1:A:232:ASP:OD2	1:A:250:GLY:N	2.52	0.42
1:A:365:HIS:HB2	1:A:504:HIS:CG	2.55	0.42
1:A:277:ARG:HH21	1:A:344:ASP:CB	2.32	0.41
1:A:393:LYS:HE2	6:A:1286:HOH:O	2.20	0.41
1:A:92:MET:HG3	3:A:803:HEM:C2D	2.54	0.41
1:A:92:MET:HG2	1:A:93:PRO:HD2	2.03	0.41
1:A:133:GLY:O	1:A:138:GLY:HA3	2.21	0.41
1:A:218:ASP:HA	6:A:1112:HOH:O	2.21	0.41
1:A:538:GLY:HA2	6:A:1157:HOH:O	2.20	0.41
1:A:71:CYS:SG	3:A:803:HEM:C3C	3.14	0.41
1:A:247:PRO:HD2	1:A:251:ALA:O	2.21	0.41
1:A:374:VAL:HB	3:A:804:HEM:CMD	2.51	0.40
1:A:203:ILE:O	1:A:204:ASN:C	2.64	0.40
1:A:4:LEU:HD11	1:A:8:HIS:HE1	1.86	0.40
1:A:136:GLY:HA3	1:A:553:ILE:HD12	2.02	0.40
1:A:47:ALA:HB2	1:A:58:HIS:HB2	2.04	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%)	532 (94%)	31 (6%)	3 (0%)	24 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	60	SER
1	A	51	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/445 (97%)	402 (94%)	28 (6%)	15	13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	49	THR
1	A	56	ASN
1	A	60	SER
1	A	65	GLU
1	A	82	CYS
1	A	91	ASN
1	A	99	LEU
1	A	113	SER
1	A	121	SER
1	A	186	THR
1	A	204	ASN
1	A	217	LYS
1	A	245	HIS
1	A	288	THR
1	A	289	VAL
1	A	368	LEU
1	A	403	ASP
1	A	424	SER
1	A	450	LEU
1	A	459	LYS
1	A	473	SER

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Mol	Chain	Res	Type
1	A	474	SER
1	A	490	ASN
1	A	510	VAL
1	A	515	LYS
1	A	522	LYS
1	A	559	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	35	GLN
1	A	56	ASN
1	A	91	ASN
1	A	204	ASN
1	A	245	HIS
1	A	256	HIS
1	A	490	ASN
1	A	543	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	1.51	12 (24%)	67,82,82	1.33	10 (14%)
3	HEM	A	802	1	50,50,50	1.24	6 (12%)	67,82,82	1.13	2 (2%)
5	TEO	A	806	-	5,8,8	4.49	3 (60%)	4,10,10	1.75	1 (25%)
3	HEM	A	804	6,1	50,50,50	1.35	7 (14%)	67,82,82	1.44	13 (19%)
3	HEM	A	803	1	50,50,50	1.30	6 (12%)	67,82,82	1.36	7 (10%)
4	FAD	A	805	-	58,58,58	1.76	12 (20%)	85,89,89	1.92	23 (27%)

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	A	802	1	-	3/14/54/54	-
5	TEO	A	806	-	1/1/3/4	4/6/8/8	-
3	HEM	A	804	6,1	-	2/14/54/54	-
3	HEM	A	803	1	-	2/14/54/54	-
4	FAD	A	805	-	-	8/34/50/50	0/6/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	806	TEO	O2-C2	-9.28	1.31	1.43
4	A	805	FAD	C2'-C3'	4.59	1.61	1.53
4	A	805	FAD	P-O3P	4.42	1.64	1.59
4	A	805	FAD	C6-C5X	4.38	1.46	1.40
4	A	805	FAD	C4'-C3'	3.59	1.59	1.53
4	A	805	FAD	O4-C4	-3.55	1.16	1.23
3	A	801	HEM	CAB-C3B	3.49	1.56	1.47
3	A	801	HEM	FE-ND	3.29	2.05	1.94
4	A	805	FAD	C2A-N3A	3.26	1.39	1.33
3	A	802	HEM	FE-NB	3.25	2.04	1.94
3	A	803	HEM	FE-NC	3.24	2.05	1.95
3	A	801	HEM	FE-NB	3.22	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	HEM	FE-ND	3.05	2.04	1.94
3	A	803	HEM	CMD-C2D	2.92	1.56	1.50
3	A	804	HEM	CAC-C3C	2.90	1.55	1.47
4	A	805	FAD	P-O1P	-2.85	1.40	1.50
4	A	805	FAD	C10-N1	-2.84	1.27	1.33
3	A	803	HEM	CMC-C2C	2.84	1.56	1.50
3	A	804	HEM	FE-NB	2.83	2.03	1.94
3	A	803	HEM	CAB-C3B	2.80	1.54	1.47
3	A	804	HEM	CAB-C3B	2.79	1.54	1.47
5	A	806	TEO	C2-C1	2.73	1.59	1.54
3	A	801	HEM	CAC-C3C	2.68	1.54	1.47
5	A	806	TEO	O1B-C1	-2.67	1.22	1.30
3	A	803	HEM	CAC-C3C	2.55	1.54	1.47
3	A	802	HEM	CAC-C3C	2.54	1.54	1.47
4	A	805	FAD	C8-C7	2.52	1.47	1.40
3	A	801	HEM	CAA-C2A	2.49	1.57	1.51
3	A	802	HEM	CAB-C3B	2.44	1.53	1.47
3	A	801	HEM	CMA-C3A	2.42	1.55	1.50
4	A	805	FAD	C9-C8	2.42	1.42	1.39
3	A	804	HEM	CAA-C2A	2.42	1.57	1.51
3	A	801	HEM	CMD-C2D	2.41	1.55	1.50
3	A	804	HEM	FE-NA	2.40	2.03	1.95
3	A	804	HEM	C2A-C3A	-2.33	1.32	1.38
3	A	802	HEM	CMC-C2C	2.30	1.55	1.50
3	A	801	HEM	C3B-C2B	-2.30	1.32	1.37
4	A	805	FAD	O2'-C2'	2.27	1.48	1.43
3	A	802	HEM	CMD-C2D	2.24	1.55	1.50
3	A	801	HEM	C2A-C3A	-2.21	1.33	1.38
3	A	801	HEM	CMB-C2B	2.18	1.55	1.50
4	A	805	FAD	O2-C2	-2.15	1.20	1.24
3	A	801	HEM	O1D-CGD	2.12	1.29	1.22
3	A	801	HEM	CMC-C2C	2.07	1.55	1.50
3	A	802	HEM	FE-ND	2.05	2.01	1.94
3	A	803	HEM	C2A-C3A	-2.00	1.33	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	HEM	CAD-CBD-CGD	5.61	128.54	113.67
4	A	805	FAD	O4'-C4'-C3'	-5.37	96.69	109.25
4	A	805	FAD	O5'-C5'-C4'	-4.92	96.22	109.36
4	A	805	FAD	O4B-C1B-C2B	-4.24	97.54	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	FAD	N3A-C4A-N9A	-4.22	119.99	127.17
3	A	804	HEM	CAA-CBA-CGA	4.09	124.51	113.67
4	A	805	FAD	C4-N3-C2	-3.99	118.55	125.64
4	A	805	FAD	O3'-C3'-C2'	-3.85	100.18	108.93
4	A	805	FAD	C5A-C4A-N9A	3.68	109.82	105.81
4	A	805	FAD	C4X-C10-N10	3.62	121.66	116.48
3	A	802	HEM	CAD-CBD-CGD	3.61	123.24	113.67
4	A	805	FAD	C4A-N9A-C8A	-3.41	102.16	105.74
4	A	805	FAD	O4'-C4'-C5'	3.36	117.40	109.99
3	A	802	HEM	C4A-CHB-C1B	-3.29	118.52	126.25
3	A	804	HEM	CMA-C3A-C2A	3.26	132.54	125.62
3	A	804	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
4	A	805	FAD	C7M-C7-C6	2.87	124.63	119.57
3	A	804	HEM	CHB-C4A-NA	2.81	128.95	123.86
4	A	805	FAD	C9A-N10-C10	-2.69	116.66	120.75
3	A	803	HEM	CHC-C4B-NB	2.67	127.30	124.42
3	A	801	HEM	C3D-C4D-ND	-2.66	107.25	110.17
4	A	805	FAD	C5'-C4'-C3'	2.62	117.17	112.22
3	A	801	HEM	CAD-CBD-CGD	2.59	120.53	113.67
3	A	803	HEM	C3B-C2B-C1B	2.58	108.35	106.41
3	A	801	HEM	O2D-CGD-CBD	2.58	122.15	114.00
3	A	801	HEM	C2A-C1A-NA	-2.56	107.31	110.15
5	A	806	TEO	O2-C2-C1	2.56	116.08	109.54
4	A	805	FAD	N3-C2-N1	2.49	124.78	119.50
3	A	801	HEM	CHA-C4D-C3D	2.48	129.81	125.23
3	A	804	HEM	CHC-C4B-NB	-2.47	121.76	124.42
3	A	804	HEM	O2A-CGA-CBA	2.46	121.77	114.00
4	A	805	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
3	A	801	HEM	O1D-CGD-CBD	-2.43	115.38	123.09
4	A	805	FAD	C5A-C4A-N3A	2.35	129.95	126.72
4	A	805	FAD	C2A-N1A-C6A	2.35	122.58	118.73
3	A	804	HEM	CMB-C2B-C1B	-2.35	121.37	125.03
3	A	801	HEM	CMD-C2D-C1D	-2.32	121.40	125.03
3	A	801	HEM	CAA-CBA-CGA	2.31	119.78	113.67
3	A	801	HEM	C3B-C2B-C1B	2.30	108.14	106.41
3	A	803	HEM	C1C-CHC-C4B	-2.27	121.19	126.02
4	A	805	FAD	O2B-C2B-C1B	-2.27	102.29	110.10
3	A	804	HEM	C4A-CHB-C1B	-2.24	120.98	126.25
3	A	803	HEM	CAA-C2A-C1A	-2.21	120.61	124.94
3	A	801	HEM	C4D-ND-C1D	2.16	107.76	105.21
3	A	803	HEM	CBB-CAB-C3B	-2.14	116.81	127.53
4	A	805	FAD	C9-C8-C7	2.13	122.81	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	HEM	CBA-CAA-C2A	-2.12	106.67	112.53
3	A	803	HEM	O1A-CGA-CBA	-2.12	116.38	123.09
3	A	804	HEM	CHC-C4B-C3B	2.11	129.29	125.07
4	A	805	FAD	N10-C10-N1	-2.11	112.31	118.51
4	A	805	FAD	C2B-C1B-N9A	-2.07	108.15	113.30
3	A	804	HEM	CHB-C4A-C3A	-2.07	121.41	127.43
3	A	804	HEM	CHA-C4D-ND	2.07	126.92	124.37
4	A	805	FAD	O4-C4-N3	-2.06	116.23	120.11
3	A	804	HEM	CHB-C1B-NB	2.03	126.88	124.37
4	A	805	FAD	C7M-C7-C8	-2.02	116.63	120.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	806	TEO	C2

All (22) torsion outliers are listed below:

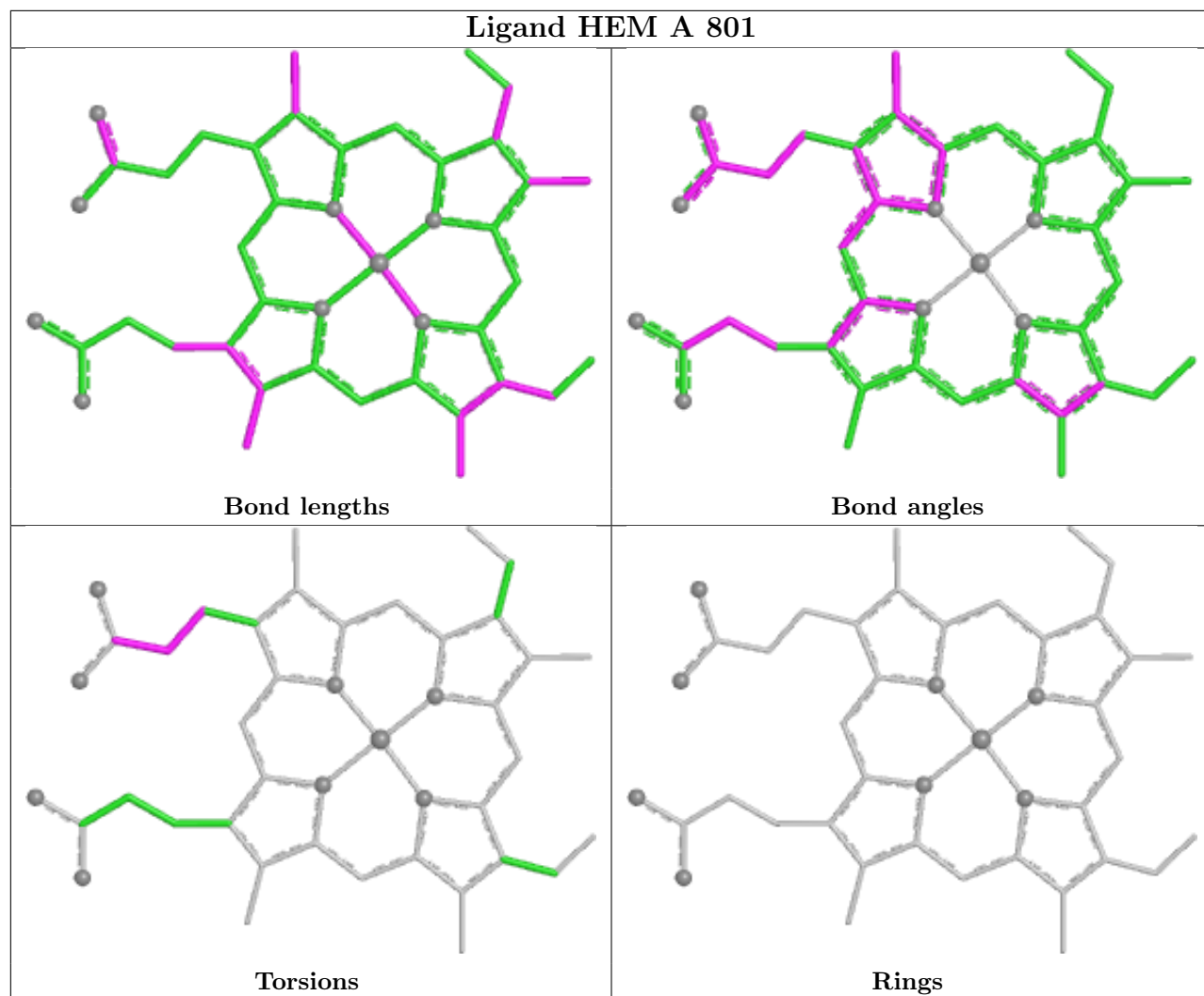
Mol	Chain	Res	Type	Atoms
4	A	805	FAD	N10-C1'-C2'-O2'
5	A	806	TEO	C1-C2-C3-C4
5	A	806	TEO	O2-C2-C3-C4
3	A	803	HEM	C2A-CAA-CBA-CGA
4	A	805	FAD	C2'-C3'-C4'-C5'
3	A	802	HEM	C3D-CAD-CBD-CGD
3	A	803	HEM	C3D-CAD-CBD-CGD
5	A	806	TEO	O1A-C1-C2-O2
5	A	806	TEO	O1B-C1-C2-O2
3	A	801	HEM	C3D-CAD-CBD-CGD
4	A	805	FAD	P-O3P-PA-O1A
4	A	805	FAD	C2B-C1B-N9A-C8A
4	A	805	FAD	C2'-C3'-C4'-O4'
4	A	805	FAD	P-O3P-PA-O2A
3	A	802	HEM	CAD-CBD-CGD-O1D
3	A	804	HEM	CAA-CBA-CGA-O2A
3	A	804	HEM	CAA-CBA-CGA-O1A
3	A	801	HEM	CAD-CBD-CGD-O1D
3	A	802	HEM	CAD-CBD-CGD-O2D
3	A	801	HEM	CAD-CBD-CGD-O2D
4	A	805	FAD	O4B-C4B-C5B-O5B
4	A	805	FAD	N10-C1'-C2'-C3'

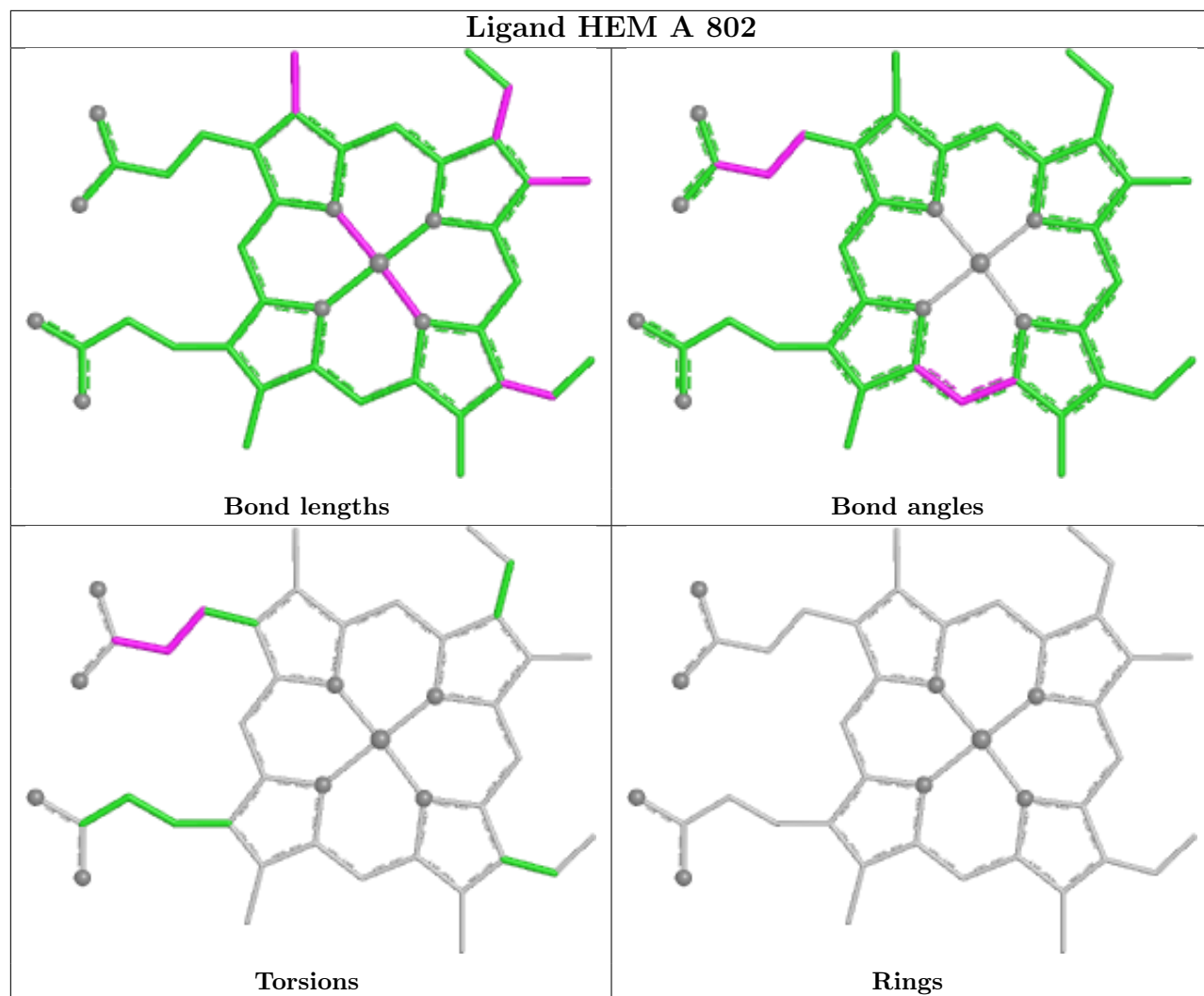
There are no ring outliers.

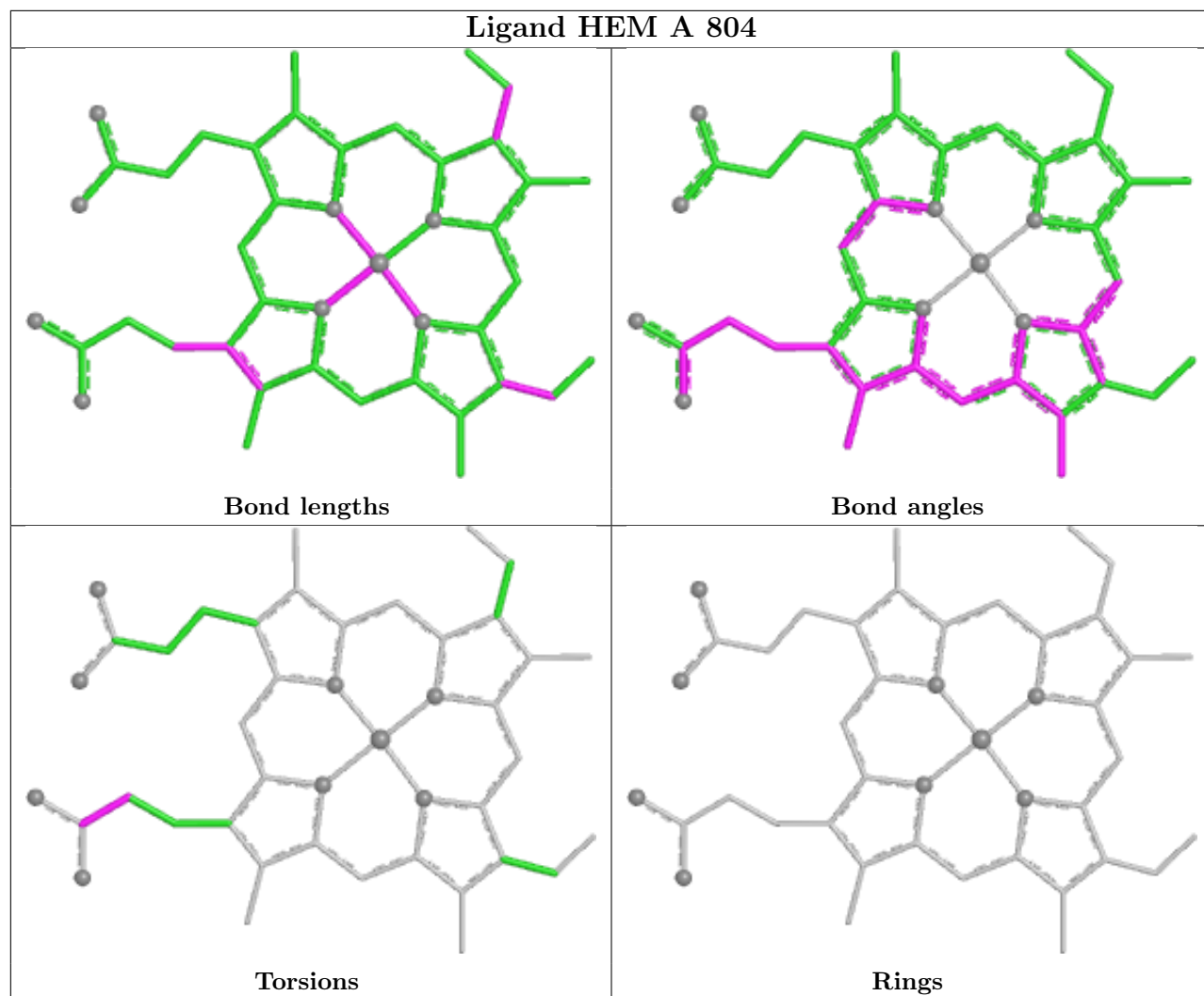
6 monomers are involved in 40 short contacts:

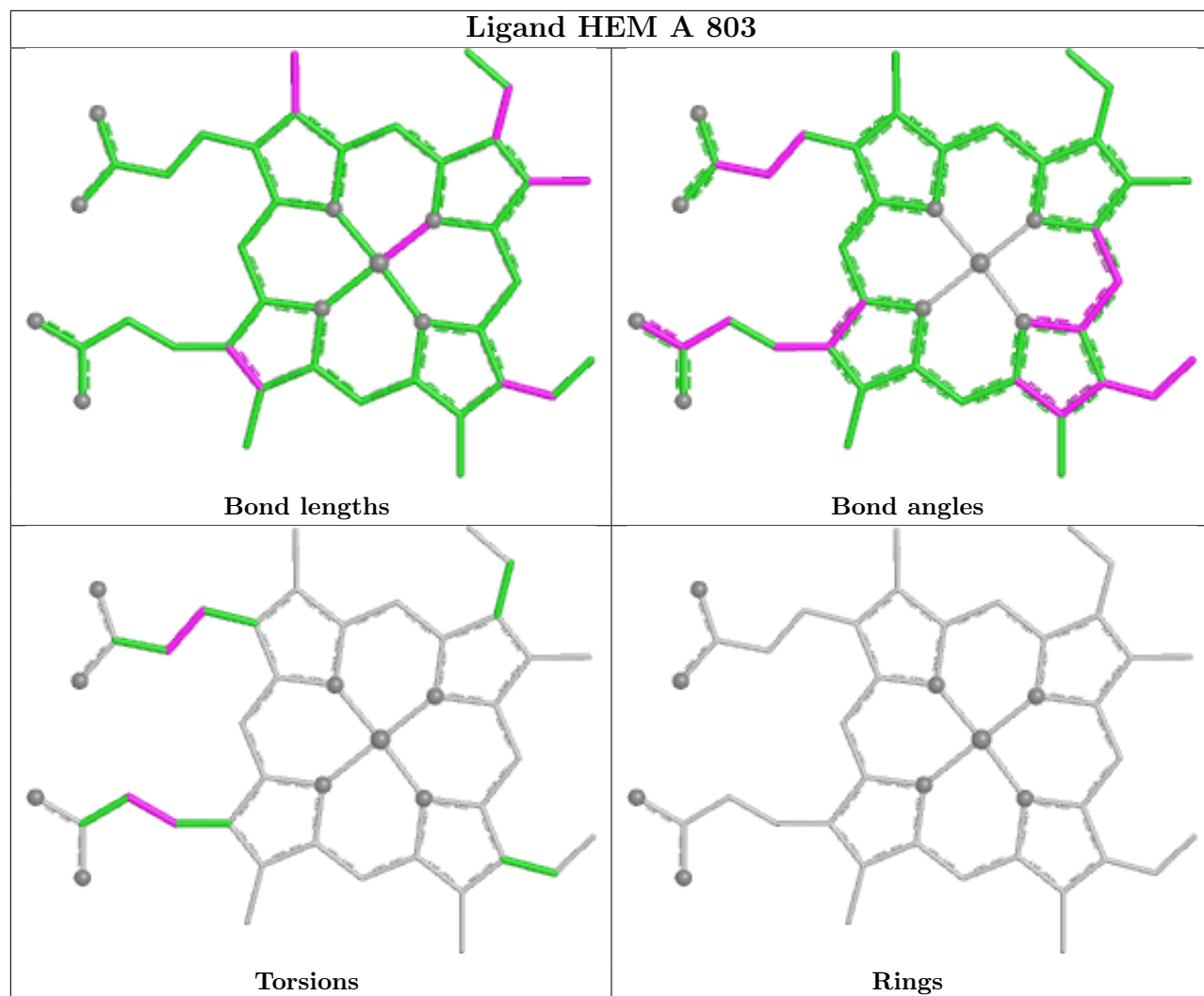
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	HEM	9	0
3	A	802	HEM	8	0
5	A	806	TEO	2	0
3	A	804	HEM	12	0
3	A	803	HEM	8	0
4	A	805	FAD	1	0

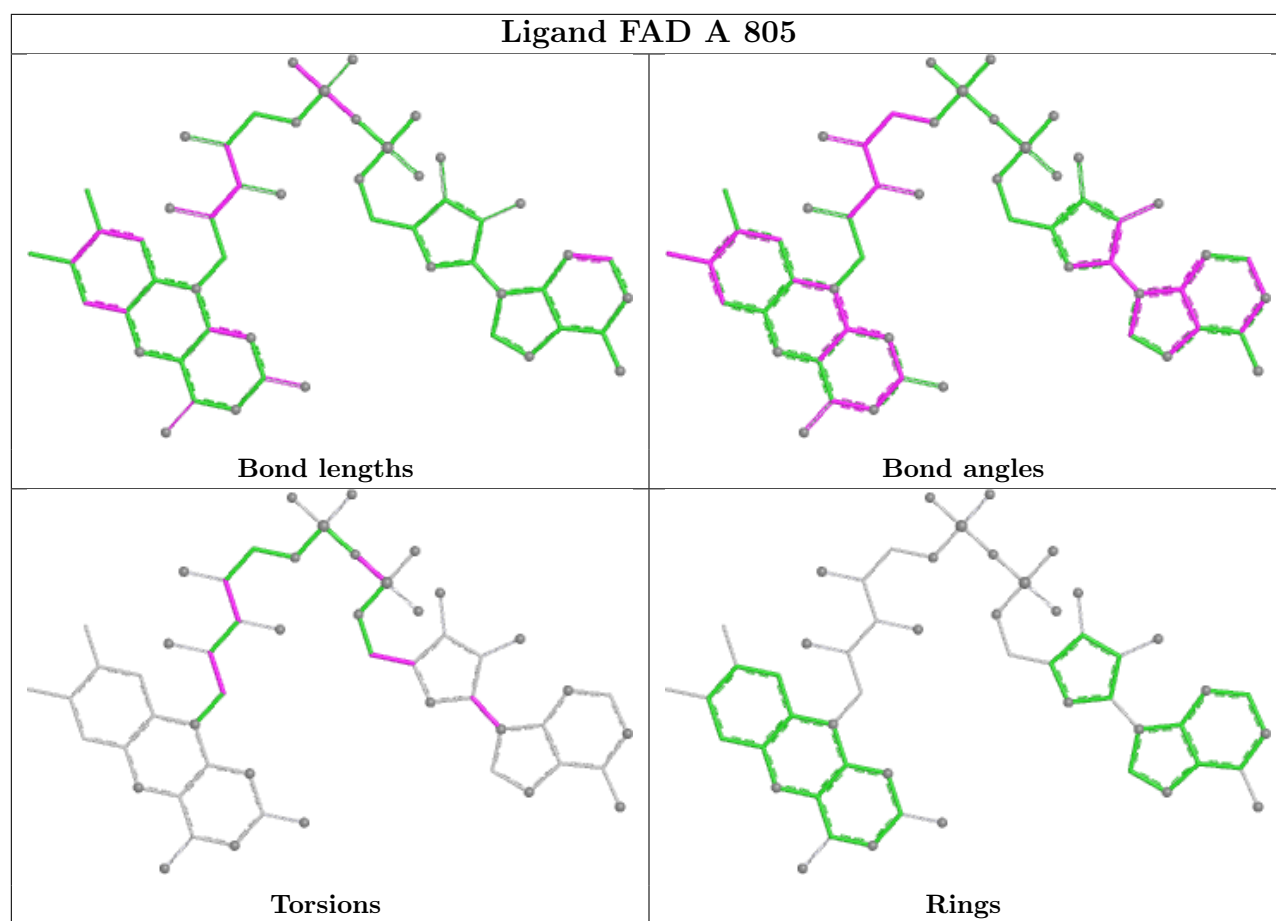
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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