



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:08 AM UTC

PDB ID : 3BK9 / pdb_00003bk9
Title : H55A mutant of tryptophan 2,3-dioxygenase from Xanthomonas campestris
Authors : Bruckmann, C.; Mowat, C.G.
Deposited on : 2007-12-06
Resolution : 2.15 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

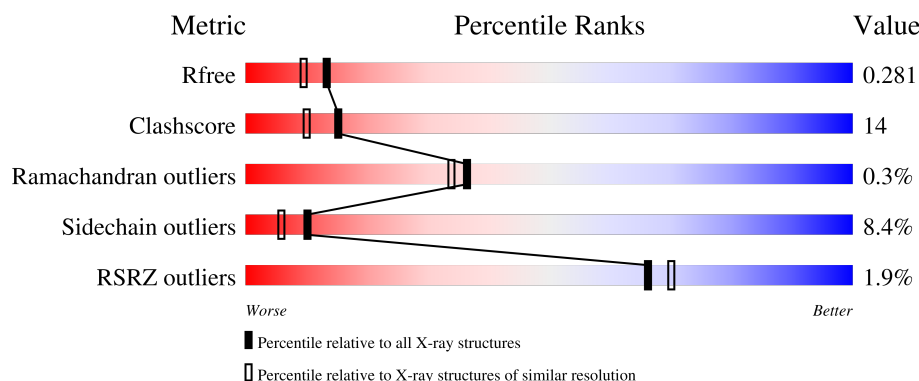
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	% 60% 23% 6% • 9%
1	B	306	56% 28% 7% • 8%
1	C	306	3% 53% 30% 6% 11%
1	D	306	55% 24% 6% 14%
1	E	306	% 50% 27% 7% • 15%

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Mol	Chain	Length	Quality of chain
1	F	306	2%53%24%5%18%
1	G	306	%48%32%5%•14%
1	H	306	4%56%25%•16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19073 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2285	1462	404	412	7			
1	B	280	Total	C	N	O	S	0	0	0
			2308	1475	408	418	7			
1	C	272	Total	C	N	O	S	0	0	0
			2244	1437	395	405	7			
1	D	262	Total	C	N	O	S	0	0	0
			2165	1389	381	388	7			
1	E	260	Total	C	N	O	S	0	0	0
			2153	1381	379	386	7			
1	F	250	Total	C	N	O	S	0	0	0
			2071	1330	362	372	7			
1	G	262	Total	C	N	O	S	0	0	0
			2172	1393	384	388	7			
1	H	257	Total	C	N	O	S	0	0	0
			2120	1362	372	379	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	HIS	engineered mutation	UNP Q8PDA8
A	299	LEU	-	expression tag	UNP Q8PDA8
A	300	GLU	-	expression tag	UNP Q8PDA8
A	301	HIS	-	expression tag	UNP Q8PDA8
A	302	HIS	-	expression tag	UNP Q8PDA8
A	303	HIS	-	expression tag	UNP Q8PDA8
A	304	HIS	-	expression tag	UNP Q8PDA8
A	305	HIS	-	expression tag	UNP Q8PDA8
A	306	HIS	-	expression tag	UNP Q8PDA8
B	55	ALA	HIS	engineered mutation	UNP Q8PDA8
B	299	LEU	-	expression tag	UNP Q8PDA8
B	300	GLU	-	expression tag	UNP Q8PDA8
B	301	HIS	-	expression tag	UNP Q8PDA8

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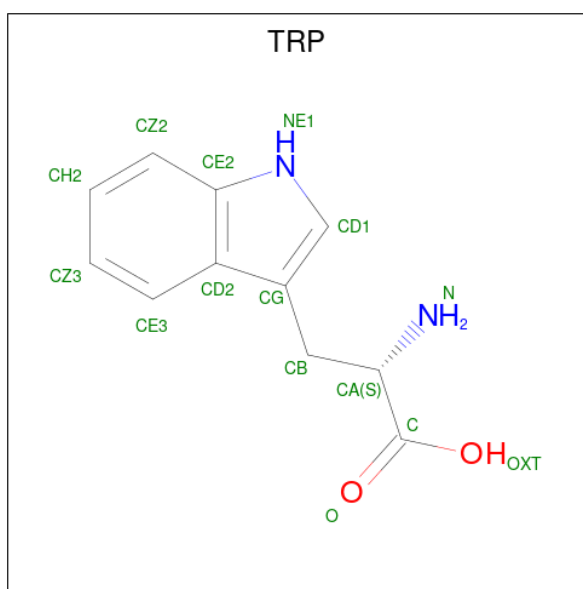
Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP Q8PDA8
B	303	HIS	-	expression tag	UNP Q8PDA8
B	304	HIS	-	expression tag	UNP Q8PDA8
B	305	HIS	-	expression tag	UNP Q8PDA8
B	306	HIS	-	expression tag	UNP Q8PDA8
C	55	ALA	HIS	engineered mutation	UNP Q8PDA8
C	299	LEU	-	expression tag	UNP Q8PDA8
C	300	GLU	-	expression tag	UNP Q8PDA8
C	301	HIS	-	expression tag	UNP Q8PDA8
C	302	HIS	-	expression tag	UNP Q8PDA8
C	303	HIS	-	expression tag	UNP Q8PDA8
C	304	HIS	-	expression tag	UNP Q8PDA8
C	305	HIS	-	expression tag	UNP Q8PDA8
C	306	HIS	-	expression tag	UNP Q8PDA8
D	55	ALA	HIS	engineered mutation	UNP Q8PDA8
D	299	LEU	-	expression tag	UNP Q8PDA8
D	300	GLU	-	expression tag	UNP Q8PDA8
D	301	HIS	-	expression tag	UNP Q8PDA8
D	302	HIS	-	expression tag	UNP Q8PDA8
D	303	HIS	-	expression tag	UNP Q8PDA8
D	304	HIS	-	expression tag	UNP Q8PDA8
D	305	HIS	-	expression tag	UNP Q8PDA8
D	306	HIS	-	expression tag	UNP Q8PDA8
E	55	ALA	HIS	engineered mutation	UNP Q8PDA8
E	299	LEU	-	expression tag	UNP Q8PDA8
E	300	GLU	-	expression tag	UNP Q8PDA8
E	301	HIS	-	expression tag	UNP Q8PDA8
E	302	HIS	-	expression tag	UNP Q8PDA8
E	303	HIS	-	expression tag	UNP Q8PDA8
E	304	HIS	-	expression tag	UNP Q8PDA8
E	305	HIS	-	expression tag	UNP Q8PDA8
E	306	HIS	-	expression tag	UNP Q8PDA8
F	55	ALA	HIS	engineered mutation	UNP Q8PDA8
F	299	LEU	-	expression tag	UNP Q8PDA8
F	300	GLU	-	expression tag	UNP Q8PDA8
F	301	HIS	-	expression tag	UNP Q8PDA8
F	302	HIS	-	expression tag	UNP Q8PDA8
F	303	HIS	-	expression tag	UNP Q8PDA8
F	304	HIS	-	expression tag	UNP Q8PDA8
F	305	HIS	-	expression tag	UNP Q8PDA8
F	306	HIS	-	expression tag	UNP Q8PDA8
G	55	ALA	HIS	engineered mutation	UNP Q8PDA8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	299	LEU	-	expression tag	UNP Q8PDA8
G	300	GLU	-	expression tag	UNP Q8PDA8
G	301	HIS	-	expression tag	UNP Q8PDA8
G	302	HIS	-	expression tag	UNP Q8PDA8
G	303	HIS	-	expression tag	UNP Q8PDA8
G	304	HIS	-	expression tag	UNP Q8PDA8
G	305	HIS	-	expression tag	UNP Q8PDA8
G	306	HIS	-	expression tag	UNP Q8PDA8
H	55	ALA	HIS	engineered mutation	UNP Q8PDA8
H	299	LEU	-	expression tag	UNP Q8PDA8
H	300	GLU	-	expression tag	UNP Q8PDA8
H	301	HIS	-	expression tag	UNP Q8PDA8
H	302	HIS	-	expression tag	UNP Q8PDA8
H	303	HIS	-	expression tag	UNP Q8PDA8
H	304	HIS	-	expression tag	UNP Q8PDA8
H	305	HIS	-	expression tag	UNP Q8PDA8
H	306	HIS	-	expression tag	UNP Q8PDA8

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



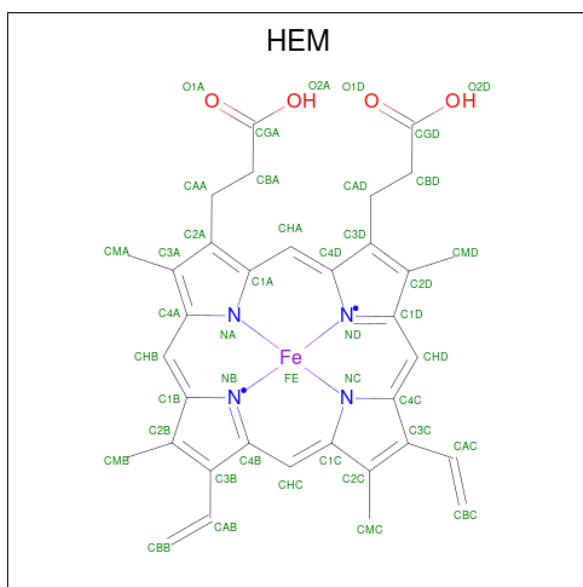
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 15	C 11	N 2	O 2	0	0
2	C	1	Total 15	C 11	N 2	O 2	0	0
2	C	1	Total 15	C 11	N 2	O 2	0	0
2	D	1	Total 15	C 11	N 2	O 2	0	0
2	D	1	Total 15	C 11	N 2	O 2	0	0
2	E	1	Total 15	C 11	N 2	O 2	0	0
2	E	1	Total 15	C 11	N 2	O 2	0	0
2	F	1	Total 15	C 11	N 2	O 2	0	0
2	G	1	Total 15	C 11	N 2	O 2	0	0
2	H	1	Total 15	C 11	N 2	O 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

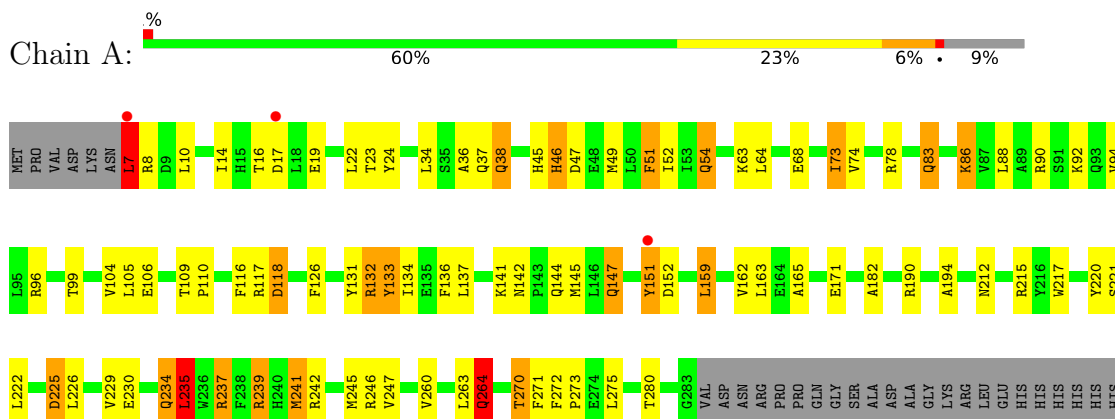
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total 170	O 170	0	0
4	B	152	Total 152	O 152	0	0
4	C	129	Total 129	O 129	0	0
4	D	124	Total 124	O 124	0	0
4	E	133	Total 133	O 133	0	0
4	F	96	Total 96	O 96	0	0
4	G	113	Total 113	O 113	0	0
4	H	99	Total 99	O 99	0	0

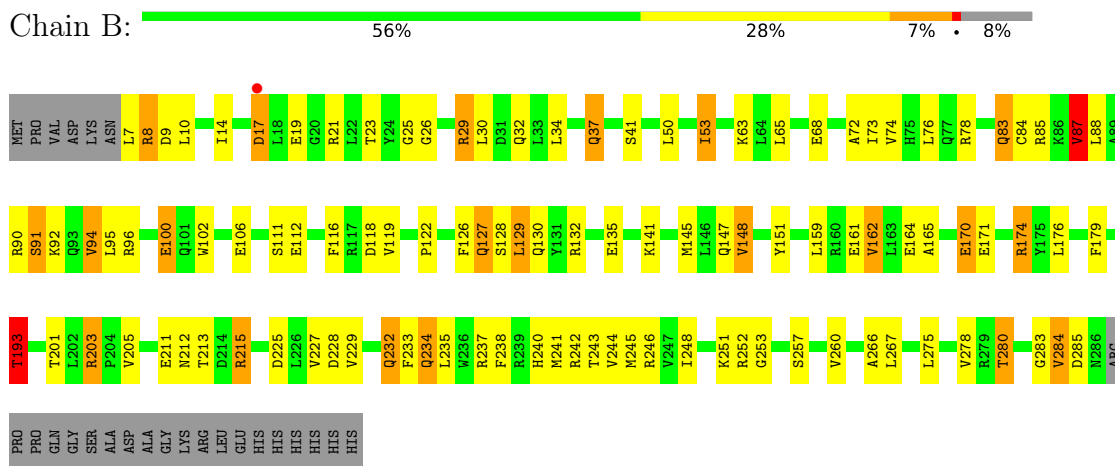
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

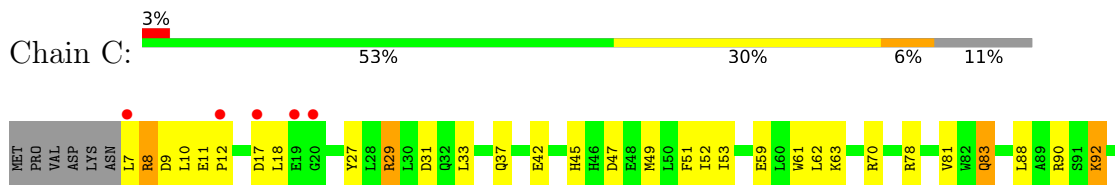
• Molecule 1: Tryptophan 2,3-dioxygenase

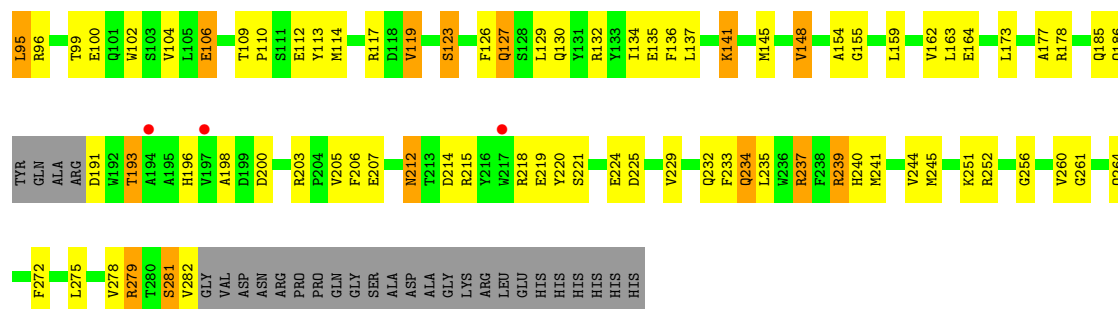


• Molecule 1: Tryptophan 2,3-dioxygenase

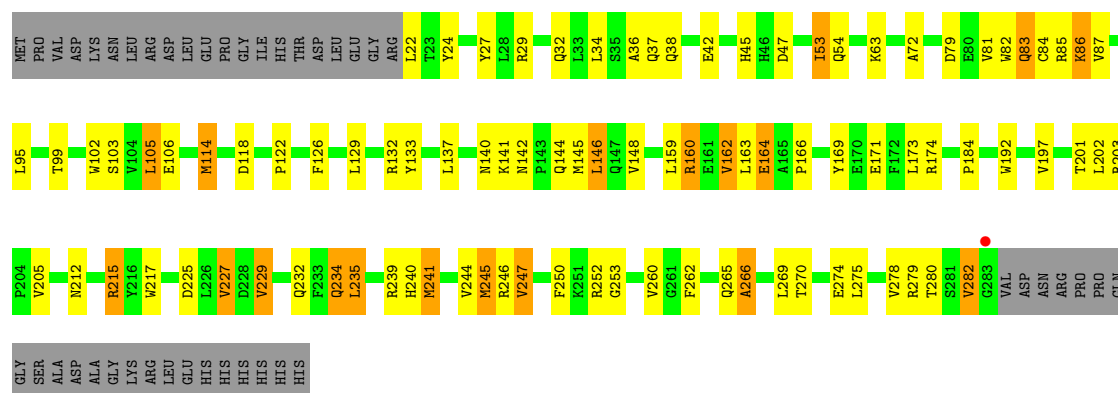


• Molecule 1: Tryptophan 2,3-dioxygenase

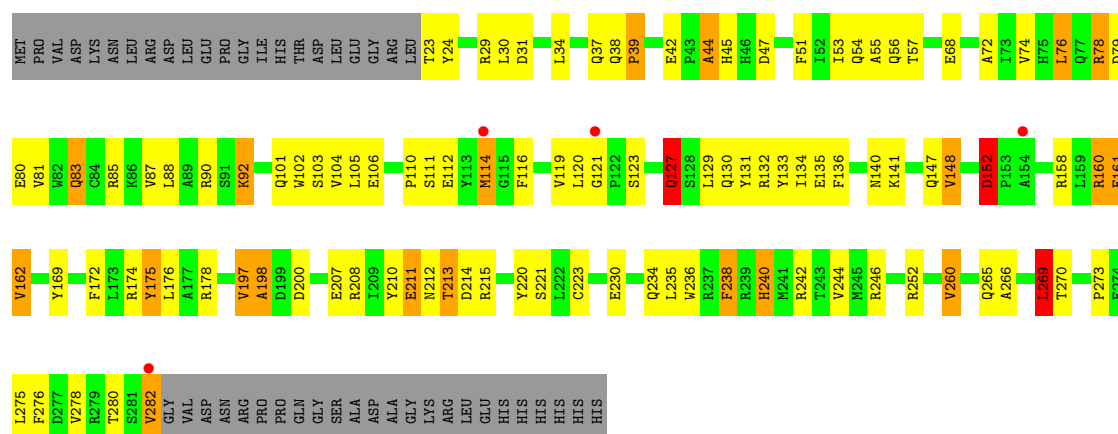




• Molecule 1: Tryptophan 2,3-dioxygenase

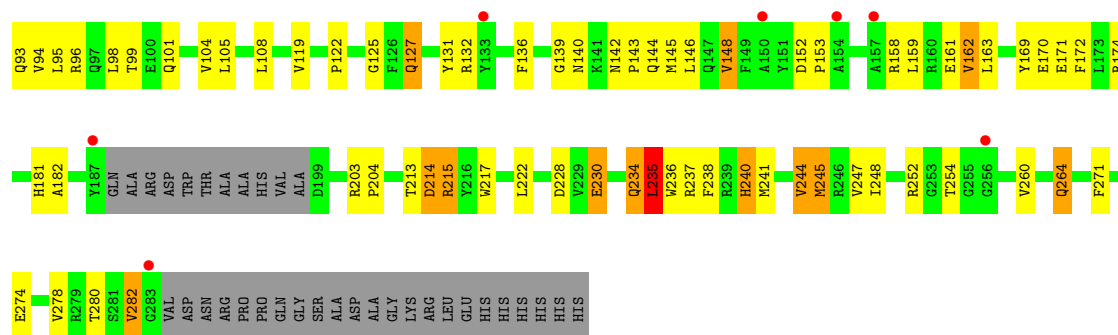


• Molecule 1: Tryptophan 2,3-dioxygenase

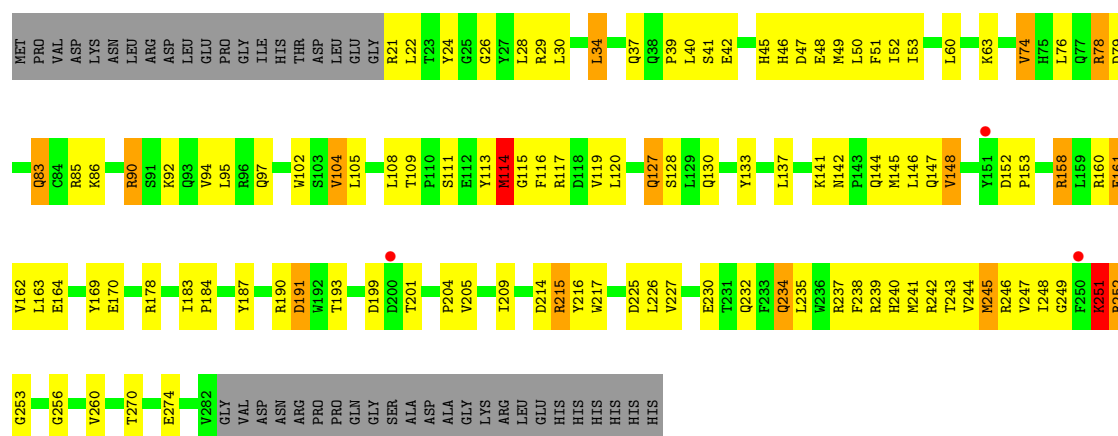


• Molecule 1: Tryptophan 2,3-dioxygenase

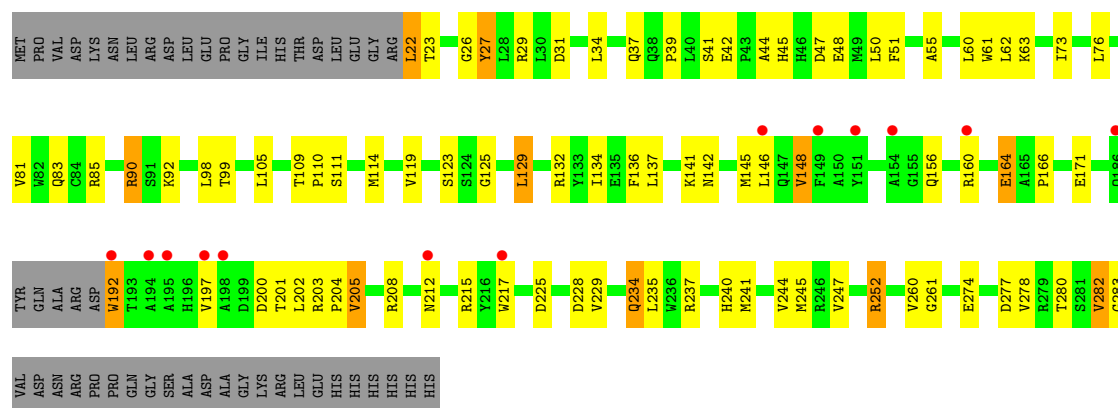




- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.22Å 117.61Å 139.28Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	54.13 – 2.15 54.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (54.13-2.15) 96.7 (54.13-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.285 0.201 , 0.281	Depositor DCC
R_{free} test set	6624 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19073	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.76	27/2342 (1.2%)	1.57	28/3174 (0.9%)
1	B	1.80	30/2365 (1.3%)	1.66	35/3206 (1.1%)
1	C	1.62	23/2299 (1.0%)	1.54	24/3115 (0.8%)
1	D	1.64	24/2220 (1.1%)	1.51	16/3009 (0.5%)
1	E	1.64	18/2208 (0.8%)	1.52	25/2993 (0.8%)
1	F	1.55	16/2122 (0.8%)	1.45	14/2872 (0.5%)
1	G	1.56	16/2227 (0.7%)	1.52	23/3018 (0.8%)
1	H	1.41	9/2173 (0.4%)	1.41	11/2944 (0.4%)
All	All	1.63	163/17956 (0.9%)	1.53	176/24331 (0.7%)

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	1	0
1	B	0	1
1	G	0	1
All	All	1	2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	97	GLN	C-O	-11.13	1.11	1.24
1	E	104	VAL	C-O	-10.11	1.12	1.24
1	E	148	VAL	CA-CB	8.95	1.67	1.54
1	E	141	LYS	N-CA	8.87	1.57	1.46
1	C	218	ARG	C-O	8.73	1.34	1.24
1	B	233	PHE	CA-CB	8.53	1.66	1.53
1	E	213	THR	C-O	-8.51	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	74	VAL	C-N	8.49	1.45	1.33
1	F	136	PHE	CA-C	8.46	1.63	1.52
1	E	104	VAL	CA-C	8.34	1.63	1.52
1	B	227	VAL	CA-CB	8.32	1.64	1.54
1	C	12	PRO	C-O	8.30	1.32	1.23
1	G	52	ILE	CA-CB	8.23	1.64	1.54
1	E	276	PHE	CA-C	8.12	1.63	1.52
1	C	233	PHE	C-O	7.98	1.33	1.24
1	B	165	ALA	CA-CB	7.98	1.66	1.53
1	D	227	VAL	CA-CB	7.92	1.64	1.54
1	B	252	ARG	CD-NE	-7.78	1.35	1.46
1	F	136	PHE	C-O	-7.69	1.15	1.24
1	D	86	LYS	N-CA	7.68	1.55	1.46
1	B	162	VAL	CA-CB	7.63	1.63	1.54
1	E	44	ALA	C-O	7.59	1.33	1.24
1	B	170	GLU	C-O	-7.51	1.15	1.24
1	F	282	VAL	CA-CB	7.49	1.62	1.54
1	E	175	TYR	N-CA	7.47	1.55	1.46
1	B	85	ARG	N-CA	-7.26	1.37	1.46
1	A	182	ALA	CA-CB	7.16	1.61	1.52
1	B	266	ALA	CA-CB	7.05	1.64	1.53
1	A	36	ALA	CA-CB	7.04	1.65	1.53
1	A	237	ARG	N-CA	6.72	1.54	1.46
1	C	95	LEU	N-CA	6.64	1.54	1.46
1	E	104	VAL	CA-CB	6.62	1.63	1.54
1	F	182	ALA	CA-CB	6.59	1.61	1.52
1	C	272	PHE	CA-CB	6.58	1.60	1.53
1	G	260	VAL	CA-CB	6.58	1.62	1.54
1	A	17	ASP	CB-CG	6.57	1.68	1.52
1	D	262	PHE	C-O	-6.46	1.16	1.24
1	B	14	ILE	CA-C	6.46	1.60	1.52
1	F	222	LEU	N-CA	6.45	1.54	1.46
1	D	229	VAL	N-CA	6.38	1.54	1.46
1	B	87	VAL	CA-CB	6.37	1.62	1.54
1	F	92	LYS	C-O	-6.37	1.16	1.24
1	A	38	GLN	CA-C	-6.36	1.46	1.52
1	G	227	VAL	CA-CB	6.33	1.62	1.54
1	E	169	TYR	C-N	6.33	1.42	1.34
1	H	148	VAL	CA-CB	6.33	1.62	1.54
1	B	159	LEU	C-N	-6.31	1.25	1.33
1	F	87	VAL	CA-CB	6.29	1.62	1.54
1	D	53	ILE	CA-CB	6.29	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	236	TRP	C-O	6.28	1.31	1.24
1	H	44	ALA	C-N	6.27	1.42	1.33
1	A	226	LEU	C-O	-6.24	1.17	1.24
1	E	134	ILE	C-O	6.23	1.31	1.24
1	E	174	ARG	C-N	-6.22	1.26	1.33
1	F	94	VAL	CA-CB	6.22	1.61	1.54
1	A	221	SER	N-CA	6.21	1.53	1.46
1	H	212	ASN	CB-CG	6.17	1.67	1.52
1	D	241	MET	C-O	-6.17	1.16	1.24
1	B	161	GLU	CG-CD	6.15	1.67	1.52
1	C	8	ARG	N-CA	6.12	1.53	1.46
1	A	212	ASN	CB-CG	6.12	1.67	1.52
1	A	136	PHE	C-O	-6.11	1.17	1.24
1	A	54	GLN	N-CA	-6.08	1.39	1.46
1	C	104	VAL	CA-CB	6.06	1.61	1.54
1	A	7	LEU	CA-C	6.05	1.65	1.52
1	C	62	LEU	N-CA	6.05	1.53	1.46
1	B	94	VAL	CA-CB	6.04	1.61	1.54
1	A	194	ALA	CA-CB	5.98	1.61	1.53
1	A	86	LYS	C-O	-5.98	1.17	1.24
1	B	238	PHE	CA-C	5.92	1.60	1.52
1	F	152	ASP	CA-C	5.91	1.58	1.52
1	G	42	GLU	N-CA	5.90	1.52	1.46
1	F	252	ARG	CA-C	5.89	1.60	1.52
1	C	239	ARG	N-CA	5.89	1.53	1.46
1	C	117	ARG	C-O	5.86	1.31	1.24
1	C	239	ARG	CD-NE	-5.86	1.38	1.46
1	H	205	VAL	CA-CB	5.84	1.60	1.54
1	C	113	TYR	N-CA	-5.79	1.38	1.46
1	A	132	ARG	C-O	-5.75	1.16	1.24
1	E	81	VAL	CA-CB	5.74	1.61	1.54
1	B	65	LEU	CA-C	5.72	1.60	1.52
1	A	49	MET	CB-CG	5.71	1.69	1.52
1	B	243	THR	C-O	-5.69	1.17	1.24
1	G	226	LEU	C-O	-5.66	1.17	1.24
1	D	162	VAL	CA-CB	5.64	1.61	1.54
1	D	27	TYR	CA-C	5.63	1.60	1.52
1	G	193	THR	N-CA	5.61	1.53	1.46
1	D	79	ASP	CA-CB	5.60	1.61	1.53
1	C	134	ILE	CA-CB	5.59	1.60	1.54
1	D	36	ALA	C-O	-5.58	1.16	1.24
1	C	205	VAL	CA-CB	5.54	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	GLU	CB-CG	5.51	1.69	1.52
1	E	198	ALA	CA-CB	5.50	1.62	1.53
1	D	173	LEU	C-O	-5.50	1.17	1.24
1	D	266	ALA	N-CA	5.50	1.53	1.46
1	A	126	PHE	CA-CB	5.49	1.62	1.53
1	F	181	HIS	C-O	5.48	1.30	1.23
1	B	37	GLN	N-CA	5.48	1.53	1.46
1	B	165	ALA	C-O	-5.47	1.17	1.23
1	H	62	LEU	C-O	-5.47	1.17	1.24
1	G	238	PHE	N-CA	-5.46	1.39	1.46
1	A	263	LEU	N-CA	5.45	1.53	1.46
1	A	133	TYR	C-O	-5.44	1.17	1.24
1	B	148	VAL	CA-CB	5.43	1.61	1.54
1	C	178	ARG	CA-C	-5.42	1.45	1.52
1	E	39	PRO	CA-C	5.42	1.58	1.52
1	A	215	ARG	CA-C	5.39	1.59	1.52
1	B	251	LYS	CE-NZ	5.38	1.65	1.49
1	D	122	PRO	CA-C	5.37	1.57	1.52
1	B	159	LEU	C-O	5.36	1.30	1.24
1	B	205	VAL	CA-C	5.36	1.59	1.52
1	A	241	MET	CB-CG	5.36	1.68	1.52
1	A	68	GLU	C-O	-5.35	1.17	1.24
1	C	33	LEU	CA-C	-5.35	1.46	1.52
1	B	251	LYS	CG-CD	5.35	1.68	1.52
1	C	212	ASN	CB-CG	5.34	1.65	1.52
1	D	282	VAL	CA-C	5.33	1.59	1.52
1	B	25	GLY	CA-C	-5.31	1.45	1.51
1	B	32	GLN	N-CA	-5.31	1.40	1.46
1	D	282	VAL	CA-CB	5.29	1.59	1.54
1	A	270	THR	CA-CB	5.27	1.63	1.53
1	D	239	ARG	C-O	-5.27	1.17	1.24
1	H	119	VAL	CA-CB	5.27	1.60	1.54
1	G	90	ARG	CA-C	5.25	1.59	1.52
1	G	246	ARG	CZ-NH2	5.25	1.40	1.33
1	F	240	HIS	C-O	-5.23	1.18	1.24
1	B	267	LEU	C-O	-5.23	1.17	1.24
1	B	232	GLN	CA-C	5.21	1.59	1.52
1	A	74	VAL	CA-CB	5.20	1.60	1.54
1	D	54	GLN	C-O	5.20	1.30	1.24
1	F	53	ILE	N-CA	5.20	1.52	1.46
1	F	238	PHE	C-O	-5.19	1.18	1.24
1	B	50	LEU	N-CA	5.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	MET	CB-CG	5.18	1.68	1.52
1	B	30	LEU	CG-CD2	5.18	1.69	1.52
1	D	159	LEU	CA-C	-5.17	1.46	1.52
1	E	55	ALA	CA-CB	5.17	1.61	1.53
1	E	208	ARG	C-O	-5.15	1.18	1.24
1	A	220	TYR	N-CA	-5.14	1.40	1.46
1	H	197	VAL	CA-CB	5.14	1.60	1.54
1	A	51	PHE	C-O	-5.13	1.18	1.24
1	G	191	ASP	CA-CB	5.13	1.59	1.52
1	F	215	ARG	CZ-NH2	-5.12	1.26	1.33
1	C	70	ARG	N-CA	5.12	1.52	1.46
1	D	140	ASN	CA-C	5.10	1.59	1.53
1	G	30	LEU	N-CA	5.10	1.52	1.46
1	C	173	LEU	C-O	5.10	1.30	1.24
1	B	128	SER	CA-C	-5.09	1.46	1.52
1	D	260	VAL	CA-CB	-5.09	1.48	1.54
1	A	73	ILE	CB-CG2	5.08	1.69	1.52
1	C	123	SER	CA-C	5.08	1.59	1.52
1	G	114	MET	N-CA	5.07	1.52	1.46
1	G	248	ILE	N-CA	5.07	1.50	1.46
1	G	141	LYS	CE-NZ	5.06	1.64	1.49
1	D	270	THR	CA-CB	5.05	1.62	1.53
1	D	105	LEU	C-O	-5.05	1.17	1.24
1	C	119	VAL	CA-CB	5.04	1.61	1.54
1	H	27	TYR	CA-C	5.04	1.59	1.52
1	C	221	SER	N-CA	5.04	1.52	1.46
1	D	245	MET	CA-C	-5.02	1.46	1.52
1	D	235	LEU	C-O	-5.01	1.18	1.24
1	A	46	HIS	N-CA	5.01	1.52	1.46
1	H	278	VAL	CA-CB	5.00	1.60	1.54

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH2	-11.75	108.62	119.20
1	B	252	ARG	CG-CD-NE	-9.23	91.69	112.00
1	H	229	VAL	N-CA-C	8.80	118.84	110.30
1	B	252	ARG	CD-NE-CZ	8.68	136.56	124.40
1	A	152	ASP	CA-C-N	8.60	128.59	119.05
1	A	152	ASP	C-N-CA	8.60	128.59	119.05
1	H	247	VAL	N-CA-C	8.42	119.28	111.45
1	D	103	SER	N-CA-C	8.37	121.33	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH1	8.33	129.83	121.50
1	C	279	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	C	81	VAL	N-CA-C	7.90	117.95	110.53
1	E	260	VAL	N-CA-C	7.79	117.90	110.42
1	E	120	LEU	N-CA-C	-7.74	100.55	110.53
1	B	251	LYS	CG-CD-CE	7.60	128.78	111.30
1	B	8	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	C	203	ARG	CA-C-N	-7.55	111.93	119.56
1	C	203	ARG	C-N-CA	-7.55	111.93	119.56
1	H	261	GLY	N-CA-C	7.50	121.98	112.83
1	D	174	ARG	N-CA-C	7.47	120.37	111.33
1	A	134	ILE	N-CA-C	7.37	118.13	110.62
1	B	29	ARG	NE-CZ-NH2	7.36	125.82	119.20
1	F	215	ARG	NE-CZ-NH1	-7.29	114.21	121.50
1	C	279	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	C	99	THR	N-CA-C	7.00	118.56	111.07
1	A	272	PHE	CA-C-N	6.96	126.20	118.97
1	A	272	PHE	C-N-CA	6.96	126.20	118.97
1	B	251	LYS	CA-CB-CG	6.92	127.94	114.10
1	C	11	GLU	CA-C-N	-6.90	112.54	119.99
1	C	11	GLU	C-N-CA	-6.90	112.54	119.99
1	G	74	VAL	O-C-N	-6.84	115.18	121.89
1	G	127	GLN	CB-CA-C	6.75	121.88	111.02
1	A	264	GLN	N-CA-C	6.73	119.45	111.71
1	B	14	ILE	N-CA-C	6.64	117.89	108.93
1	E	120	LEU	CA-C-N	-6.62	111.48	121.87
1	E	120	LEU	C-N-CA	-6.62	111.48	121.87
1	F	222	LEU	N-CA-C	6.61	118.49	111.28
1	B	30	LEU	N-CA-C	6.57	119.44	111.82
1	G	152	ASP	CA-C-N	-6.57	113.44	120.47
1	G	152	ASP	C-N-CA	-6.57	113.44	120.47
1	B	203	ARG	NE-CZ-NH1	-6.55	114.94	121.50
1	H	44	ALA	CA-C-O	6.55	128.16	120.69
1	E	121	GLY	CA-C-N	6.53	127.36	120.12
1	E	121	GLY	C-N-CA	6.53	127.36	120.12
1	E	215	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	F	136	PHE	O-C-N	6.45	129.06	122.09
1	G	252	ARG	N-CA-C	6.44	119.81	110.28
1	A	16	THR	CA-C-N	-6.44	111.73	122.17
1	A	16	THR	C-N-CA	-6.44	111.73	122.17
1	A	221	SER	CA-CB-OG	-6.44	98.22	111.10
1	A	17	ASP	CB-CA-C	6.40	121.86	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ARG	CA-C-N	-6.40	111.71	120.28
1	D	85	ARG	C-N-CA	-6.40	111.71	120.28
1	H	129	LEU	CA-CB-CG	6.38	138.62	116.30
1	F	235	LEU	CA-CB-CG	6.37	138.61	116.30
1	D	260	VAL	N-CA-C	6.35	117.03	110.36
1	A	225	ASP	N-CA-C	6.34	117.85	111.07
1	D	118	ASP	N-CA-C	6.31	118.96	111.71
1	C	224	GLU	N-CA-C	6.30	118.23	111.36
1	B	275	LEU	N-CA-C	6.29	117.81	111.07
1	B	76	LEU	N-CA-C	6.27	118.64	111.11
1	D	53	ILE	N-CA-C	6.26	117.01	110.62
1	B	129	LEU	N-CA-C	6.21	118.56	111.11
1	A	17	ASP	N-CA-C	6.20	118.89	108.23
1	C	27	TYR	N-CA-C	6.17	118.00	111.28
1	B	29	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	B	179	PHE	N-CA-C	6.14	119.72	112.72
1	E	238	PHE	N-CA-C	6.10	117.93	111.28
1	G	114	MET	CB-CG-SD	6.08	130.95	112.70
1	D	270	THR	CB-CA-C	6.07	120.81	109.71
1	A	23	THR	CB-CA-C	-6.06	98.85	110.24
1	A	104	VAL	CB-CA-C	-6.06	103.96	112.14
1	F	152	ASP	CA-C-N	5.99	127.33	119.84
1	F	152	ASP	C-N-CA	5.99	127.33	119.84
1	B	53	ILE	N-CA-C	5.97	118.52	111.05
1	E	223	CYS	N-CA-CB	5.97	118.66	110.01
1	B	84	CYS	N-CA-C	5.95	118.25	111.11
1	E	129	LEU	CA-C-N	5.94	128.16	120.44
1	E	129	LEU	C-N-CA	5.94	128.16	120.44
1	A	104	VAL	N-CA-C	5.93	116.67	110.62
1	C	52	ILE	N-CA-C	5.92	116.10	110.42
1	E	269	LEU	CA-CB-CG	5.90	136.97	116.30
1	C	8	ARG	N-CA-C	5.89	118.34	108.73
1	G	109	THR	CA-C-N	-5.88	113.57	119.56
1	G	109	THR	C-N-CA	-5.88	113.57	119.56
1	C	252	ARG	CG-CD-NE	-5.87	99.08	112.00
1	H	62	LEU	N-CA-C	5.87	117.67	111.28
1	B	248	ILE	N-CA-C	5.84	118.77	113.10
1	B	193	THR	N-CA-C	5.83	119.65	112.54
1	D	164	GLU	N-CA-C	5.83	120.23	113.18
1	C	154	ALA	CA-C-N	5.81	126.27	119.94
1	C	154	ALA	C-N-CA	5.81	126.27	119.94
1	E	178	ARG	N-CA-C	5.78	119.86	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	ILE	N-CA-C	5.77	116.50	110.62
1	F	162	VAL	N-CA-C	-5.72	103.94	111.09
1	A	17	ASP	N-CA-CB	5.70	118.51	110.24
1	H	134	ILE	N-CA-C	5.69	116.15	110.23
1	B	91	SER	N-CA-C	5.61	117.85	111.11
1	F	248	ILE	CB-CA-C	-5.60	104.82	111.65
1	A	237	ARG	NE-CZ-NH2	-5.57	114.18	119.20
1	B	174	ARG	CA-C-N	5.57	127.67	120.44
1	B	174	ARG	C-N-CA	5.57	127.67	120.44
1	D	279	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	D	250	PHE	N-CA-C	5.56	119.69	113.02
1	G	104	VAL	N-CA-C	-5.54	105.32	110.53
1	B	41	SER	N-CA-C	5.53	118.03	110.24
1	B	176	LEU	N-CA-C	5.46	117.24	111.28
1	D	215	ARG	N-CA-C	5.44	116.89	111.07
1	B	159	LEU	CA-C-O	-5.44	114.78	120.55
1	G	46	HIS	N-CA-C	5.43	117.63	111.11
1	B	8	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	235	LEU	CA-CB-CG	5.42	135.27	116.30
1	B	201	THR	N-CA-C	5.41	119.14	112.54
1	C	256	GLY	N-CA-C	5.38	122.51	115.36
1	E	215	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	G	217	TRP	N-CA-C	5.38	117.14	111.28
1	E	152	ASP	CA-C-N	5.36	124.87	119.19
1	E	152	ASP	C-N-CA	5.36	124.87	119.19
1	F	244	VAL	CB-CA-C	-5.35	105.03	112.04
1	A	52	ILE	N-CA-C	5.35	115.55	110.42
1	C	92	LYS	O-C-N	5.34	127.79	122.12
1	B	17	ASP	N-CA-C	5.34	118.14	107.62
1	E	260	VAL	N-CA-CB	5.33	116.78	110.55
1	A	78	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	270	THR	CA-C-N	5.30	127.33	120.44
1	A	270	THR	C-N-CA	5.30	127.33	120.44
1	B	251	LYS	CD-CE-NZ	5.30	128.87	111.90
1	B	284	VAL	CB-CA-C	5.30	119.98	111.29
1	H	29	ARG	N-CA-C	5.28	118.71	111.54
1	H	148	VAL	N-CA-C	5.27	115.99	110.62
1	C	206	PHE	N-CA-C	5.26	117.02	111.28
1	A	14	ILE	N-CA-C	5.25	115.77	108.84
1	G	120	LEU	CA-C-N	-5.24	113.64	121.87
1	G	120	LEU	C-N-CA	-5.24	113.64	121.87
1	E	127	GLN	CB-CA-C	5.23	119.55	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	PHE	CA-C-O	5.22	125.75	119.43
1	G	178	ARG	N-CA-C	5.22	119.12	112.34
1	H	41	SER	N-CA-C	5.21	118.19	110.48
1	H	90	ARG	N-CA-C	5.21	116.64	111.07
1	B	211	GLU	CA-C-N	-5.20	116.06	123.03
1	B	211	GLU	C-N-CA	-5.20	116.06	123.03
1	A	131	TYR	CA-C-N	5.19	128.21	120.31
1	A	131	TYR	C-N-CA	5.19	128.21	120.31
1	E	121	GLY	N-CA-C	-5.19	101.75	112.34
1	G	170	GLU	N-CA-C	5.19	116.94	111.28
1	B	87	VAL	N-CA-C	5.19	115.96	110.72
1	E	240	HIS	N-CA-C	5.19	116.62	111.07
1	E	176	LEU	N-CA-C	5.19	116.93	111.28
1	A	8	ARG	N-CA-C	5.17	117.16	108.73
1	G	34	LEU	N-CA-C	-5.17	106.57	112.92
1	G	248	ILE	CA-C-O	5.17	123.63	118.98
1	C	281	SER	N-CA-C	5.14	120.54	113.97
1	E	197	VAL	CB-CA-C	-5.13	103.56	111.31
1	F	213	THR	CA-C-N	5.13	127.46	120.54
1	F	213	THR	C-N-CA	5.13	127.46	120.54
1	F	214	ASP	N-CA-C	5.12	117.25	111.11
1	G	183	ILE	CA-C-N	-5.12	114.67	119.89
1	G	183	ILE	C-N-CA	-5.12	114.67	119.89
1	A	239	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	G	128	SER	CA-C-N	5.10	127.07	120.44
1	G	128	SER	C-N-CA	5.10	127.07	120.44
1	A	222	LEU	N-CA-C	5.09	116.91	111.36
1	D	169	TYR	N-CA-C	5.09	116.64	111.14
1	D	247	VAL	N-CA-C	5.09	116.19	111.45
1	D	81	VAL	N-CA-C	5.09	115.32	110.53
1	C	219	GLU	CA-C-N	5.08	127.40	120.54
1	C	219	GLU	C-N-CA	5.08	127.40	120.54
1	G	215	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	G	247	VAL	CB-CA-C	5.06	118.55	111.92
1	B	205	VAL	N-CA-C	5.06	115.67	110.36
1	C	12	PRO	N-CA-C	-5.06	102.67	111.32
1	E	208	ARG	CA-C-N	5.06	126.93	120.56
1	E	208	ARG	C-N-CA	5.06	126.93	120.56
1	C	61	TRP	N-CA-C	5.05	116.48	111.07
1	C	261	GLY	N-CA-C	5.05	118.75	112.64
1	F	101	GLN	N-CA-C	5.03	118.68	112.54
1	E	172	PHE	N-CA-C	5.02	117.13	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	17	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	283	GLY	Peptide
1	G	251	LYS	Peptide

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	2285	0	2240	72	0
1	B	2308	0	2259	63	0
1	C	2244	0	2201	70	0
1	D	2165	0	2123	66	0
1	E	2153	0	2109	70	0
1	F	2071	0	2033	57	0
1	G	2172	0	2133	79	0
1	H	2120	0	2083	61	0
2	A	30	0	18	3	0
2	B	30	0	18	0	0
2	C	30	0	18	3	0
2	D	30	0	18	0	0
2	E	30	0	18	1	0
2	F	15	0	9	0	0
2	G	15	0	9	1	0
2	H	15	0	9	2	0
3	A	43	0	30	1	0
3	B	43	0	30	4	0
3	C	43	0	30	2	0
3	D	43	0	30	4	0
3	E	43	0	30	7	0
3	F	43	0	30	5	0
3	G	43	0	30	3	0
3	H	43	0	30	5	0
4	A	170	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	152	0	0	6	0
4	C	129	0	0	7	0
4	D	124	0	0	5	0
4	E	133	0	0	6	0
4	F	96	0	0	2	0
4	G	113	0	0	11	0
4	H	99	0	0	1	0
All	All	19073	0	17538	483	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 14.

All (483) 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:E:114:MET:SD	1:H:283:GLY:HA2	1.77	1.24
1:E:38:GLN:NE2	1:F:29:ARG:HH11	1.37	1.23
1:C:241:MET:SD	1:C:245:MET:HE3	1.79	1.22
1:F:241:MET:SD	1:F:245:MET:HE1	1.78	1.22
1:E:38:GLN:HE22	1:F:29:ARG:NH1	1.38	1.20
1:A:241:MET:CE	1:A:245:MET:HE2	1.74	1.17
1:C:241:MET:SD	1:C:245:MET:CE	2.37	1.13
1:D:266:ALA:HA	1:D:269:LEU:HD13	1.33	1.04
1:A:241:MET:HE2	1:A:260:VAL:HG13	1.40	1.02
1:B:241:MET:SD	1:B:245:MET:HE2	2.00	1.01
1:A:241:MET:SD	1:A:245:MET:CE	2.49	1.00
1:E:54:GLN:HE21	1:E:101:GLN:HE21	1.06	1.00
1:C:130:GLN:HE21	1:D:34:LEU:HD13	1.22	0.98
1:A:241:MET:HE1	1:A:245:MET:HE2	1.42	0.98
1:G:37:GLN:HE21	1:H:63:LYS:HZ3	1.02	0.98
1:G:241:MET:SD	1:G:245:MET:HE1	2.03	0.98
1:A:241:MET:SD	1:A:245:MET:HE3	2.03	0.97
3:H:401:HEM:HMB1	3:H:401:HEM:HBB2	1.49	0.93
1:D:114:MET:HE2	1:D:114:MET:HA	1.47	0.93
1:G:153:PRO:HD2	4:G:1151:HOH:O	1.70	0.90
1:D:212:ASN:OD1	4:D:635:HOH:O	1.91	0.89
1:H:22:LEU:HD22	1:H:27:TYR:HB2	1.54	0.88
1:H:241:MET:SD	1:H:245:MET:CE	2.62	0.88
1:B:203:ARG:NH1	1:B:280:THR:HG22	1.88	0.87
1:G:83:GLN:H	1:G:83:GLN:HE21	1.23	0.86
1:A:234:GLN:HE21	1:A:234:GLN:HA	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ASP:OD1	4:G:1481:HOH:O	1.93	0.85
1:H:114:MET:HE2	1:H:114:MET:HA	1.59	0.85
1:E:54:GLN:NE2	1:E:101:GLN:HE21	1.76	0.84
1:C:130:GLN:NE2	1:D:34:LEU:HD13	1.94	0.83
1:D:241:MET:SD	1:D:245:MET:HE3	2.19	0.83
1:B:29:ARG:NH1	4:B:1518:HOH:O	2.11	0.83
1:A:235:LEU:HD21	1:C:239:ARG:HD3	1.61	0.81
1:A:241:MET:CE	1:A:245:MET:CE	2.55	0.81
1:D:241:MET:SD	1:D:245:MET:CE	2.69	0.80
1:A:241:MET:HE1	1:A:245:MET:CE	2.12	0.80
1:C:212:ASN:HB2	4:C:832:HOH:O	1.81	0.79
1:A:241:MET:HE1	4:A:1149:HOH:O	1.83	0.79
1:A:54:GLN:HG2	1:A:105:LEU:HD22	1.64	0.79
1:A:83:GLN:H	1:A:83:GLN:HE21	1.29	0.78
1:E:207:GLU:O	1:E:211:GLU:HG3	1.84	0.78
3:H:401:HEM:HBB2	3:H:401:HEM:CMB	2.13	0.78
1:A:109:THR:HG21	1:C:220:TYR:OH	1.84	0.78
1:E:114:MET:SD	1:H:283:GLY:CA	2.69	0.78
1:G:133:TYR:CD1	1:G:158:ARG:NH1	2.52	0.78
1:E:212:ASN:HB2	4:E:1430:HOH:O	1.82	0.77
1:A:144:GLN:O	1:A:147:GLN:HG2	1.85	0.77
1:D:83:GLN:H	1:D:83:GLN:HE21	1.29	0.77
1:G:40:LEU:HD11	1:H:22:LEU:HD21	1.65	0.77
1:B:116:PHE:O	1:B:119:VAL:HG22	1.84	0.77
1:A:241:MET:HE3	1:A:264:GLN:NE2	2.00	0.77
1:H:160:ARG:O	1:H:164:GLU:HG2	1.84	0.77
1:F:83:GLN:NE2	4:F:1379:HOH:O	2.00	0.76
1:G:133:TYR:HD1	1:G:158:ARG:NH1	1.84	0.76
1:H:166:PRO:HG3	1:H:192:TRP:CZ2	2.20	0.76
1:A:241:MET:SD	1:A:245:MET:HE2	2.20	0.76
1:C:45:HIS:HD2	1:C:47:ASP:H	1.31	0.76
1:F:217:TRP:HH2	1:H:217:TRP:HH2	1.34	0.76
1:C:234:GLN:HA	1:C:234:GLN:HE21	1.51	0.75
1:E:79:ASP:OD1	4:E:902:HOH:O	2.05	0.75
1:A:241:MET:HE2	1:A:260:VAL:CG1	2.13	0.75
1:H:23:THR:HG23	1:H:26:GLY:H	1.50	0.74
1:H:92:LYS:NZ	1:H:225:ASP:OD1	2.21	0.74
1:E:160:ARG:HG3	1:E:160:ARG:HH11	1.53	0.74
1:C:207:GLU:OE2	1:C:281:SER:HB2	1.88	0.74
1:B:241:MET:SD	1:B:245:MET:CE	2.75	0.73
1:B:126:PHE:HE1	1:B:145:MET:HE1	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLN:HE21	1:F:63:LYS:NZ	1.87	0.73
1:E:51:PHE:HE1	3:E:401:HEM:HBB2	1.53	0.72
1:C:63:LYS:HZ3	1:D:37:GLN:HE21	1.36	0.72
1:E:45:HIS:HE1	4:E:1024:HOH:O	1.71	0.72
4:A:767:HOH:O	1:B:23:THR:HA	1.89	0.72
1:H:45:HIS:HD2	1:H:47:ASP:H	1.38	0.72
1:G:29:ARG:NH1	4:G:1292:HOH:O	2.23	0.71
1:E:111:SER:O	1:E:114:MET:HG2	1.90	0.71
1:D:102:TRP:O	1:D:106:GLU:HG3	1.91	0.71
1:D:29:ARG:HH21	1:D:32:GLN:NE2	1.88	0.71
1:C:109:THR:HB	1:C:110:PRO:HD2	1.72	0.71
1:C:241:MET:SD	1:C:245:MET:HE1	2.29	0.70
1:E:160:ARG:HG3	1:E:160:ARG:NH1	2.05	0.70
1:E:38:GLN:NE2	1:F:29:ARG:HD3	2.06	0.70
1:D:146:LEU:HD11	1:D:163:LEU:HD22	1.74	0.70
1:H:99:THR:HG21	1:H:235:LEU:HG	1.72	0.69
1:E:29:ARG:HG3	1:F:38:GLN:NE2	2.06	0.69
1:B:88:LEU:O	1:B:92:LYS:HG3	1.91	0.69
1:H:241:MET:SD	1:H:245:MET:HE3	2.32	0.69
1:G:26:GLY:O	1:G:29:ARG:HD3	1.93	0.69
1:A:19:GLU:HG3	1:B:151:TYR:HB2	1.75	0.68
1:A:37:GLN:HE21	1:B:63:LYS:NZ	1.91	0.68
1:E:103:SER:HA	1:E:106:GLU:HG2	1.76	0.68
1:C:102:TRP:O	1:C:106:GLU:HG3	1.94	0.68
1:E:133:TYR:CZ	1:E:162:VAL:HG21	2.28	0.68
1:E:88:LEU:O	1:E:92:LYS:HG3	1.93	0.68
1:F:230:GLU:O	1:F:230:GLU:HG3	1.94	0.67
1:C:96:ARG:O	1:C:100:GLU:HG2	1.94	0.67
1:C:88:LEU:O	1:C:92:LYS:HG3	1.93	0.67
1:A:45:HIS:HD2	1:A:47:ASP:H	1.43	0.67
1:G:137:LEU:HG	1:G:162:VAL:HG21	1.77	0.67
1:D:45:HIS:HD2	1:D:47:ASP:H	1.42	0.66
1:C:278:VAL:O	1:C:282:VAL:HG13	1.96	0.66
1:E:116:PHE:O	1:E:119:VAL:HG22	1.95	0.66
1:B:234:GLN:HA	1:B:234:GLN:HE21	1.61	0.66
1:H:34:LEU:HA	1:H:37:GLN:HE22	1.61	0.65
1:D:234:GLN:HE21	1:D:234:GLN:HA	1.60	0.65
1:G:234:GLN:HE22	1:G:237:ARG:HH21	1.42	0.65
1:F:260:VAL:HG12	1:F:264:GLN:OE1	1.95	0.65
1:H:146:LEU:HD13	1:H:160:ARG:HD2	1.78	0.65
1:C:63:LYS:NZ	1:D:37:GLN:HE21	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ALA:O	1:E:269:LEU:HD22	1.97	0.65
1:B:126:PHE:CE1	1:B:145:MET:HE1	2.31	0.65
1:C:159:LEU:O	1:C:162:VAL:HG12	1.96	0.65
1:E:136:PHE:HB3	1:E:162:VAL:HG12	1.78	0.64
1:A:86:LYS:NZ	1:B:112:GLU:OE2	2.26	0.64
1:F:132:ARG:HD2	1:F:145:MET:HG3	1.80	0.64
1:C:132:ARG:HD2	1:C:145:MET:HG3	1.80	0.64
1:A:151:TYR:HB2	1:B:19:GLU:HG2	1.80	0.64
1:G:113:TYR:CE1	1:G:117:ARG:HD3	2.33	0.64
1:D:83:GLN:NE2	4:D:1513:HOH:O	2.08	0.64
1:D:99:THR:HG21	1:D:235:LEU:HG	1.80	0.64
1:A:88:LEU:O	1:A:92:LYS:HG3	1.98	0.63
1:E:45:HIS:HD2	1:E:47:ASP:H	1.46	0.63
1:D:203:ARG:NH2	4:D:780:HOH:O	2.29	0.63
1:G:133:TYR:HD1	1:G:158:ARG:HH11	1.45	0.63
1:G:237:ARG:HD2	4:G:1364:HOH:O	1.98	0.63
1:H:109:THR:HB	1:H:110:PRO:HD2	1.79	0.63
1:C:130:GLN:HE21	1:D:34:LEU:CD1	2.03	0.63
1:G:239:ARG:HD2	4:G:957:HOH:O	1.99	0.62
1:H:61:TRP:HB2	1:H:98:LEU:HD21	1.82	0.62
1:C:63:LYS:NZ	1:D:37:GLN:NE2	2.48	0.62
1:C:191:ASP:N	4:C:726:HOH:O	2.33	0.61
1:G:146:LEU:CD2	1:G:160:ARG:HG2	2.30	0.61
1:A:22:LEU:O	1:B:122:PRO:HG2	2.01	0.61
1:F:240:HIS:O	1:F:244:VAL:HG23	1.99	0.61
1:E:132:ARG:NH2	3:E:401:HEM:O1D	2.26	0.61
1:D:114:MET:HA	1:D:114:MET:CE	2.25	0.61
1:E:112:GLU:OE2	1:F:86:LYS:NZ	2.33	0.61
1:G:137:LEU:HG	1:G:162:VAL:CG2	2.30	0.61
3:H:401:HEM:HMB1	3:H:401:HEM:CBB	2.29	0.61
1:E:83:GLN:H	1:E:83:GLN:HE21	1.48	0.60
1:G:161:GLU:O	1:G:161:GLU:HG2	2.01	0.60
1:H:39:PRO:HB2	4:H:1245:HOH:O	2.00	0.60
1:E:37:GLN:HE21	1:F:63:LYS:HZ3	1.47	0.60
1:A:110:PRO:HB2	1:C:282:VAL:HG21	1.83	0.60
1:D:265:GLN:O	1:D:269:LEU:HD12	2.02	0.60
1:E:207:GLU:O	1:E:211:GLU:CG	2.50	0.59
1:H:146:LEU:CD1	1:H:160:ARG:HH11	2.15	0.59
1:B:212:ASN:HB2	4:B:871:HOH:O	2.02	0.59
1:D:252:ARG:HD3	4:D:1280:HOH:O	2.01	0.59
1:F:54:GLN:HG2	1:F:105:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:PHE:O	1:G:119:VAL:HG22	2.03	0.59
1:B:242:ARG:HD2	1:B:245:MET:HE3	1.85	0.59
1:C:83:GLN:NE2	4:C:1326:HOH:O	2.27	0.59
1:E:106:GLU:OE1	1:E:246:ARG:NH1	2.36	0.59
1:B:245:MET:HG2	1:B:260:VAL:HG21	1.85	0.58
1:G:242:ARG:HA	1:G:245:MET:HE3	1.85	0.58
1:H:208:ARG:NH1	1:H:215:ARG:HH22	2.01	0.58
1:E:51:PHE:HE1	3:E:401:HEM:CBB	2.15	0.58
1:G:234:GLN:NE2	1:G:237:ARG:HH21	2.02	0.57
1:H:132:ARG:NE	1:H:145:MET:HE2	2.18	0.57
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.18	0.57
1:D:160:ARG:NH1	1:D:164:GLU:OE2	2.36	0.57
1:H:202:LEU:O	1:H:205:VAL:HB	2.05	0.57
1:D:202:LEU:O	1:D:205:VAL:HB	2.04	0.57
1:A:37:GLN:HE21	1:B:63:LYS:HZ3	1.53	0.57
1:C:37:GLN:HE21	1:D:63:LYS:NZ	2.02	0.57
3:G:401:HEM:HBC2	3:G:401:HEM:HH2	1.86	0.56
1:B:141:LYS:HE2	4:B:1338:HOH:O	2.05	0.56
1:G:237:ARG:CD	4:G:1411:HOH:O	2.54	0.56
1:F:83:GLN:H	1:F:83:GLN:HE21	1.54	0.56
1:H:51:PHE:CZ	2:H:402:TRP:CE2	2.93	0.56
1:D:266:ALA:CA	1:D:269:LEU:HD13	2.23	0.56
1:F:247:VAL:HG11	3:F:401:HEM:HBB2	1.88	0.56
1:G:50:LEU:HD11	1:G:104:VAL:HG12	1.86	0.56
1:H:105:LEU:HD21	3:H:401:HEM:HAB	1.87	0.56
1:A:34:LEU:HA	1:A:37:GLN:HE22	1.71	0.56
1:A:99:THR:HG21	1:A:235:LEU:HD12	1.88	0.56
1:H:240:HIS:O	1:H:244:VAL:HG23	2.06	0.56
1:E:160:ARG:HH11	1:E:160:ARG:CG	2.19	0.55
1:B:102:TRP:CZ2	1:B:240:HIS:HB2	2.42	0.55
1:D:253:GLY:HA3	3:D:401:HEM:O2A	2.06	0.55
1:G:63:LYS:HZ3	1:H:37:GLN:HE21	1.54	0.55
1:A:144:GLN:HE22	1:B:9:ASP:HA	1.72	0.55
1:G:63:LYS:NZ	1:H:37:GLN:HE21	2.04	0.55
1:F:234:GLN:NE2	1:F:237:ARG:HH21	2.04	0.55
1:D:145:MET:SD	4:D:1169:HOH:O	2.59	0.55
1:C:110:PRO:O	1:C:114:MET:HG2	2.06	0.55
1:C:214:ASP:HB3	4:C:1208:HOH:O	2.06	0.55
1:B:34:LEU:HA	1:B:37:GLN:HE22	1.72	0.54
1:C:8:ARG:HB2	1:D:269:LEU:HD11	1.90	0.54
1:E:240:HIS:O	1:E:244:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HD12	1:D:148:VAL:O	2.07	0.54
1:C:123:SER:HA	1:C:127:GLN:OE1	2.06	0.54
1:D:72:ALA:HB2	1:D:87:VAL:CG2	2.37	0.54
1:G:146:LEU:HD21	1:G:160:ARG:HG2	1.89	0.54
1:G:74:VAL:O	1:G:78:ARG:HD3	2.07	0.54
1:G:215:ARG:NH2	1:G:216:TYR:OH	2.40	0.54
1:D:95:LEU:HB3	1:D:232:GLN:HG2	1.89	0.54
1:D:105:LEU:HD21	3:D:401:HEM:HAB	1.88	0.54
1:A:241:MET:CE	1:A:264:GLN:NE2	2.69	0.53
1:H:203:ARG:HB3	1:H:204:PRO:HD2	1.90	0.53
1:C:59:GLU:OE1	1:C:130:GLN:HG3	2.08	0.53
1:B:235:LEU:HD11	1:D:235:LEU:HD11	1.90	0.53
1:C:31:ASP:HB2	4:C:693:HOH:O	2.08	0.53
1:C:37:GLN:HE21	1:D:63:LYS:HZ3	1.57	0.53
1:E:39:PRO:HB2	4:E:1230:HOH:O	2.08	0.53
1:G:111:SER:O	1:G:114:MET:CG	2.57	0.53
1:G:160:ARG:O	1:G:163:LEU:HB3	2.08	0.53
1:G:237:ARG:HD3	4:G:1411:HOH:O	2.09	0.53
1:C:207:GLU:OE2	1:C:281:SER:CB	2.56	0.53
1:E:213:THR:HB	1:E:220:TYR:CD2	2.44	0.53
1:E:135:GLU:OE1	1:E:140:ASN:ND2	2.31	0.53
1:C:145:MET:O	1:C:148:VAL:HG13	2.08	0.53
1:B:203:ARG:HH12	1:B:280:THR:HG22	1.70	0.52
1:G:113:TYR:CZ	1:G:117:ARG:HD3	2.44	0.52
1:F:73:ILE:HG23	1:F:171:GLU:HG2	1.90	0.52
1:F:234:GLN:HE21	1:F:234:GLN:HA	1.73	0.52
1:G:160:ARG:O	1:G:164:GLU:HG3	2.10	0.52
1:E:136:PHE:HB3	1:E:162:VAL:CG1	2.40	0.52
1:G:28:LEU:HD11	1:H:55:ALA:HB1	1.91	0.52
1:H:208:ARG:HH12	1:H:215:ARG:HH22	1.57	0.52
1:A:90:ARG:O	1:A:94:VAL:HG23	2.10	0.52
1:A:242:ARG:HD2	1:A:245:MET:HE3	1.91	0.52
1:G:34:LEU:HA	1:G:37:GLN:HE22	1.74	0.52
1:G:251:LYS:HB3	1:G:251:LYS:HZ2	1.75	0.52
2:A:402:TRP:HA	3:A:401:HEM:C1B	2.45	0.52
1:B:72:ALA:HB2	1:B:87:VAL:HG23	1.92	0.52
1:D:29:ARG:NH2	1:D:32:GLN:NE2	2.58	0.52
3:B:401:HEM:HBC2	3:B:401:HEM:HHD	1.91	0.52
1:G:102:TRP:CH2	1:G:240:HIS:HD2	2.28	0.52
1:G:111:SER:O	1:G:114:MET:HG3	2.09	0.51
1:H:203:ARG:NH1	1:H:277:ASP:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:N	1:A:7:LEU:HD23	2.25	0.51
1:E:270:THR:HG21	1:E:273:PRO:HB3	1.91	0.51
1:F:217:TRP:HH2	1:H:217:TRP:CH2	2.23	0.51
1:A:106:GLU:OE1	1:A:246:ARG:NH1	2.44	0.51
1:A:142:ASN:HD21	1:A:144:GLN:HE21	1.57	0.51
1:B:203:ARG:NH1	1:B:280:THR:CG2	2.67	0.51
1:F:50:LEU:HD11	1:F:104:VAL:HG12	1.93	0.51
1:H:241:MET:SD	1:H:245:MET:HE1	2.50	0.51
1:E:54:GLN:HG2	1:E:105:LEU:HD22	1.92	0.51
1:E:51:PHE:CE1	3:E:401:HEM:HBB2	2.39	0.51
1:B:203:ARG:HH12	1:B:280:THR:CG2	2.24	0.51
1:H:73:ILE:HG23	1:H:171:GLU:HG3	1.92	0.51
1:E:72:ALA:HB2	1:E:87:VAL:CG1	2.42	0.50
1:A:241:MET:HE3	1:A:264:GLN:CD	2.35	0.50
1:E:24:TYR:H	1:F:127:GLN:NE2	2.08	0.50
1:F:75:HIS:O	1:F:80:GLU:HB2	2.11	0.50
1:D:133:TYR:HE2	1:D:137:LEU:HD11	1.77	0.50
1:G:187:TYR:OH	1:G:199:ASP:OD2	2.15	0.50
1:G:199:ASP:OD1	1:G:201:THR:OG1	2.29	0.50
1:C:29:ARG:NE	1:D:38:GLN:HG3	2.27	0.50
1:G:95:LEU:HB3	1:G:232:GLN:HG2	1.94	0.50
1:G:133:TYR:HB2	1:G:158:ARG:HH12	1.76	0.50
1:B:244:VAL:HG22	3:B:401:HEM:CHB	2.42	0.50
1:F:278:VAL:O	1:F:278:VAL:HG22	2.12	0.50
1:C:136:PHE:HD2	1:C:162:VAL:HG13	1.77	0.49
1:H:203:ARG:HB3	1:H:204:PRO:CD	2.42	0.49
1:C:245:MET:HE2	1:C:260:VAL:HG11	1.93	0.49
1:H:51:PHE:CZ	2:H:402:TRP:NE1	2.81	0.49
1:B:212:ASN:OD1	1:B:215:ARG:HD2	2.12	0.49
1:C:83:GLN:HE21	1:C:83:GLN:H	1.60	0.49
1:G:47:ASP:OD1	1:H:90:ARG:NH1	2.38	0.49
1:G:48:GLU:O	1:G:51:PHE:HB3	2.11	0.49
2:A:403:TRP:CE3	1:D:86:LYS:HE2	2.48	0.49
1:C:29:ARG:HH11	1:C:29:ARG:HG3	1.78	0.49
1:F:99:THR:HG21	1:F:235:LEU:HG	1.95	0.49
1:G:49:MET:O	1:G:53:ILE:HG12	2.12	0.49
1:H:114:MET:HA	1:H:114:MET:CE	2.37	0.49
1:D:247:VAL:HG11	3:D:401:HEM:HBB2	1.95	0.49
1:G:60:LEU:HD12	1:H:60:LEU:HD12	1.93	0.49
1:B:130:GLN:HB3	4:B:508:HOH:O	2.13	0.49
1:C:234:GLN:NE2	1:C:237:ARG:HE	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:HD3	4:B:987:HOH:O	2.12	0.48
1:C:163:LEU:HG	1:C:193:THR:HB	1.94	0.48
1:D:202:LEU:HB2	1:D:274:GLU:HG2	1.95	0.48
1:F:241:MET:O	1:F:245:MET:HE3	2.13	0.48
1:C:51:PHE:HZ	2:C:402:TRP:CG	2.30	0.48
1:D:265:GLN:O	1:D:269:LEU:CD1	2.60	0.48
1:A:241:MET:CE	1:A:264:GLN:HE22	2.26	0.48
1:A:63:LYS:NZ	1:B:37:GLN:HE21	2.09	0.48
2:E:403:TRP:CE3	1:G:86:LYS:HE2	2.48	0.48
1:F:131:TYR:CD2	3:F:401:HEM:HMD2	2.48	0.48
1:A:225:ASP:O	1:A:229:VAL:HG23	2.12	0.48
1:E:76:LEU:HD22	1:E:175:TYR:HB2	1.95	0.48
1:H:245:MET:HG3	1:H:260:VAL:HG21	1.96	0.48
1:A:73:ILE:HG23	1:A:171:GLU:HG3	1.96	0.48
1:D:29:ARG:NH2	1:D:32:GLN:HE21	2.11	0.48
1:D:132:ARG:HD2	1:D:145:MET:HG3	1.94	0.48
1:B:95:LEU:HB3	1:B:232:GLN:HG3	1.94	0.48
1:C:126:PHE:CZ	1:C:145:MET:HE1	2.48	0.48
1:E:85:ARG:HD2	1:E:221:SER:HB3	1.94	0.48
1:C:51:PHE:CZ	2:C:402:TRP:CD1	3.02	0.48
1:E:135:GLU:CD	1:E:140:ASN:HD22	2.20	0.48
1:F:92:LYS:HD3	1:F:228:ASP:HB3	1.95	0.47
1:H:252:ARG:NH1	1:H:252:ARG:HG2	2.28	0.47
1:A:132:ARG:NE	1:A:145:MET:HE2	2.28	0.47
1:F:203:ARG:N	1:F:204:PRO:HD2	2.30	0.47
1:E:74:VAL:O	1:E:78:ARG:HD3	2.15	0.47
1:G:83:GLN:HE21	1:G:83:GLN:N	2.02	0.47
1:E:158:ARG:HA	1:E:161:GLU:HG2	1.97	0.47
1:F:169:TYR:OH	1:F:274:GLU:OE1	2.32	0.47
1:B:73:ILE:HG23	1:B:171:GLU:HG3	1.97	0.47
1:E:30:LEU:O	1:E:31:ASP:C	2.57	0.47
1:E:68:GLU:CD	1:E:90:ARG:HD2	2.39	0.47
1:A:159:LEU:HA	1:A:162:VAL:HG12	1.96	0.47
1:C:95:LEU:HB3	1:C:232:GLN:HG3	1.96	0.47
1:D:126:PHE:CZ	1:D:145:MET:HE1	2.49	0.47
1:E:270:THR:CG2	1:E:273:PRO:HB3	2.45	0.47
1:G:105:LEU:HD23	1:G:243:THR:HG21	1.97	0.47
1:H:142:ASN:HB3	1:H:145:MET:HG2	1.97	0.47
1:E:80:GLU:HB3	1:E:83:GLN:NE2	2.30	0.47
1:E:133:TYR:CE1	1:E:162:VAL:HG21	2.50	0.47
1:B:253:GLY:HA3	3:B:401:HEM:HMA1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:LEU:CD1	1:H:160:ARG:HD2	2.44	0.46
1:H:171:GLU:HA	1:H:171:GLU:OE2	2.15	0.46
1:B:244:VAL:HG22	3:B:401:HEM:C1B	2.49	0.46
1:D:72:ALA:HB2	1:D:87:VAL:HG23	1.96	0.46
1:G:237:ARG:HD2	4:G:1411:HOH:O	2.14	0.46
1:A:116:PHE:O	1:A:117:ARG:C	2.58	0.46
3:C:401:HEM:CBC	3:C:401:HEM:HHD	2.45	0.46
1:F:146:LEU:HD11	1:F:163:LEU:HD22	1.97	0.46
1:F:169:TYR:CE1	1:F:274:GLU:OE1	2.68	0.46
1:B:132:ARG:HD2	1:B:145:MET:HG3	1.97	0.46
1:B:225:ASP:O	1:B:229:VAL:HG23	2.15	0.46
1:E:45:HIS:CD2	1:E:47:ASP:H	2.30	0.46
1:H:92:LYS:HD3	1:H:228:ASP:HB3	1.96	0.46
1:C:129:LEU:HD21	1:C:155:GLY:HA3	1.98	0.46
3:E:401:HEM:HBC2	3:E:401:HEM:HHD	1.98	0.46
1:G:51:PHE:CZ	2:G:402:TRP:CE2	3.04	0.46
1:G:253:GLY:HA3	3:G:401:HEM:O2A	2.16	0.46
1:A:24:TYR:H	1:B:127:GLN:NE2	2.14	0.46
1:G:145:MET:O	1:G:148:VAL:HG13	2.15	0.46
1:C:95:LEU:HB2	1:C:232:GLN:HG2	1.97	0.46
1:C:137:LEU:HA	1:C:137:LEU:HD23	1.27	0.46
1:G:244:VAL:HG22	3:G:401:HEM:C1B	2.51	0.46
1:H:45:HIS:CD2	1:H:47:ASP:H	2.25	0.46
1:H:202:LEU:HD12	1:H:274:GLU:CD	2.40	0.46
1:B:26:GLY:O	1:B:29:ARG:HD2	2.16	0.46
1:C:275:LEU:O	1:C:278:VAL:HG12	2.16	0.46
1:H:48:GLU:O	1:H:51:PHE:HB3	2.16	0.46
1:A:141:LYS:NZ	1:A:165:ALA:O	2.41	0.45
1:C:240:HIS:O	1:C:244:VAL:HG23	2.16	0.45
1:C:49:MET:HG3	1:C:53:ILE:HD12	1.98	0.45
1:E:72:ALA:HB2	1:E:87:VAL:HG12	1.97	0.45
1:F:122:PRO:HA	1:F:254:THR:O	2.16	0.45
1:A:234:GLN:HA	1:A:234:GLN:NE2	2.18	0.45
1:A:234:GLN:NE2	1:A:237:ARG:HH21	2.13	0.45
1:B:68:GLU:CD	1:B:90:ARG:HD2	2.41	0.45
1:A:37:GLN:HE21	1:B:63:LYS:HZ2	1.64	0.45
1:B:242:ARG:NH1	1:B:245:MET:HE1	2.31	0.45
1:F:65:LEU:HD21	1:F:95:LEU:HD21	1.99	0.45
1:G:45:HIS:HD2	1:G:47:ASP:H	1.65	0.45
1:F:140:ASN:HB2	1:F:271:PHE:CE1	2.52	0.45
1:B:83:GLN:H	1:B:83:GLN:HE21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:MET:O	1:G:249:GLY:HA2	2.17	0.45
1:A:51:PHE:CZ	2:A:402:TRP:CD1	3.05	0.45
1:A:234:GLN:HE21	1:A:234:GLN:CA	2.16	0.45
1:B:83:GLN:NE2	4:B:1192:HOH:O	2.35	0.45
1:F:142:ASN:OD1	1:F:144:GLN:HG3	2.17	0.45
1:F:245:MET:HE3	1:F:245:MET:HB2	1.26	0.45
1:A:142:ASN:HD21	1:A:144:GLN:NE2	2.16	0.44
1:C:225:ASP:O	1:C:229:VAL:HG23	2.18	0.44
1:E:275:LEU:O	1:E:278:VAL:HG12	2.18	0.44
3:E:401:HEM:HHD	3:E:401:HEM:CBC	2.48	0.44
1:F:217:TRP:CH2	1:H:217:TRP:HH2	2.23	0.44
3:C:401:HEM:HHD	3:C:401:HEM:HBC2	1.99	0.44
1:D:240:HIS:O	1:D:244:VAL:HG23	2.17	0.44
1:H:208:ARG:NH1	1:H:215:ARG:NH2	2.65	0.44
1:B:90:ARG:O	1:B:94:VAL:HG23	2.17	0.44
1:C:102:TRP:CZ2	1:C:240:HIS:HB2	2.53	0.44
1:E:85:ARG:CD	1:E:221:SER:HB3	2.47	0.44
1:E:238:PHE:O	1:E:242:ARG:HG2	2.18	0.44
1:G:95:LEU:HB3	1:G:232:GLN:CG	2.48	0.44
1:G:142:ASN:HB3	1:G:145:MET:HG2	2.00	0.44
1:C:10:LEU:HB2	1:D:144:GLN:OE1	2.18	0.44
1:A:234:GLN:HE22	1:A:237:ARG:HH21	1.66	0.44
1:B:164:GLU:HA	1:B:193:THR:HG22	2.00	0.44
1:C:135:GLU:OE2	1:C:237:ARG:NH1	2.50	0.44
1:D:84:CYS:O	1:D:87:VAL:HG22	2.18	0.44
1:G:39:PRO:HB3	1:G:48:GLU:CD	2.43	0.44
1:F:169:TYR:HE1	1:F:274:GLU:OE1	2.00	0.44
1:C:63:LYS:HZ2	1:D:37:GLN:NE2	2.15	0.43
1:G:41:SER:HA	1:G:119:VAL:HG11	2.00	0.43
1:G:130:GLN:HE21	1:H:34:LEU:HD13	1.83	0.43
1:H:132:ARG:HD2	1:H:145:MET:HG3	1.99	0.43
1:B:88:LEU:HA	1:B:91:SER:HB2	2.00	0.43
1:B:135:GLU:OE2	1:B:237:ARG:NH1	2.51	0.43
1:D:142:ASN:OD1	1:D:144:GLN:HB2	2.18	0.43
1:D:166:PRO:HB2	1:D:171:GLU:HG2	2.00	0.43
1:D:72:ALA:HB2	1:D:87:VAL:HG21	2.00	0.43
1:E:131:TYR:CG	3:E:401:HEM:HMD1	2.53	0.43
1:E:198:ALA:HB3	4:E:1065:HOH:O	2.17	0.43
1:G:144:GLN:O	1:G:147:GLN:HG2	2.18	0.43
1:E:53:ILE:O	1:E:57:THR:HG23	2.18	0.43
1:F:203:ARG:HH11	1:F:280:THR:HB	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:LYS:NZ	1:G:225:ASP:OD1	2.47	0.43
1:G:108:LEU:HD12	1:G:108:LEU:HA	1.86	0.43
1:A:239:ARG:HD2	4:A:1091:HOH:O	2.18	0.43
1:G:215:ARG:HD3	1:G:216:TYR:CZ	2.53	0.43
1:E:123:SER:HA	1:E:127:GLN:OE1	2.18	0.43
1:F:235:LEU:CD2	1:G:239:ARG:HD3	2.48	0.43
1:A:96:ARG:HH22	1:B:100:GLU:HG3	1.84	0.42
1:C:109:THR:O	1:C:112:GLU:HB2	2.19	0.42
1:F:108:LEU:HD23	3:F:401:HEM:HBB1	1.99	0.42
1:A:110:PRO:HB3	1:A:247:VAL:O	2.19	0.42
1:F:139:GLY:HA3	4:F:728:HOH:O	2.17	0.42
1:G:90:ARG:O	1:G:94:VAL:HG23	2.20	0.42
1:B:74:VAL:O	1:B:78:ARG:HG3	2.20	0.42
1:F:42:GLU:HA	1:F:43:PRO:C	2.44	0.42
1:A:245:MET:HG2	1:A:260:VAL:HG21	2.01	0.42
1:D:141:LYS:HB3	1:D:163:LEU:HD12	2.02	0.42
1:G:85:ARG:HG2	1:G:225:ASP:OD2	2.19	0.42
1:A:133:TYR:CE2	1:A:137:LEU:HD22	2.55	0.42
1:H:81:VAL:O	1:H:85:ARG:HG3	2.20	0.42
1:A:45:HIS:CD2	1:A:47:ASP:HB2	2.55	0.42
1:F:93:GLN:HE22	1:F:96:ARG:HE	1.68	0.42
1:G:230:GLU:O	1:G:234:GLN:HG2	2.19	0.42
1:A:37:GLN:NE2	1:B:63:LYS:HZ2	2.18	0.42
1:A:45:HIS:CD2	1:A:47:ASP:H	2.29	0.42
1:C:177:ALA:HB3	4:C:1319:HOH:O	2.18	0.42
1:F:143:PRO:HB3	1:F:163:LEU:HD21	2.01	0.42
1:H:156:GLN:O	1:H:160:ARG:HG2	2.19	0.42
1:D:225:ASP:O	1:D:229:VAL:HG23	2.20	0.42
1:D:244:VAL:HG22	3:D:401:HEM:C1B	2.55	0.42
1:G:252:ARG:NH1	1:G:256:GLY:O	2.52	0.42
1:H:136:PHE:O	1:H:141:LYS:NZ	2.52	0.42
1:A:217:TRP:HH2	1:D:217:TRP:CH2	2.38	0.42
1:D:99:THR:CG2	1:D:235:LEU:HG	2.48	0.42
1:E:44:ALA:HA	4:E:1230:HOH:O	2.20	0.42
1:F:125:GLY:HA3	3:F:401:HEM:C1D	2.55	0.42
1:A:24:TYR:H	1:B:127:GLN:HE21	1.68	0.41
1:B:213:THR:HG23	1:B:285:ASP:OD1	2.20	0.41
1:F:170:GLU:O	1:F:174:ARG:HG3	2.20	0.41
1:H:244:VAL:HG22	3:H:401:HEM:C1B	2.54	0.41
1:C:141:LYS:HB3	1:C:163:LEU:HD12	2.02	0.41
1:F:61:TRP:HB2	1:F:98:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:LEU:HD23	1:F:98:LEU:HA	1.91	0.41
1:A:230:GLU:O	1:A:230:GLU:HG3	2.20	0.41
1:B:170:GLU:O	1:B:174:ARG:HD3	2.20	0.41
1:G:45:HIS:CE1	1:G:115:GLY:HA3	2.55	0.41
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.85	0.41
1:B:228:ASP:OD1	1:D:246:ARG:NH2	2.49	0.41
1:E:110:PRO:HB2	1:H:282:VAL:HG11	2.03	0.41
1:C:51:PHE:HZ	2:C:402:TRP:CD1	2.39	0.41
1:A:64:LEU:HB2	1:B:53:ILE:HD13	2.01	0.41
1:D:166:PRO:HG3	1:D:192:TRP:CE2	2.55	0.41
1:E:102:TRP:CH2	1:E:240:HIS:HD2	2.38	0.41
1:C:237:ARG:HD3	4:C:1308:HOH:O	2.20	0.41
1:A:46:HIS:NE2	1:B:68:GLU:OE1	2.46	0.41
1:A:63:LYS:HZ3	1:B:37:GLN:HE21	1.69	0.41
1:A:147:GLN:HE21	1:A:147:GLN:HB3	1.60	0.41
1:B:132:ARG:CZ	1:B:145:MET:HE3	2.50	0.41
1:E:236:TRP:CD2	1:E:236:TRP:C	2.99	0.41
1:F:230:GLU:O	1:F:234:GLN:HG2	2.20	0.41
1:A:271:PHE:C	1:A:273:PRO:HD3	2.46	0.41
1:F:41:SER:HA	1:F:119:VAL:HG11	2.03	0.41
3:F:401:HEM:HBB2	3:F:401:HEM:HMB1	2.02	0.41
1:G:242:ARG:HB3	4:G:742:HOH:O	2.19	0.41
1:B:106:GLU:OE1	1:B:246:ARG:NH1	2.52	0.41
1:C:123:SER:HB2	1:D:24:TYR:N	2.36	0.41
1:E:54:GLN:NE2	1:E:101:GLN:NE2	2.57	0.41
1:E:56:GLN:HG2	1:F:33:LEU:HD22	2.03	0.41
1:F:142:ASN:HA	1:F:143:PRO:HD3	1.92	0.41
1:G:24:TYR:CE2	1:H:125:GLY:HA2	2.56	0.41
1:G:205:VAL:O	1:G:209:ILE:HG13	2.20	0.41
1:H:234:GLN:NE2	1:H:237:ARG:HE	2.19	0.41
1:D:227:VAL:HG23	1:D:275:LEU:HD13	2.04	0.40
1:F:278:VAL:O	1:F:282:VAL:HG23	2.21	0.40
1:G:78:ARG:O	1:G:79:ASP:HB2	2.20	0.40
1:E:152:ASP:OD1	1:E:152:ASP:C	2.64	0.40
1:A:280:THR:HA	1:C:251:LYS:HD3	2.03	0.40
1:F:169:TYR:O	1:F:172:PHE:HB3	2.20	0.40
1:G:169:TYR:OH	1:G:274:GLU:OE2	2.27	0.40
1:G:190:ARG:NH2	4:G:1173:HOH:O	2.53	0.40
1:C:63:LYS:HZ3	1:D:37:GLN:NE2	2.06	0.40
1:C:90:ARG:NH1	1:D:47:ASP:OD1	2.48	0.40
1:E:210:TYR:CB	1:E:282:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:NE2	1:B:63:LYS:NZ	2.65	0.40
1:A:110:PRO:HG3	1:C:279:ARG:HG3	2.04	0.40
1:C:245:MET:HG2	1:C:260:VAL:HG21	2.03	0.40
1:D:266:ALA:O	1:D:269:LEU:HB2	2.22	0.40
1:E:34:LEU:HA	1:E:37:GLN:HE22	1.86	0.40
1:G:214:ASP:OD1	4:G:936:HOH:O	2.22	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	275/306 (90%)	269 (98%)	5 (2%)	1 (0%)	30	26
1	B	278/306 (91%)	268 (96%)	9 (3%)	1 (0%)	30	26
1	C	268/306 (88%)	258 (96%)	9 (3%)	1 (0%)	30	26
1	D	260/306 (85%)	250 (96%)	9 (4%)	1 (0%)	30	26
1	E	258/306 (84%)	245 (95%)	13 (5%)	0	100	100
1	F	246/306 (80%)	235 (96%)	9 (4%)	2 (1%)	16	10
1	G	260/306 (85%)	247 (95%)	12 (5%)	1 (0%)	30	26
1	H	253/306 (83%)	241 (95%)	12 (5%)	0	100	100
All	All	2098/2448 (86%)	2013 (96%)	78 (4%)	7 (0%)	36	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	VAL
1	A	118	ASP
1	G	114	MET
1	C	198	ALA

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Mol	Chain	Res	Type
1	D	184	PRO
1	F	148	VAL
1	F	153	PRO

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	241/266 (91%)	227 (94%)	14 (6%)	18	14
1	B	244/266 (92%)	223 (91%)	21 (9%)	10	5
1	C	238/266 (90%)	216 (91%)	22 (9%)	8	4
1	D	228/266 (86%)	211 (92%)	17 (8%)	12	8
1	E	227/266 (85%)	200 (88%)	27 (12%)	5	2
1	F	220/266 (83%)	202 (92%)	18 (8%)	10	6
1	G	229/266 (86%)	213 (93%)	16 (7%)	14	9
1	H	224/266 (84%)	205 (92%)	19 (8%)	10	6
All	All	1851/2128 (87%)	1697 (92%)	154 (8%)	10	6

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU
1	A	38	GLN
1	A	83	GLN
1	A	118	ASP
1	A	147	GLN
1	A	151	TYR
1	A	159	LEU
1	A	163	LEU
1	A	190	ARG
1	A	234	GLN
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	264	GLN
1	A	270	THR
1	B	7	LEU
1	B	8	ARG
1	B	10	LEU
1	B	17	ASP
1	B	21	ARG
1	B	83	GLN
1	B	87	VAL
1	B	100	GLU
1	B	111	SER
1	B	118	ASP
1	B	127	GLN
1	B	129	LEU
1	B	147	GLN
1	B	148	VAL
1	B	162	VAL
1	B	193	THR
1	B	215	ARG
1	B	234	GLN
1	B	257	SER
1	B	278	VAL
1	B	280	THR
1	C	7	LEU
1	C	9	ASP
1	C	17	ASP
1	C	29	ARG
1	C	42	GLU
1	C	78	ARG
1	C	83	GLN
1	C	119	VAL
1	C	127	GLN
1	C	141	LYS
1	C	148	VAL
1	C	164	GLU
1	C	185	GLN
1	C	186	GLN
1	C	193	THR
1	C	196	HIS
1	C	200	ASP
1	C	215	ARG
1	C	234	GLN

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Mol	Chain	Res	Type
1	C	235	LEU
1	C	237	ARG
1	C	264	GLN
1	D	22	LEU
1	D	42	GLU
1	D	53	ILE
1	D	82	TRP
1	D	83	GLN
1	D	114	MET
1	D	129	LEU
1	D	146	LEU
1	D	160	ARG
1	D	162	VAL
1	D	197	VAL
1	D	201	THR
1	D	215	ARG
1	D	234	GLN
1	D	278	VAL
1	D	280	THR
1	D	282	VAL
1	E	23	THR
1	E	42	GLU
1	E	76	LEU
1	E	78	ARG
1	E	83	GLN
1	E	92	LYS
1	E	127	GLN
1	E	130	GLN
1	E	147	GLN
1	E	148	VAL
1	E	152	ASP
1	E	160	ARG
1	E	161	GLU
1	E	162	VAL
1	E	197	VAL
1	E	200	ASP
1	E	211	GLU
1	E	214	ASP
1	E	230	GLU
1	E	234	GLN
1	E	235	LEU
1	E	252	ARG

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Mol	Chain	Res	Type
1	E	260	VAL
1	E	265	GLN
1	E	269	LEU
1	E	280	THR
1	E	282	VAL
1	F	53	ILE
1	F	76	LEU
1	F	78	ARG
1	F	83	GLN
1	F	87	VAL
1	F	127	GLN
1	F	148	VAL
1	F	158	ARG
1	F	159	LEU
1	F	161	GLU
1	F	162	VAL
1	F	214	ASP
1	F	215	ARG
1	F	230	GLU
1	F	234	GLN
1	F	235	LEU
1	F	245	MET
1	F	264	GLN
1	G	21	ARG
1	G	22	LEU
1	G	76	LEU
1	G	78	ARG
1	G	83	GLN
1	G	127	GLN
1	G	148	VAL
1	G	158	ARG
1	G	161	GLU
1	G	184	PRO
1	G	204	PRO
1	G	234	GLN
1	G	235	LEU
1	G	245	MET
1	G	251	LYS
1	G	270	THR
1	H	22	LEU
1	H	31	ASP
1	H	42	GLU

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Mol	Chain	Res	Type
1	H	50	LEU
1	H	76	LEU
1	H	83	GLN
1	H	111	SER
1	H	123	SER
1	H	129	LEU
1	H	137	LEU
1	H	148	VAL
1	H	164	GLU
1	H	192	TRP
1	H	200	ASP
1	H	201	THR
1	H	234	GLN
1	H	252	ARG
1	H	280	THR
1	H	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLN
1	A	45	HIS
1	A	83	GLN
1	A	144	GLN
1	A	147	GLN
1	A	156	GLN
1	A	234	GLN
1	A	264	GLN
1	B	32	GLN
1	B	37	GLN
1	B	83	GLN
1	B	93	GLN
1	B	127	GLN
1	B	130	GLN
1	B	140	ASN
1	B	147	GLN
1	B	234	GLN
1	C	32	GLN
1	C	37	GLN
1	C	45	HIS
1	C	83	GLN

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Mol	Chain	Res	Type
1	C	130	GLN
1	C	147	GLN
1	C	156	GLN
1	C	186	GLN
1	C	212	ASN
1	C	234	GLN
1	C	264	GLN
1	C	265	GLN
1	D	32	GLN
1	D	37	GLN
1	D	45	HIS
1	D	83	GLN
1	D	97	GLN
1	D	130	GLN
1	D	212	ASN
1	D	234	GLN
1	D	265	GLN
1	E	32	GLN
1	E	37	GLN
1	E	38	GLN
1	E	45	HIS
1	E	54	GLN
1	E	83	GLN
1	E	156	GLN
1	E	186	GLN
1	E	188	GLN
1	E	234	GLN
1	E	264	GLN
1	F	32	GLN
1	F	37	GLN
1	F	38	GLN
1	F	83	GLN
1	F	93	GLN
1	F	101	GLN
1	F	127	GLN
1	F	185	GLN
1	F	212	ASN
1	F	234	GLN
1	G	37	GLN
1	G	45	HIS
1	G	83	GLN
1	G	93	GLN

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Mol	Chain	Res	Type
1	G	130	GLN
1	G	142	ASN
1	G	156	GLN
1	G	188	GLN
1	G	234	GLN
1	G	264	GLN
1	H	37	GLN
1	H	45	HIS
1	H	75	HIS
1	H	83	GLN
1	H	97	GLN
1	H	130	GLN
1	H	234	GLN

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](#)

21 ligands are modelled in this entry.

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	$\# Z > 2$
2	TRP	E	403	-	15,16,16	1.76	5 (33%)	18,22,22	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	A	402	-	15,16,16	2.13	3 (20%)	18,22,22	1.15	1 (5%)
2	TRP	A	403	-	15,16,16	1.55	2 (13%)	18,22,22	0.51	0
2	TRP	H	402	-	15,16,16	1.59	3 (20%)	18,22,22	0.73	0
3	HEM	C	401	1	50,50,50	2.13	13 (26%)	67,82,82	1.82	18 (26%)
3	HEM	H	401	1	50,50,50	2.39	10 (20%)	67,82,82	2.00	24 (35%)
2	TRP	D	403	-	15,16,16	1.60	4 (26%)	18,22,22	0.90	1 (5%)
2	TRP	B	403	-	15,16,16	1.04	1 (6%)	18,22,22	0.79	1 (5%)
2	TRP	E	402	-	15,16,16	1.97	4 (26%)	18,22,22	1.22	2 (11%)
2	TRP	F	402	-	15,16,16	1.62	4 (26%)	18,22,22	1.10	1 (5%)
3	HEM	F	401	1	50,50,50	2.67	10 (20%)	67,82,82	2.06	17 (25%)
2	TRP	G	402	-	15,16,16	1.62	2 (13%)	18,22,22	0.71	1 (5%)
3	HEM	D	401	1	50,50,50	2.06	14 (28%)	67,82,82	1.81	23 (34%)
3	HEM	B	401	1,4	50,50,50	2.07	16 (32%)	67,82,82	1.84	19 (28%)
2	TRP	C	403	-	15,16,16	1.44	2 (13%)	18,22,22	0.79	1 (5%)
2	TRP	C	402	-	15,16,16	2.05	3 (20%)	18,22,22	0.93	1 (5%)
3	HEM	A	401	1	50,50,50	2.07	14 (28%)	67,82,82	2.00	19 (28%)
2	TRP	D	402	-	15,16,16	2.19	4 (26%)	18,22,22	1.00	1 (5%)
3	HEM	G	401	1	50,50,50	2.22	10 (20%)	67,82,82	2.01	20 (29%)
3	HEM	E	401	1,4	50,50,50	2.54	11 (22%)	67,82,82	2.09	18 (26%)
2	TRP	B	402	-	15,16,16	2.12	5 (33%)	18,22,22	0.75	0

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
2	TRP	E	403	-	-	1/8/8/8	0/2/2/2
2	TRP	A	402	-	-	5/8/8/8	0/2/2/2
2	TRP	A	403	-	-	0/8/8/8	0/2/2/2
2	TRP	H	402	-	-	5/8/8/8	0/2/2/2
3	HEM	C	401	1	-	2/14/54/54	-
3	HEM	H	401	1	-	5/14/54/54	-
2	TRP	D	403	-	-	0/8/8/8	0/2/2/2
2	TRP	B	403	-	-	0/8/8/8	0/2/2/2
2	TRP	E	402	-	-	3/8/8/8	0/2/2/2
2	TRP	F	402	-	-	6/8/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	F	401	1	-	4/14/54/54	-
2	TRP	G	402	-	-	5/8/8/8	0/2/2/2
3	HEM	D	401	1	-	3/14/54/54	-
3	HEM	B	401	1,4	-	6/14/54/54	-
2	TRP	C	403	-	-	0/8/8/8	0/2/2/2
2	TRP	C	402	-	-	6/8/8/8	0/2/2/2
3	HEM	A	401	1	-	6/14/54/54	-
2	TRP	D	402	-	-	5/8/8/8	0/2/2/2
3	HEM	G	401	1	-	4/14/54/54	-
3	HEM	E	401	1,4	-	4/14/54/54	-
2	TRP	B	402	-	-	5/8/8/8	0/2/2/2

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	HEM	FE-ND	10.61	2.27	1.94
3	E	401	HEM	FE-ND	10.32	2.26	1.94
3	H	401	HEM	C3D-C2D	8.76	1.55	1.36
3	F	401	HEM	C3D-C2D	8.66	1.55	1.36
3	E	401	HEM	C3D-C2D	8.29	1.54	1.36
3	F	401	HEM	FE-NB	8.20	2.20	1.94
3	H	401	HEM	FE-ND	7.69	2.18	1.94
3	G	401	HEM	FE-NC	7.17	2.18	1.95
3	A	401	HEM	C3D-C2D	6.87	1.51	1.36
3	C	401	HEM	C3D-C2D	6.73	1.51	1.36
2	A	402	TRP	CD1-NE1	6.55	1.47	1.37
3	A	401	HEM	FE-NA	6.07	2.15	1.95
3	G	401	HEM	C3D-C2D	6.04	1.49	1.36
2	C	402	TRP	CD1-NE1	6.00	1.46	1.37
3	E	401	HEM	FE-NB	5.90	2.13	1.94
3	G	401	HEM	FE-ND	5.84	2.12	1.94
3	D	401	HEM	C3D-C2D	5.81	1.49	1.36
3	B	401	HEM	C3D-C2D	5.79	1.49	1.36
2	D	402	TRP	CD1-NE1	5.62	1.46	1.37
3	H	401	HEM	FE-NA	5.31	2.12	1.95
3	H	401	HEM	FE-NB	5.13	2.10	1.94
3	C	401	HEM	FE-NC	5.12	2.12	1.95
3	G	401	HEM	FE-NB	5.10	2.10	1.94
3	E	401	HEM	FE-NA	4.96	2.11	1.95
3	H	401	HEM	FE-NC	4.95	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	HEM	FE-NA	4.66	2.10	1.95
3	D	401	HEM	CMB-C2B	4.52	1.60	1.50
3	D	401	HEM	FE-NC	4.47	2.09	1.95
2	B	402	TRP	CZ3-CE3	-4.43	1.31	1.38
3	B	401	HEM	C3C-C2C	-4.38	1.28	1.37
2	E	402	TRP	CD1-NE1	4.30	1.44	1.37
3	C	401	HEM	CMB-C2B	4.29	1.59	1.50
2	A	403	TRP	CB-CG	4.28	1.58	1.50
3	A	401	HEM	FE-NC	4.09	2.08	1.95
3	B	401	HEM	FE-NC	4.05	2.08	1.95
3	F	401	HEM	FE-NC	3.95	2.08	1.95
3	B	401	HEM	FE-NA	3.94	2.08	1.95
3	E	401	HEM	FE-NC	3.93	2.08	1.95
2	B	402	TRP	CD1-NE1	3.86	1.43	1.37
2	C	403	TRP	CB-CG	3.79	1.57	1.50
3	F	401	HEM	CAC-C3C	3.73	1.57	1.47
3	C	401	HEM	FE-NA	3.73	2.07	1.95
3	D	401	HEM	CAC-C3C	3.60	1.57	1.47
2	B	402	TRP	CH2-CZ3	3.58	1.46	1.38
2	F	402	TRP	CB-CG	-3.56	1.43	1.50
2	G	402	TRP	CD1-NE1	3.49	1.42	1.37
2	E	403	TRP	CB-CG	3.48	1.56	1.50
3	C	401	HEM	CHA-C1A	-3.47	1.31	1.39
3	G	401	HEM	CAC-C3C	3.46	1.56	1.47
3	E	401	HEM	CAC-C3C	3.42	1.56	1.47
2	D	402	TRP	OXT-C	-3.36	1.19	1.30
2	F	402	TRP	OXT-C	-3.31	1.20	1.30
2	E	402	TRP	CD2-CE2	3.29	1.45	1.41
3	B	401	HEM	CAC-C3C	3.28	1.56	1.47
2	H	402	TRP	CH2-CZ3	3.27	1.45	1.38
3	H	401	HEM	CAB-C3B	3.25	1.56	1.47
3	C	401	HEM	CAC-C3C	3.25	1.56	1.47
3	D	401	HEM	CAB-C3B	3.23	1.56	1.47
3	F	401	HEM	CMA-C3A	3.16	1.57	1.50
3	B	401	HEM	C4D-C3D	-3.14	1.39	1.45
2	A	402	TRP	CD1-CG	-3.10	1.32	1.36
3	C	401	HEM	C1D-ND	3.08	1.44	1.38
3	C	401	HEM	CBA-CGA	3.07	1.57	1.50
3	A	401	HEM	CMA-C3A	3.05	1.57	1.50
2	C	402	TRP	OXT-C	-3.03	1.21	1.30
3	D	401	HEM	FE-ND	-2.99	1.85	1.94
3	G	401	HEM	CAB-C3B	2.99	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	HEM	C1B-C2B	-2.98	1.38	1.44
2	D	403	TRP	CH2-CZ3	2.96	1.44	1.38
3	A	401	HEM	CAA-C2A	2.95	1.58	1.51
3	H	401	HEM	CMA-C3A	2.90	1.56	1.50
3	D	401	HEM	CMC-C2C	2.86	1.56	1.50
2	B	402	TRP	CB-CG	2.83	1.55	1.50
3	C	401	HEM	FE-NB	-2.81	1.86	1.94
3	A	401	HEM	CAC-C3C	2.81	1.54	1.47
3	B	401	HEM	CAB-C3B	2.79	1.54	1.47
3	B	401	HEM	CAD-C3D	2.79	1.58	1.51
3	D	401	HEM	C2A-C3A	-2.79	1.31	1.38
3	F	401	HEM	CAB-C3B	2.78	1.54	1.47
2	E	402	TRP	CH2-CZ3	2.77	1.44	1.38
2	A	402	TRP	OXT-C	-2.77	1.21	1.30
3	C	401	HEM	CAB-C3B	2.73	1.54	1.47
3	G	401	HEM	O1D-CGD	2.71	1.31	1.22
3	D	401	HEM	FE-NB	-2.67	1.86	1.94
3	G	401	HEM	CMC-C2C	2.67	1.56	1.50
3	C	401	HEM	CMC-C2C	2.67	1.56	1.50
3	B	401	HEM	C1C-C2C	-2.66	1.40	1.45
3	H	401	HEM	CMC-C2C	2.61	1.56	1.50
3	A	401	HEM	CAB-C3B	2.59	1.54	1.47
2	C	403	TRP	CD1-CG	-2.59	1.32	1.36
3	F	401	HEM	CMC-C2C	2.58	1.56	1.50
3	B	401	HEM	C3B-C4B	-2.56	1.40	1.44
2	H	402	TRP	CD1-NE1	2.54	1.41	1.37
2	E	403	TRP	CZ3-CE3	2.54	1.43	1.38
3	F	401	HEM	C1B-NB	-2.53	1.35	1.40
2	D	403	TRP	CZ2-CE2	2.52	1.43	1.39
3	B	401	HEM	C3B-C2B	-2.52	1.32	1.37
2	C	402	TRP	CD2-CG	2.52	1.48	1.44
3	A	401	HEM	C4A-NA	-2.48	1.34	1.39
3	D	401	HEM	FE-NA	2.48	2.03	1.95
2	H	402	TRP	CD2-CE2	2.47	1.44	1.41
2	E	403	TRP	O-C	2.46	1.29	1.22
3	A	401	HEM	O1D-CGD	2.44	1.30	1.22
2	D	403	TRP	CE3-CD2	2.44	1.43	1.39
2	E	403	TRP	CH2-CZ3	2.42	1.43	1.38
2	D	402	TRP	CD2-CG	2.41	1.47	1.44
2	F	402	TRP	CD1-NE1	2.39	1.41	1.37
3	D	401	HEM	CAA-C2A	2.39	1.57	1.51
3	B	401	HEM	C3C-C4C	-2.38	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	HEM	C4D-ND	2.37	1.44	1.40
2	D	403	TRP	OXT-C	-2.37	1.23	1.30
2	G	402	TRP	CZ3-CE3	2.36	1.42	1.38
3	D	401	HEM	C1B-NB	2.36	1.44	1.40
3	B	401	HEM	C4D-ND	2.35	1.44	1.40
3	E	401	HEM	CAB-C3B	2.34	1.53	1.47
3	D	401	HEM	CHA-C4D	-2.28	1.33	1.38
3	E	401	HEM	CHC-C1C	2.26	1.42	1.38
3	A	401	HEM	CBA-CGA	2.26	1.55	1.50
3	E	401	HEM	O1D-CGD	2.25	1.29	1.22
2	A	403	TRP	O-C	2.24	1.28	1.22
3	E	401	HEM	CMA-C3A	2.23	1.55	1.50
3	F	401	HEM	CMB-C2B	2.23	1.55	1.50
3	H	401	HEM	CAA-C2A	2.19	1.57	1.51
3	H	401	HEM	CAC-C3C	2.19	1.53	1.47
2	B	403	TRP	CZ3-CE3	2.19	1.42	1.38
3	B	401	HEM	C4C-NC	-2.18	1.35	1.39
3	G	401	HEM	CMB-C2B	2.16	1.55	1.50
3	A	401	HEM	CMD-C2D	2.16	1.55	1.50
2	F	402	TRP	CD2-CE2	2.14	1.44	1.41
2	E	402	TRP	CB-CG	2.14	1.54	1.50
3	A	401	HEM	C4B-NB	2.13	1.43	1.38
3	B	401	HEM	FE-NB	-2.13	1.88	1.94
2	D	402	TRP	CZ2-CE2	2.11	1.43	1.39
3	A	401	HEM	C4C-NC	-2.09	1.35	1.39
3	D	401	HEM	CMA-C3A	2.08	1.55	1.50
3	C	401	HEM	C3B-C4B	-2.07	1.40	1.44
2	E	403	TRP	CD1-CG	2.06	1.39	1.36
2	B	402	TRP	CD2-CG	2.04	1.47	1.44
3	E	401	HEM	CMB-C2B	2.04	1.55	1.50
3	C	401	HEM	CHB-C4A	-2.04	1.34	1.39

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HEM	C4D-ND-C1D	8.55	115.33	105.21
3	E	401	HEM	C4D-ND-C1D	7.70	114.33	105.21
3	G	401	HEM	C4D-ND-C1D	7.27	113.81	105.21
3	E	401	HEM	C3B-C4B-NB	-7.11	104.36	109.47
3	H	401	HEM	C4D-ND-C1D	7.04	113.54	105.21
3	E	401	HEM	C1B-NB-C4B	5.44	111.65	105.21
3	G	401	HEM	CHD-C1D-ND	5.16	129.97	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HEM	C1B-NB-C4B	5.05	111.19	105.21
3	A	401	HEM	CHA-C4D-ND	5.02	130.58	124.37
3	C	401	HEM	CHC-C4B-NB	5.00	129.81	124.42
3	F	401	HEM	C3B-C4B-NB	-4.93	105.93	109.47
3	H	401	HEM	C3B-C4B-NB	-4.85	105.99	109.47
3	B	401	HEM	CHC-C4B-NB	4.81	129.60	124.42
3	A	401	HEM	CMD-C2D-C1D	4.75	132.46	125.03
3	G	401	HEM	C1B-NB-C4B	4.60	110.65	105.21
3	D	401	HEM	C3B-C2B-C1B	-4.57	102.98	106.41
3	B	401	HEM	C4B-C3B-C2B	4.43	111.35	107.28
3	A	401	HEM	CAD-C3D-C4D	4.31	132.21	124.70
3	C	401	HEM	CHA-C4D-ND	4.25	129.62	124.37
3	A	401	HEM	CAD-C3D-C2D	-4.17	120.06	127.87
3	B	401	HEM	CHC-C1C-NC	4.13	128.95	124.45
3	H	401	HEM	C3D-C4D-ND	-4.09	105.69	110.17
3	A	401	HEM	CMA-C3A-C2A	4.08	134.27	125.62
3	A	401	HEM	CAA-C2A-C1A	-4.02	117.09	124.94
3	H	401	HEM	C1B-NB-C4B	3.93	109.86	105.21
2	E	402	TRP	OXT-C-O	-3.92	115.19	124.08
2	F	402	TRP	OXT-C-O	-3.89	115.26	124.08
3	A	401	HEM	CBD-CAD-C3D	-3.85	101.88	112.53
3	G	401	HEM	C2D-C1D-ND	-3.76	105.56	109.90
3	C	401	HEM	CMA-C3A-C4A	-3.75	119.71	125.42
3	E	401	HEM	CBD-CAD-C3D	-3.67	102.39	112.53
3	B	401	HEM	CHA-C4D-ND	3.65	128.88	124.37
3	G	401	HEM	C3B-C4B-NB	-3.63	106.86	109.47
3	F	401	HEM	C3D-C4D-ND	-3.46	106.37	110.17
3	C	401	HEM	CMA-C3A-C2A	3.46	132.96	125.62
3	D	401	HEM	C2B-C1B-NB	3.44	113.79	109.84
2	D	402	TRP	OXT-C-O	-3.43	116.30	124.08
3	B	401	HEM	CMA-C3A-C2A	3.36	132.75	125.62
3	G	401	HEM	CHB-C1B-NB	3.34	128.50	124.37
3	D	401	HEM	CHA-C4D-C3D	-3.34	119.07	125.23
3	F	401	HEM	CAD-C3D-C4D	3.31	130.47	124.70
3	F	401	HEM	CHD-C4C-NC	3.29	128.04	124.45
3	A	401	HEM	CAA-C2A-C3A	3.28	134.44	127.07
3	C	401	HEM	C4B-C3B-C2B	3.27	110.29	107.28
3	H	401	HEM	C2A-C1A-NA	-3.22	106.58	110.15
3	F	401	HEM	C2D-C1D-ND	-3.21	106.19	109.90
3	B	401	HEM	C1C-CHC-C4B	-3.16	119.31	126.02
3	B	401	HEM	CMA-C3A-C4A	-3.16	120.61	125.42
3	A	401	HEM	CMA-C3A-C4A	-3.15	120.62	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	HEM	C3B-C4B-NB	-3.09	107.25	109.47
3	D	401	HEM	CHD-C4C-NC	-3.07	121.11	124.45
3	D	401	HEM	CAA-C2A-C3A	3.02	133.85	127.07
3	D	401	HEM	CHA-C4D-ND	3.01	128.09	124.37
3	D	401	HEM	O2A-CGA-O1A	-3.01	115.59	123.33
2	A	402	TRP	OXT-C-O	-2.99	117.31	124.08
3	G	401	HEM	C4C-CHD-C1D	2.98	132.36	126.02
3	E	401	HEM	C4C-NC-C1C	2.97	110.66	105.82
3	H	401	HEM	O1A-CGA-CBA	-2.97	113.69	123.09
3	H	401	HEM	CHD-C4C-NC	2.94	127.65	124.45
3	F	401	HEM	CBA-CAA-C2A	-2.93	104.44	112.53
3	C	401	HEM	CHA-C4D-C3D	-2.92	119.84	125.23
3	G	401	HEM	C2B-C1B-NB	-2.91	106.49	109.84
3	H	401	HEM	O2A-CGA-CBA	2.91	123.18	114.00
3	E	401	HEM	CHD-C4C-NC	2.91	127.62	124.45
3	B	401	HEM	CMB-C2B-C1B	2.90	129.57	125.03
3	D	401	HEM	CMA-C3A-C4A	-2.89	121.03	125.42
3	C	401	HEM	CHC-C4B-C3B	-2.87	119.34	125.07
3	C	401	HEM	CMD-C2D-C1D	2.87	129.52	125.03
3	C	401	HEM	C3B-C2B-C1B	-2.85	104.27	106.41
2	D	403	TRP	OXT-C-O	-2.82	117.69	124.08
3	B	401	HEM	CBD-CAD-C3D	-2.82	104.75	112.53
3	D	401	HEM	CAA-C2A-C1A	-2.80	119.48	124.94
3	F	401	HEM	CHA-C1A-NA	2.79	128.91	123.86
3	A	401	HEM	CBC-CAC-C3C	-2.77	113.70	127.53
3	A	401	HEM	C4D-ND-C1D	2.74	108.45	105.21
3	A	401	HEM	O2A-CGA-CBA	2.73	122.62	114.00
3	A	401	HEM	C3D-C4D-ND	-2.72	107.19	110.17
3	H	401	HEM	O2D-CGD-CBD	2.71	122.57	114.00
3	D	401	HEM	O2A-CGA-CBA	2.71	122.57	114.00
3	D	401	HEM	C1C-CHC-C4B	2.71	131.78	126.02
3	A	401	HEM	C4B-C3B-C2B	2.71	109.77	107.28
3	D	401	HEM	CAD-C3D-C4D	2.70	129.41	124.70
3	B	401	HEM	CAC-C3C-C4C	2.70	131.26	124.82
3	D	401	HEM	C4B-C3B-C2B	2.70	109.76	107.28
3	B	401	HEM	C2A-C1A-NA	-2.69	107.17	110.15
3	H	401	HEM	CBC-CAC-C3C	-2.69	114.09	127.53
3	G	401	HEM	CBD-CAD-C3D	-2.64	105.23	112.53
3	E	401	HEM	C4C-CHD-C1D	2.64	131.62	126.02
3	E	401	HEM	CHD-C1D-C2D	2.62	129.17	125.03
3	H	401	HEM	CHA-C4D-ND	2.62	127.61	124.37
3	F	401	HEM	C4C-C3C-C2C	2.62	109.08	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	HEM	CBC-CAC-C3C	-2.62	114.46	127.53
3	E	401	HEM	C2B-C1B-NB	-2.60	106.85	109.84
3	C	401	HEM	O2D-CGD-CBD	2.58	122.16	114.00
3	E	401	HEM	C2C-C1C-NC	-2.58	104.87	109.64
3	E	401	HEM	C3D-C4D-ND	-2.55	107.37	110.17
3	B	401	HEM	CAC-C3C-C2C	-2.55	120.14	128.43
3	D	401	HEM	CHD-C1D-ND	2.55	127.16	124.42
3	G	401	HEM	C4A-C3A-C2A	2.53	109.72	106.82
3	D	401	HEM	CHD-C1D-C2D	-2.53	121.03	125.03
3	E	401	HEM	C3B-C2B-C1B	2.53	108.31	106.41
3	D	401	HEM	CMA-C3A-C2A	2.52	130.98	125.62
3	D	401	HEM	CHD-C4C-C3C	2.50	129.43	125.21
3	C	401	HEM	O2A-CGA-O1A	-2.50	116.89	123.33
3	G	401	HEM	CAD-C3D-C4D	2.50	129.05	124.70
3	G	401	HEM	C3A-C4A-NA	-2.50	106.14	110.14
3	H	401	HEM	CHC-C4B-NB	2.49	127.10	124.42
3	G	401	HEM	C2A-C1A-NA	-2.48	107.40	110.15
3	G	401	HEM	C4C-NC-C1C	2.46	109.83	105.82
2	E	402	TRP	CA-CB-CG	2.46	118.16	113.49
3	G	401	HEM	C3D-C4D-ND	-2.44	107.49	110.17
2	C	403	TRP	OXT-C-O	-2.44	118.54	124.08
3	G	401	HEM	CHA-C4D-ND	2.42	127.36	124.37
3	H	401	HEM	C4A-NA-C1A	2.42	109.76	105.82
3	H	401	HEM	C4C-C3C-C2C	2.38	108.88	106.81
3	D	401	HEM	CAA-CBA-CGA	2.36	119.94	113.67
3	D	401	HEM	C3D-C4D-ND	2.36	112.76	110.17
3	E	401	HEM	C2D-C1D-ND	-2.35	107.19	109.90
3	H	401	HEM	C4B-C3B-C2B	2.34	109.43	107.28
3	H	401	HEM	O1D-CGD-CBD	-2.33	115.70	123.09
3	A	401	HEM	C1D-C2D-C3D	-2.33	104.53	106.98
3	G	401	HEM	C3B-C2B-C1B	2.33	108.16	106.41
3	F	401	HEM	CHD-C1D-C2D	2.33	128.70	125.03
3	F	401	HEM	CAD-C3D-C2D	-2.32	123.51	127.87
3	B	401	HEM	C3C-C2C-C1C	2.32	109.24	107.05
3	H	401	HEM	CHD-C1D-ND	2.31	126.91	124.42
3	A	401	HEM	CHD-C1D-C2D	-2.31	121.38	125.03
3	C	401	HEM	CHA-C1A-NA	-2.30	119.69	123.86
3	C	401	HEM	CHD-C1D-ND	2.29	126.89	124.42
3	H	401	HEM	CMC-C2C-C1C	2.29	128.76	124.73
2	C	402	TRP	OXT-C-O	-2.28	118.90	124.08
3	A	401	HEM	CAA-CBA-CGA	-2.28	107.63	113.67
3	D	401	HEM	CHC-C1C-NC	-2.26	121.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	402	TRP	OXT-C-O	-2.26	118.95	124.08
3	A	401	HEM	C3B-C4B-NB	-2.26	107.85	109.47
3	F	401	HEM	C2A-C1A-NA	-2.26	107.65	110.15
3	C	401	HEM	CAB-C3B-C4B	-2.24	114.47	124.39
3	E	401	HEM	CBA-CAA-C2A	-2.24	106.34	112.53
3	E	401	HEM	CHC-C4B-C3B	2.22	129.50	125.07
3	C	401	HEM	C1C-CHC-C4B	-2.21	121.32	126.02
3	F	401	HEM	CHA-C4D-C3D	2.19	129.27	125.23
3	B	401	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
3	B	401	HEM	O2A-CGA-CBA	2.19	120.91	114.00
3	F	401	HEM	CAD-CBD-CGD	-2.18	107.88	113.67
3	E	401	HEM	C3C-C2C-C1C	2.17	109.10	107.05
3	B	401	HEM	CBC-CAC-C3C	-2.14	116.83	127.53
3	G	401	HEM	CAD-CBD-CGD	-2.13	108.01	113.67
3	H	401	HEM	CAD-CBD-CGD	-2.11	108.06	113.67
3	H	401	HEM	CMC-C2C-C3C	-2.11	123.32	128.43
3	H	401	HEM	CMB-C2B-C1B	2.11	128.33	125.03
3	F	401	HEM	O2D-CGD-CBD	2.11	120.65	114.00
3	G	401	HEM	CHD-C4C-C3C	2.11	128.76	125.21
3	H	401	HEM	CMD-C2D-C3D	2.10	131.83	126.15
3	D	401	HEM	O2D-CGD-O1D	-2.10	117.94	123.33
2	B	403	TRP	OXT-C-O	-2.09	119.33	124.08
3	G	401	HEM	CHC-C1C-C2C	2.09	129.83	125.49
3	C	401	HEM	CAB-C3B-C2B	2.08	135.21	128.43
3	E	401	HEM	C4C-C3C-C2C	2.07	108.61	106.81
3	H	401	HEM	C2B-C1B-NB	-2.04	107.49	109.84
3	B	401	HEM	CMC-C2C-C3C	-2.03	123.51	128.43
3	F	401	HEM	CBD-CAD-C3D	-2.03	106.92	112.53
3	C	401	HEM	CAA-C2A-C3A	2.03	131.62	127.07
3	H	401	HEM	C4C-NC-C1C	2.03	109.13	105.82
3	B	401	HEM	O2D-CGD-CBD	2.02	120.37	114.00
3	E	401	HEM	O1D-CGD-CBD	-2.02	116.70	123.09
3	D	401	HEM	C1B-NB-C4B	-2.01	102.83	105.21
3	D	401	HEM	C4D-C3D-C2D	-2.00	103.97	106.89
3	A	401	HEM	O2A-CGA-O1A	-2.00	118.18	123.33

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	HEM	C2B-C3B-CAB-CBB
3	B	401	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	E	401	HEM	C2B-C3B-CAB-CBB
3	E	401	HEM	C4B-C3B-CAB-CBB
3	H	401	HEM	C2C-C3C-CAC-CBC
3	H	401	HEM	C4C-C3C-CAC-CBC
3	A	401	HEM	C2C-C3C-CAC-CBC
3	B	401	HEM	C4B-C3B-CAB-CBB
2	G	402	TRP	N-CA-CB-CG
2	E	402	TRP	CA-CB-CG-CD2
2	H	402	TRP	CA-CB-CG-CD2
2	A	402	TRP	CA-CB-CG-CD1
2	C	402	TRP	CA-CB-CG-CD1
2	F	402	TRP	CA-CB-CG-CD2
2	B	402	TRP	CA-CB-CG-CD1
2	H	402	TRP	CA-CB-CG-CD1
3	G	401	HEM	C2B-C3B-CAB-CBB
2	B	402	TRP	CA-CB-CG-CD2
2	D	402	TRP	CA-CB-CG-CD1
2	E	402	TRP	CA-CB-CG-CD1
2	F	402	TRP	CA-CB-CG-CD1
3	A	401	HEM	C4B-C3B-CAB-CBB
2	C	402	TRP	OXT-C-CA-CB
2	D	402	TRP	CA-CB-CG-CD2
2	A	402	TRP	N-CA-CB-CG
2	B	402	TRP	N-CA-CB-CG
2	C	402	TRP	N-CA-CB-CG
2	E	402	TRP	N-CA-CB-CG
2	F	402	TRP	N-CA-CB-CG
2	H	402	TRP	N-CA-CB-CG
2	C	402	TRP	CA-CB-CG-CD2
2	A	402	TRP	CA-CB-CG-CD2
2	A	402	TRP	O-C-CA-CB
2	B	402	TRP	O-C-CA-CB
2	A	402	TRP	OXT-C-CA-CB
2	C	402	TRP	O-C-CA-CB
2	D	402	TRP	O-C-CA-CB
2	D	402	TRP	OXT-C-CA-CB
3	F	401	HEM	C2C-C3C-CAC-CBC
2	B	402	TRP	OXT-C-CA-CB
2	F	402	TRP	OXT-C-CA-CB
2	H	402	TRP	O-C-CA-CB
3	A	401	HEM	C4C-C3C-CAC-CBC
3	G	401	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	E	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	C2A-CAA-CBA-CGA
3	A	401	HEM	CAA-CBA-CGA-O1A
3	G	401	HEM	CAA-CBA-CGA-O1A
3	F	401	HEM	CAA-CBA-CGA-O2A
2	D	402	TRP	N-CA-CB-CG
2	G	402	TRP	O-C-CA-N
3	D	401	HEM	CAA-CBA-CGA-O2A
3	H	401	HEM	CAA-CBA-CGA-O2A
3	B	401	HEM	CAA-CBA-CGA-O2A
3	F	401	HEM	CAA-CBA-CGA-O1A
2	F	402	TRP	O-C-CA-CB
2	H	402	TRP	OXT-C-CA-CB
3	G	401	HEM	CAA-CBA-CGA-O2A
3	E	401	HEM	CAA-CBA-CGA-O1A
3	A	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAA-CBA-CGA-O1A
3	H	401	HEM	CAA-CBA-CGA-O1A
3	B	401	HEM	CAA-CBA-CGA-O1A
3	C	401	HEM	CAA-CBA-CGA-O2A
3	B	401	HEM	CAD-CBD-CGD-O2D
2	F	402	TRP	C-CA-CB-CG
2	G	402	TRP	C-CA-CB-CG
3	C	401	HEM	CAA-CBA-CGA-O1A
2	G	402	TRP	CA-CB-CG-CD2
2	G	402	TRP	CA-CB-CG-CD1
3	B	401	HEM	CAD-CBD-CGD-O1D
2	C	402	TRP	OXT-C-CA-N
3	F	401	HEM	CAD-CBD-CGD-O2D
2	E	403	TRP	OXT-C-CA-N
3	H	401	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

14 monomers are involved in 40 short contacts:

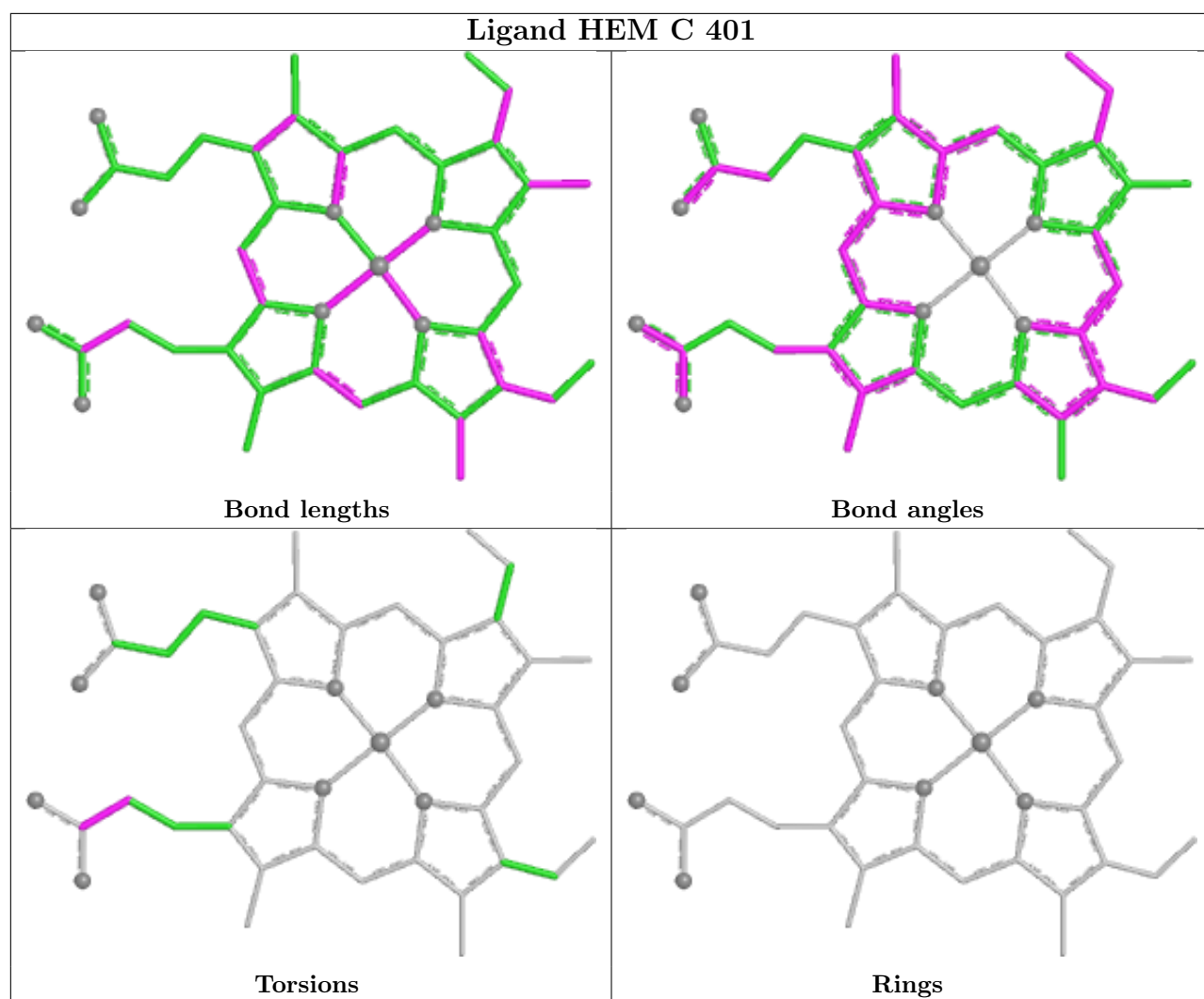
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	403	TRP	1	0
2	A	402	TRP	2	0
2	A	403	TRP	1	0
2	H	402	TRP	2	0
3	C	401	HEM	2	0
3	H	401	HEM	5	0

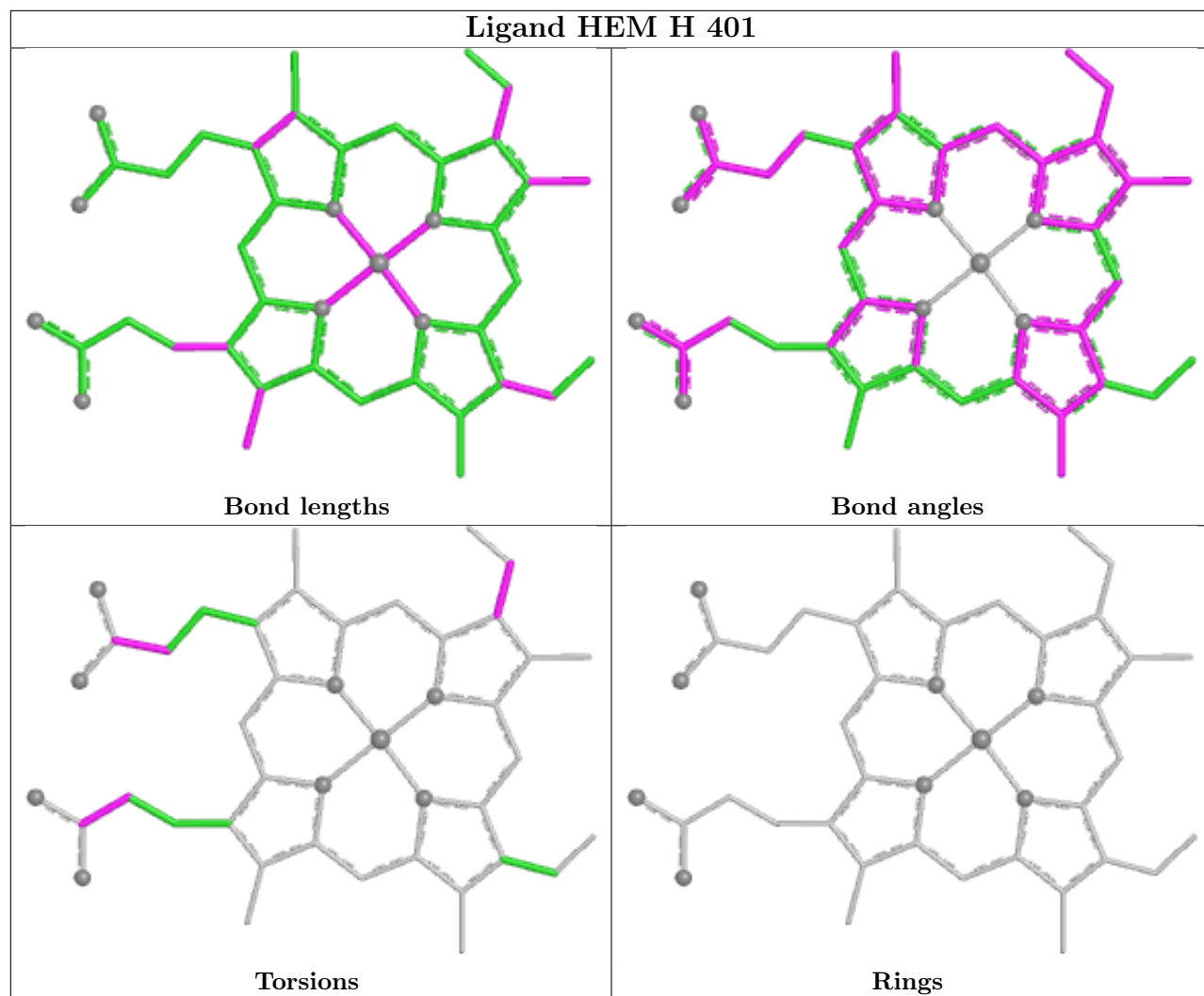
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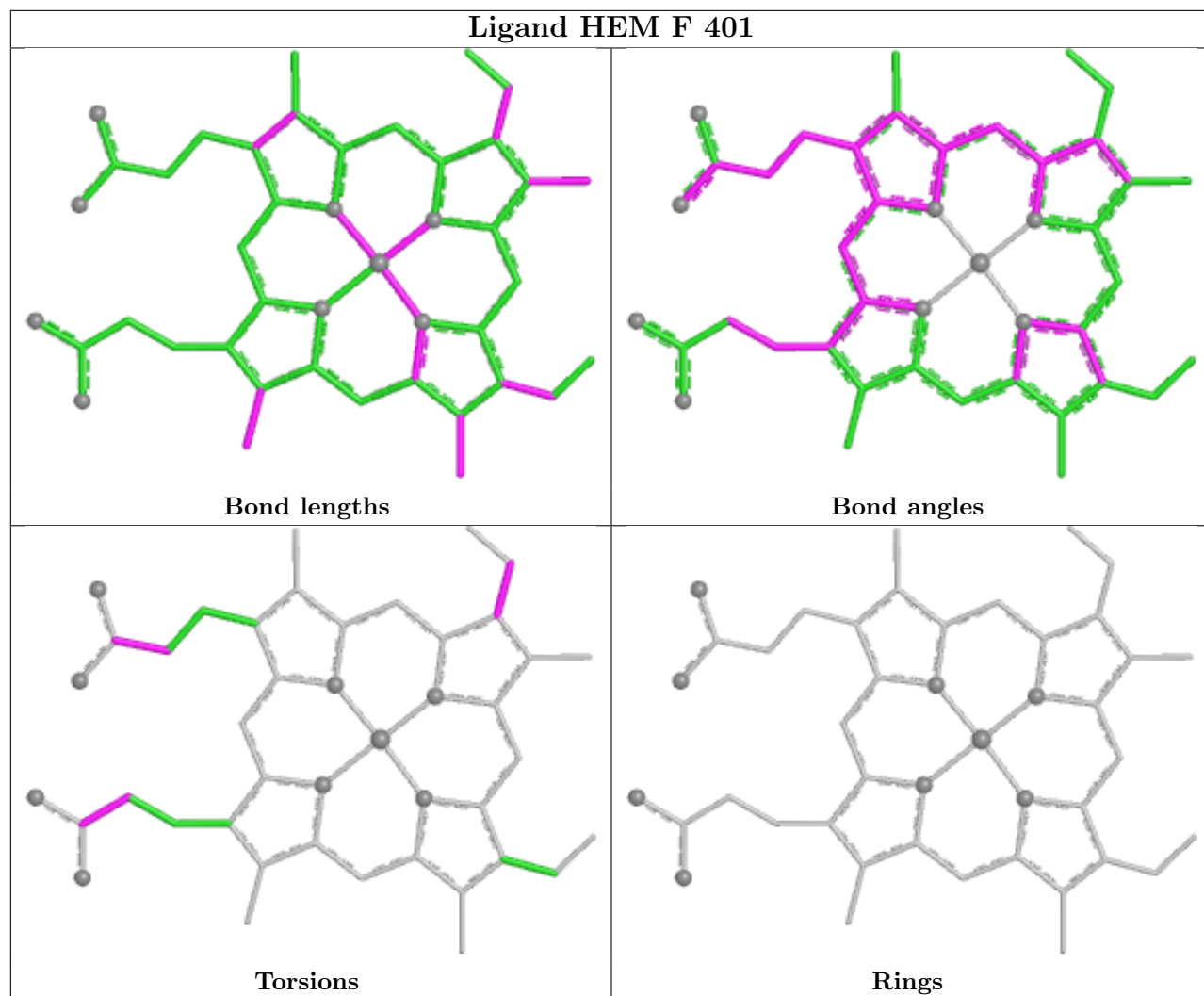
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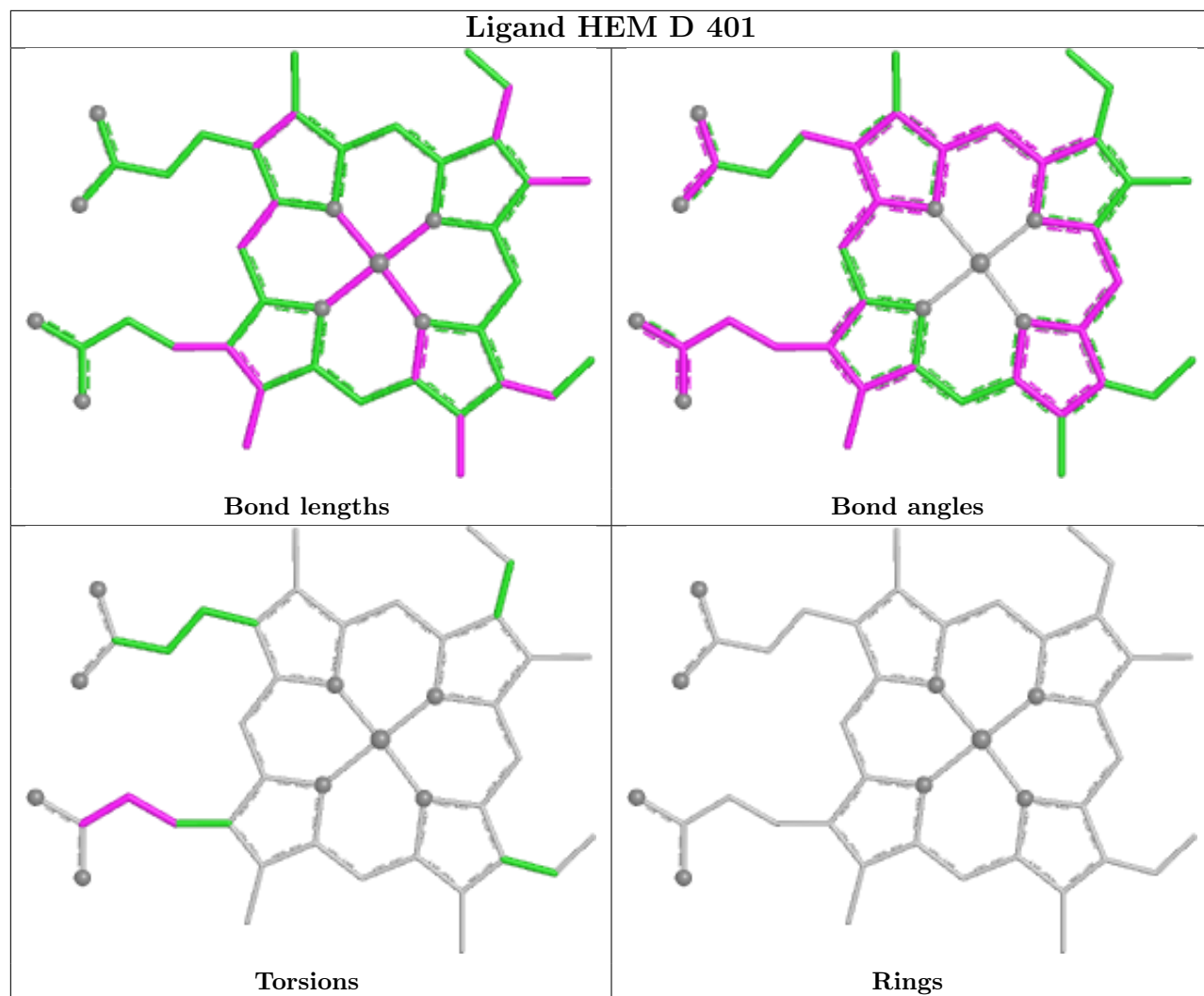
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	HEM	5	0
2	G	402	TRP	1	0
3	D	401	HEM	4	0
3	B	401	HEM	4	0
2	C	402	TRP	3	0
3	A	401	HEM	1	0
3	G	401	HEM	3	0
3	E	401	HEM	7	0

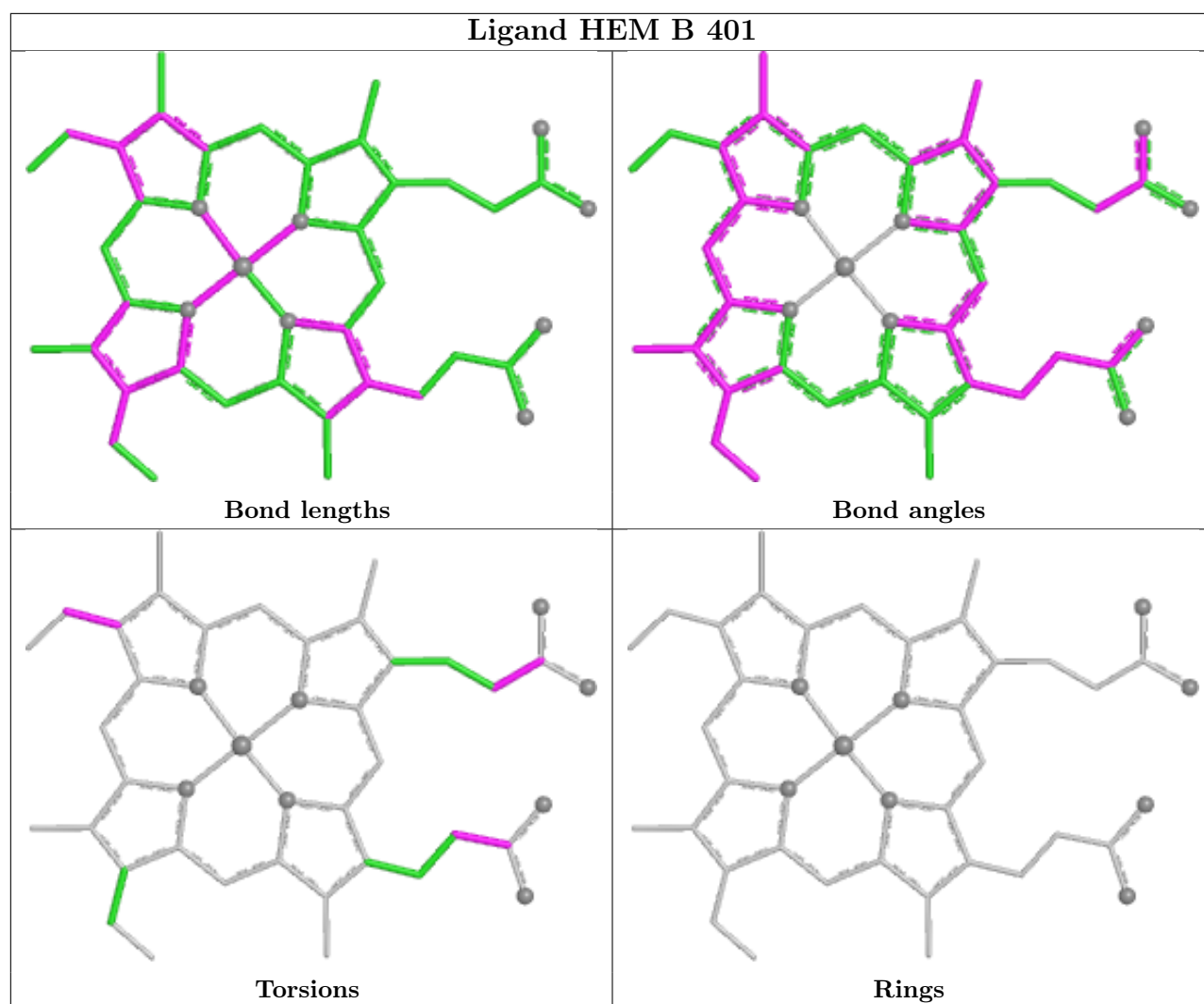
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

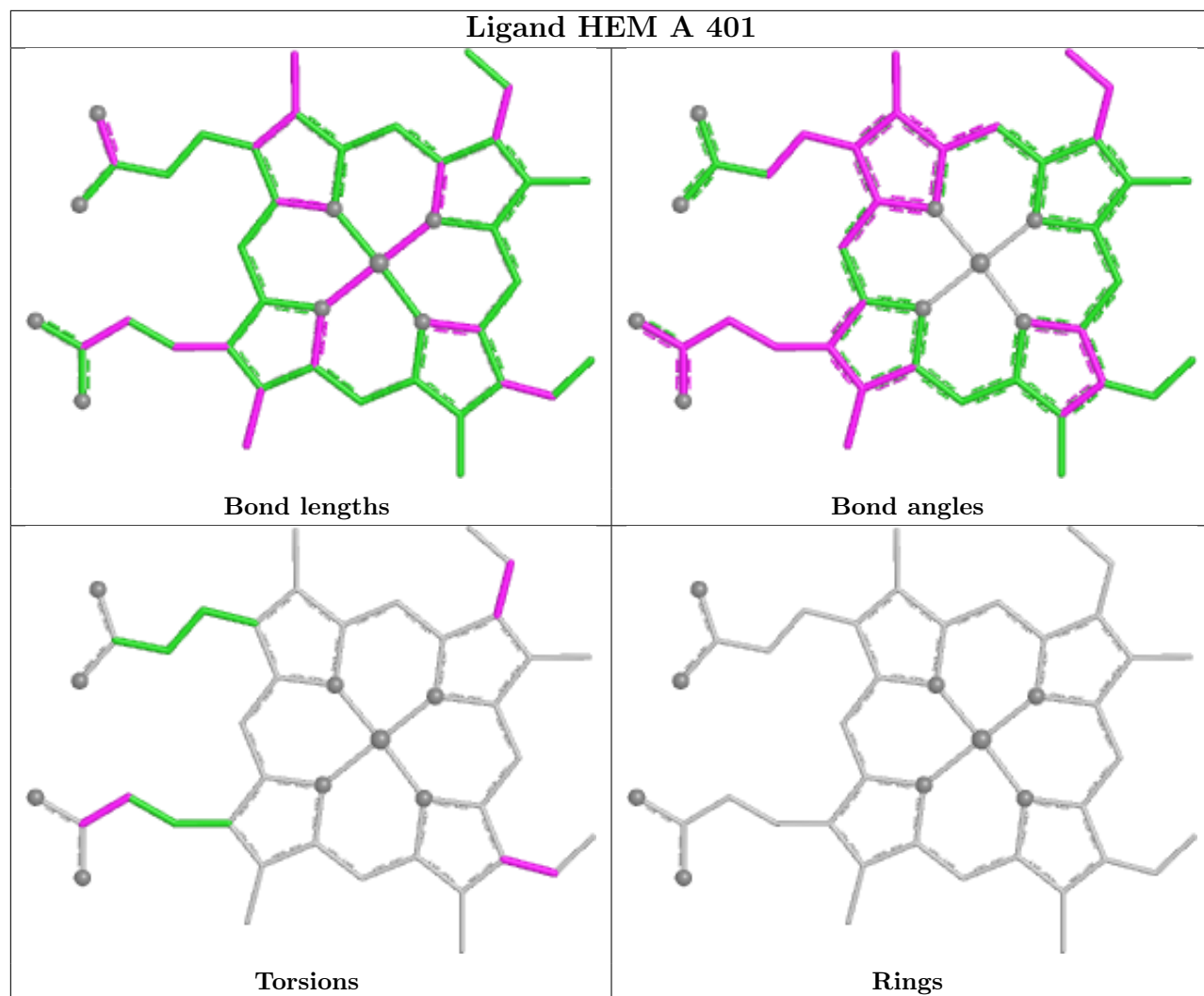


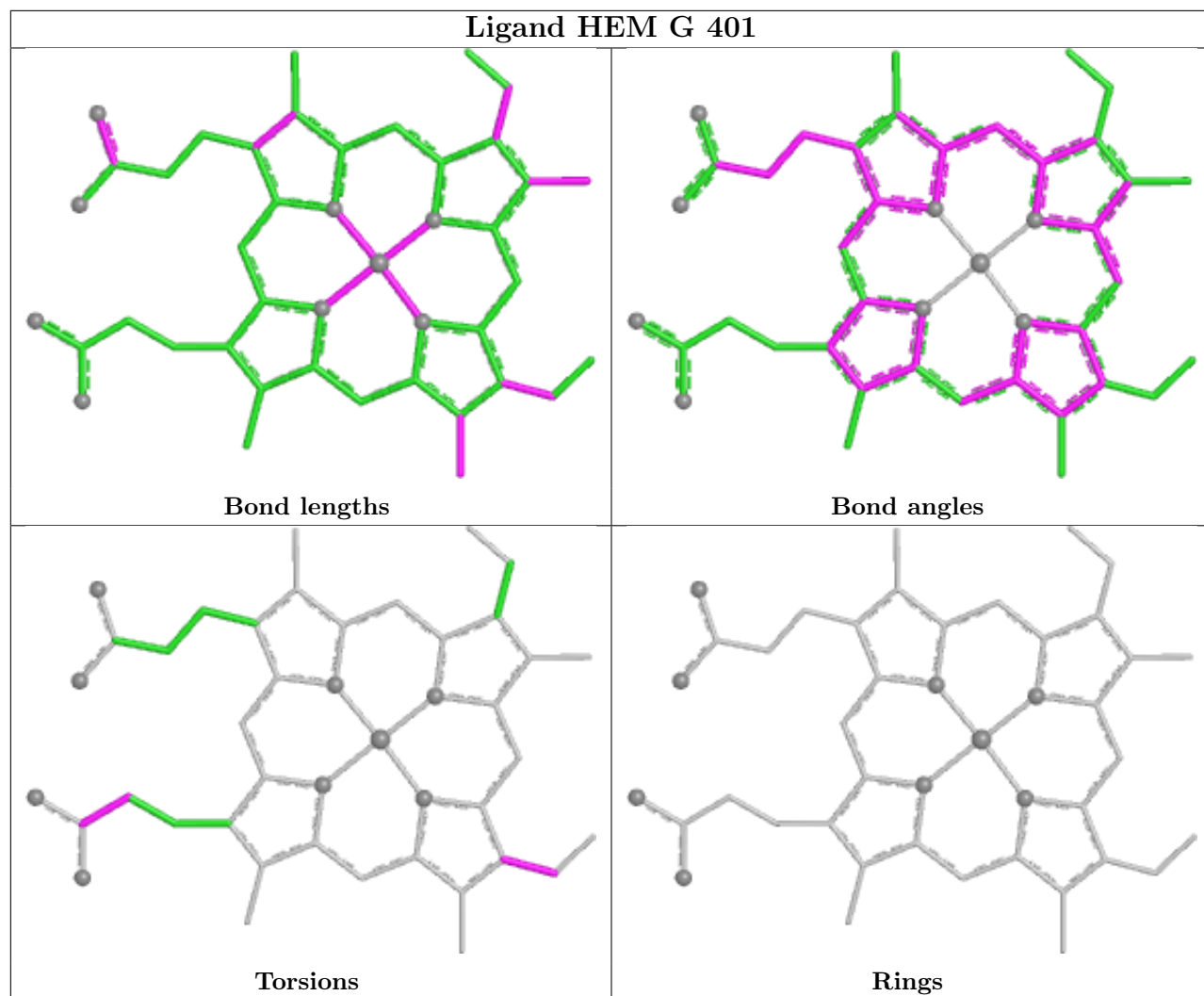


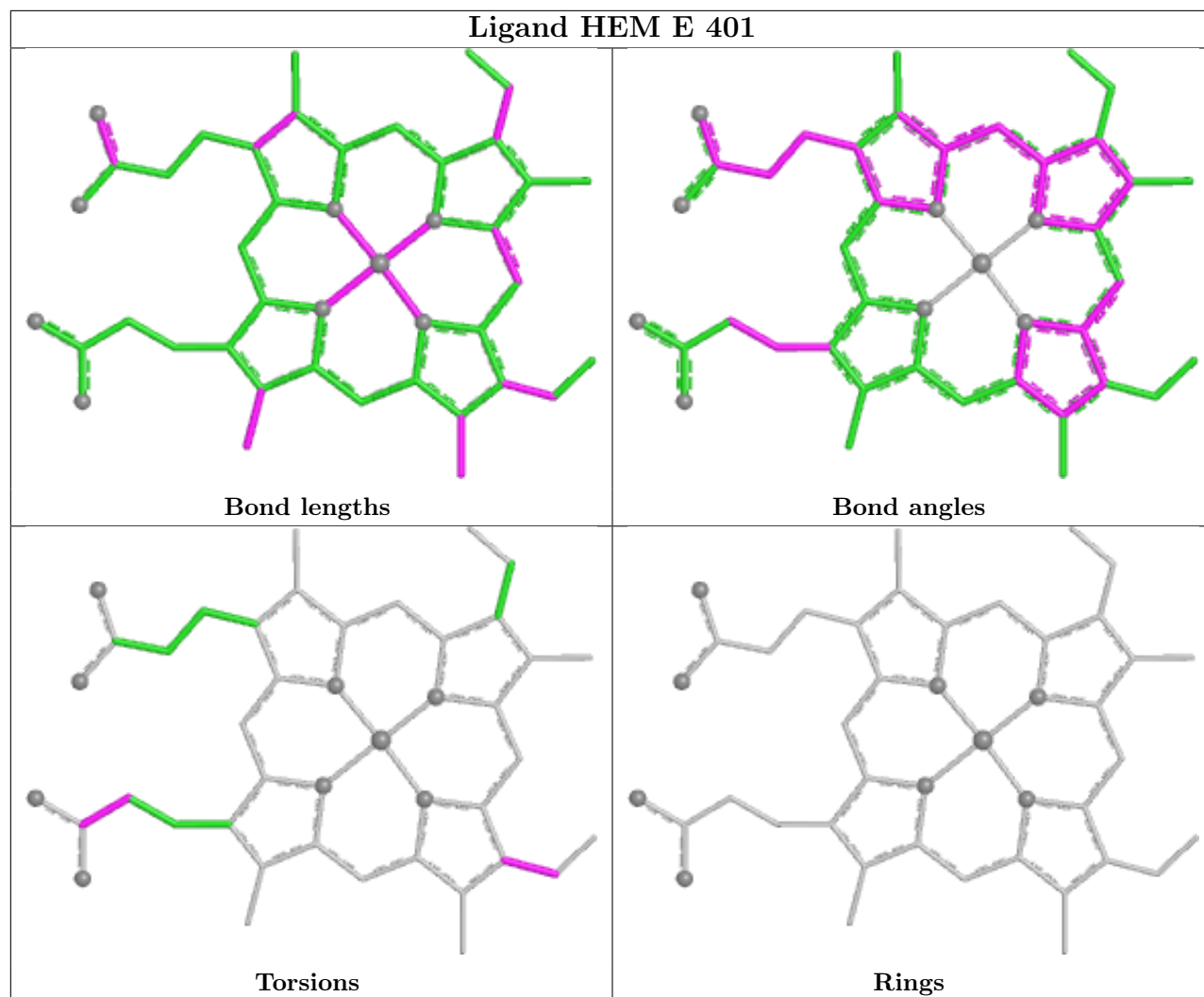












5.7 Other polymers [i](#)

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/306 (90%)	-0.32	3 (1%) 78 80	5, 15, 27, 45	0
1	B	280/306 (91%)	-0.27	1 (0%) 88 90	4, 15, 31, 42	0
1	C	272/306 (88%)	-0.06	8 (2%) 53 57	10, 19, 41, 54	0
1	D	262/306 (85%)	-0.16	1 (0%) 88 90	9, 19, 38, 44	0
1	E	260/306 (84%)	-0.02	4 (1%) 72 76	9, 24, 37, 43	0
1	F	250/306 (81%)	0.19	7 (2%) 55 59	15, 26, 45, 55	0
1	G	262/306 (85%)	0.08	3 (1%) 78 80	9, 25, 42, 47	0
1	H	257/306 (83%)	0.37	13 (5%) 33 37	16, 31, 52, 63	0
All	All	2120/2448 (86%)	-0.03	40 (1%) 66 70	4, 22, 41, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	LEU	4.4
1	C	19	GLU	3.8
1	H	192	TRP	3.6
1	A	7	LEU	3.4
1	G	250	PHE	3.3
1	E	114	MET	3.1
1	C	12	PRO	3.1
1	A	151	TYR	3.0
1	H	197	VAL	3.0
1	H	151	TYR	2.9
1	H	212	ASN	2.8
1	C	17	ASP	2.8
1	F	157	ALA	2.7
1	B	17	ASP	2.7
1	H	198	ALA	2.6
1	C	217	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	154	ALA	2.4
1	F	187	TYR	2.4
1	F	150	ALA	2.4
1	H	154	ALA	2.4
1	H	149	PHE	2.4
1	H	186	GLN	2.4
1	A	17	ASP	2.4
1	C	20	GLY	2.3
1	H	160	ARG	2.3
1	H	194	ALA	2.3
1	H	195	ALA	2.3
1	G	151	TYR	2.3
1	H	146	LEU	2.2
1	F	283	GLY	2.2
1	C	194	ALA	2.2
1	D	283	GLY	2.1
1	E	121	GLY	2.1
1	H	217	TRP	2.1
1	C	197	VAL	2.1
1	E	282	VAL	2.1
1	G	200	ASP	2.1
1	F	133	TYR	2.0
1	F	256	GLY	2.0
1	E	154	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

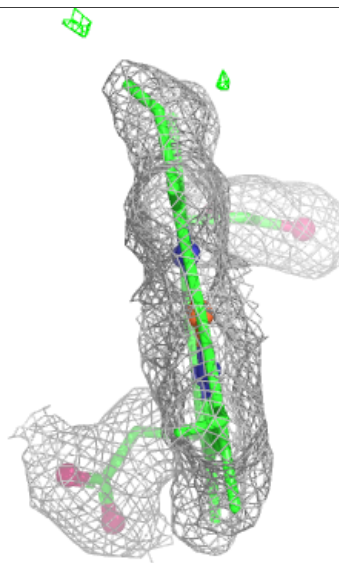
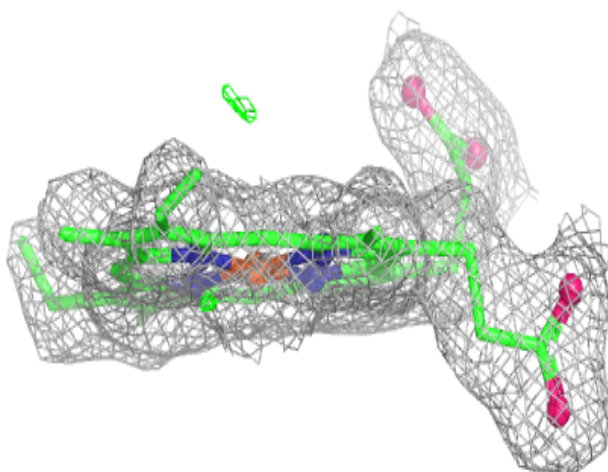
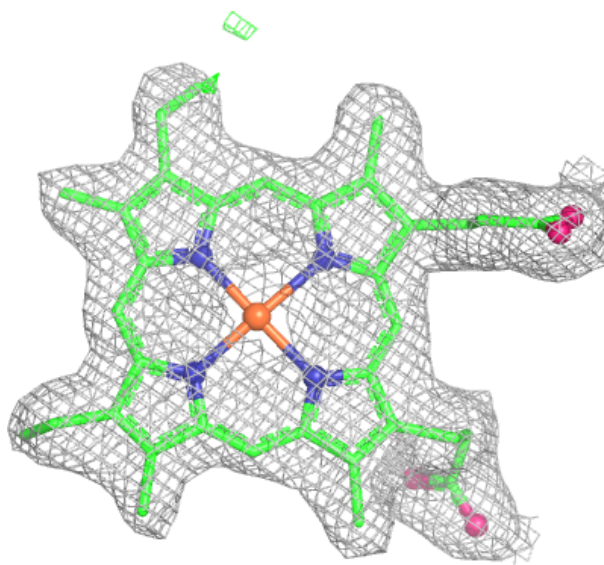
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	H	402	15/15	0.79	0.16	32,36,40,41	0
2	TRP	E	402	15/15	0.82	0.13	29,31,33,36	0
2	TRP	G	402	15/15	0.84	0.13	30,35,40,43	0
2	TRP	E	403	15/15	0.86	0.11	24,27,38,39	0
2	TRP	F	402	15/15	0.91	0.09	25,27,32,35	0
2	TRP	C	403	15/15	0.91	0.08	14,18,27,28	0
2	TRP	D	402	15/15	0.91	0.09	14,18,25,26	0
2	TRP	B	403	15/15	0.92	0.07	12,20,26,26	0
2	TRP	C	402	15/15	0.92	0.09	13,21,28,31	0
2	TRP	A	402	15/15	0.92	0.08	14,16,23,25	0
2	TRP	A	403	15/15	0.93	0.08	14,21,28,28	0
2	TRP	D	403	15/15	0.94	0.07	11,15,27,30	0
2	TRP	B	402	15/15	0.95	0.07	7,9,18,18	0
3	HEM	E	401	43/43	0.96	0.07	11,23,27,34	0
3	HEM	F	401	43/43	0.96	0.08	13,20,27,34	0
3	HEM	G	401	43/43	0.96	0.07	20,25,31,38	0
3	HEM	H	401	43/43	0.96	0.07	17,23,27,28	0
3	HEM	A	401	43/43	0.98	0.06	2,8,13,17	0
3	HEM	B	401	43/43	0.98	0.05	2,5,10,13	0
3	HEM	C	401	43/43	0.98	0.06	4,10,16,19	0
3	HEM	D	401	43/43	0.98	0.05	2,9,17,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

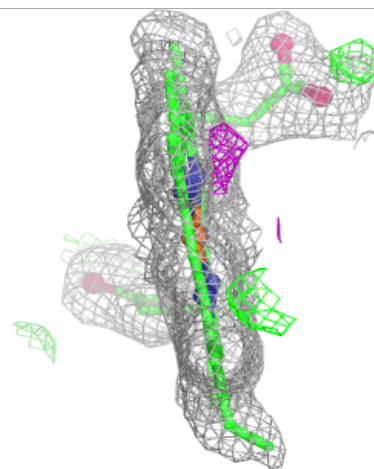
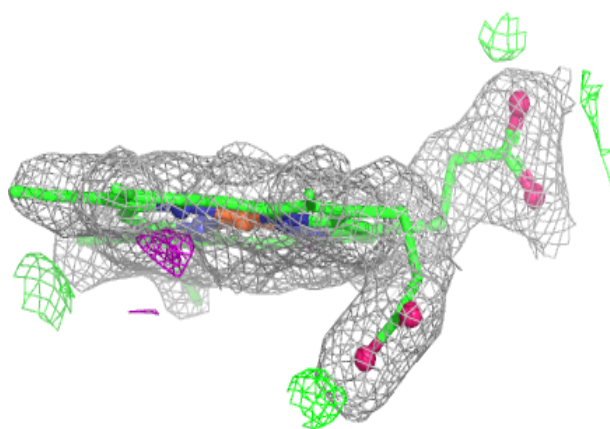
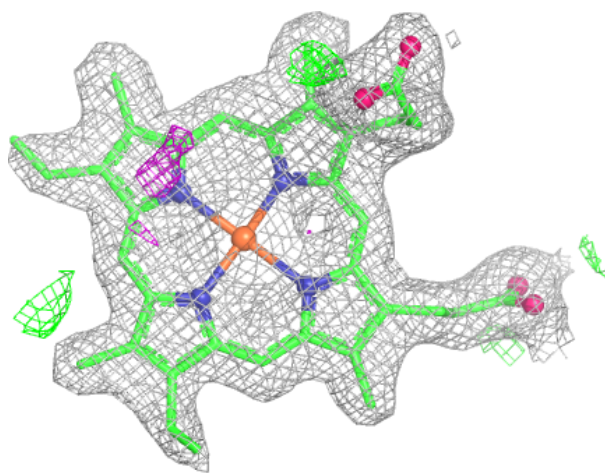
Electron density around HEM E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



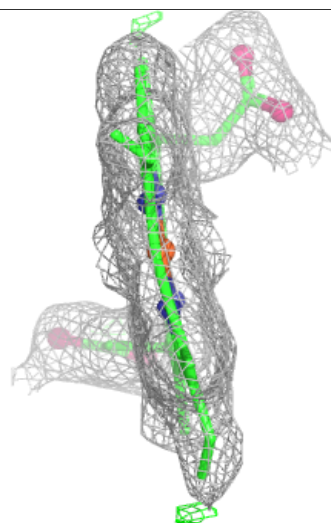
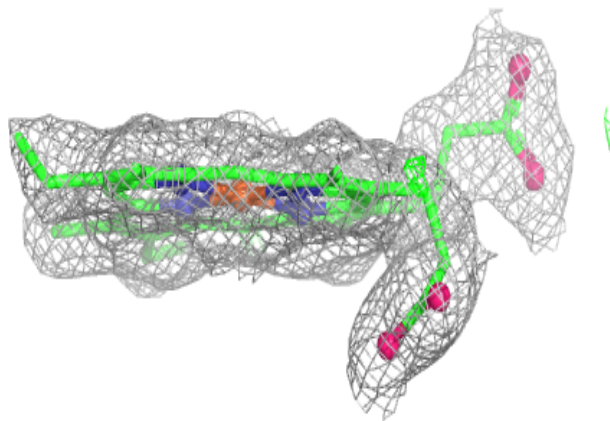
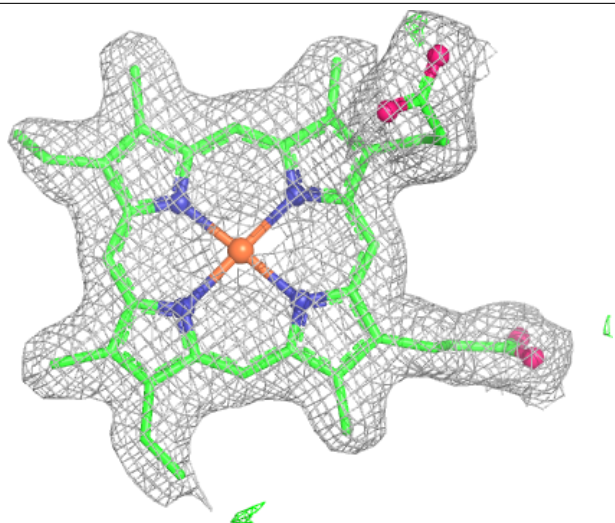
Electron density around HEM F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



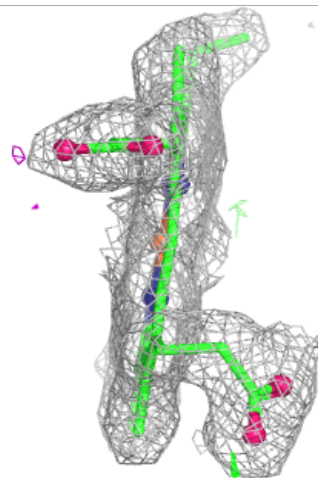
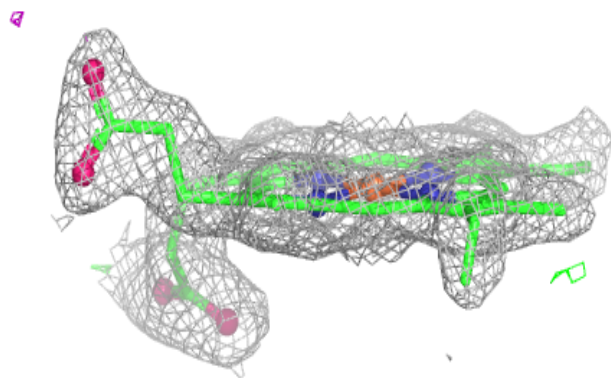
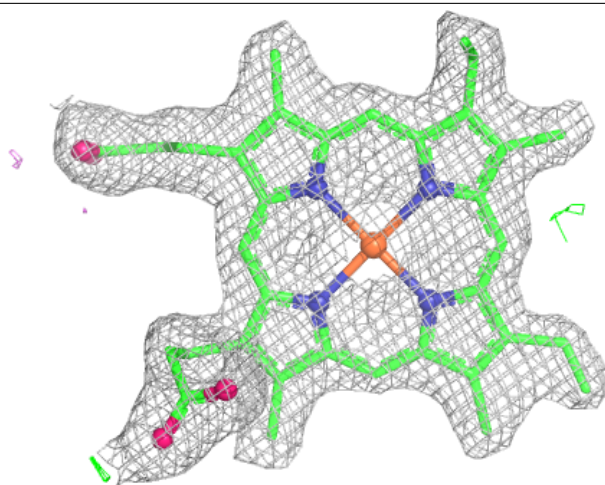
Electron density around HEM G 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



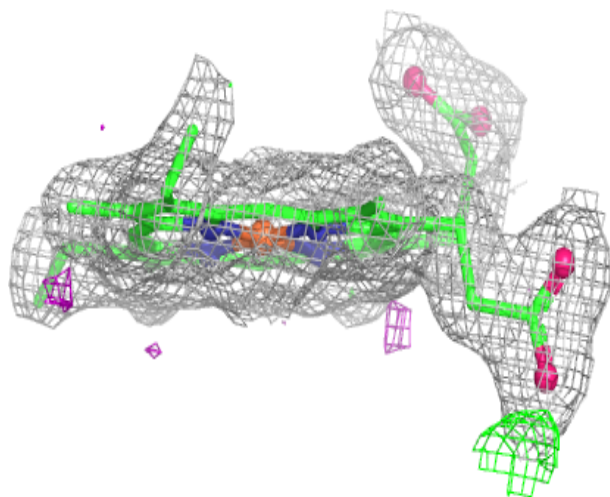
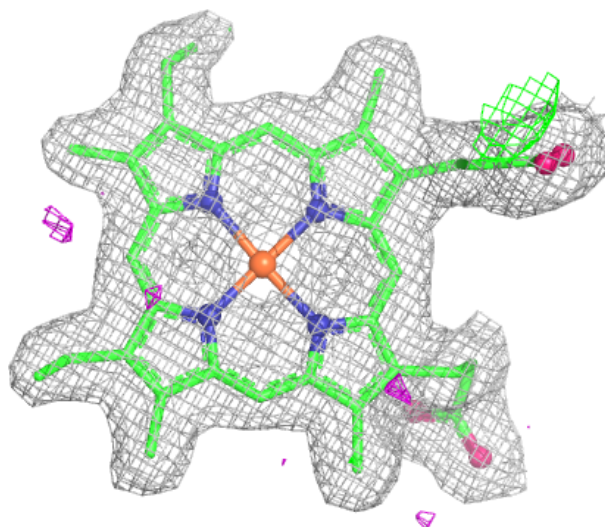
Electron density around HEM H 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



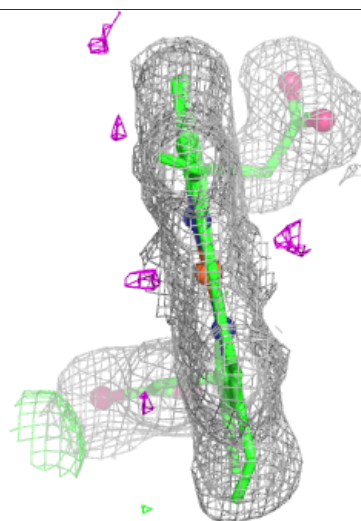
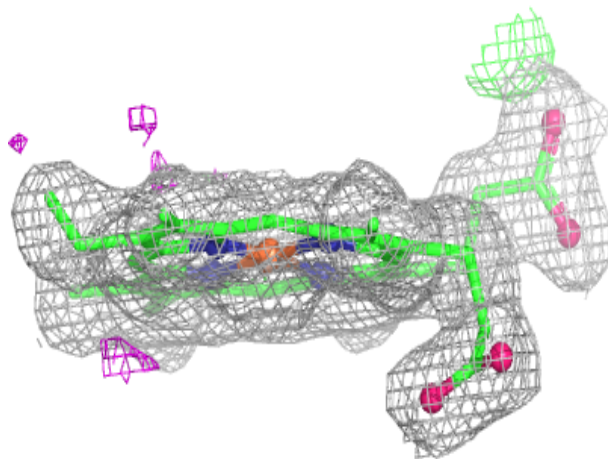
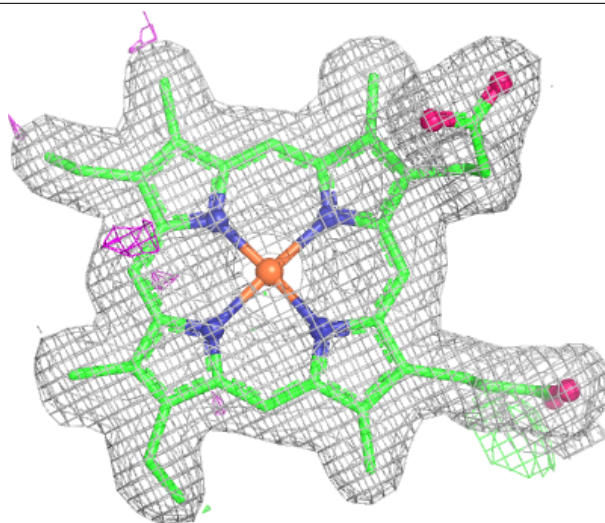
Electron density around HEM A 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



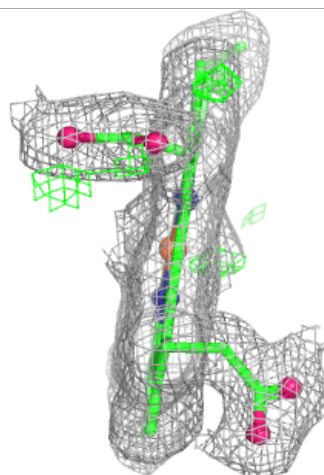
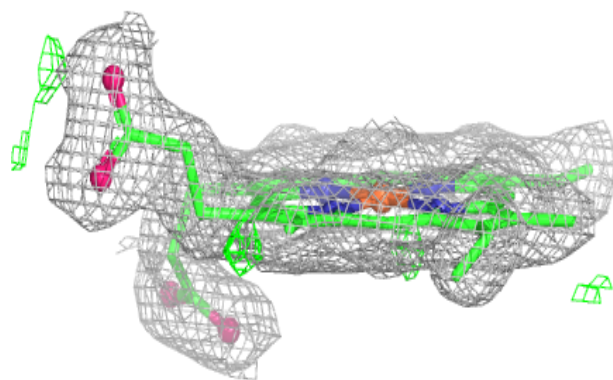
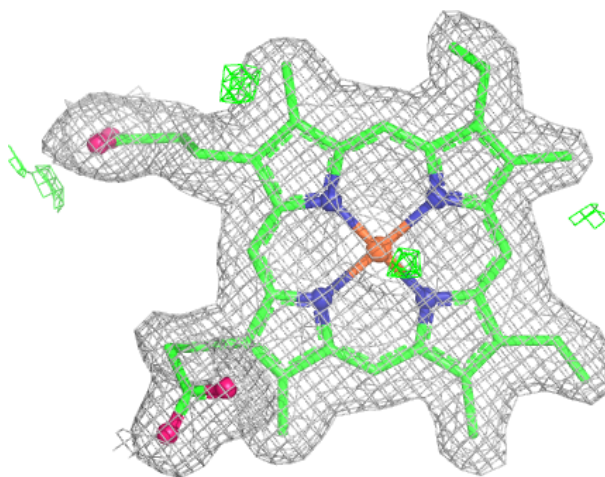
Electron density around HEM B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



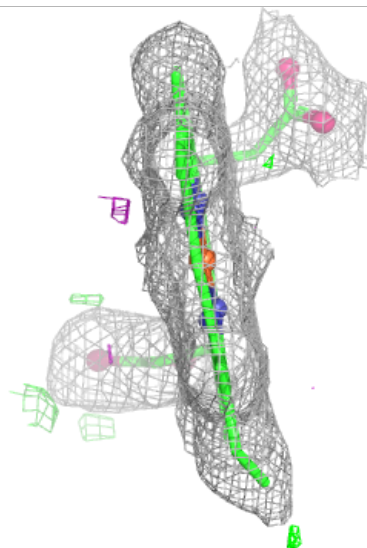
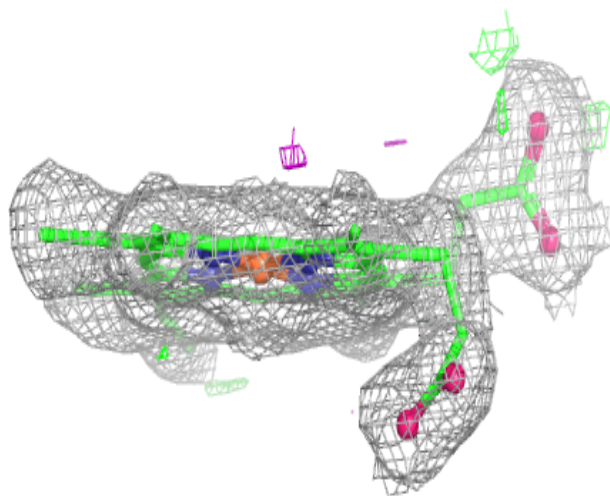
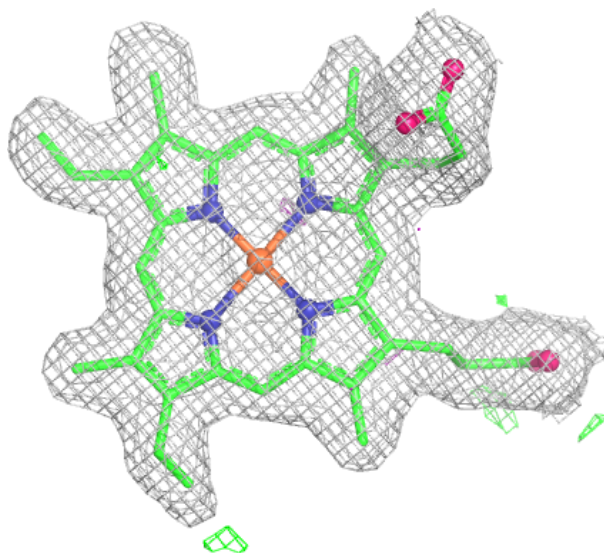
Electron density around HEM C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.