



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 05:42 AM EDT

PDB ID : 3BK9  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

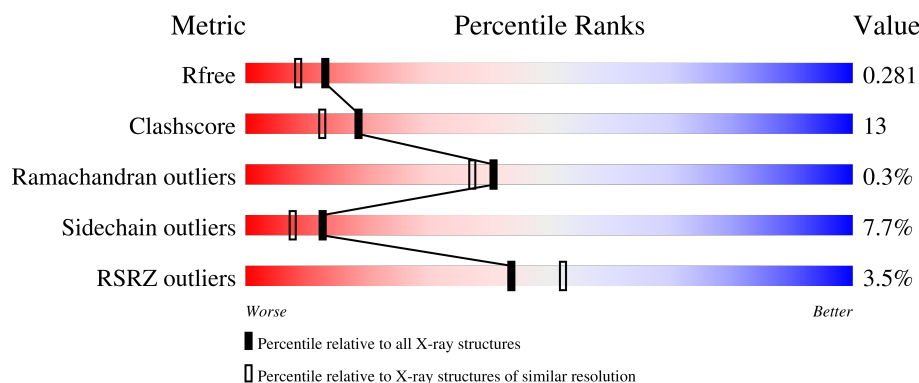
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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  $\geq 3$ , 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	<div> <div>0%</div> <div>64%</div> <div>20%</div> <div>6%</div> <div>9%</div> </div>
1	B	306	<div> <div>2%</div> <div>60%</div> <div>25%</div> <div>6%</div> <div>8%</div> </div>
1	C	306	<div> <div>2%</div> <div>58%</div> <div>25%</div> <div>5%</div> <div>11%</div> </div>
1	D	306	<div> <div>59%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
1	E	306	<div> <div>2%</div> <div>53%</div> <div>26%</div> <div>5%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	306	<div><div><div></div><div></div><div></div><div></div></div><div>4%55%23%••18%</div></div>
1	G	306	<div><div><div></div><div></div><div></div><div></div></div><div>5%53%27%5%•14%</div></div>
1	H	306	<div><div><div></div><div></div><div></div><div></div></div><div>9%59%21%•16%</div></div>

## 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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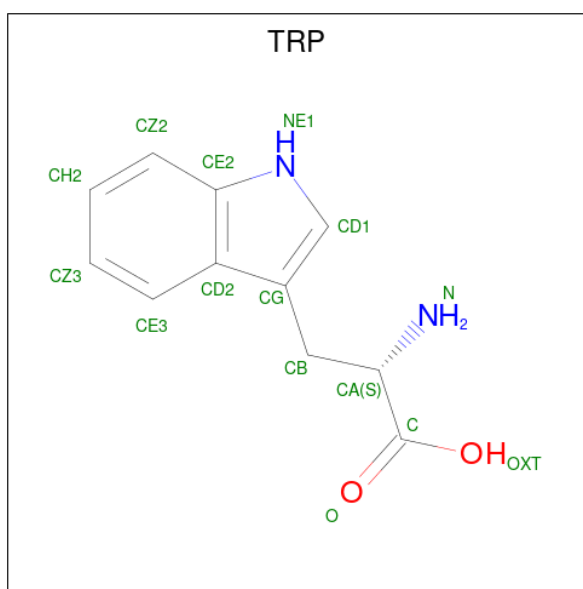
Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP Q8PDA8
B	303	HIS	-	expression tag	UNP Q8PDA8
B	304	HIS	-	expression tag	UNP Q8PDA8
B	305	HIS	-	expression tag	UNP Q8PDA8
B	306	HIS	-	expression tag	UNP Q8PDA8
C	55	ALA	HIS	engineered mutation	UNP Q8PDA8
C	299	LEU	-	expression 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 (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



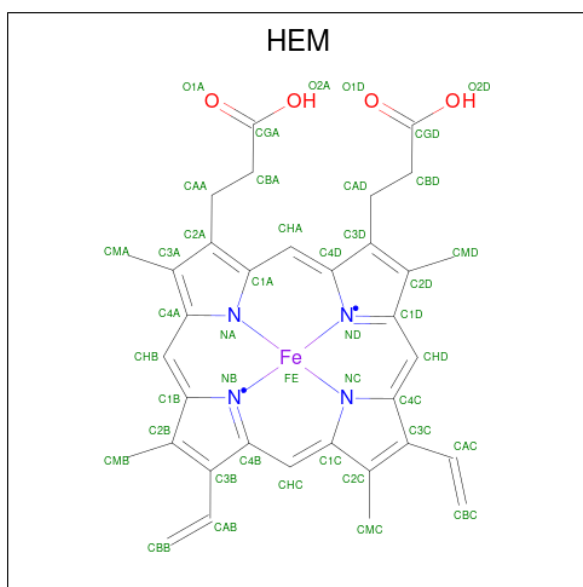
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

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

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



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

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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.

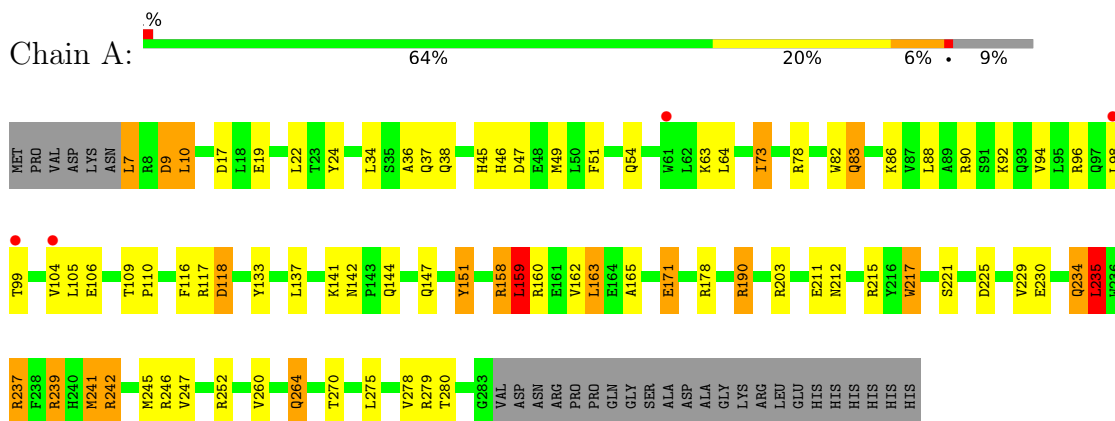
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total 170	O 170	0	0
4	B	152	Total 152	O 152	0	0
4	C	129	Total 129	O 129	0	0
4	D	124	Total 124	O 124	0	0
4	E	133	Total 133	O 133	0	0
4	F	96	Total 96	O 96	0	0
4	G	113	Total 113	O 113	0	0
4	H	99	Total 99	O 99	0	0



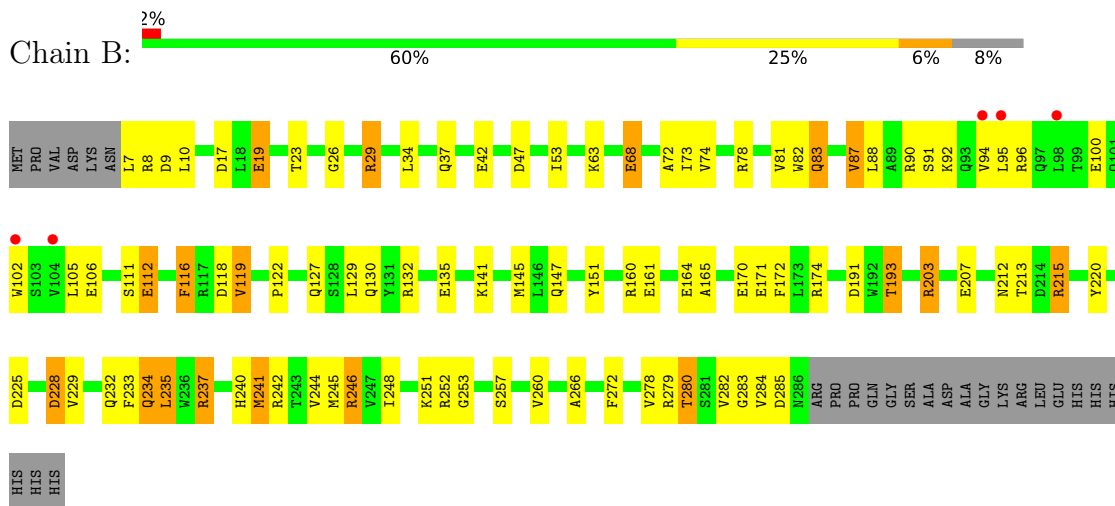
### 3 Residue-property plots [i](#)

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.

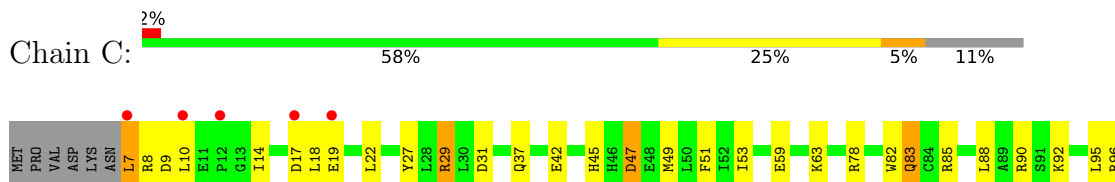
#### • Molecule 1: Tryptophan 2,3-dioxygenase



#### • Molecule 1: Tryptophan 2,3-dioxygenase



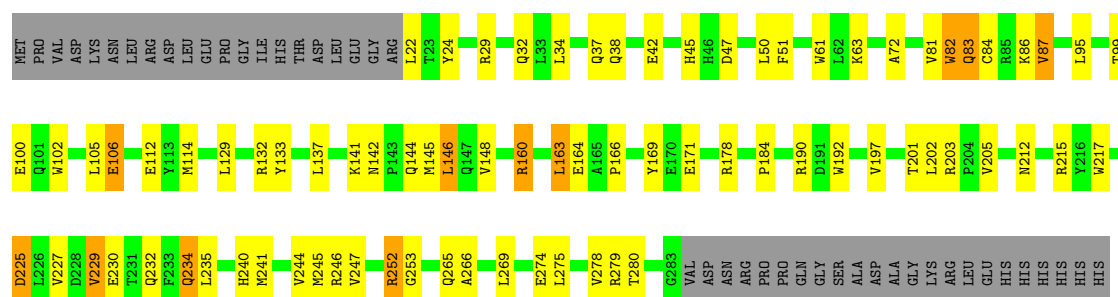
#### • Molecule 1: Tryptophan 2,3-dioxygenase





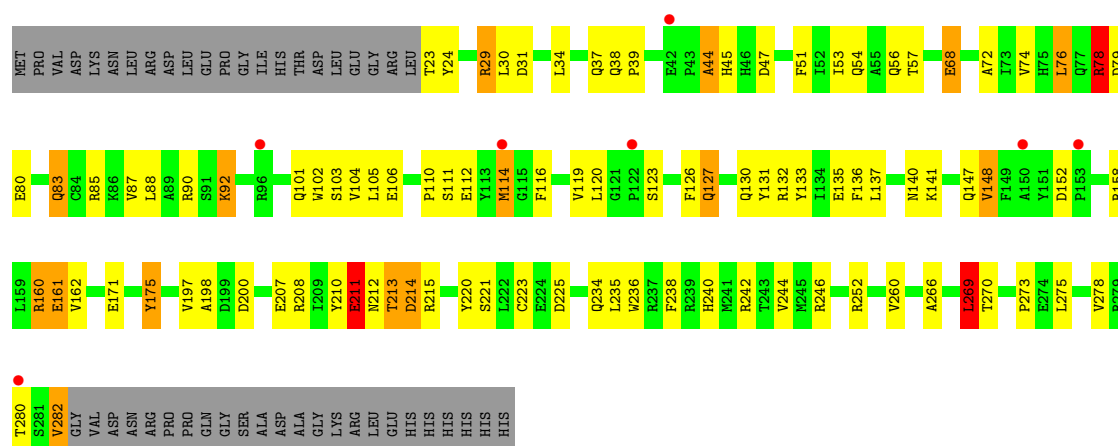
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D: 59% 23% 14%



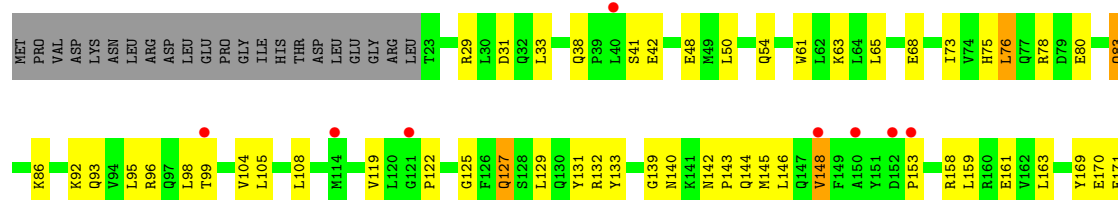
• Molecule 1: Tryptophan 2,3-dioxygenase

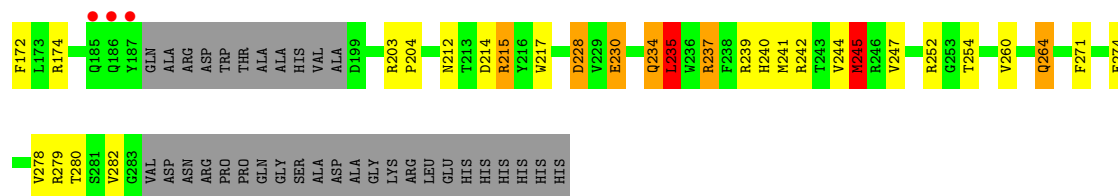
Chain E: 53% 26% 5% 15%



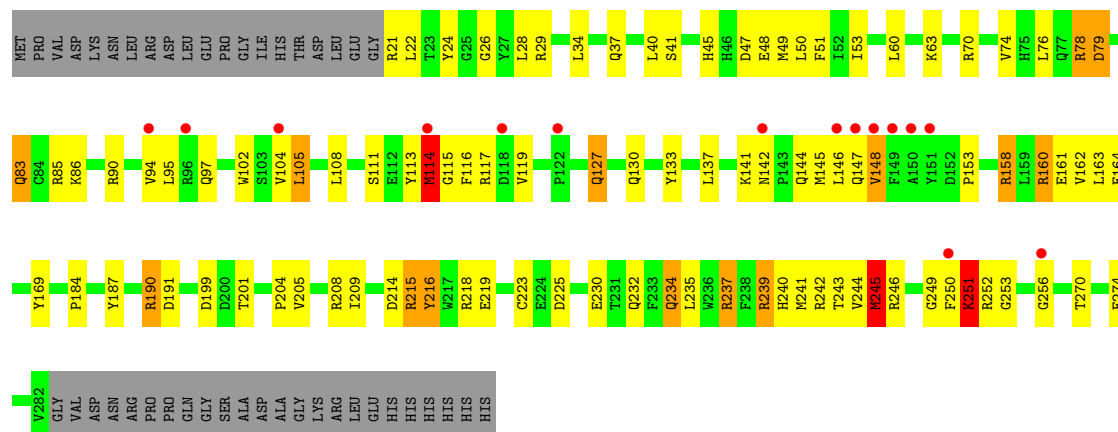
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain F: 55% 23% 18%

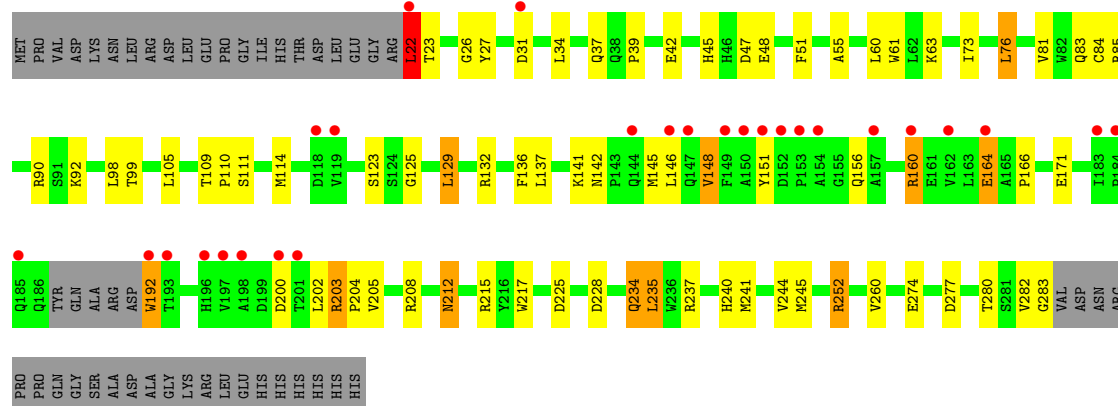




• Molecule 1: Tryptophan 2,3-dioxygenase



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.46	15/2342 (0.6%)	1.35	26/3174 (0.8%)
1	B	1.52	27/2365 (1.1%)	1.50	24/3206 (0.7%)
1	C	1.35	13/2299 (0.6%)	1.31	19/3115 (0.6%)
1	D	1.41	12/2220 (0.5%)	1.17	9/3009 (0.3%)
1	E	1.36	14/2208 (0.6%)	1.24	14/2993 (0.5%)
1	F	1.28	5/2122 (0.2%)	1.16	13/2872 (0.5%)
1	G	1.27	5/2227 (0.2%)	1.21	14/3018 (0.5%)
1	H	1.18	2/2173 (0.1%)	1.05	5/2944 (0.2%)
All	All	1.36	93/17956 (0.5%)	1.26	124/24331 (0.5%)

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 (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	GLU	CG-CD	10.31	1.67	1.51
1	C	106	GLU	CB-CG	8.86	1.69	1.52
1	A	17	ASP	CB-CG	7.96	1.68	1.51
1	D	106	GLU	CB-CG	7.73	1.66	1.52
1	D	106	GLU	CD-OE2	7.31	1.33	1.25
1	H	212	ASN	CB-CG	7.15	1.67	1.51
1	A	212	ASN	CB-CG	7.08	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	84	CYS	CB-SG	-7.08	1.70	1.82
1	A	217	TRP	CB-CG	7.04	1.62	1.50
1	A	221	SER	CB-OG	-6.98	1.33	1.42
1	D	106	GLU	CG-CD	6.96	1.62	1.51
1	E	223	CYS	CB-SG	-6.93	1.70	1.82
1	B	19	GLU	CD-OE2	6.78	1.33	1.25
1	C	282	VAL	CB-CG2	6.72	1.67	1.52
1	C	106	GLU	CD-OE2	6.68	1.32	1.25
1	A	171	GLU	CG-CD	6.65	1.61	1.51
1	D	100	GLU	CG-CD	6.61	1.61	1.51
1	B	165	ALA	CA-CB	6.59	1.66	1.52
1	B	251	LYS	CE-NZ	6.58	1.65	1.49
1	D	229	VAL	CB-CG1	6.57	1.66	1.52
1	D	230	GLU	CD-OE2	6.54	1.32	1.25
1	B	252	ARG	CD-NE	-6.53	1.35	1.46
1	G	219	GLU	CG-CD	6.51	1.61	1.51
1	B	19	GLU	CG-CD	6.50	1.61	1.51
1	A	171	GLU	CB-CG	6.48	1.64	1.52
1	D	169	TYR	CE1-CZ	6.47	1.47	1.38
1	F	68	GLU	CG-CD	6.41	1.61	1.51
1	A	211	GLU	CD-OE1	6.39	1.32	1.25
1	G	97	GLN	C-O	-6.34	1.11	1.23
1	C	212	ASN	CB-CG	6.24	1.65	1.51
1	B	220	TYR	CD1-CE1	6.22	1.48	1.39
1	E	68	GLU	CG-CD	6.21	1.61	1.51
1	G	141	LYS	CE-NZ	6.19	1.64	1.49
1	A	36	ALA	CA-CB	6.17	1.65	1.52
1	B	252	ARG	CG-CD	6.17	1.67	1.51
1	G	216	TYR	CB-CG	-6.16	1.42	1.51
1	F	42	GLU	CG-CD	6.06	1.61	1.51
1	B	119	VAL	CB-CG1	-6.04	1.40	1.52
1	E	148	VAL	CA-CB	6.04	1.67	1.54
1	B	172	PHE	CD1-CE1	-6.04	1.27	1.39
1	B	19	GLU	CD-OE1	5.99	1.32	1.25
1	D	61	TRP	CE3-CZ3	5.99	1.48	1.38
1	E	171	GLU	CG-CD	5.93	1.60	1.51
1	B	112	GLU	CG-CD	5.92	1.60	1.51
1	B	233	PHE	CA-CB	5.86	1.66	1.53
1	E	211	GLU	CB-CG	5.82	1.63	1.52
1	C	218	ARG	C-O	5.82	1.34	1.23
1	B	87	VAL	CB-CG2	-5.77	1.40	1.52
1	D	82	TRP	CB-CG	5.75	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	ALA	CA-CB	5.73	1.64	1.52
1	A	104	VAL	CB-CG1	5.72	1.64	1.52
1	A	49	MET	CB-CG	5.69	1.69	1.51
1	C	27	TYR	CD2-CE2	5.68	1.47	1.39
1	B	282	VAL	CB-CG1	-5.63	1.41	1.52
1	A	278	VAL	CB-CG1	5.60	1.64	1.52
1	E	141	LYS	N-CA	5.58	1.57	1.46
1	B	207	GLU	CB-CG	-5.55	1.41	1.52
1	G	246	ARG	CZ-NH2	5.55	1.40	1.33
1	A	104	VAL	CB-CG2	-5.54	1.41	1.52
1	F	133	TYR	CB-CG	-5.54	1.43	1.51
1	B	251	LYS	CB-CG	5.51	1.67	1.52
1	D	112	GLU	CG-CD	5.51	1.60	1.51
1	B	42	GLU	CG-CD	5.50	1.60	1.51
1	E	104	VAL	C-O	-5.47	1.12	1.23
1	E	213	THR	C-O	-5.43	1.13	1.23
1	E	175	TYR	CD1-CE1	5.41	1.47	1.39
1	B	116	PHE	CB-CG	5.40	1.60	1.51
1	E	44	ALA	C-O	5.37	1.33	1.23
1	A	241	MET	CB-CG	5.37	1.68	1.51
1	A	73	ILE	CB-CG2	5.31	1.69	1.52
1	A	82	TRP	CB-CG	5.30	1.59	1.50
1	E	175	TYR	CD2-CE2	5.29	1.47	1.39
1	C	233	PHE	C-O	5.27	1.33	1.23
1	F	31	ASP	CB-CG	5.27	1.62	1.51
1	C	82	TRP	CD2-CE3	-5.25	1.32	1.40
1	C	19	GLU	CG-CD	5.24	1.59	1.51
1	B	68	GLU	CG-CD	5.21	1.59	1.51
1	E	114	MET	CB-CG	5.20	1.68	1.51
1	B	82	TRP	CE3-CZ3	5.20	1.47	1.38
1	B	42	GLU	CB-CG	5.16	1.61	1.52
1	F	48	GLU	CD-OE2	5.15	1.31	1.25
1	C	161	GLU	CB-CG	5.14	1.61	1.52
1	B	251	LYS	CD-CE	5.13	1.64	1.51
1	C	14	ILE	CB-CG2	5.12	1.68	1.52
1	C	131	TYR	CD2-CE2	5.12	1.47	1.39
1	B	272	PHE	CD2-CE2	5.12	1.49	1.39
1	E	236	TRP	CE3-CZ3	5.11	1.47	1.38
1	C	133	TYR	CD1-CE1	5.11	1.47	1.39
1	B	81	VAL	CB-CG1	5.09	1.63	1.52
1	D	81	VAL	CB-CG2	5.07	1.63	1.52
1	D	51	PHE	CE2-CZ	5.07	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	126	PHE	CE1-CZ	5.04	1.47	1.37
1	B	82	TRP	CB-CG	5.02	1.59	1.50

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH2	-23.35	108.62	120.30
1	B	252	ARG	NE-CZ-NH1	19.05	129.83	120.30
1	B	8	ARG	NE-CZ-NH2	-15.85	112.38	120.30
1	B	8	ARG	NE-CZ-NH1	13.25	126.92	120.30
1	C	279	ARG	NE-CZ-NH2	12.71	126.65	120.30
1	A	239	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	A	237	ARG	NE-CZ-NH1	12.37	126.49	120.30
1	A	237	ARG	NE-CZ-NH2	-12.23	114.18	120.30
1	F	215	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	C	279	ARG	NE-CZ-NH1	-11.60	114.50	120.30
1	B	29	ARG	NE-CZ-NH2	11.05	125.82	120.30
1	B	237	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	B	203	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	A	239	ARG	NE-CZ-NH2	-10.53	115.04	120.30
1	H	129	LEU	CA-CB-CG	10.14	138.62	115.30
1	F	235	LEU	CA-CB-CG	10.13	138.61	115.30
1	E	78	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	B	29	ARG	NE-CZ-NH1	-9.93	115.34	120.30
1	B	237	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	B	252	ARG	CG-CD-NE	-9.58	91.69	111.80
1	A	160	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	E	215	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	E	269	LEU	CA-CB-CG	9.42	136.97	115.30
1	B	252	ARG	CD-NE-CZ	9.26	136.56	123.60
1	C	131	TYR	CG-CD2-CE2	-9.12	114.01	121.30
1	C	239	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	178	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	279	ARG	NE-CZ-NH1	-8.73	115.93	120.30
1	A	235	LEU	CA-CB-CG	8.68	135.27	115.30
1	E	215	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	160	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	G	239	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	E	78	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	178	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	F	279	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	D	225	ASP	CB-CG-OD1	7.52	125.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	LYS	CD-CE-NZ	7.46	128.87	111.70
1	A	78	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	158	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	237	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	G	239	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	E	225	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	275	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	F	237	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	F	237	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	47	ASP	CB-CG-OD2	7.10	124.69	118.30
1	H	76	LEU	CA-CB-CG	7.08	131.58	115.30
1	G	215	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	C	237	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	158	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	F	252	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	225	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	22	LEU	CB-CG-CD2	-6.76	99.51	111.00
1	F	252	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	242	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	239	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	G	70	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	163	LEU	CB-CG-CD2	-6.67	99.66	111.00
1	E	29	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	79	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	251	LYS	CA-CB-CG	6.61	127.94	113.40
1	E	214	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	252	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	B	246	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	D	178	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	E	29	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	203	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	E	137	LEU	CA-CB-CG	6.41	130.05	115.30
1	B	47	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	F	239	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	C	245	MET	CG-SD-CE	-6.24	90.22	100.20
1	C	7	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	279	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	E	225	ASP	CB-CG-OD1	6.18	123.86	118.30
1	G	114	MET	CB-CG-SD	6.18	130.95	112.40
1	E	214	ASP	CB-CG-OD1	6.16	123.84	118.30
1	H	22	LEU	CA-CB-CG	6.12	129.38	115.30
1	E	208	ARG	NE-CZ-NH1	6.11	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LEU	CB-CG-CD2	6.09	121.36	111.00
1	C	252	ARG	CG-CD-NE	-6.06	99.08	111.80
1	A	98	LEU	CB-CG-CD1	6.00	121.20	111.00
1	A	279	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	C	22	LEU	CA-CB-CG	5.93	128.93	115.30
1	B	160	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	G	105	LEU	CA-CB-CG	5.81	128.65	115.30
1	A	190	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	G	127	GLN	CB-CA-C	5.74	121.88	110.40
1	A	17	ASP	CB-CA-C	5.73	121.86	110.40
1	B	279	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	50	LEU	CB-CG-CD2	5.63	120.58	111.00
1	B	251	LYS	CG-CD-CE	5.63	128.78	111.90
1	B	235	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	78	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	G	245	MET	CG-SD-CE	-5.55	91.33	100.20
1	A	10	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	159	LEU	CB-CG-CD1	5.53	120.41	111.00
1	F	235	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	A	203	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	105	LEU	CB-CG-CD2	5.48	120.32	111.00
1	G	190	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	163	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	C	176	LEU	CB-CG-CD1	-5.42	101.80	111.00
1	G	190	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	223	CYS	CA-CB-SG	5.39	123.70	114.00
1	G	218	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	245	MET	CG-SD-CE	-5.35	91.65	100.20
1	B	248	ILE	CG1-CB-CG2	5.34	123.14	111.40
1	D	252	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	129	LEU	CA-CB-CG	5.29	127.48	115.30
1	D	87	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	H	203	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	85	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	163	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	9	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	228	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	178	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	F	76	LEU	CB-CG-CD2	5.16	119.77	111.00
1	E	120	LEU	C-N-CA	-5.15	111.48	122.30
1	H	235	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	C	131	TYR	CB-CG-CD2	-5.11	117.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	228	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	241	MET	CA-CB-CG	5.03	121.84	113.30
1	A	212	ASN	N-CA-CB	5.02	119.64	110.60
1	G	237	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	70	0
1	B	2308	0	2259	58	0
1	C	2244	0	2201	66	0
1	D	2165	0	2123	64	0
1	E	2153	0	2109	69	0
1	F	2071	0	2033	58	0
1	G	2172	0	2133	77	0
1	H	2120	0	2083	60	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
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	470	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 13.

All (470) 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:E:38:GLN:HE22	1:F:29:ARG:NH1	1.38	1.20
1:A:241:MET:CE	1:A:245:MET:HE2	1.75	1.16
1:C:241:MET:SD	1:C:245:MET:HE3	1.86	1.15
1:C:241:MET:SD	1:C:245:MET:CE	2.37	1.13
1:A:241:MET:HE2	1:A:245:MET:HE2	1.29	1.07
1:D:266:ALA:HA	1:D:269:LEU:HD13	1.33	1.04
1:A:241:MET:SD	1:A:245:MET:HE3	1.97	1.03
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:F:241:MET:SD	1:F:245:MET:HE1	2.07	0.95
3:H:401:HEM:HMB1	3:H:401:HEM:HBB2	1.49	0.93
1:B:241:MET:SD	1:B:245:MET:HE2	2.09	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:191:ASP:OD1	4:G:1481:HOH:O	1.93	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: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:C:241:MET:SD	1:C:245:MET:HE2	2.20	0.80
1:C:212:ASN:HB2	4:C:832:HOH:O	1.81	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: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: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:D:241:MET:SD	1:D:245:MET:HE3	2.25	0.75
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: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:F:241:MET:SD	1:F:245:MET:CE	2.75	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:E:37:GLN:HE21	1:F:63:LYS:NZ	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:PHE:HE1	3:E:401:HEM:HBB2	1.53	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: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:G:37:GLN:HE21	1:H:63:LYS:NZ	1.91	0.69
1:B:88:LEU:O	1:B:92:LYS:HG3	1.91	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:A:241:MET:SD	1:A:245:MET:HE2	2.27	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:A:37:GLN:HE21	1:B:63:LYS:HZ3	1.42	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:G:37:GLN:HE21	1:H:63:LYS:HZ3	1.44	0.66
1:B:234:GLN:HA	1:B:234:GLN:HE21	1.61	0.66
1:D:114:MET:HA	1:D:114:MET:CE	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:NZ	1:D:37:GLN:HE21	1.94	0.65
1:E:266:ALA:O	1:E:269:LEU:HD22	1.97	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:G:241:MET:SD	1:G:245:MET:HE1	2.37	0.64
1:F:132:ARG:HD2	1:F:145:MET:HG3	1.80	0.64
1:H:241:MET:SD	1:H:245:MET:HE3	2.36	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:A:86:LYS:NZ	1:B:112:GLU:OE2	2.26	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: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:112:GLU:OE2	1:F:86:LYS:NZ	2.33	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:B:242:ARG:NH1	1:B:245:MET:HE1	2.16	0.60
1:E:37:GLN:HE21	1:F:63:LYS:HZ3	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:HZ3	1:D:37:GLN:HE21	1.49	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
1:G:116:PHE:O	1:G:119:VAL:HG22	2.03	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:A:241:MET:CE	1:A:260:VAL:HG13	2.34	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: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:G:241:MET:SD	1:G:245:MET:CE	2.92	0.57
1:C:63:LYS:HZ2	1:D:37:GLN:NE2	2.01	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:C:37:GLN:HE21	1:D:63:LYS:NZ	2.02	0.57
3:G:401:HEM:HBC2	3:G:401:HEM:HHD	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:A:241:MET:HE1	1:A:264:GLN:HE22	1.71	0.55
1:A:144:GLN:HE22	1:B:9:ASP:HA	1.72	0.55
1:A:241:MET:CE	1:A:264:GLN:NE2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:MET:SD	1:H:245:MET:HE1	2.44	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
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:A:241:MET:HE2	1:A:260:VAL:HG13	1.90	0.54
1:H:114:MET:CE	1:H:114:MET:HA	2.37	0.54
1:D:105:LEU:HD21	3:D:401:HEM:HAB	1.88	0.54
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: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:H:145:MET:HE3	1:H:148:VAL:HG11	1.90	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:D:114:MET:HA	1:D:114:MET:HE3	1.89	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:G:34:LEU:HA	1:G:37:GLN:HE22	1.74	0.52
1:D:241:MET:SD	1:D:245:MET:HE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:E:37:GLN:NE2	1:F:63:LYS:HZ3	2.07	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:F:242:ARG:HA	1:F:245:MET:HE3	1.95	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: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: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:F:203:ARG:N	1:F:204:PRO:HD2	2.30	0.47
1:A:241:MET:HE2	1:A:260:VAL:CG1	2.44	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:B:73:ILE:HG23	1:B:171:GLU:HG3	1.97	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:ARG:HD2	4:G:1411:HOH:O	2.14	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:A:241:MET:HE1	1:A:264:GLN:NE2	2.30	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:B:242:ARG:HD2	1:B:245:MET:HE3	1.96	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: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: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:A:241:MET:HE3	1:A:264:GLN:NE2	2.32	0.45
1:B:83:GLN:H	1:B:83:GLN:HE21	1.64	0.45
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:A:142:ASN:HD21	1:A:144:GLN:NE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:242:ARG:HD2	1:A:245:MET:HE3	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:F:169:TYR:HE1	1:F:274:GLU:OE1	2.00	0.44
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:A:241:MET:CE	4:A:1149:HOH:O	2.66	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
1:E:135:GLU:CD	1:E:140:ASN:HD22	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:30:LEU:O	1:E:31:ASP:C	2.57	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:E:68:GLU:CD	1:E:90:ARG:HD2	2.39	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: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:A:116:PHE:O	1:A:117:ARG:C	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:202:LEU:HD12	1:H:274:GLU:CD	2.40	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:A:245:MET:HE2	4:A:1149:HOH:O	2.21	0.41
1:F:230:GLU:O	1:F:234:GLN:HG2	2.20	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:G:251:LYS:HZ3	1:G:252:ARG:H	1.69	0.41
1:B:68:GLU:CD	1:B:90:ARG:HD2	2.41	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:245:MET:HE3	1:F:245:MET:HB2	1.80	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: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: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
1:F:241:MET:O	1:F:245:MET:HE3	2.21	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	29
1	B	278/306 (91%)	268 (96%)	9 (3%)	1 (0%)	34	29
1	C	268/306 (88%)	258 (96%)	9 (3%)	1 (0%)	34	29
1	D	260/306 (85%)	250 (96%)	9 (4%)	1 (0%)	34	29
1	E	258/306 (84%)	245 (95%)	13 (5%)	0	100	100
1	F	246/306 (80%)	235 (96%)	9 (4%)	2 (1%)	19	12
1	G	260/306 (85%)	247 (95%)	12 (5%)	1 (0%)	34	29
1	H	253/306 (83%)	241 (95%)	12 (5%)	0	100	100
All	All	2098/2448 (86%)	2013 (96%)	78 (4%)	7 (0%)	41	37

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
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%)	225 (93%)	16 (7%)	16	11
1	B	244/266 (92%)	229 (94%)	15 (6%)	18	14
1	C	238/266 (90%)	220 (92%)	18 (8%)	13	8
1	D	228/266 (86%)	214 (94%)	14 (6%)	18	14
1	E	227/266 (85%)	204 (90%)	23 (10%)	7	4
1	F	220/266 (83%)	204 (93%)	16 (7%)	14	9
1	G	229/266 (86%)	211 (92%)	18 (8%)	12	7
1	H	224/266 (84%)	205 (92%)	19 (8%)	10	6
All	All	1851/2128 (87%)	1712 (92%)	139 (8%)	13	8

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	ASP
1	A	10	LEU
1	A	38	GLN
1	A	83	GLN
1	A	118	ASP
1	A	151	TYR
1	A	158	ARG
1	A	159	LEU
1	A	163	LEU
1	A	190	ARG
1	A	215	ARG
1	A	234	GLN
1	A	235	LEU
1	A	264	GLN
1	A	270	THR
1	B	7	LEU
1	B	10	LEU
1	B	17	ASP

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Mol	Chain	Res	Type
1	B	83	GLN
1	B	111	SER
1	B	118	ASP
1	B	129	LEU
1	B	147	GLN
1	B	191	ASP
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	127	GLN
1	C	164	GLU
1	C	185	GLN
1	C	186	GLN
1	C	193	THR
1	C	200	ASP
1	C	215	ARG
1	C	234	GLN
1	C	235	LEU
1	C	257	SER
1	C	264	GLN
1	D	22	LEU
1	D	42	GLU
1	D	82	TRP
1	D	83	GLN
1	D	129	LEU
1	D	146	LEU
1	D	160	ARG
1	D	190	ARG
1	D	197	VAL
1	D	201	THR
1	D	215	ARG
1	D	234	GLN

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Mol	Chain	Res	Type
1	D	278	VAL
1	D	280	THR
1	E	23	THR
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	197	VAL
1	E	200	ASP
1	E	211	GLU
1	E	214	ASP
1	E	234	GLN
1	E	235	LEU
1	E	252	ARG
1	E	260	VAL
1	E	269	LEU
1	E	280	THR
1	E	282	VAL
1	F	76	LEU
1	F	78	ARG
1	F	83	GLN
1	F	127	GLN
1	F	148	VAL
1	F	158	ARG
1	F	159	LEU
1	F	161	GLU
1	F	212	ASN
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

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Mol	Chain	Res	Type
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	160	ARG
1	G	184	PRO
1	G	204	PRO
1	G	208	ARG
1	G	234	GLN
1	G	235	LEU
1	G	245	MET
1	G	250	PHE
1	G	251	LYS
1	G	270	THR
1	H	22	LEU
1	H	31	ASP
1	H	42	GLU
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	151	TYR
1	H	160	ARG
1	H	164	GLU
1	H	192	TRP
1	H	200	ASP
1	H	212	ASN
1	H	234	GLN
1	H	252	ARG
1	H	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	45	HIS
1	A	83	GLN
1	A	93	GLN
1	A	130	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	147	GLN
1	B	234	GLN
1	C	32	GLN
1	C	37	GLN
1	C	38	GLN
1	C	45	HIS
1	C	83	GLN
1	C	101	GLN
1	C	130	GLN
1	C	186	GLN
1	C	212	ASN
1	C	234	GLN
1	C	264	GLN
1	D	32	GLN
1	D	37	GLN
1	D	38	GLN
1	D	45	HIS
1	D	83	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

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Mol	Chain	Res	Type
1	E	54	GLN
1	E	83	GLN
1	E	147	GLN
1	E	156	GLN
1	E	188	GLN
1	E	234	GLN
1	F	32	GLN
1	F	37	GLN
1	F	38	GLN
1	F	93	GLN
1	F	101	GLN
1	F	127	GLN
1	F	130	GLN
1	F	185	GLN
1	F	234	GLN
1	G	37	GLN
1	G	45	HIS
1	G	83	GLN
1	G	130	GLN
1	G	144	GLN
1	G	156	GLN
1	G	188	GLN
1	G	234	GLN
1	H	37	GLN
1	H	45	HIS
1	H	83	GLN
1	H	93	GLN
1	H	130	GLN
1	H	232	GLN
1	H	234	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	402	-	12,16,16	1.58	3 (25%)	12,22,22	0.86	0
3	HEM	E	401	4,1	27,50,50	2.01	6 (22%)	17,82,82	2.29	7 (41%)
3	HEM	H	401	1	27,50,50	2.24	10 (37%)	17,82,82	2.07	7 (41%)
2	TRP	C	403	-	12,16,16	1.19	1 (8%)	12,22,22	0.97	0
2	TRP	B	402	-	12,16,16	1.61	3 (25%)	12,22,22	1.29	2 (16%)
2	TRP	C	402	-	12,16,16	1.58	1 (8%)	12,22,22	0.82	1 (8%)
2	TRP	G	402	-	12,16,16	1.41	2 (16%)	12,22,22	0.75	0
3	HEM	A	401	1	27,50,50	2.33	9 (33%)	17,82,82	3.00	10 (58%)
3	HEM	F	401	1	27,50,50	2.30	8 (29%)	17,82,82	2.23	9 (52%)
2	TRP	H	402	-	12,16,16	1.29	2 (16%)	12,22,22	0.94	1 (8%)
2	TRP	D	403	-	12,16,16	1.35	1 (8%)	12,22,22	0.93	1 (8%)
2	TRP	F	402	-	12,16,16	1.36	3 (25%)	12,22,22	1.00	0
3	HEM	G	401	1	27,50,50	1.86	6 (22%)	17,82,82	1.97	5 (29%)
2	TRP	A	403	-	12,16,16	1.30	2 (16%)	12,22,22	0.81	0
3	HEM	B	401	4,1	27,50,50	2.70	6 (22%)	17,82,82	2.21	4 (23%)
2	TRP	E	403	-	12,16,16	1.27	2 (16%)	12,22,22	0.93	0
3	HEM	D	401	1	27,50,50	2.28	10 (37%)	17,82,82	2.27	7 (41%)
2	TRP	B	403	-	12,16,16	1.03	1 (8%)	12,22,22	1.11	2 (16%)
2	TRP	D	402	-	12,16,16	1.84	4 (33%)	12,22,22	0.74	0
2	TRP	A	402	-	12,16,16	1.76	1 (8%)	12,22,22	1.30	1 (8%)
3	HEM	C	401	1	27,50,50	2.53	11 (40%)	17,82,82	2.15	3 (17%)

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	402	-	-	3/3/8/8	0/2/2/2
3	HEM	E	401	4,1	-	0/6/54/54	-
3	HEM	H	401	1	-	0/6/54/54	-
2	TRP	C	403	-	-	0/3/8/8	0/2/2/2
2	TRP	B	402	-	-	3/3/8/8	0/2/2/2
2	TRP	C	402	-	-	3/3/8/8	0/2/2/2
2	TRP	G	402	-	-	3/3/8/8	0/2/2/2
3	HEM	A	401	1	-	0/6/54/54	-
3	HEM	F	401	1	-	0/6/54/54	-
2	TRP	H	402	-	-	3/3/8/8	0/2/2/2
2	TRP	D	403	-	-	0/3/8/8	0/2/2/2
2	TRP	F	402	-	-	3/3/8/8	0/2/2/2
3	HEM	G	401	1	-	0/6/54/54	-
2	TRP	A	403	-	-	0/3/8/8	0/2/2/2
3	HEM	B	401	4,1	-	0/6/54/54	-
2	TRP	E	403	-	-	0/3/8/8	0/2/2/2
3	HEM	D	401	1	-	0/6/54/54	-
2	TRP	B	403	-	-	0/3/8/8	0/2/2/2
2	TRP	D	402	-	-	3/3/8/8	0/2/2/2
2	TRP	A	402	-	-	3/3/8/8	0/2/2/2
3	HEM	C	401	1	-	0/6/54/54	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	HEM	C3C-C2C	-8.72	1.28	1.40
3	H	401	HEM	C3D-C2D	6.07	1.55	1.37
3	B	401	HEM	C3B-C2B	-6.00	1.32	1.40
3	F	401	HEM	C3D-C2D	6.00	1.55	1.37
3	E	401	HEM	C3D-C2D	5.73	1.54	1.37
2	A	402	TRP	CD1-NE1	5.42	1.47	1.36
3	C	401	HEM	C3B-C2B	-5.20	1.33	1.40
3	A	401	HEM	C3C-C2C	-5.18	1.33	1.40
2	C	402	TRP	CD1-NE1	4.99	1.46	1.36
3	A	401	HEM	C3D-C2D	4.69	1.51	1.37
2	D	402	TRP	CD1-NE1	4.69	1.46	1.36
3	A	401	HEM	CAA-C2A	4.68	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	HEM	C3C-CAC	4.65	1.57	1.47
3	C	401	HEM	C3D-C2D	4.60	1.51	1.37
3	D	401	HEM	C3C-CAC	4.48	1.57	1.47
3	D	401	HEM	C3C-C2C	-4.39	1.34	1.40
3	G	401	HEM	C3C-CAC	4.30	1.56	1.47
3	E	401	HEM	C3C-CAC	4.24	1.56	1.47
3	C	401	HEM	C1D-ND	4.24	1.44	1.36
3	G	401	HEM	C3D-C2D	4.09	1.49	1.37
3	B	401	HEM	C3C-CAC	4.07	1.56	1.47
3	C	401	HEM	C3C-CAC	4.02	1.56	1.47
3	F	401	HEM	C3C-C2C	-4.02	1.34	1.40
3	H	401	HEM	C3B-CAB	3.99	1.56	1.47
3	D	401	HEM	C3B-CAB	3.96	1.56	1.47
3	H	401	HEM	C3C-C2C	-3.95	1.34	1.40
3	C	401	HEM	C3C-C2C	-3.94	1.34	1.40
3	D	401	HEM	C3D-C2D	3.93	1.49	1.37
3	B	401	HEM	C3D-C2D	3.91	1.49	1.37
3	D	401	HEM	CAA-C2A	3.70	1.57	1.52
2	E	402	TRP	CD1-NE1	3.65	1.44	1.36
3	G	401	HEM	C3B-CAB	3.65	1.55	1.47
3	B	401	HEM	CAD-C3D	3.59	1.58	1.52
3	D	401	HEM	CMB-C2B	3.56	1.60	1.51
3	A	401	HEM	C3C-CAC	3.45	1.54	1.47
3	B	401	HEM	C3B-CAB	3.39	1.54	1.47
3	E	401	HEM	C3B-C2B	-3.38	1.35	1.40
3	F	401	HEM	C3B-CAB	3.37	1.54	1.47
3	C	401	HEM	C1A-CHA	-3.37	1.31	1.41
3	C	401	HEM	CMB-C2B	3.36	1.59	1.51
3	H	401	HEM	CAA-C2A	3.36	1.57	1.52
3	A	401	HEM	C4B-NB	3.33	1.43	1.36
3	C	401	HEM	C3B-CAB	3.31	1.54	1.47
3	F	401	HEM	C1A-NA	3.31	1.43	1.36
3	H	401	HEM	C3B-C2B	-3.30	1.35	1.40
2	B	402	TRP	CD1-NE1	3.30	1.43	1.36
3	A	401	HEM	C3B-CAB	3.12	1.54	1.47
2	B	402	TRP	CH2-CZ3	3.06	1.46	1.38
2	G	402	TRP	CD1-NE1	3.01	1.42	1.36
3	C	401	HEM	CAA-C2A	2.98	1.56	1.52
2	F	402	TRP	CB-CG	-2.90	1.43	1.51
2	E	403	TRP	CZ3-CE3	2.88	1.43	1.36
3	G	401	HEM	CAA-C2A	2.80	1.56	1.52
3	E	401	HEM	C3B-CAB	2.80	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	402	TRP	CH2-CZ3	2.80	1.45	1.38
2	G	402	TRP	CZ3-CE3	2.74	1.42	1.36
3	A	401	HEM	C3B-C2B	-2.74	1.36	1.40
3	F	401	HEM	CMA-C3A	2.69	1.57	1.51
3	G	401	HEM	C3C-C2C	-2.66	1.36	1.40
3	H	401	HEM	C3C-CAC	2.64	1.53	1.47
2	B	403	TRP	CZ3-CE3	2.61	1.42	1.36
3	G	401	HEM	C1A-NA	2.60	1.41	1.36
3	E	401	HEM	C3C-C2C	-2.60	1.36	1.40
3	A	401	HEM	CMA-C3A	2.59	1.57	1.51
2	D	403	TRP	CH2-CZ3	2.54	1.44	1.38
3	E	401	HEM	CAA-C2A	2.52	1.55	1.52
2	A	403	TRP	CB-CG	2.52	1.58	1.51
3	F	401	HEM	C1C-C2C	2.51	1.48	1.42
3	A	401	HEM	C1D-ND	2.51	1.41	1.36
3	F	401	HEM	C4A-NA	2.50	1.41	1.36
3	H	401	HEM	CMA-C3A	2.44	1.56	1.51
3	H	401	HEM	C1C-C2C	2.41	1.48	1.42
2	E	402	TRP	CH2-CZ3	2.39	1.44	1.38
2	D	402	TRP	CZ3-CE3	2.38	1.42	1.36
3	D	401	HEM	C1D-ND	2.37	1.41	1.36
2	B	402	TRP	CZ3-CE3	-2.35	1.31	1.36
3	H	401	HEM	C1B-C2B	2.33	1.47	1.42
2	A	403	TRP	CZ3-CE3	2.31	1.42	1.36
2	H	402	TRP	CD1-NE1	2.27	1.41	1.36
3	C	401	HEM	CAD-C3D	2.21	1.56	1.52
3	C	401	HEM	C4A-CHB	-2.21	1.34	1.41
2	C	403	TRP	CB-CG	2.19	1.57	1.51
2	F	402	TRP	CD1-NE1	2.15	1.41	1.36
3	D	401	HEM	CMC-C2C	2.13	1.56	1.51
2	D	402	TRP	CA-N	2.10	1.51	1.47
2	E	403	TRP	CH2-CZ3	2.09	1.43	1.38
2	D	402	TRP	CH2-CZ2	2.09	1.41	1.36
2	E	402	TRP	CZ3-CE3	2.08	1.41	1.36
3	D	401	HEM	C3B-C2B	-2.07	1.37	1.40
2	F	402	TRP	CZ3-CE3	2.05	1.41	1.36
3	D	401	HEM	C2A-C3A	-2.04	1.31	1.37
3	H	401	HEM	C4B-NB	2.01	1.40	1.36

All (60) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	HEM	CBD-CAD-C3D	-5.75	101.88	112.48
3	C	401	HEM	CMA-C3A-C4A	-5.70	119.71	128.46
3	E	401	HEM	CBD-CAD-C3D	-5.48	102.39	112.48
3	B	401	HEM	CMA-C3A-C4A	-5.11	120.61	128.46
3	A	401	HEM	CMA-C3A-C4A	-5.10	120.62	128.46
3	A	401	HEM	CMA-C3A-C2A	4.95	134.27	124.94
3	D	401	HEM	CMA-C3A-C4A	-4.84	121.03	128.46
3	F	401	HEM	CBA-CAA-C2A	-4.36	104.44	112.49
3	D	401	HEM	CAA-CBA-CGA	4.33	119.94	112.67
3	C	401	HEM	CMA-C3A-C2A	4.25	132.96	124.94
3	B	401	HEM	CBD-CAD-C3D	-4.20	104.75	112.48
3	B	401	HEM	CMA-C3A-C2A	4.14	132.75	124.94
3	H	401	HEM	CMD-C2D-C1D	-3.94	122.41	128.46
3	G	401	HEM	CBD-CAD-C3D	-3.93	105.23	112.48
3	G	401	HEM	C4A-C3A-C2A	3.91	109.72	107.00
3	E	401	HEM	C3B-C4B-NB	-3.75	104.36	109.21
3	H	401	HEM	CMD-C2D-C3D	3.65	131.83	124.94
3	A	401	HEM	C1D-C2D-C3D	-3.55	104.53	107.00
2	A	402	TRP	CB-CA-C	-3.49	105.05	110.69
3	F	401	HEM	CMA-C3A-C4A	-3.47	123.13	128.46
3	E	401	HEM	CBA-CAA-C2A	-3.33	106.34	112.49
3	D	401	HEM	CMA-C3A-C2A	3.20	130.98	124.94
3	D	401	HEM	CMB-C2B-C3B	3.20	130.66	124.68
3	F	401	HEM	C4C-C3C-C2C	3.13	109.08	106.90
3	F	401	HEM	CBD-CAD-C3D	-3.02	106.92	112.48
3	A	401	HEM	CAA-CBA-CGA	-3.01	107.63	112.67
3	A	401	HEM	C4A-C3A-C2A	-2.91	104.97	107.00
3	F	401	HEM	CAD-CBD-CGD	-2.86	107.88	112.67
3	H	401	HEM	C4C-C3C-C2C	2.83	108.88	106.90
3	G	401	HEM	CAD-CBD-CGD	-2.78	108.01	112.67
3	H	401	HEM	CAD-CBD-CGD	-2.75	108.06	112.67
2	B	402	TRP	CH2-CZ2-CE2	-2.75	116.13	120.08
3	A	401	HEM	CBA-CAA-C2A	-2.74	107.43	112.49
3	D	401	HEM	CMD-C2D-C1D	-2.67	124.36	128.46
3	A	401	HEM	CMD-C2D-C1D	2.60	132.46	128.46
3	F	401	HEM	C3B-C4B-NB	-2.54	105.93	109.21
3	A	401	HEM	CAA-C2A-C3A	2.50	134.44	127.25
3	A	401	HEM	CAD-C3D-C2D	-2.50	120.06	127.25
3	H	401	HEM	C3B-C4B-NB	-2.49	105.99	109.21
3	H	401	HEM	CBD-CAD-C3D	-2.48	107.91	112.48
3	E	401	HEM	C4C-C3C-C2C	2.46	108.61	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	HEM	CMB-C2B-C3B	2.45	129.26	124.68
3	F	401	HEM	CMA-C3A-C2A	2.37	129.42	124.94
3	B	401	HEM	C4C-C3C-C2C	2.31	108.51	106.90
3	C	401	HEM	CBD-CAD-C3D	-2.30	108.23	112.48
3	D	401	HEM	CAA-C2A-C3A	2.30	133.85	127.25
3	E	401	HEM	C3C-C4C-NC	-2.22	106.75	110.94
2	H	402	TRP	CH2-CZ2-CE2	-2.22	116.89	120.08
3	G	401	HEM	C1D-C2D-C3D	2.21	108.53	107.00
3	D	401	HEM	CMD-C2D-C3D	2.20	129.09	124.94
3	F	401	HEM	C3C-C4C-NC	-2.18	106.83	110.94
2	B	402	TRP	CB-CG-CD1	-2.15	125.31	127.97
2	B	403	TRP	CZ3-CE3-CD2	-2.14	117.92	120.89
3	E	401	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
3	E	401	HEM	CMD-C2D-C1D	-2.09	125.25	128.46
3	F	401	HEM	CMB-C2B-C3B	2.09	128.59	124.68
2	B	403	TRP	CH2-CZ2-CE2	-2.08	117.08	120.08
3	H	401	HEM	C3C-C4C-NC	-2.05	107.07	110.94
2	D	403	TRP	CH2-CZ2-CE2	-2.03	117.16	120.08
2	C	402	TRP	CH2-CZ2-CE2	-2.02	117.18	120.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	TRP	C-CA-CB-CG
2	B	402	TRP	C-CA-CB-CG
2	D	402	TRP	C-CA-CB-CG
2	E	402	TRP	C-CA-CB-CG
2	F	402	TRP	C-CA-CB-CG
2	G	402	TRP	C-CA-CB-CG
2	G	402	TRP	CA-CB-CG-CD1
2	H	402	TRP	C-CA-CB-CG
2	C	402	TRP	N-CA-CB-CG
2	G	402	TRP	N-CA-CB-CG
2	A	402	TRP	CA-CB-CG-CD1
2	B	402	TRP	CA-CB-CG-CD1
2	C	402	TRP	CA-CB-CG-CD1
2	D	402	TRP	CA-CB-CG-CD1
2	E	402	TRP	CA-CB-CG-CD1
2	F	402	TRP	CA-CB-CG-CD1
2	H	402	TRP	CA-CB-CG-CD1
2	A	402	TRP	N-CA-CB-CG

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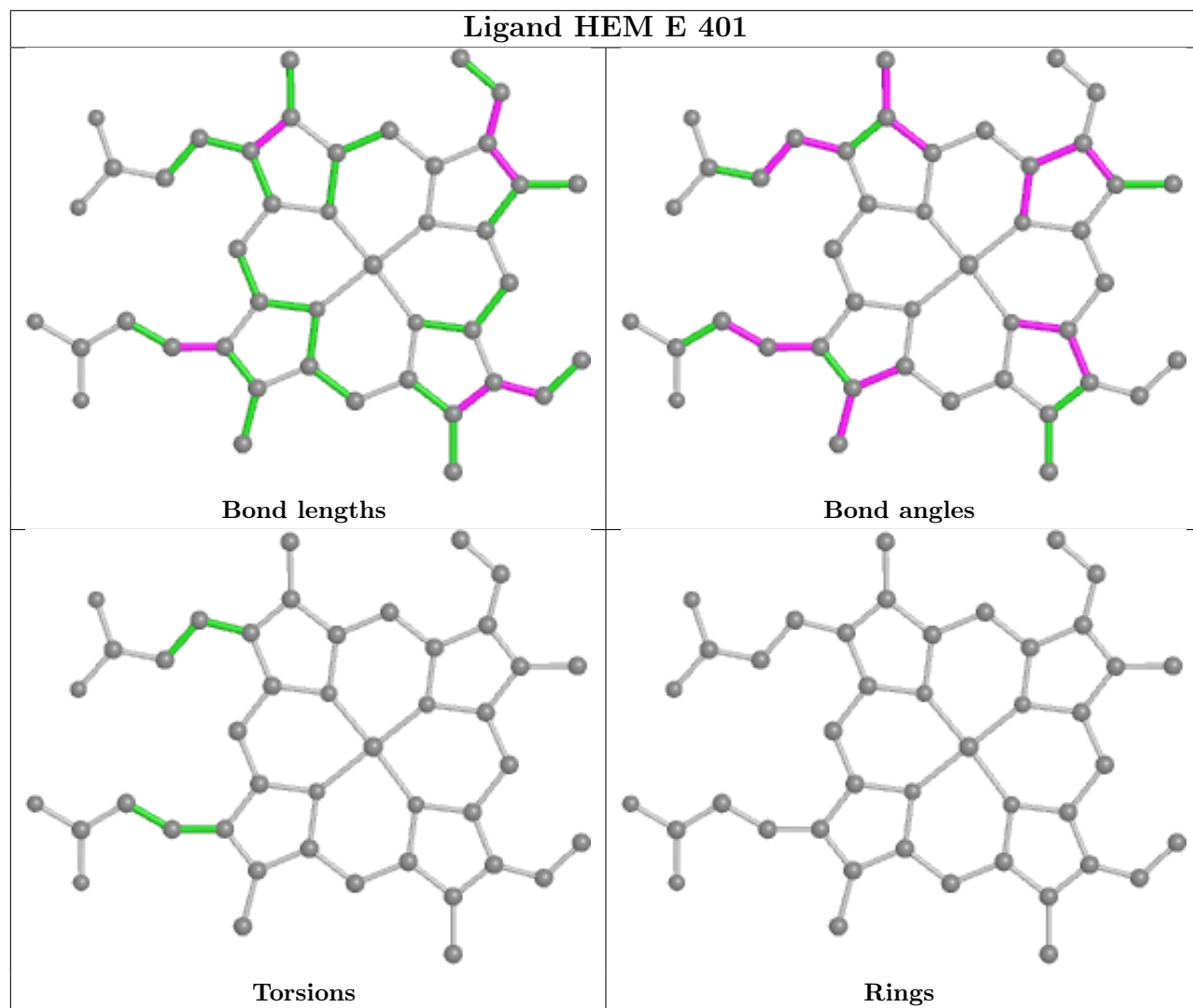
Mol	Chain	Res	Type	Atoms
2	B	402	TRP	N-CA-CB-CG
2	D	402	TRP	N-CA-CB-CG
2	E	402	TRP	N-CA-CB-CG
2	F	402	TRP	N-CA-CB-CG
2	H	402	TRP	N-CA-CB-CG
2	C	402	TRP	C-CA-CB-CG

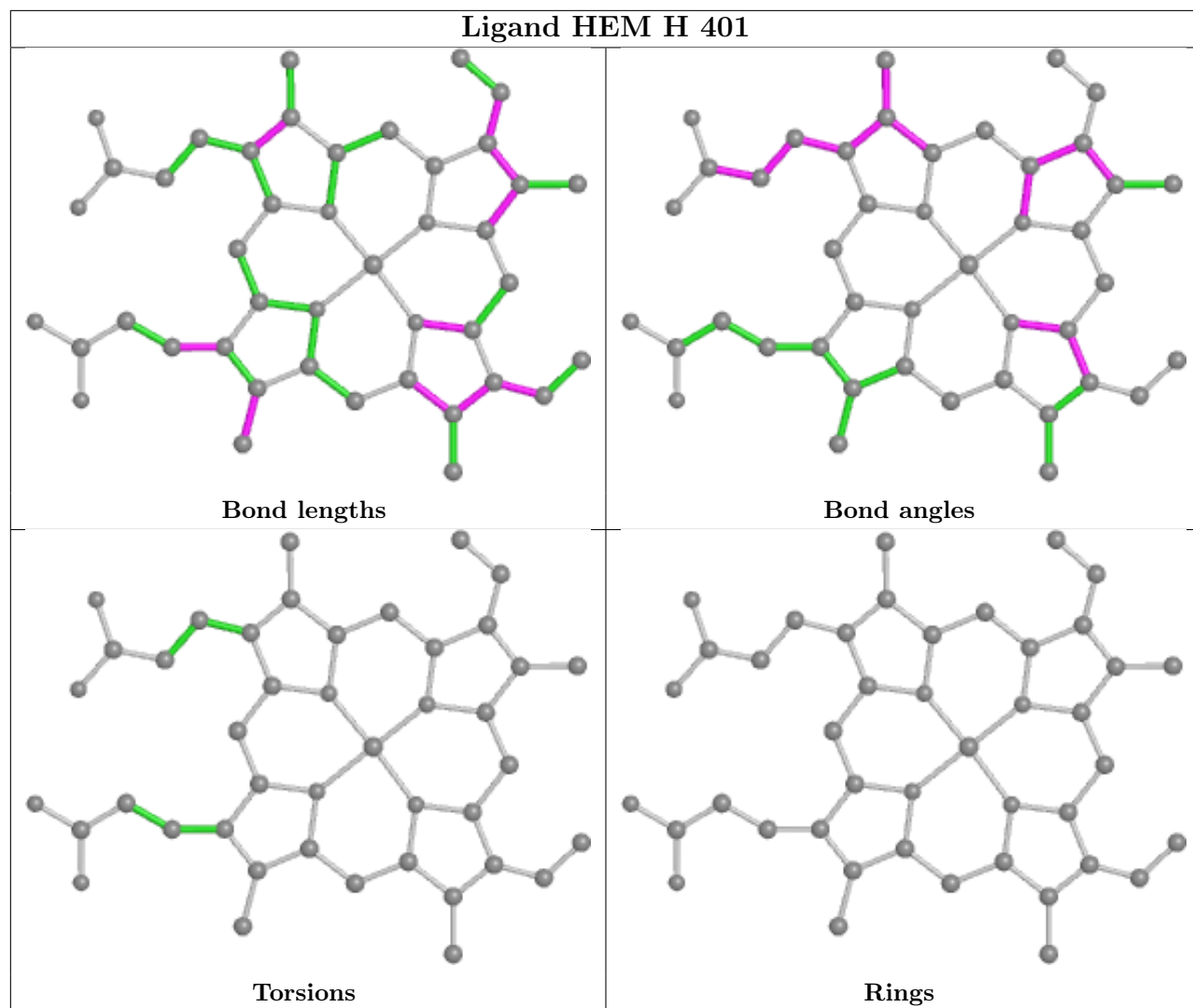
There are no ring outliers.

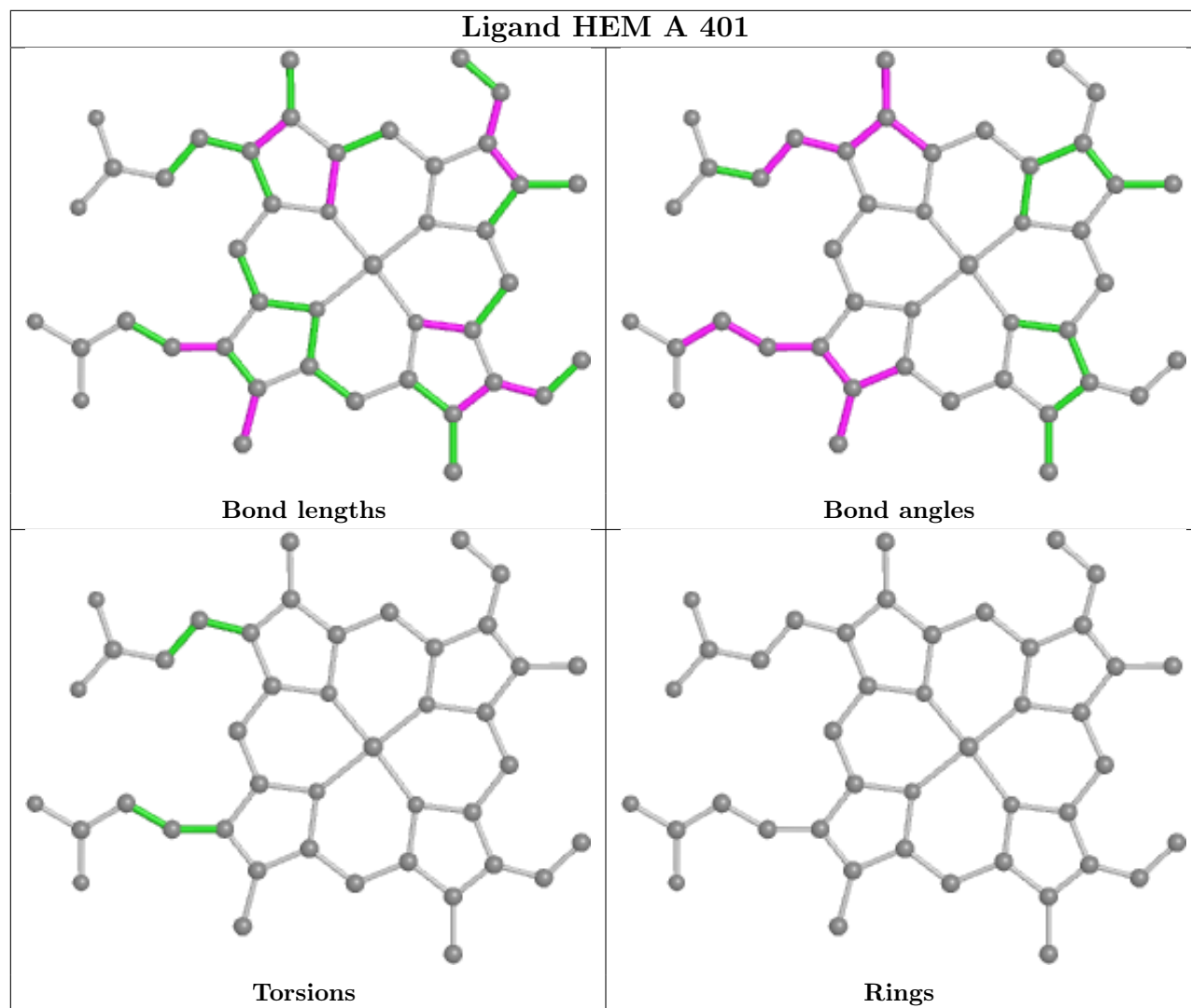
14 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	HEM	7	0
3	H	401	HEM	5	0
2	C	402	TRP	3	0
2	G	402	TRP	1	0
3	A	401	HEM	1	0
3	F	401	HEM	5	0
2	H	402	TRP	2	0
3	G	401	HEM	3	0
2	A	403	TRP	1	0
3	B	401	HEM	4	0
2	E	403	TRP	1	0
3	D	401	HEM	4	0
2	A	402	TRP	2	0
3	C	401	HEM	2	0

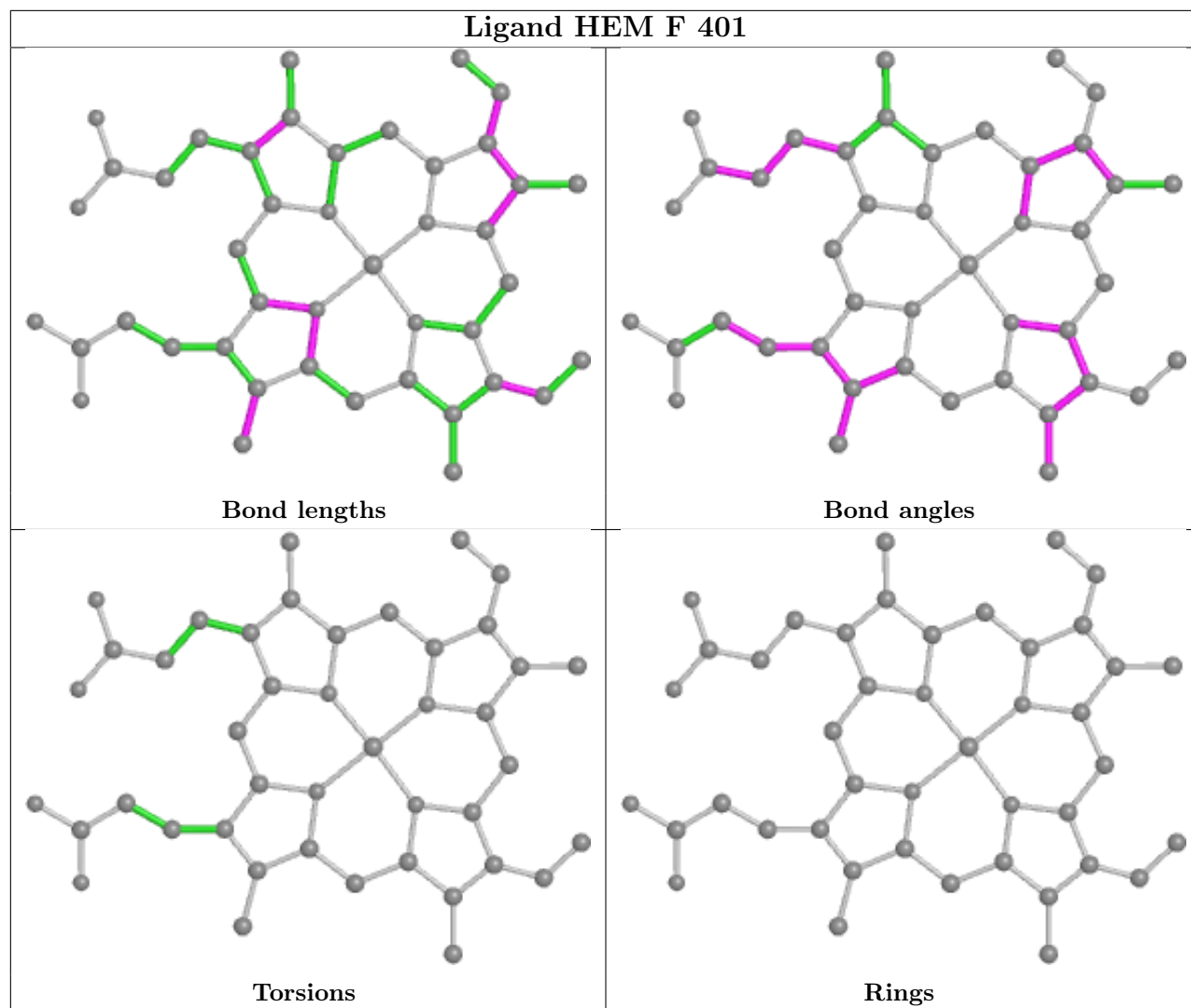
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

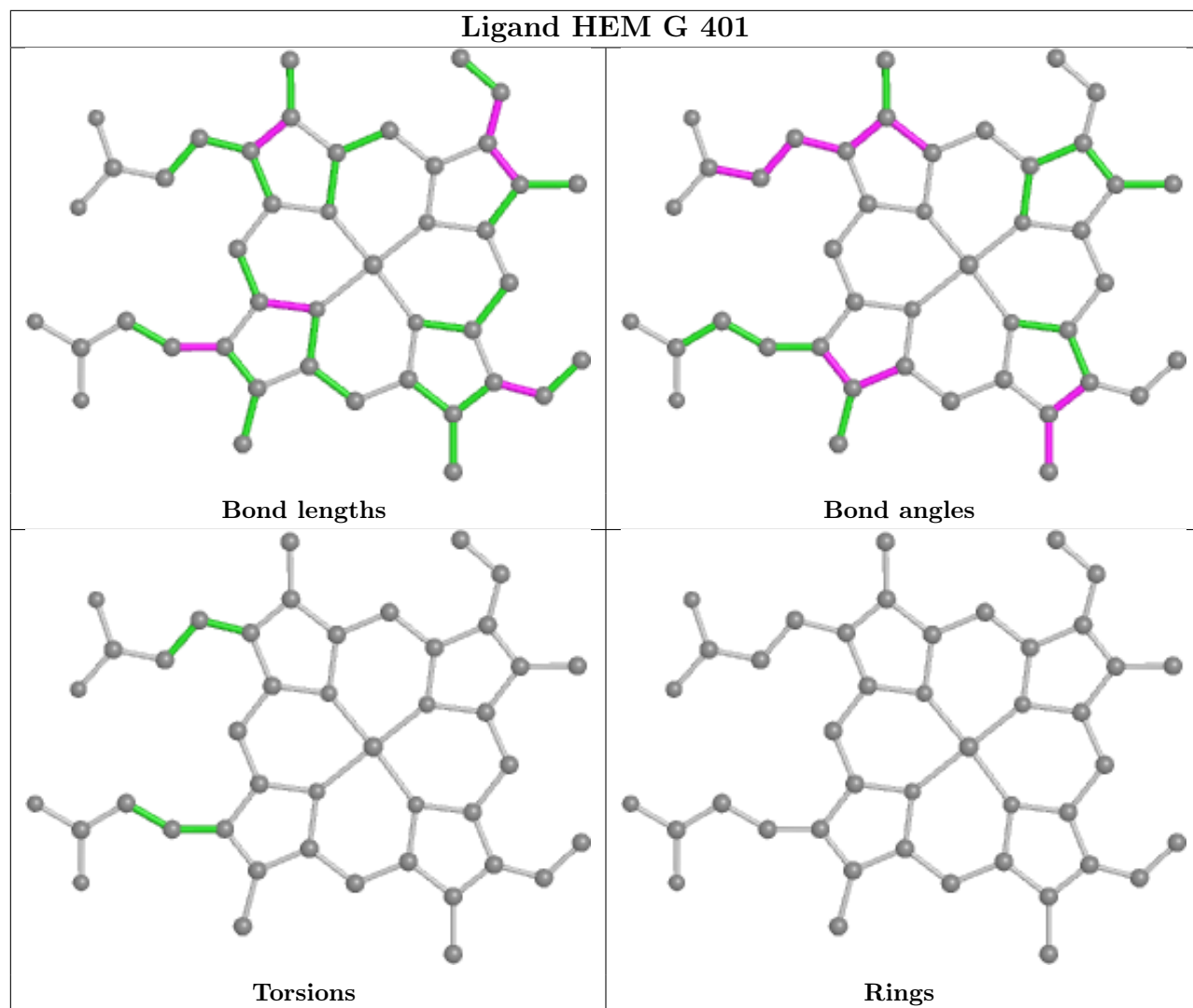


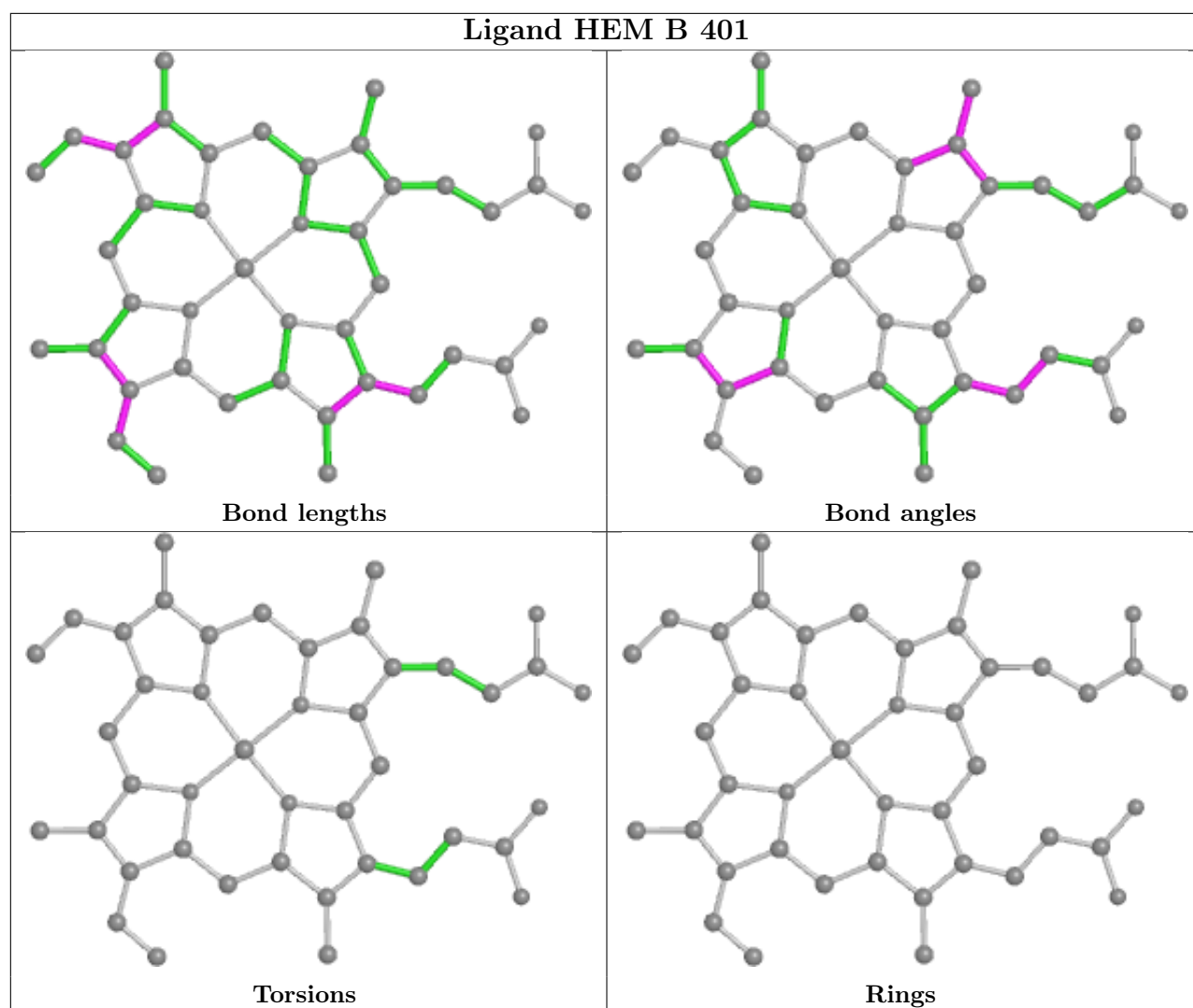


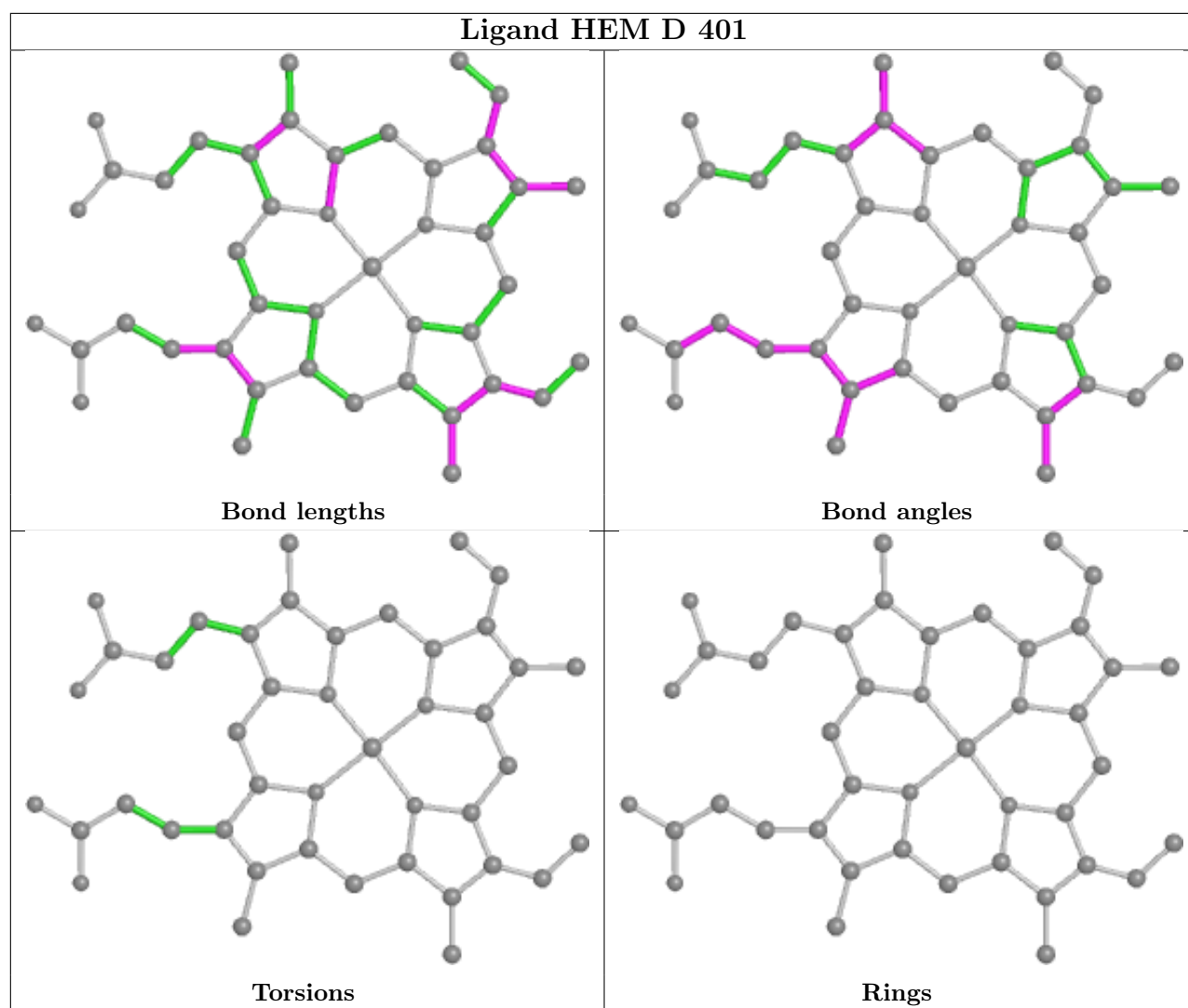


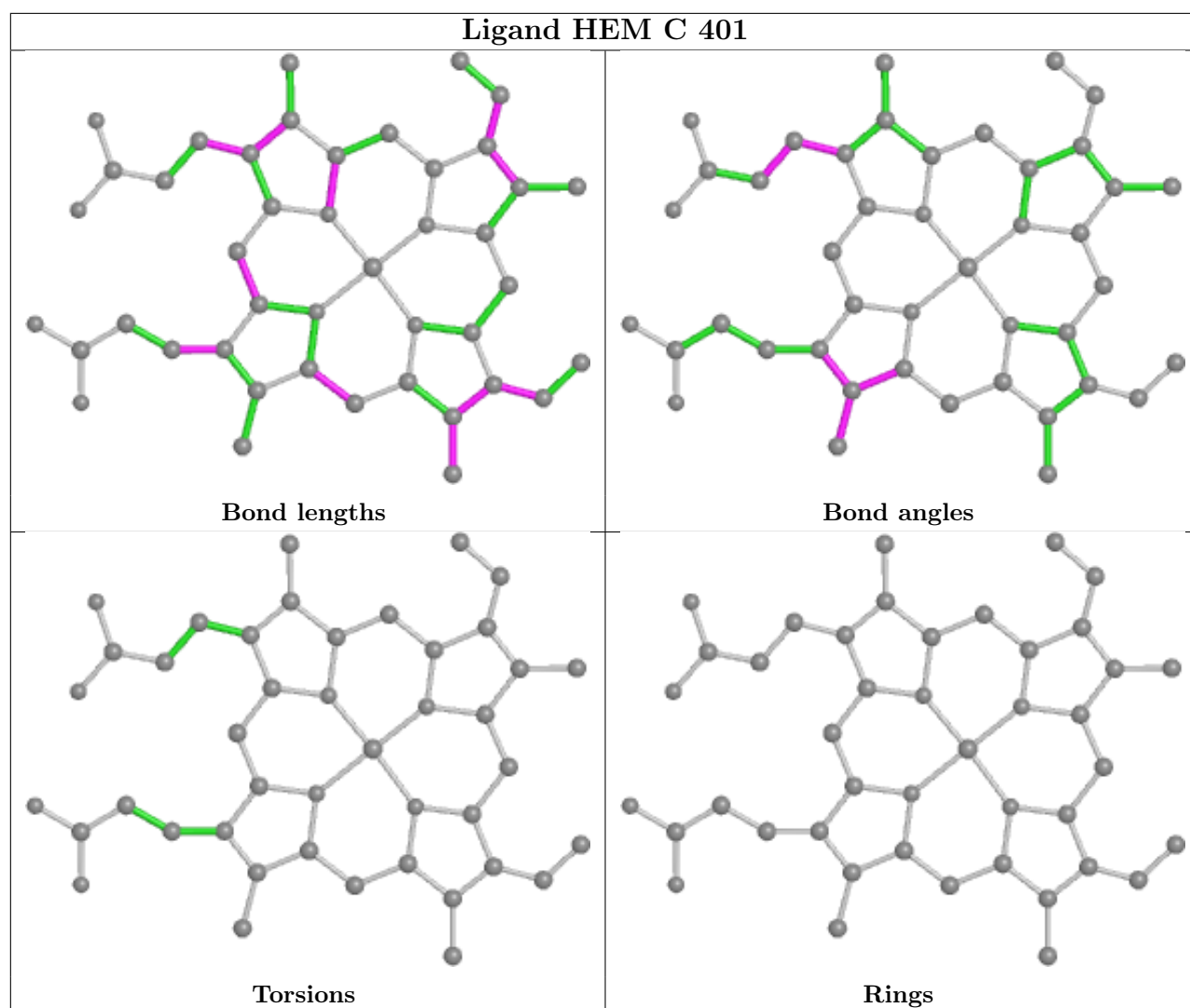












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/306 (90%)	-0.07	4 (1%) 75 80	5, 15, 27, 45	0
1	B	280/306 (91%)	-0.03	5 (1%) 68 75	4, 15, 31, 42	0
1	C	272/306 (88%)	0.06	6 (2%) 62 69	10, 19, 41, 54	0
1	D	262/306 (85%)	0.01	0 100 100	9, 19, 38, 44	0
1	E	260/306 (84%)	0.12	7 (2%) 54 63	9, 24, 37, 43	0
1	F	250/306 (81%)	0.32	11 (4%) 34 43	15, 26, 45, 55	0
1	G	262/306 (85%)	0.21	15 (5%) 23 32	9, 25, 42, 47	0
1	H	257/306 (83%)	0.63	27 (10%) 6 9	16, 31, 52, 63	0
All	All	2120/2448 (86%)	0.15	75 (3%) 44 52	4, 22, 41, 63	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	185	GLN	4.6
1	H	119	VAL	4.4
1	C	19	GLU	4.3
1	H	150	ALA	4.3
1	H	192	TRP	4.3
1	G	250	PHE	4.2
1	H	197	VAL	3.9
1	A	104	VAL	3.8
1	H	151	TYR	3.8
1	E	42	GLU	3.4
1	F	185	GLN	3.3
1	H	154	ALA	3.2
1	C	191	ASP	3.2
1	H	193	THR	3.1
1	F	186	GLN	3.1
1	H	22	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	184	PRO	3.0
1	H	201	THR	2.9
1	H	198	ALA	2.9
1	G	122	PRO	2.9
1	H	31	ASP	2.8
1	H	152	ASP	2.8
1	C	7	LEU	2.8
1	G	114	MET	2.8
1	H	196	HIS	2.8
1	G	147	GLN	2.8
1	H	183	ILE	2.7
1	G	151	TYR	2.7
1	H	118	ASP	2.7
1	F	150	ALA	2.7
1	C	17	ASP	2.7
1	G	150	ALA	2.7
1	C	12	PRO	2.6
1	F	121	GLY	2.6
1	F	40	LEU	2.6
1	H	144	GLN	2.6
1	B	95	LEU	2.5
1	F	114	MET	2.5
1	B	98	LEU	2.5
1	H	164	GLU	2.5
1	H	157	ALA	2.5
1	F	99	THR	2.4
1	G	94	VAL	2.4
1	G	118	ASP	2.4
1	F	187	TYR	2.4
1	E	122	PRO	2.4
1	H	146	LEU	2.4
1	F	153	PRO	2.3
1	F	148	VAL	2.3
1	B	102	TRP	2.3
1	H	149	PHE	2.3
1	E	280	THR	2.3
1	H	147	GLN	2.3
1	E	150	ALA	2.3
1	E	153	PRO	2.3
1	B	94	VAL	2.2
1	H	153	PRO	2.2
1	G	146	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	149	PHE	2.2
1	H	162	VAL	2.2
1	E	114	MET	2.2
1	A	99	THR	2.2
1	A	98	LEU	2.1
1	B	104	VAL	2.1
1	H	200	ASP	2.1
1	G	148	VAL	2.1
1	G	142	ASN	2.1
1	F	152	ASP	2.1
1	H	160	ARG	2.1
1	E	96	ARG	2.1
1	C	10	LEU	2.0
1	G	256	GLY	2.0
1	A	61	TRP	2.0
1	G	96	ARG	2.0
1	G	104	VAL	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 monosaccharides 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, 95<sup>th</sup> 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	0.82	0.24	32,36,40,41	0
2	TRP	E	402	15/15	0.84	0.20	29,31,33,36	0
2	TRP	G	402	15/15	0.85	0.24	30,35,40,43	0
2	TRP	E	403	15/15	0.86	0.19	24,27,38,39	0
2	TRP	C	402	15/15	0.92	0.15	13,21,28,31	0
2	TRP	D	402	15/15	0.92	0.16	14,18,25,26	0

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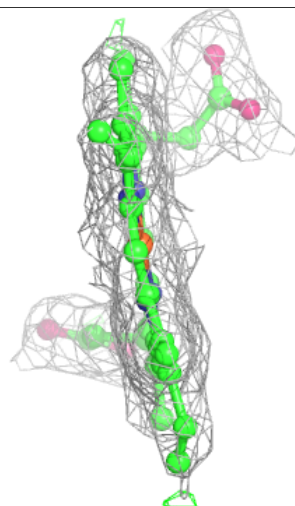
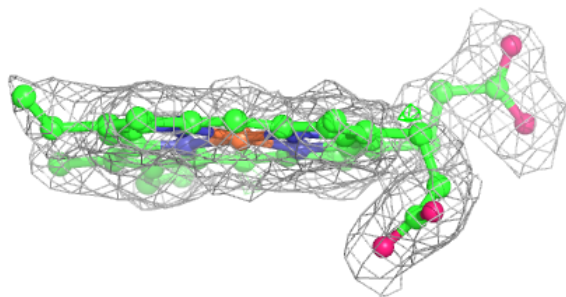
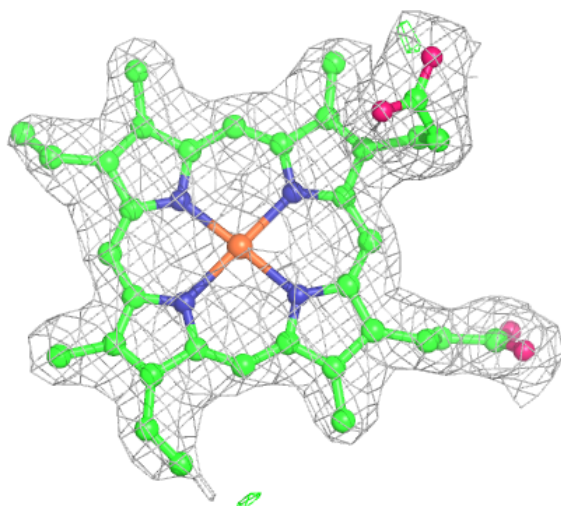
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TRP	C	403	15/15	0.94	0.13	14,18,27,28	0
2	TRP	F	402	15/15	0.94	0.18	25,27,32,35	0
2	TRP	B	403	15/15	0.94	0.11	12,20,26,26	0
2	TRP	A	402	15/15	0.94	0.12	14,16,23,25	0
2	TRP	A	403	15/15	0.95	0.13	14,21,28,28	0
3	HEM	G	401	43/43	0.95	0.11	20,25,31,38	0
2	TRP	B	402	15/15	0.96	0.11	7,9,18,18	0
3	HEM	E	401	43/43	0.96	0.11	11,23,27,34	0
3	HEM	F	401	43/43	0.96	0.12	13,20,27,34	0
2	TRP	D	403	15/15	0.96	0.10	11,15,27,30	0
3	HEM	H	401	43/43	0.96	0.12	17,23,27,28	0
3	HEM	C	401	43/43	0.97	0.11	4,10,16,19	0
3	HEM	D	401	43/43	0.97	0.12	2,9,17,21	0
3	HEM	A	401	43/43	0.98	0.12	2,8,13,17	0
3	HEM	B	401	43/43	0.98	0.12	2,5,10,13	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.

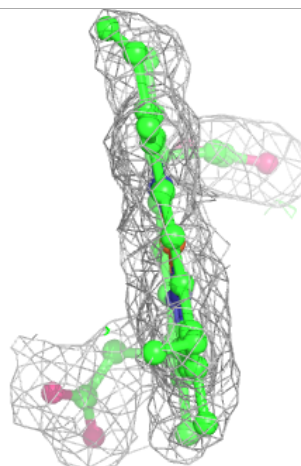
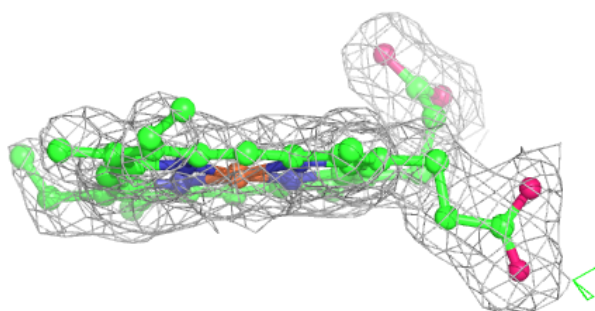
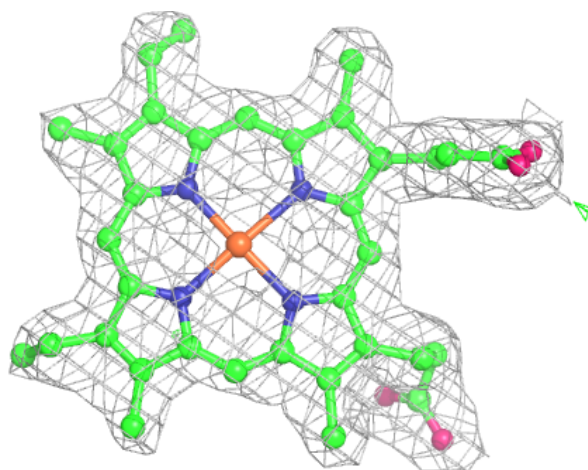
**Electron density around HEM G 401:**

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



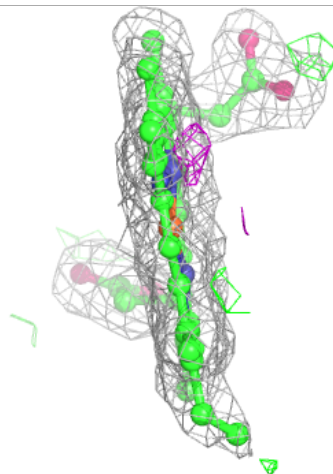
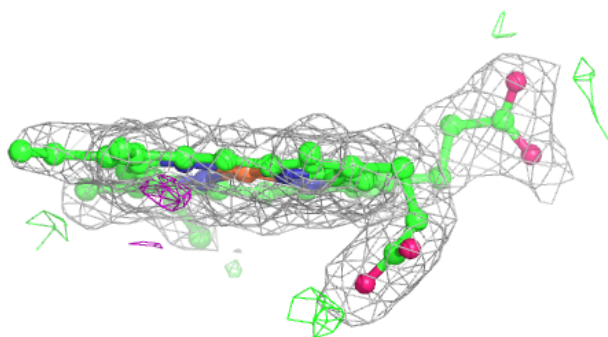
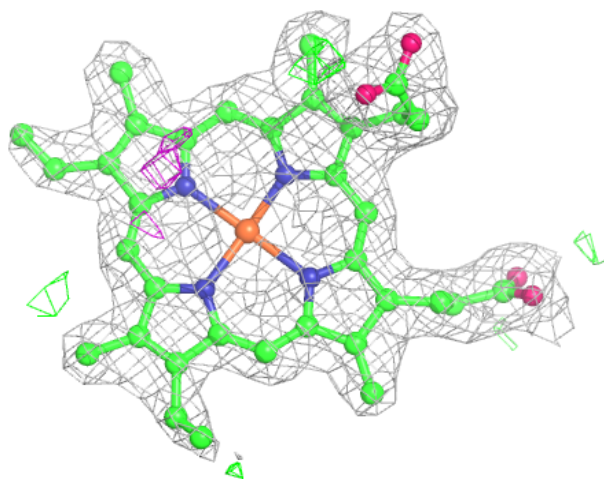
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



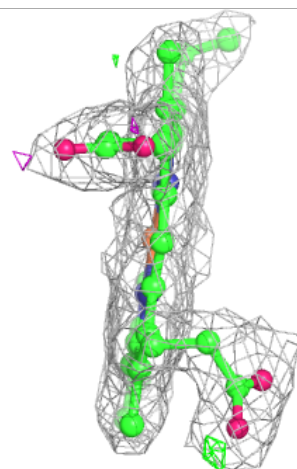
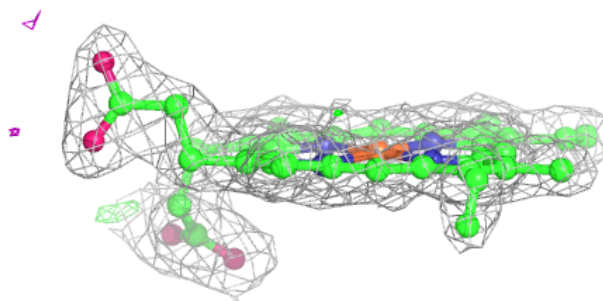
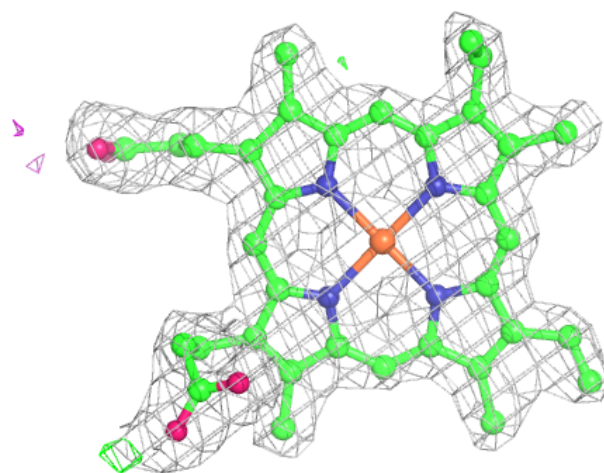
**Electron density around HEM F 401:**

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



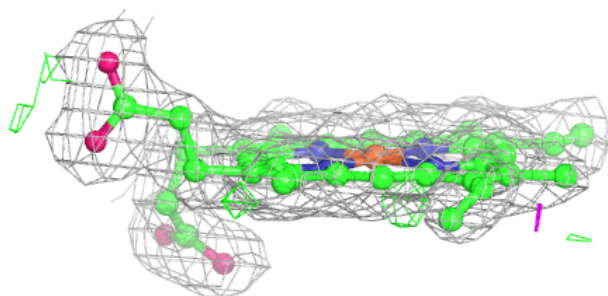
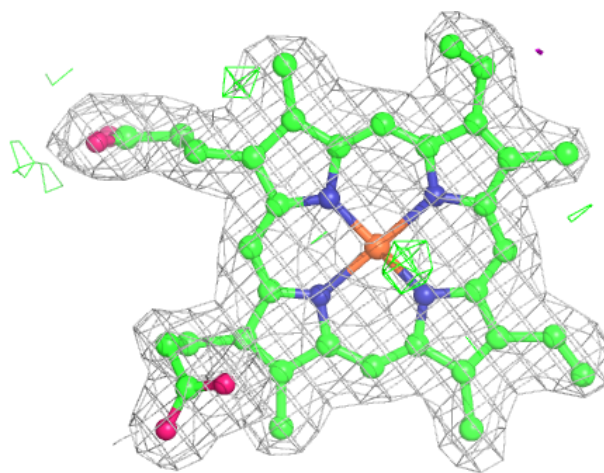
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and green (positive)



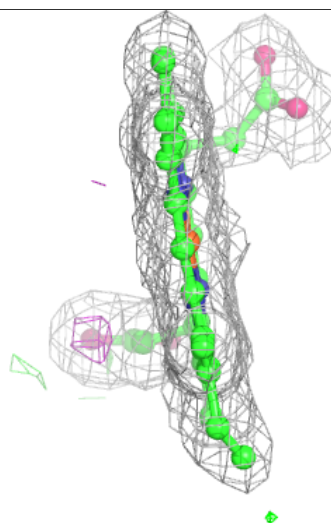
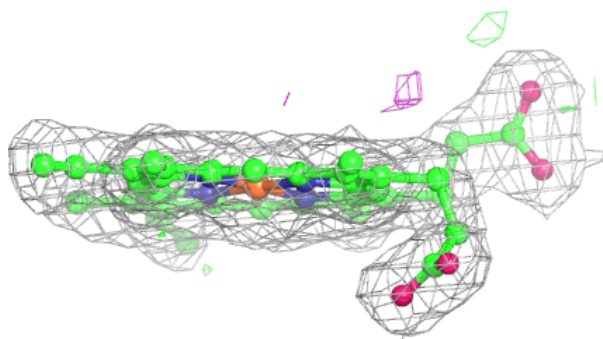
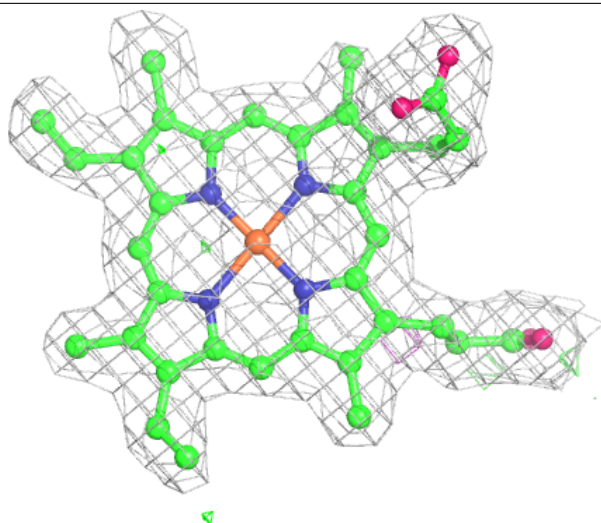
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and green (positive)



**Electron density around HEM D 401:**

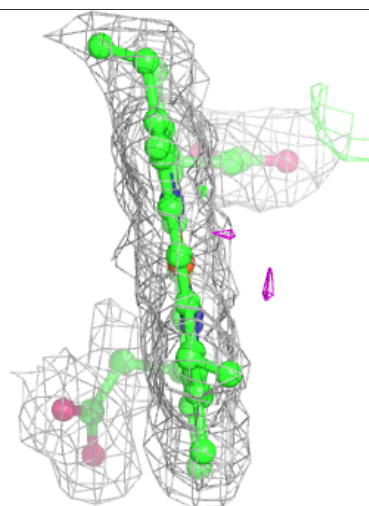
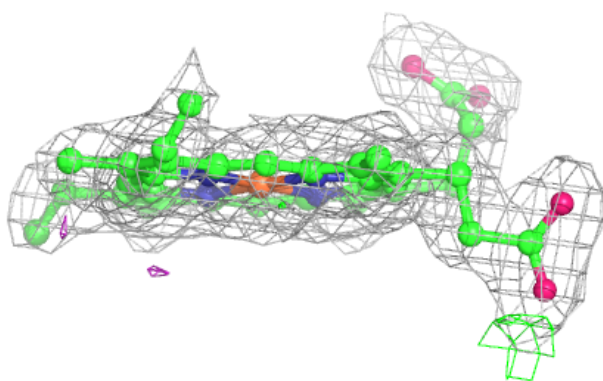
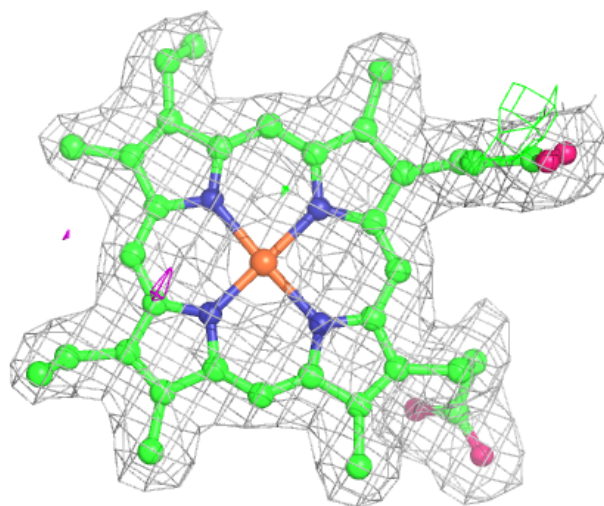
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM A 401:**

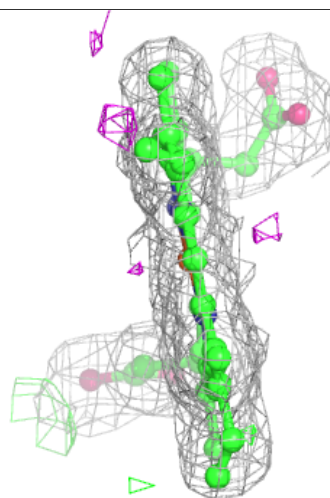
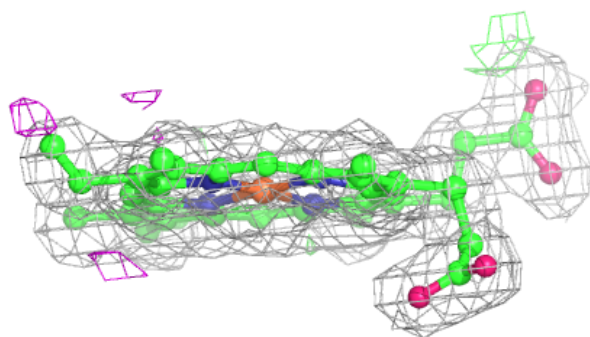
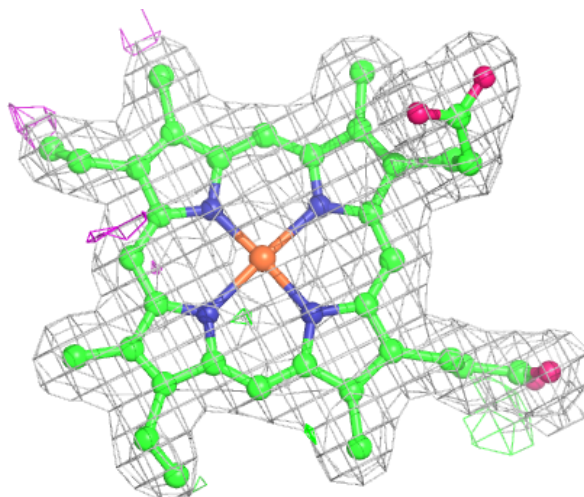
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM B 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.