



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:47 AM EDT

PDB ID : 8W1Y / pdb_00008w1y
Title : 2.30 angstrom resolution intermediate crystal structure of KatG from Mycobacterium tuberculosis with an MYW-OOH cofactor soaked with peroxide for 1 minute
Authors : Li, J.; Duan, R.; Liu, A.
Deposited on : 2024-02-19
Resolution : 2.30 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

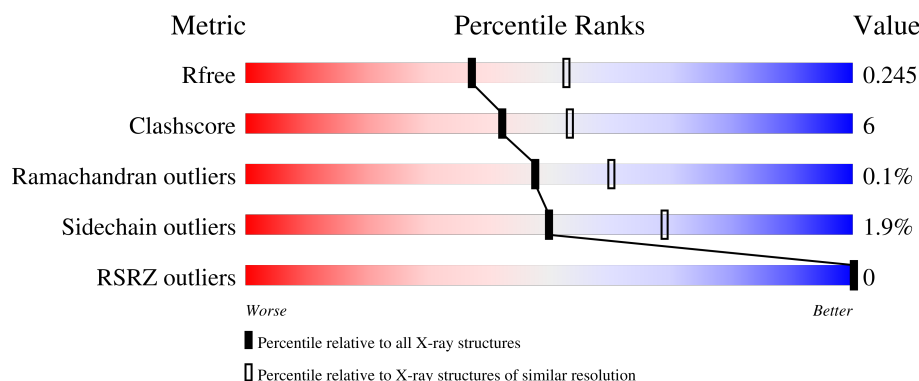
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	741	 75% 21% ..
1	B	741	 88% 8% ..
1	C	741	 76% 20% ..
1	D	741	 87% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23617 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.

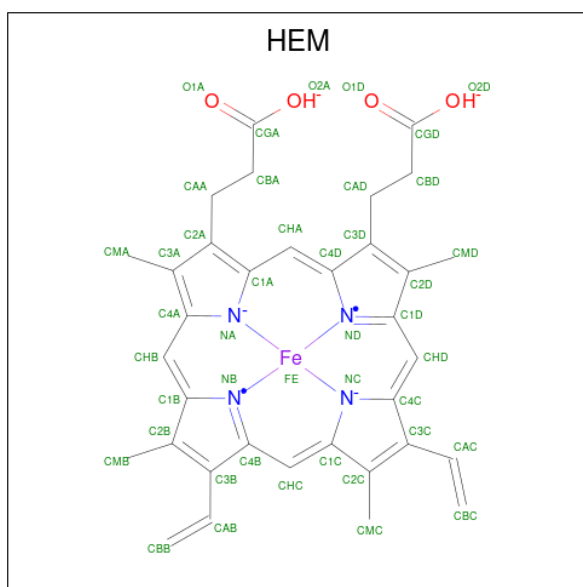
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	1	0
			5532	3515	953	1045	19			
1	B	717	Total	C	N	O	S	0	1	0
			5532	3515	953	1045	19			
1	C	717	Total	C	N	O	S	0	1	0
			5532	3515	953	1045	19			
1	D	717	Total	C	N	O	S	0	1	0
			5532	3515	953	1045	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A0D5ZBI4
A	1	HIS	-	expression tag	UNP A0A0D5ZBI4
B	0	GLY	-	expression tag	UNP A0A0D5ZBI4
B	1	HIS	-	expression tag	UNP A0A0D5ZBI4
C	0	GLY	-	expression tag	UNP A0A0D5ZBI4
C	1	HIS	-	expression tag	UNP A0A0D5ZBI4
D	0	GLY	-	expression tag	UNP A0A0D5ZBI4
D	1	HIS	-	expression tag	UNP A0A0D5ZBI4

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

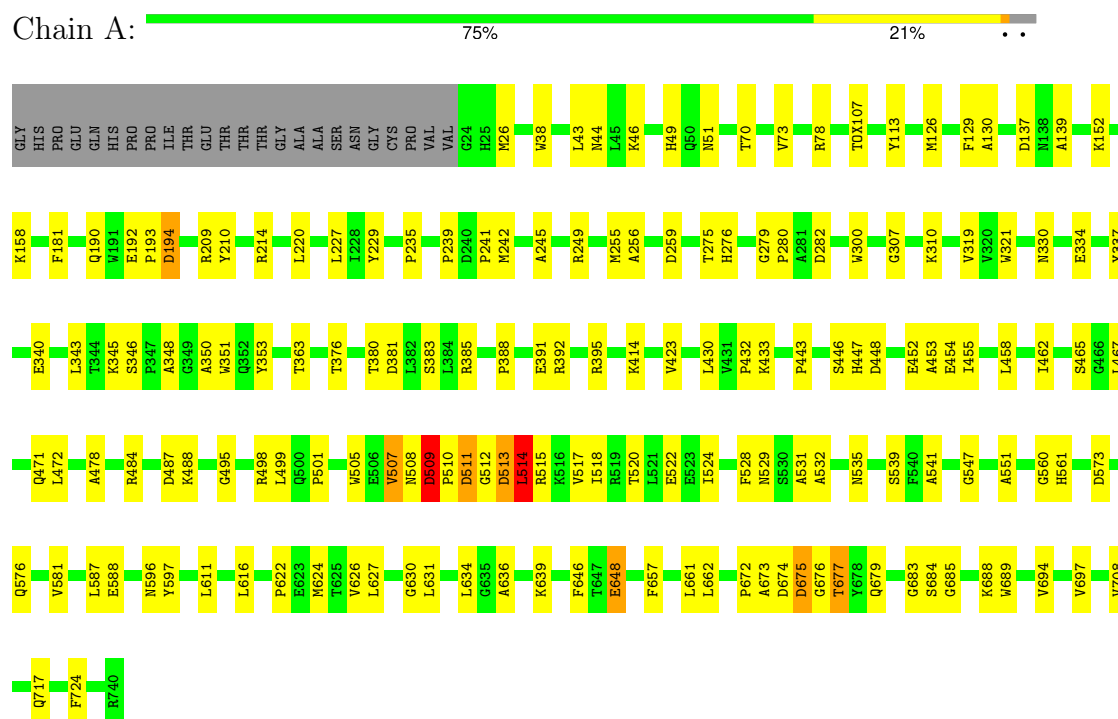
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	238	Total	O	0	0
			238	238		
5	B	395	Total	O	0	0
			395	395		
5	C	265	Total	O	0	0
			265	265		
5	D	391	Total	O	0	0
			391	391		

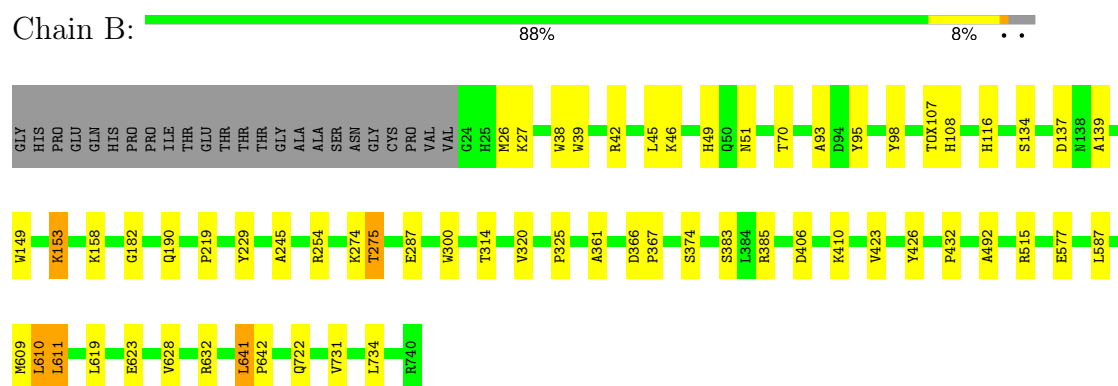
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Catalase-peroxidase

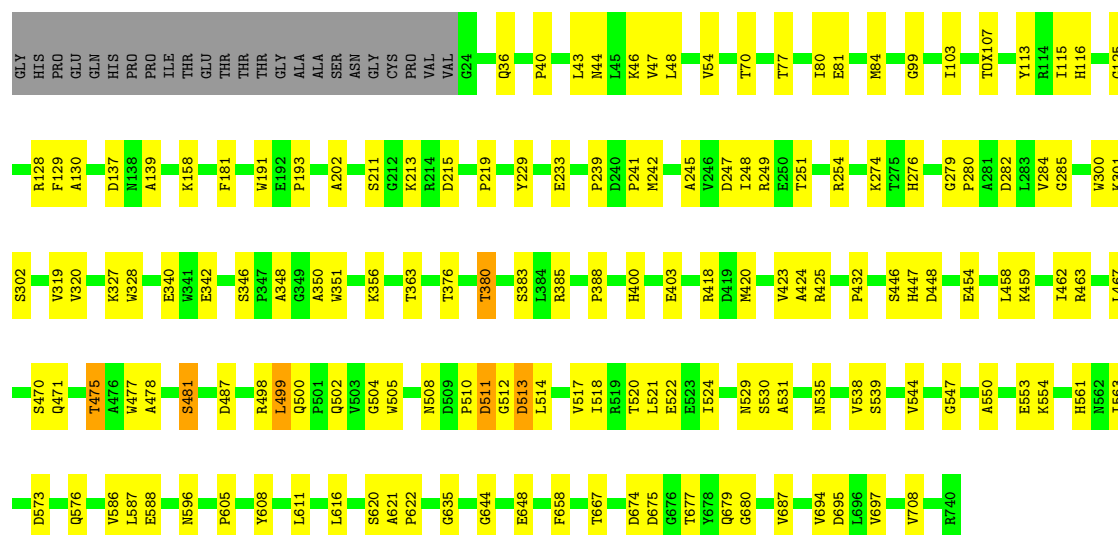


• Molecule 1: Catalase-peroxidase



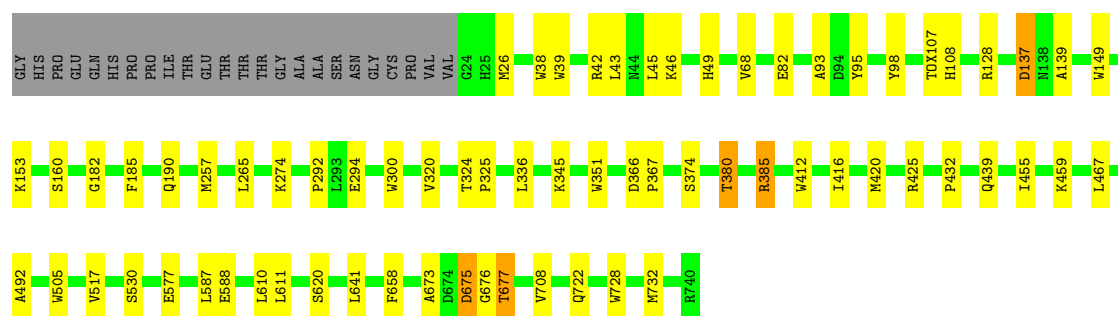
• Molecule 1: Catalase-peroxidase

Chain C:  76% 20% ..



● Molecule 1: Catalase-peroxidase

Chain D:  87% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	150.51Å 150.51Å 155.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.30 48.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.93-2.30) 87.2 (48.93-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.247 0.192 , 0.245	Depositor DCC
R_{free} test set	1978 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.011 for -h,l,k 0.013 for l,-k,h 0.017 for -l,-k,-h 0.457 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23617	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, HEM, TOX, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	13/5663 (0.2%)	0.69	10/7706 (0.1%)
1	B	0.66	15/5663 (0.3%)	0.62	4/7706 (0.1%)
1	C	0.52	9/5663 (0.2%)	0.65	8/7706 (0.1%)
1	D	0.43	1/5663 (0.0%)	0.60	2/7706 (0.0%)
All	All	0.58	38/22652 (0.2%)	0.64	24/30824 (0.1%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	611	LEU	C-O	-14.19	1.07	1.24
1	B	254	ARG	C-O	-13.87	1.03	1.24
1	B	609	MET	C-O	-13.51	1.07	1.24
1	A	673	ALA	C-O	-11.16	1.09	1.24
1	A	674	ASP	C-O	-10.67	1.10	1.23
1	B	610	LEU	C-O	-10.55	1.11	1.24
1	C	674	ASP	C-O	-10.02	1.11	1.23
1	B	609	MET	SD-CE	-9.88	1.54	1.79
1	A	677	THR	C-O	-9.48	1.11	1.23
1	A	514	LEU	C-O	-8.68	1.14	1.24
1	B	254	ARG	CZ-NH2	-8.45	1.22	1.33
1	B	254	ARG	CZ-NH1	-8.12	1.21	1.32
1	B	254	ARG	CD-NE	-8.01	1.35	1.46
1	C	677	THR	C-O	-8.00	1.13	1.23
1	A	676	GLY	C-O	-7.70	1.14	1.24
1	A	513	ASP	CG-OD2	-7.60	1.10	1.25
1	C	675	ASP	CG-OD1	-7.58	1.10	1.25
1	A	675	ASP	CG-OD2	-7.51	1.11	1.25
1	A	512	GLY	C-O	-7.51	1.13	1.23
1	B	611	LEU	N-CA	-7.45	1.37	1.46
1	B	609	MET	N-CA	-6.80	1.37	1.46
1	A	513	ASP	CA-C	6.71	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	610	LEU	CA-CB	-6.61	1.42	1.53
1	A	675	ASP	C-O	-6.40	1.15	1.24
1	C	675	ASP	CB-CG	-6.28	1.36	1.52
1	A	515	ARG	C-O	-6.23	1.16	1.24
1	C	675	ASP	N-CA	-6.19	1.37	1.46
1	A	675	ASP	N-CA	-6.15	1.38	1.46
1	C	675	ASP	CG-OD2	-5.85	1.14	1.25
1	C	284	VAL	C-O	-5.81	1.17	1.24
1	D	677	THR	C-O	-5.77	1.16	1.23
1	B	610	LEU	N-CA	-5.73	1.39	1.46
1	A	513	ASP	C-O	-5.64	1.16	1.24
1	B	722	GLN	C-O	-5.63	1.17	1.24
1	B	254	ARG	NE-CZ	-5.55	1.26	1.33
1	C	677	THR	N-CA	-5.23	1.39	1.45
1	B	609	MET	CG-SD	-5.20	1.67	1.80
1	C	675	ASP	CA-CB	-5.08	1.45	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	ASP	N-CA-C	8.65	123.59	112.34
1	C	675	ASP	N-CA-CB	-7.64	98.52	110.44
1	C	674	ASP	N-CA-CB	7.11	121.79	111.62
1	C	511	ASP	N-CA-C	-6.85	96.21	110.80
1	D	676	GLY	N-CA-C	-6.62	104.89	115.08
1	D	675	ASP	N-CA-C	6.60	120.55	112.23
1	A	194	ASP	N-CA-C	-6.59	99.28	109.76
1	A	676	GLY	N-CA-C	-6.57	105.60	115.32
1	C	675	ASP	CB-CA-C	-6.56	96.23	109.55
1	C	677	THR	N-CA-CB	-6.26	101.06	111.20
1	B	254	ARG	CD-NE-CZ	5.72	132.41	124.40
1	A	675	ASP	CB-CA-C	-5.69	98.77	110.38
1	C	677	THR	CA-CB-CG2	5.63	120.08	110.50
1	A	675	ASP	N-CA-CB	-5.55	101.75	110.30
1	B	610	LEU	CB-CG-CD2	5.51	127.24	110.70
1	C	191	TRP	N-CA-C	5.42	120.77	113.72
1	A	514	LEU	N-CA-C	5.34	117.53	111.02
1	B	611	LEU	N-CA-CB	5.29	117.90	110.12
1	A	363	THR	CB-CA-C	-5.28	99.58	109.72
1	A	363	THR	N-CA-C	5.25	119.68	113.28
1	B	609	MET	CB-CG-SD	5.22	128.37	112.70
1	C	276	HIS	N-CA-C	5.18	116.77	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ASP	O-C-N	5.16	124.84	121.23
1	A	648	GLU	N-CA-C	-5.08	107.14	113.38

There are no chirality outliers.

There are no planarity outliers.

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	5532	0	5347	104	0
1	B	5532	0	5347	43	0
1	C	5532	0	5347	88	0
1	D	5532	0	5347	38	0
2	A	43	0	30	6	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0
2	D	43	0	30	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	1	0
5	A	238	0	0	6	0
5	B	395	0	0	4	0
5	C	265	0	0	3	0
5	D	391	0	0	2	0
All	All	23617	0	21540	275	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 6.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:HD21	1:A:46:LYS:HD3	1.43	0.82
1:A:509:ASP:HB2	1:A:514:LEU:HB2	1.60	0.81
1:C:129:PHE:HB3	1:C:193:PRO:HG3	1.67	0.77
1:C:513:ASP:N	1:C:513:ASP:OD1	2.12	0.77
1:B:149:TRP:CZ2	1:B:153:LYS:HG3	2.24	0.73
1:C:248:ILE:HD11	1:C:380:THR:HG22	1.69	0.73
1:C:478:ALA:HB1	1:C:508:ASN:ND2	2.05	0.72
1:D:43:LEU:HD22	1:D:611:LEU:HD12	1.72	0.71
1:C:471:GLN:NE2	1:C:513:ASP:OD2	2.23	0.70
1:D:675:ASP:HB3	1:D:677:THR:HG23	1.72	0.70
1:B:274:LYS:HB2	1:B:320:VAL:HG22	1.73	0.70
1:C:459:LYS:HG2	1:C:550:ALA:HB2	1.71	0.70
1:B:51:ASN:ND2	1:B:190:GLN:HG2	2.07	0.69
1:A:471:GLN:NE2	1:A:513:ASP:OD1	2.26	0.69
1:A:478:ALA:HB1	1:A:508:ASN:ND2	2.08	0.69
1:A:510:PRO:O	1:A:511:ASP:HB2	1.90	0.68
1:C:463:ARG:HD3	1:C:554:LYS:HD3	1.74	0.68
1:B:39:TRP:HB2	1:B:42:ARG:HD2	1.74	0.68
1:D:46:LYS:HG2	1:D:49:HIS:CE1	2.29	0.68
1:A:129:PHE:HB3	1:A:193:PRO:HG3	1.75	0.67
1:C:504:GLY:HA2	1:C:510:PRO:HG3	1.77	0.66
1:C:115:ILE:HG13	1:C:586:VAL:HG11	1.78	0.66
1:A:44:ASN:HD21	1:A:46:LYS:CD	2.09	0.65
1:D:439:GLN:NE2	5:D:901:HOH:O	2.23	0.63
1:C:518:ILE:O	1:C:522:GLU:HG3	2.00	0.62
1:D:39:TRP:HB2	1:D:42:ARG:HD2	1.81	0.62
1:A:392:ARG:NH2	5:A:903:HOH:O	2.28	0.62
1:A:458:LEU:HD11	1:A:528:PHE:CE1	2.35	0.61
1:D:45:LEU:HD13	1:D:611:LEU:HD11	1.83	0.60
1:A:510:PRO:HB2	1:A:639:LYS:NZ	2.17	0.60
1:C:70:THR:OG1	1:C:158:LYS:NZ	2.22	0.60
1:D:26:MET:HE3	1:D:38:TRP:CE2	2.37	0.60
2:D:801:HEM:HMB2	2:D:801:HEM:HBB2	1.83	0.59
1:C:447:HIS:HB3	1:C:535:ASN:O	2.01	0.59
1:B:139:ALA:HA	1:B:300:TRP:CZ3	2.36	0.59
1:A:507:VAL:HG22	1:A:597:TYR:CE2	2.38	0.58
1:A:518:ILE:O	1:A:522:GLU:HG3	2.03	0.58
1:A:43:LEU:HG	1:A:611:LEU:HD11	1.86	0.58
1:C:520:THR:O	1:C:524:ILE:HD12	2.03	0.58
1:A:447:HIS:HB3	1:A:535:ASN:O	2.04	0.58
1:A:126:MET:HE3	1:A:194:ASP:HB2	1.84	0.57
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:PRO:O	1:C:241:PRO:HD3	2.05	0.56
1:A:239:PRO:O	1:A:241:PRO:HD3	2.05	0.56
1:A:242:MET:HE1	1:A:388:PRO:HD2	1.88	0.55
1:A:276:HIS:ND1	2:A:801:HEM:O2A	2.34	0.55
1:B:39:TRP:O	1:B:42:ARG:HB2	2.06	0.55
1:B:26:MET:HE3	1:B:38:TRP:CE2	2.41	0.55
1:C:211:SER:O	1:C:215:ASP:HB2	2.06	0.55
1:C:242:MET:HE1	1:C:388:PRO:HD2	1.88	0.55
1:D:274:LYS:HB2	1:D:320:VAL:HG22	1.89	0.55
1:C:539:SER:HB2	1:C:573:ASP:OD1	2.07	0.54
1:A:70:THR:OG1	1:A:158:LYS:NZ	2.23	0.54
1:A:319:VAL:HG22	1:A:376:THR:HB	1.90	0.54
1:A:467:LEU:HD22	1:A:517:VAL:HG22	1.89	0.54
1:C:400:HIS:HB3	1:C:403:GLU:HG3	1.89	0.54
2:A:801:HEM:HBB2	2:A:801:HEM:HMB2	1.89	0.54
1:C:502:GLN:HG2	1:C:505:TRP:CZ3	2.43	0.54
1:B:149:TRP:O	1:B:153:LYS:HB2	2.07	0.54
1:C:319:VAL:HG22	1:C:376:THR:HB	1.90	0.53
1:A:391:GLU:O	1:A:395:ARG:HB2	2.07	0.53
1:C:249:ARG:HG2	5:C:993:HOH:O	2.07	0.53
1:C:520:THR:HG22	1:C:524:ILE:HD11	1.91	0.53
1:A:245:ALA:HB2	1:A:383:SER:HB3	1.89	0.53
1:A:505:TRP:CG	1:A:588:GLU:HG3	2.43	0.53
4:C:803:GOL:H31	5:C:1068:HOH:O	2.08	0.53
1:A:675:ASP:HB3	1:A:677:THR:HG23	1.91	0.53
1:C:340:GLU:OE2	1:C:385:ARG:NH2	2.41	0.52
1:D:46:LYS:HG2	1:D:49:HIS:NE2	2.23	0.52
1:A:498:ARG:HG3	1:A:499:LEU:HD12	1.91	0.52
1:A:539:SER:HB2	1:A:573:ASP:OD1	2.09	0.52
5:B:1051:HOH:O	1:C:424:ALA:HB1	2.10	0.52
1:A:488:LYS:HE2	5:A:921:HOH:O	2.10	0.52
1:C:327:LYS:HE2	1:C:328:TRP:O	2.10	0.52
1:C:285:GLY:N	1:C:301:LYS:O	2.36	0.51
1:D:380:THR:HG21	2:D:801:HEM:CMB	2.41	0.51
1:A:181:PHE:CE2	1:A:432:PRO:HG2	2.44	0.51
1:A:310:LYS:O	1:A:310:LYS:HD3	2.10	0.51
1:B:46:LYS:HG2	1:B:49:HIS:NE2	2.26	0.51
1:A:51:ASN:ND2	1:A:190:GLN:HG2	2.26	0.50
1:A:560:GLY:C	1:A:561:HIS:HD2	2.19	0.50
1:B:361:ALA:HA	1:B:374:SER:HB3	1.94	0.50
1:A:501:PRO:HD3	1:A:581:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HH11	1:B:515:ARG:HG2	1.77	0.50
1:A:484:ARG:HB2	1:A:616:LEU:HD22	1.93	0.50
1:D:139:ALA:HA	1:D:300:TRP:CZ3	2.46	0.50
1:D:658:PHE:HD1	1:D:708:VAL:HG13	1.77	0.50
1:A:214:ARG:NH2	1:A:235:PRO:HB3	2.27	0.49
1:C:181:PHE:CE2	1:C:432:PRO:HG2	2.47	0.49
1:A:130:ALA:O	1:A:193:PRO:HB3	2.12	0.49
1:C:510:PRO:O	1:C:512:GLY:N	2.45	0.49
1:A:694:VAL:O	1:A:697:VAL:HG12	2.12	0.49
1:C:454:GLU:O	1:C:458:LEU:HB2	2.13	0.49
1:D:257:MET:HE3	1:D:265:LEU:HD11	1.95	0.49
1:C:462:ILE:HG21	1:C:547:GLY:HA2	1.94	0.49
1:C:54:VAL:HG22	1:D:620:SER:HB3	1.94	0.49
1:A:688:LYS:HG3	1:A:688:LYS:O	2.10	0.49
1:A:340:GLU:OE2	1:A:385:ARG:NH2	2.40	0.48
1:D:336:LEU:HD21	1:D:385:ARG:HB3	1.94	0.48
1:C:274:LYS:HB2	1:C:320:VAL:HG22	1.95	0.48
1:A:380:THR:HG21	2:A:801:HEM:HMB1	1.95	0.48
1:C:43:LEU:HG	1:C:611:LEU:HD11	1.96	0.48
1:C:553:GLU:HG2	1:C:563:ILE:O	2.14	0.48
1:A:343:LEU:HD13	1:A:353:TYR:CZ	2.49	0.47
1:A:672:PRO:HD2	1:A:679:GLN:NE2	2.28	0.47
1:A:280:PRO:HB2	1:A:282:ASP:OD1	2.15	0.47
1:C:470:SER:HB2	1:C:635:GLY:HA3	1.96	0.47
1:C:505:TRP:CG	1:C:588:GLU:HG3	2.49	0.47
1:A:454:GLU:O	1:A:458:LEU:HD12	2.15	0.47
1:A:510:PRO:HB2	1:A:639:LYS:HZ1	1.79	0.47
1:A:662:LEU:HD11	1:A:708:VAL:HG12	1.96	0.47
1:B:45:LEU:HD23	1:B:611:LEU:HD21	1.96	0.47
1:B:116:HIS:ND1	1:B:219:PRO:HB3	2.29	0.47
1:A:611:LEU:CD2	1:A:624:MET:HE1	2.44	0.47
1:B:275:THR:HB	2:B:801:HEM:HAA2	1.97	0.47
1:C:44:ASN:HD21	1:C:46:LYS:HB3	1.79	0.47
1:D:380:THR:HG21	2:D:801:HEM:HMB2	1.97	0.47
1:A:209:ARG:CZ	1:A:220:LEU:HD13	2.45	0.47
1:C:510:PRO:O	1:C:511:ASP:C	2.57	0.47
1:D:93:ALA:HB2	1:D:98:TYR:CZ	2.50	0.47
1:C:463:ARG:HH11	1:C:554:LYS:HD3	1.80	0.47
1:A:520:THR:O	1:A:524:ILE:HG13	2.15	0.46
1:B:149:TRP:CE2	1:B:153:LYS:HG3	2.50	0.46
1:A:462:ILE:HG22	1:A:472:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLY:O	1:C:128:ARG:HG2	2.15	0.46
1:D:95:TYR:CZ	1:D:325:PRO:HG2	2.50	0.46
1:B:577:GLU:CD	1:B:577:GLU:H	2.24	0.46
1:A:472:LEU:HD23	1:A:551:ALA:HB2	1.96	0.46
1:C:418:ARG:HD2	1:C:418:ARG:HA	1.66	0.46
1:A:330:ASN:O	1:A:334:GLU:HG3	2.15	0.46
1:A:448:ASP:OD1	1:A:535:ASN:HB3	2.16	0.46
1:C:47:VAL:HG23	1:C:48:LEU:HD13	1.98	0.46
1:C:644:GLY:HA3	1:C:695:ASP:OD1	2.15	0.46
1:A:622:PRO:O	1:A:626:VAL:HG22	2.16	0.46
1:D:366:ASP:CG	1:D:367:PRO:HD2	2.40	0.46
1:D:728:TRP:CE2	1:D:732:MET:HE3	2.51	0.46
1:A:78:ARG:HD3	5:A:1063:HOH:O	2.16	0.46
5:A:985:HOH:O	1:B:42:ARG:HG3	2.14	0.46
1:C:521:LEU:HA	1:C:524:ILE:HD12	1.98	0.46
1:A:256:ALA:O	1:A:414:LYS:NZ	2.46	0.46
1:B:182:GLY:HA3	1:B:432:PRO:HD3	1.98	0.46
1:C:80:ILE:O	1:C:84:MET:HG3	2.16	0.46
1:C:467:LEU:HA	1:C:471:GLN:OE1	2.16	0.46
1:A:279:GLY:O	1:A:348:ALA:HB2	2.17	0.45
1:A:346:SER:OG	1:A:350:ALA:HB3	2.16	0.45
1:C:513:ASP:O	1:C:517:VAL:HG12	2.16	0.45
1:A:152:LYS:NZ	4:A:803:GOL:H31	2.31	0.45
1:B:139:ALA:HA	1:B:300:TRP:CH2	2.51	0.45
1:B:492:ALA:HB3	5:B:924:HOH:O	2.16	0.45
1:A:443:PRO:HG2	1:A:573:ASP:O	2.16	0.45
1:C:605:PRO:HD2	1:C:608:TYR:CD1	2.51	0.45
1:A:275:THR:HG22	2:A:801:HEM:HAA1	1.98	0.45
1:D:160:SER:HA	4:D:803:GOL:H12	1.98	0.45
1:A:509:ASP:C	1:A:511:ASP:H	2.23	0.45
1:C:529:ASN:O	1:C:531:ALA:N	2.50	0.45
1:C:498:ARG:HG3	1:C:499:LEU:HD12	1.99	0.45
1:D:182:GLY:HA3	1:D:432:PRO:HD3	1.99	0.45
1:B:619:LEU:HD22	1:B:623:GLU:HB3	1.99	0.44
1:C:529:ASN:C	1:C:531:ALA:H	2.26	0.44
1:A:49:HIS:O	1:A:49:HIS:ND1	2.48	0.44
1:A:249:ARG:NH1	1:A:259:ASP:OD1	2.50	0.44
1:A:495:GLY:N	1:A:541:ALA:HB2	2.32	0.44
1:B:95:TYR:CZ	1:B:325:PRO:HG2	2.52	0.44
1:C:499:LEU:HB3	1:C:576:GLN:OE1	2.16	0.44
1:A:627:LEU:O	1:A:631:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:803:GOL:H32	5:A:1018:HOH:O	2.17	0.44
1:C:478:ALA:HB1	1:C:508:ASN:HD22	1.81	0.44
1:A:446:SER:HB2	1:A:447:HIS:ND1	2.33	0.44
1:A:646:PHE:CE1	1:A:689:TRP:HB3	2.53	0.44
1:C:498:ARG:NH1	1:C:522:GLU:OE2	2.46	0.44
1:C:130:ALA:O	1:C:193:PRO:HB3	2.18	0.44
1:D:728:TRP:O	1:D:732:MET:HG2	2.18	0.44
1:A:560:GLY:C	1:A:561:HIS:CD2	2.96	0.43
1:C:139:ALA:HA	1:C:300:TRP:CH2	2.52	0.43
1:B:27:LYS:HE3	1:B:27:LYS:HB2	1.72	0.43
1:B:134:SER:HB3	1:B:287:GLU:HG3	1.99	0.43
1:D:420:MET:O	1:D:425:ARG:HD3	2.19	0.43
2:A:801:HEM:HMC1	2:A:801:HEM:HBC2	1.99	0.43
1:B:314:THR:HB	2:B:801:HEM:O1A	2.18	0.43
1:B:515:ARG:HG2	1:B:515:ARG:NH1	2.33	0.43
1:C:77:THR:O	1:C:81:GLU:HG3	2.18	0.43
1:C:477:TRP:O	1:C:481:SER:HB3	2.19	0.43
1:A:452:GLU:O	1:A:453:ALA:C	2.61	0.43
1:B:731:VAL:HA	1:B:734:LEU:HG	1.99	0.43
1:C:448:ASP:OD1	1:C:535:ASN:HB3	2.18	0.43
1:B:108:HIS:CE1	1:B:137:ASP:O	2.71	0.43
1:C:346:SER:OG	1:C:350:ALA:HB3	2.18	0.43
1:C:420:MET:O	1:C:425:ARG:HD3	2.19	0.43
1:C:458:LEU:HD12	1:C:458:LEU:HA	1.89	0.43
1:D:412:TRP:O	1:D:416:ILE:HG12	2.19	0.43
1:A:44:ASN:ND2	1:A:46:LYS:HD3	2.22	0.43
1:C:48:LEU:HD23	1:C:621:ALA:HA	2.00	0.43
1:C:202:ALA:HA	1:D:26:MET:HE2	2.00	0.43
1:D:467:LEU:HD22	1:D:517:VAL:HG22	1.99	0.43
1:A:229:TYR:HD1	1:A:255:MET:HE3	1.70	0.43
1:C:44:ASN:ND2	1:C:46:LYS:H	2.16	0.43
1:A:510:PRO:HB2	1:A:639:LYS:HZ3	1.82	0.43
1:A:630:GLY:O	1:A:634:LEU:HG	2.18	0.43
1:D:108:HIS:CE1	1:D:137:ASP:O	2.72	0.43
1:B:51:ASN:HD21	1:B:190:GLN:HG2	1.81	0.43
1:B:423:VAL:HG23	5:B:1112:HOH:O	2.18	0.42
1:C:279:GLY:O	1:C:348:ALA:HB2	2.19	0.42
1:D:455:ILE:O	1:D:459:LYS:HG3	2.18	0.42
1:D:128:ARG:NH2	1:D:190:GLN:O	2.52	0.42
1:A:657:PHE:O	1:A:661:LEU:HB2	2.19	0.42
1:C:620:SER:HB2	1:C:622:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:GLN:HB3	1:C:687:VAL:HG13	2.01	0.42
1:D:149:TRP:CE2	1:D:153:LYS:HD2	2.54	0.42
1:D:292:PRO:HB2	1:D:294:GLU:CD	2.45	0.42
1:A:321:TRP:NE1	1:A:381:ASP:OD2	2.48	0.42
1:D:345:LYS:HE2	1:D:351:TRP:CZ3	2.54	0.42
1:C:342:GLU:HB3	1:C:356:LYS:HG2	2.02	0.42
1:C:538:VAL:HA	5:C:915:HOH:O	2.19	0.42
1:A:113:TYR:OH	1:A:487:ASP:OD2	2.34	0.42
1:B:274:LYS:HG3	1:B:275:THR:O	2.20	0.42
1:A:499:LEU:HB3	1:A:576:GLN:OE1	2.20	0.42
1:A:529:ASN:C	1:A:531:ALA:H	2.27	0.42
1:B:70:THR:OG1	1:B:158:LYS:NZ	2.35	0.42
1:B:245:ALA:HB2	1:B:383:SER:HB3	2.02	0.42
1:A:26:MET:HE3	1:A:38:TRP:CE2	2.55	0.42
1:A:631:LEU:HB3	1:A:636:ALA:CB	2.49	0.42
1:B:42:ARG:NH1	5:B:923:HOH:O	2.50	0.42
1:B:93:ALA:HB2	1:B:98:TYR:CE1	2.55	0.42
1:C:36:GLN:O	1:C:40:PRO:HA	2.19	0.42
1:C:247:ASP:O	1:C:251:THR:HG23	2.19	0.42
1:C:667:THR:O	1:C:680:GLY:HA2	2.19	0.42
1:A:433:LYS:HE2	1:A:433:LYS:HB2	1.98	0.42
1:A:113:TYR:HE1	1:A:487:ASP:HB3	1.84	0.41
1:A:337:TYR:CE1	1:A:385:ARG:HG3	2.55	0.41
1:C:510:PRO:HA	1:C:514:LEU:HB3	2.01	0.41
1:D:577:GLU:H	1:D:577:GLU:CD	2.25	0.41
1:A:44:ASN:HD21	1:A:46:LYS:CE	2.33	0.41
1:B:93:ALA:HB2	1:B:98:TYR:CZ	2.55	0.41
1:B:406:ASP:O	1:B:410:LYS:HG3	2.21	0.41
1:C:116:HIS:ND1	1:C:219:PRO:HB3	2.35	0.41
1:C:280:PRO:HB2	1:C:282:ASP:OD1	2.19	0.41
1:A:139:ALA:HA	1:A:300:TRP:CZ3	2.55	0.41
1:A:345:LYS:HE2	1:A:351:TRP:CH2	2.55	0.41
1:B:366:ASP:CG	1:B:367:PRO:HD2	2.45	0.41
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.76	0.41
1:C:658:PHE:HD1	1:C:708:VAL:HG13	1.85	0.41
1:A:307:GLY:HA2	5:A:908:HOH:O	2.19	0.41
1:A:509:ASP:C	1:A:511:ASP:N	2.79	0.41
1:C:529:ASN:C	1:C:531:ALA:N	2.79	0.41
1:B:641:LEU:HB2	1:B:642:PRO:HD2	2.03	0.41
1:C:113:TYR:HE1	1:C:487:ASP:HB3	1.86	0.41
1:C:233:GLU:OE2	1:C:351:TRP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:SER:C	1:A:467:LEU:H	2.29	0.41
1:A:471:GLN:CD	1:A:513:ASP:OD1	2.64	0.41
1:C:115:ILE:HG23	1:C:254:ARG:O	2.21	0.41
1:C:616:LEU:HD23	1:C:616:LEU:HA	1.69	0.41
1:A:380:THR:HG21	2:A:801:HEM:CMB	2.50	0.41
1:A:630:GLY:HA3	1:A:724:PHE:CE1	2.56	0.41
1:A:73:VAL:HG11	1:A:430:LEU:HD11	2.02	0.40
1:A:192:GLU:OE2	1:B:49:HIS:HE1	2.04	0.40
1:A:683:GLY:C	1:A:685:GLY:H	2.29	0.40
1:B:628:VAL:O	1:B:632:ARG:HG2	2.21	0.40
1:C:245:ALA:HB2	1:C:383:SER:HB3	2.03	0.40
1:C:475:THR:HG22	1:C:544:VAL:HG13	2.03	0.40
1:D:68:VAL:HG21	1:D:185:PHE:HB3	2.03	0.40
1:C:694:VAL:O	1:C:697:VAL:HG12	2.21	0.40
1:D:324:THR:O	1:D:324:THR:OG1	2.34	0.40
1:D:505:TRP:CE2	1:D:588:GLU:HB2	2.57	0.40
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.87	0.40
1:A:458:LEU:HD11	1:A:528:PHE:CD1	2.55	0.40
1:A:505:TRP:CD1	1:A:588:GLU:HG3	2.56	0.40
1:A:661:LEU:HD12	1:A:661:LEU:HA	1.92	0.40
1:C:99:GLY:O	1:C:103:ILE:HG13	2.22	0.40
1:C:213:LYS:H	1:C:213:LYS:HG2	1.74	0.40
1:D:492:ALA:HB3	5:D:1028:HOH:O	2.21	0.40
1:A:528:PHE:O	1:A:532:ALA:HB2	2.20	0.40
1:A:472:LEU:HG	1:A:547:GLY:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	714/741 (96%)	680 (95%)	33 (5%)	1 (0%)	48 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	714/741 (96%)	697 (98%)	17 (2%)	0	100	100
1	C	714/741 (96%)	676 (95%)	37 (5%)	1 (0%)	48	60
1	D	714/741 (96%)	695 (97%)	18 (2%)	1 (0%)	48	60
All	All	2856/2964 (96%)	2748 (96%)	105 (4%)	3 (0%)	48	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	530	SER
1	D	673	ALA
1	A	684	SER

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	564/583 (97%)	553 (98%)	11 (2%)	48	67
1	B	564/583 (97%)	557 (99%)	7 (1%)	63	79
1	C	564/583 (97%)	549 (97%)	15 (3%)	39	58
1	D	564/583 (97%)	554 (98%)	10 (2%)	51	70
All	All	2256/2332 (97%)	2213 (98%)	43 (2%)	50	69

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	423	VAL
1	A	455	ILE
1	A	507	VAL
1	A	509	ASP
1	A	511	ASP
1	A	514	LEU
1	A	587	LEU

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Mol	Chain	Res	Type
1	A	596	ASN
1	A	648	GLU
1	A	717	GLN
1	B	153	LYS
1	B	275	THR
1	B	385	ARG
1	B	426	TYR
1	B	587	LEU
1	B	610	LEU
1	B	641	LEU
1	C	137	ASP
1	C	302	SER
1	C	363	THR
1	C	380	THR
1	C	423	VAL
1	C	446	SER
1	C	475	THR
1	C	481	SER
1	C	499	LEU
1	C	500	GLN
1	C	513	ASP
1	C	561	HIS
1	C	587	LEU
1	C	596	ASN
1	C	648	GLU
1	D	82	GLU
1	D	137	ASP
1	D	374	SER
1	D	380	THR
1	D	385	ARG
1	D	530	SER
1	D	587	LEU
1	D	610	LEU
1	D	641	LEU
1	D	722	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	44	ASN
1	A	50	GLN

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Mol	Chain	Res	Type
1	A	236	ASN
1	A	471	GLN
1	A	500	GLN
1	A	561	HIS
1	A	596	ASN
1	A	602	ASN
1	A	717	GLN
1	B	49	HIS
1	B	295	GLN
1	B	400	HIS
1	B	717	GLN
1	B	722	GLN
1	C	500	GLN
1	C	596	ASN
1	D	439	GLN
1	D	722	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TOX	C	107[A]	2	14,17,18	2.88	2 (14%)	12,23,25	1.65	3 (25%)
1	TOX	B	107[B]	-	14,17,18	2.94	2 (14%)	12,23,25	1.76	3 (25%)
1	TOX	D	107[A]	2	14,17,18	3.00	2 (14%)	12,23,25	1.90	5 (41%)
1	TOX	B	107[A]	2	14,17,18	2.94	2 (14%)	12,23,25	1.76	3 (25%)
1	TOX	D	107[B]	-	14,17,18	3.00	2 (14%)	12,23,25	1.90	5 (41%)
1	TOX	A	107[B]	-	14,17,18	3.02	2 (14%)	12,23,25	1.74	5 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	A	107[A]	2	14,17,18	3.02	2 (14%)	12,23,25	1.74	5 (41%)
1	TOX	C	107[B]	-	14,17,18	2.88	2 (14%)	12,23,25	1.65	3 (25%)

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
1	TOX	C	107[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	107[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	D	107[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	107[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	D	107[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	107[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	107[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	C	107[B]	-	-	2/5/8/10	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107[A]	TOX	O1-NE1	9.96	1.52	1.39
1	A	107[B]	TOX	O1-NE1	9.96	1.52	1.39
1	D	107[A]	TOX	O1-NE1	9.73	1.51	1.39
1	D	107[B]	TOX	O1-NE1	9.73	1.51	1.39
1	B	107[A]	TOX	O1-NE1	9.55	1.51	1.39
1	B	107[B]	TOX	O1-NE1	9.55	1.51	1.39
1	C	107[A]	TOX	O1-NE1	9.30	1.51	1.39
1	C	107[B]	TOX	O1-NE1	9.30	1.51	1.39
1	A	107[A]	TOX	CD2-CG	-3.79	1.37	1.44
1	A	107[B]	TOX	CD2-CG	-3.79	1.37	1.44
1	C	107[A]	TOX	CD2-CG	-3.76	1.37	1.44
1	C	107[B]	TOX	CD2-CG	-3.76	1.37	1.44
1	B	107[A]	TOX	CD2-CG	-3.27	1.38	1.44
1	B	107[B]	TOX	CD2-CG	-3.27	1.38	1.44
1	D	107[A]	TOX	CD2-CG	-3.05	1.39	1.44
1	D	107[B]	TOX	CD2-CG	-3.05	1.39	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107[A]	TOX	CZ2-CE2-CD2	-3.27	118.30	121.95
1	D	107[B]	TOX	CZ2-CE2-CD2	-3.27	118.30	121.95
1	B	107[A]	TOX	CZ2-CE2-CD2	-3.04	118.56	121.95
1	B	107[B]	TOX	CZ2-CE2-CD2	-3.04	118.56	121.95
1	D	107[A]	TOX	CZ3-CH2-CZ2	-2.80	116.79	120.24
1	D	107[B]	TOX	CZ3-CH2-CZ2	-2.80	116.79	120.24
1	D	107[A]	TOX	CZ2-CE2-NE1	2.78	133.81	129.37
1	D	107[B]	TOX	CZ2-CE2-NE1	2.78	133.81	129.37
1	B	107[A]	TOX	CZ2-CE2-NE1	2.70	133.68	129.37
1	B	107[B]	TOX	CZ2-CE2-NE1	2.70	133.68	129.37
1	B	107[A]	TOX	CB-CG-CD1	-2.68	122.94	126.67
1	B	107[B]	TOX	CB-CG-CD1	-2.68	122.94	126.67
1	A	107[A]	TOX	CZ2-CE2-CD2	-2.49	119.17	121.95
1	A	107[B]	TOX	CZ2-CE2-CD2	-2.49	119.17	121.95
1	D	107[A]	TOX	CH2-CZ2-CE2	2.41	123.14	118.28
1	D	107[B]	TOX	CH2-CZ2-CE2	2.41	123.14	118.28
1	C	107[A]	TOX	CB-CG-CD1	-2.31	123.46	126.67
1	C	107[B]	TOX	CB-CG-CD1	-2.31	123.46	126.67
1	A	107[A]	TOX	CE3-CD2-CG	-2.27	130.46	133.85
1	A	107[B]	TOX	CE3-CD2-CG	-2.27	130.46	133.85
1	A	107[A]	TOX	CZ2-CE2-NE1	2.15	132.79	129.37
1	A	107[B]	TOX	CZ2-CE2-NE1	2.15	132.79	129.37
1	A	107[A]	TOX	CZ3-CH2-CZ2	-2.11	117.64	120.24
1	A	107[B]	TOX	CZ3-CH2-CZ2	-2.11	117.64	120.24
1	C	107[A]	TOX	CZ2-CE2-NE1	2.10	132.71	129.37
1	C	107[B]	TOX	CZ2-CE2-NE1	2.10	132.71	129.37
1	D	107[A]	TOX	CB-CG-CD1	-2.07	123.80	126.67
1	D	107[B]	TOX	CB-CG-CD1	-2.07	123.80	126.67
1	C	107[A]	TOX	CE3-CD2-CG	-2.06	130.79	133.85
1	C	107[B]	TOX	CE3-CD2-CG	-2.06	130.79	133.85
1	A	107[A]	TOX	CE2-CD2-CG	2.05	109.28	107.39
1	A	107[B]	TOX	CE2-CD2-CG	2.05	109.28	107.39

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	107[A]	TOX	N-CA-CB-CG
1	A	107[A]	TOX	C-CA-CB-CG
1	A	107[B]	TOX	N-CA-CB-CG
1	A	107[B]	TOX	C-CA-CB-CG
1	B	107[A]	TOX	N-CA-CB-CG
1	B	107[A]	TOX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	107[B]	TOX	N-CA-CB-CG
1	B	107[B]	TOX	C-CA-CB-CG
1	C	107[A]	TOX	N-CA-CB-CG
1	C	107[A]	TOX	C-CA-CB-CG
1	C	107[B]	TOX	N-CA-CB-CG
1	C	107[B]	TOX	C-CA-CB-CG
1	D	107[A]	TOX	N-CA-CB-CG
1	D	107[A]	TOX	C-CA-CB-CG
1	D	107[B]	TOX	N-CA-CB-CG
1	D	107[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	801	1	50,50,50	1.43	7 (14%)	67,82,82	1.15	5 (7%)
2	HEM	C	801	1	50,50,50	1.56	9 (18%)	67,82,82	1.21	7 (10%)
4	GOL	D	803	-	5,5,5	0.79	0	5,5,5	0.51	0
2	HEM	A	801	1	50,50,50	1.52	8 (16%)	67,82,82	1.26	8 (11%)
4	GOL	B	803	-	5,5,5	0.74	0	5,5,5	1.39	0
2	HEM	B	801	1	50,50,50	2.15	21 (42%)	67,82,82	1.96	22 (32%)
4	GOL	C	803	-	5,5,5	0.56	0	5,5,5	1.66	1 (20%)
4	GOL	A	803	-	5,5,5	1.27	0	5,5,5	0.86	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	HEM	D	801	1	-	2/14/54/54	-
2	HEM	C	801	1	-	4/14/54/54	-
4	GOL	D	803	-	-	2/4/4/4	-
2	HEM	A	801	1	-	6/14/54/54	-
4	GOL	B	803	-	-	4/4/4/4	-
2	HEM	B	801	1	-	8/14/54/54	-
4	GOL	C	803	-	-	2/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-6.17	1.29	1.40
2	C	801	HEM	FE-NC	5.17	2.12	1.95
2	C	801	HEM	FE-ND	4.77	2.09	1.94
2	A	801	HEM	FE-NC	4.59	2.10	1.95
2	A	801	HEM	FE-ND	4.44	2.08	1.94
2	B	801	HEM	C4B-NB	-4.37	1.30	1.38
2	B	801	HEM	FE-NB	4.01	2.07	1.94
2	D	801	HEM	FE-ND	3.88	2.06	1.94
2	D	801	HEM	CAC-C3C	3.56	1.56	1.47
2	B	801	HEM	C3C-C4C	-3.55	1.39	1.46
2	B	801	HEM	C1A-C2A	-3.53	1.37	1.44
2	B	801	HEM	C4A-NA	-3.28	1.33	1.39
2	A	801	HEM	CAC-C3C	3.27	1.56	1.47
2	B	801	HEM	C1C-C2C	-3.26	1.38	1.45
2	B	801	HEM	C3D-C2D	-3.23	1.29	1.36
2	C	801	HEM	CAB-C3B	3.20	1.55	1.47
2	B	801	HEM	C4D-ND	-3.17	1.34	1.40
2	D	801	HEM	CAB-C3B	3.06	1.55	1.47
2	A	801	HEM	CAB-C3B	2.99	1.55	1.47
2	C	801	HEM	CAC-C3C	2.98	1.55	1.47
2	D	801	HEM	FE-NB	2.90	2.03	1.94
2	B	801	HEM	C1C-NC	-2.88	1.34	1.39
2	D	801	HEM	CMC-C2C	2.86	1.56	1.50
2	C	801	HEM	FE-NB	2.86	2.03	1.94
2	B	801	HEM	O2A-CGA	-2.77	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NA	2.72	2.04	1.95
2	B	801	HEM	FE-NC	2.68	2.04	1.95
2	B	801	HEM	C2A-C3A	-2.67	1.31	1.38
2	B	801	HEM	FE-ND	-2.67	1.86	1.94
2	B	801	HEM	C1B-C2B	-2.67	1.39	1.44
2	B	801	HEM	O2D-CGD	-2.62	1.22	1.30
2	B	801	HEM	C4C-NC	-2.52	1.34	1.39
2	B	801	HEM	C3B-C2B	-2.49	1.32	1.37
2	B	801	HEM	C1D-ND	-2.29	1.34	1.38
2	A	801	HEM	FE-NB	2.27	2.01	1.94
2	D	801	HEM	CMB-C2B	2.23	1.55	1.50
2	B	801	HEM	C4A-C3A	-2.22	1.37	1.43
2	A	801	HEM	CMB-C2B	2.18	1.55	1.50
2	A	801	HEM	C2A-C3A	-2.17	1.33	1.38
2	C	801	HEM	FE-NA	2.15	2.02	1.95
2	C	801	HEM	CMD-C2D	2.12	1.55	1.50
2	D	801	HEM	CMD-C2D	2.07	1.55	1.50
2	C	801	HEM	CMB-C2B	2.06	1.55	1.50
2	B	801	HEM	C1A-NA	-2.05	1.35	1.39
2	C	801	HEM	CMC-C2C	2.04	1.55	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAD-C3D-C4D	4.78	133.03	124.70
2	B	801	HEM	C1B-NB-C4B	4.71	110.79	105.21
2	B	801	HEM	CHC-C4B-NB	3.76	128.47	124.42
2	B	801	HEM	C3B-C4B-NB	-3.60	106.88	109.47
2	B	801	HEM	CHB-C1B-NB	3.38	128.55	124.37
2	B	801	HEM	CAD-C3D-C2D	-3.33	121.62	127.87
2	A	801	HEM	C2A-C1A-NA	-3.24	106.56	110.15
2	B	801	HEM	CMD-C2D-C1D	3.22	130.06	125.03
4	C	803	GOL	C3-C2-C1	-3.17	100.19	111.80
2	D	801	HEM	CAA-CBA-CGA	-3.11	105.42	113.67
2	B	801	HEM	O2D-CGD-O1D	-3.09	115.38	123.33
2	B	801	HEM	CHD-C1D-ND	3.06	127.71	124.42
2	B	801	HEM	CBD-CAD-C3D	3.04	120.93	112.53
2	B	801	HEM	O2D-CGD-CBD	2.96	123.36	114.00
2	B	801	HEM	CHD-C4C-NC	2.93	127.64	124.45
2	D	801	HEM	CAD-C3D-C4D	2.88	129.71	124.70
2	B	801	HEM	O2A-CGA-O1A	-2.85	116.01	123.33
2	D	801	HEM	CAD-C3D-C2D	-2.73	122.75	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	CHC-C4B-NB	2.63	127.26	124.42
2	B	801	HEM	CHD-C1D-C2D	-2.62	120.89	125.03
2	B	801	HEM	O2A-CGA-CBA	2.59	122.18	114.00
2	A	801	HEM	CHD-C1D-ND	2.52	127.13	124.42
2	B	801	HEM	C1A-CHA-C4D	-2.46	120.47	126.25
2	C	801	HEM	C4D-ND-C1D	2.39	108.03	105.21
2	A	801	HEM	CAA-CBA-CGA	-2.32	107.51	113.67
2	A	801	HEM	O2D-CGD-CBD	2.28	121.20	114.00
2	B	801	HEM	CHA-C4D-C3D	-2.27	121.04	125.23
2	D	801	HEM	CAD-CBD-CGD	-2.25	107.69	113.67
2	C	801	HEM	C4A-C3A-C2A	2.20	109.33	106.82
2	A	801	HEM	C4D-ND-C1D	2.20	107.81	105.21
2	C	801	HEM	CAA-CBA-CGA	-2.19	107.85	113.67
2	C	801	HEM	C2A-C1A-NA	-2.19	107.72	110.15
2	B	801	HEM	CMC-C2C-C1C	2.19	128.59	124.73
2	A	801	HEM	CAA-C2A-C1A	2.17	129.18	124.94
2	C	801	HEM	C3D-C4D-ND	-2.13	107.83	110.17
2	A	801	HEM	CAA-C2A-C3A	-2.12	122.32	127.07
2	C	801	HEM	C3A-C4A-NA	-2.11	106.76	110.14
2	B	801	HEM	C4C-NC-C1C	2.10	109.24	105.82
2	D	801	HEM	C2A-C1A-NA	-2.09	107.83	110.15
2	B	801	HEM	CHA-C4D-ND	2.08	126.95	124.37
2	A	801	HEM	CHC-C4B-NB	2.02	126.60	124.42
2	B	801	HEM	CMB-C2B-C1B	2.02	128.19	125.03
2	B	801	HEM	C4C-CHD-C1D	-2.00	121.76	126.02

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	C1-C2-C3-O3
4	B	803	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	D	803	GOL	C1-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
4	B	803	GOL	O2-C2-C3-O3
4	C	803	GOL	O1-C1-C2-O2
2	A	801	HEM	C1A-C2A-CAA-CBA
4	C	803	GOL	O2-C2-C3-O3
4	D	803	GOL	O2-C2-C3-O3
2	B	801	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O2-C2-C3-O3
2	A	801	HEM	C3A-C2A-CAA-CBA
2	D	801	HEM	CAA-CBA-CGA-O1A
2	D	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	C	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4C-C3C-CAC-CBC
2	A	801	HEM	CAA-CBA-CGA-O2A
4	B	803	GOL	O1-C1-C2-O2
2	C	801	HEM	CAD-CBD-CGD-O2D
2	C	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	C2C-C3C-CAC-CBC
2	B	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D

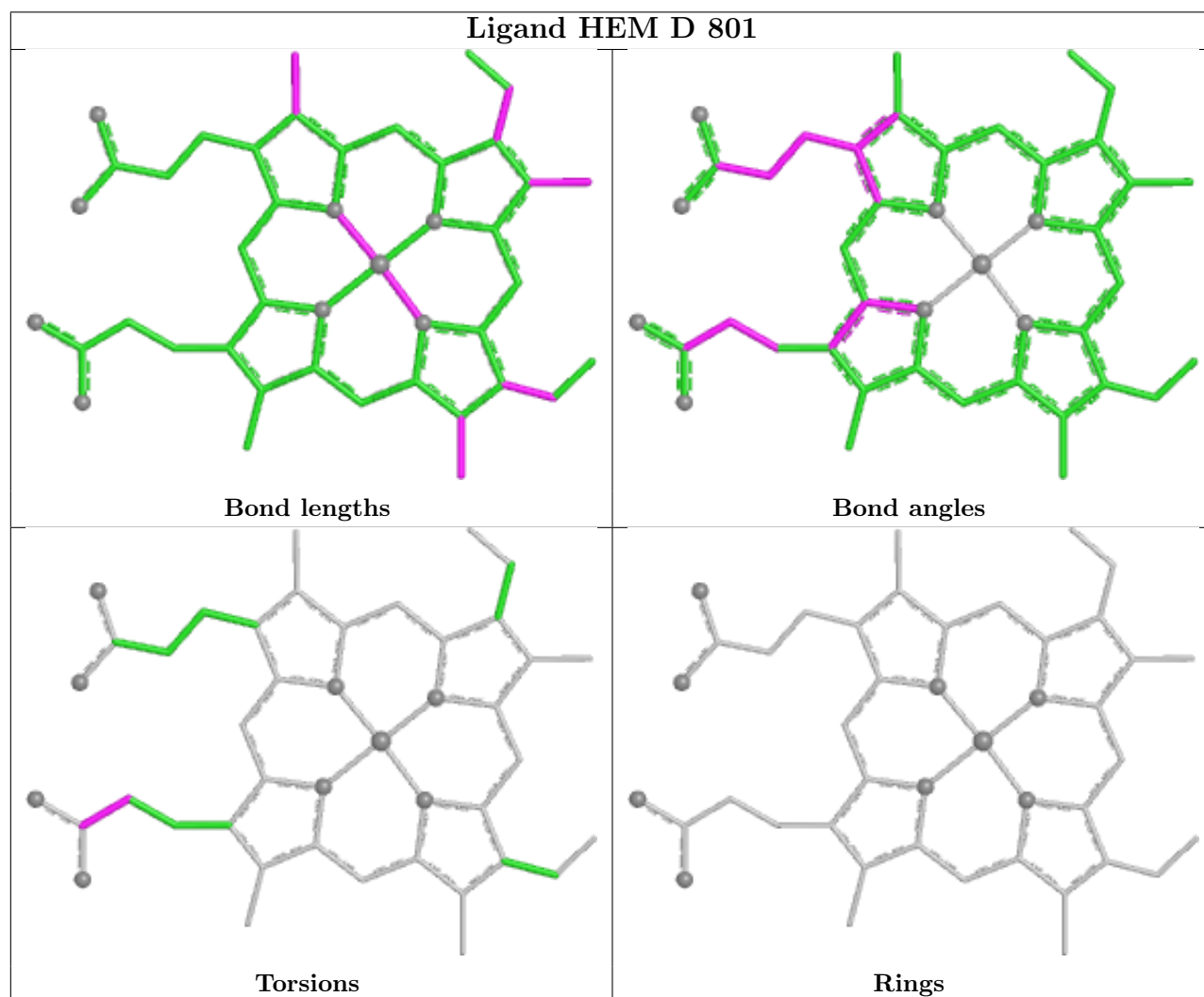
There are no ring outliers.

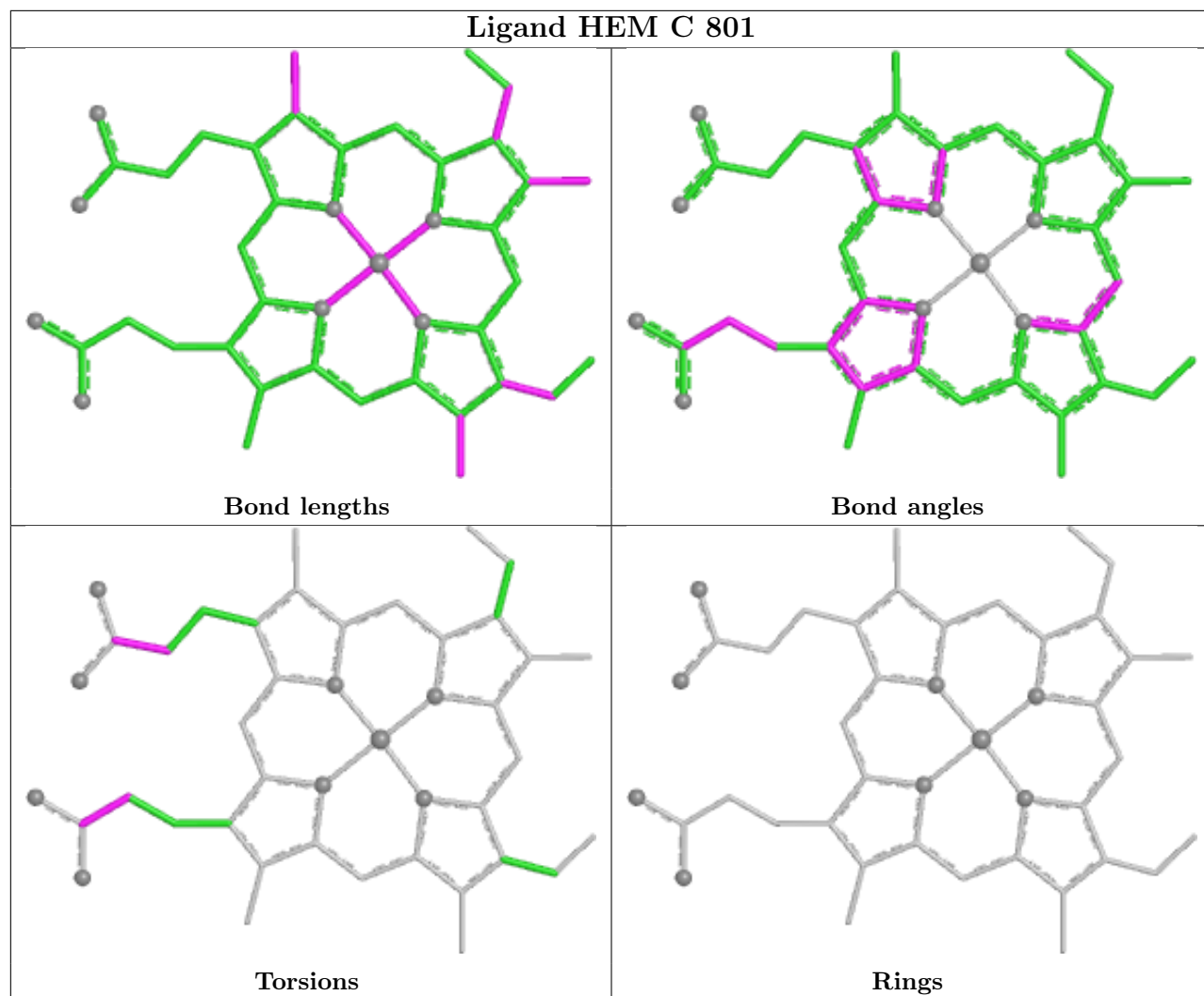
6 monomers are involved in 15 short contacts:

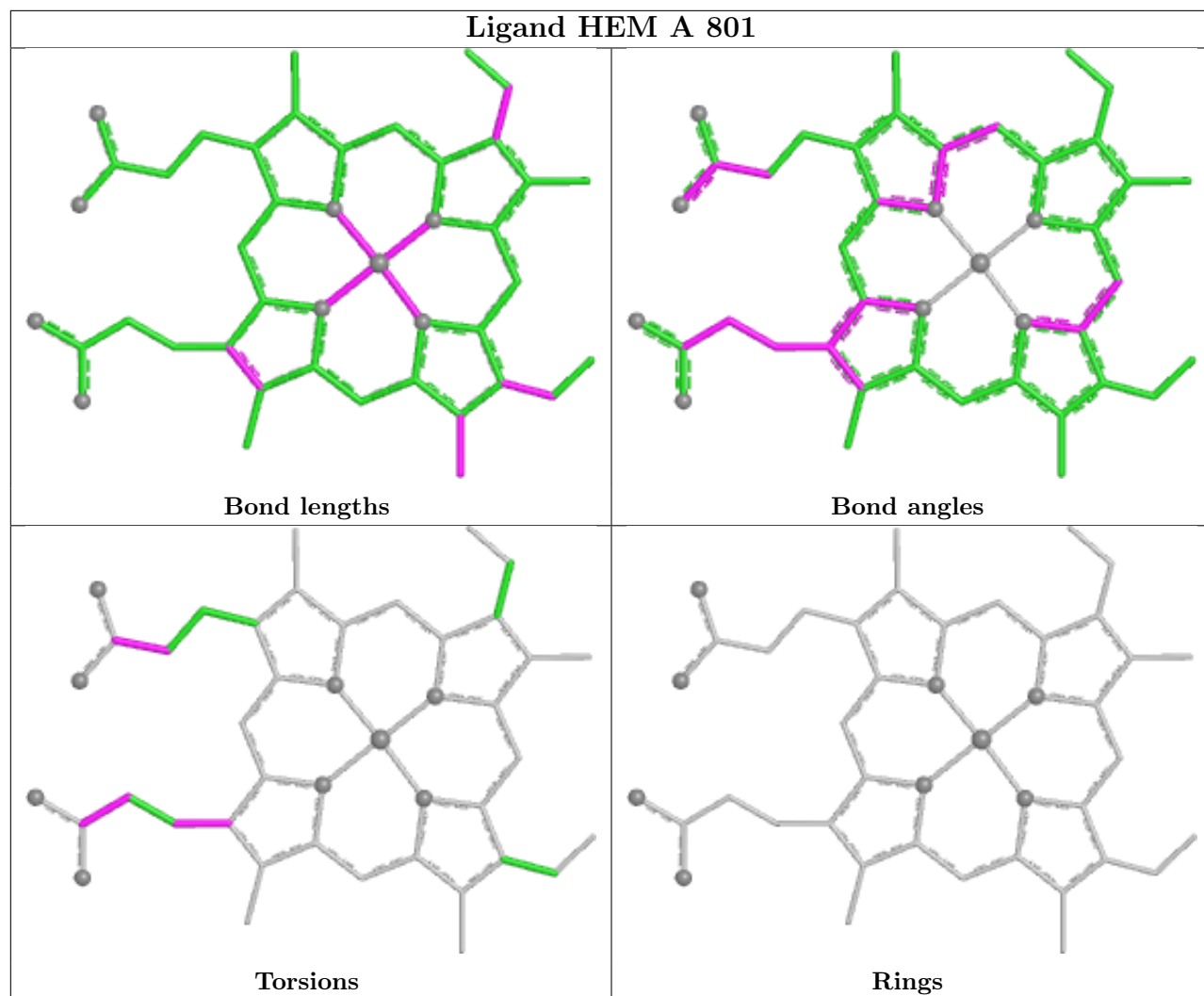
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	HEM	3	0
4	D	803	GOL	1	0
2	A	801	HEM	6	0
2	B	801	HEM	2	0
4	C	803	GOL	1	0
4	A	803	GOL	2	0

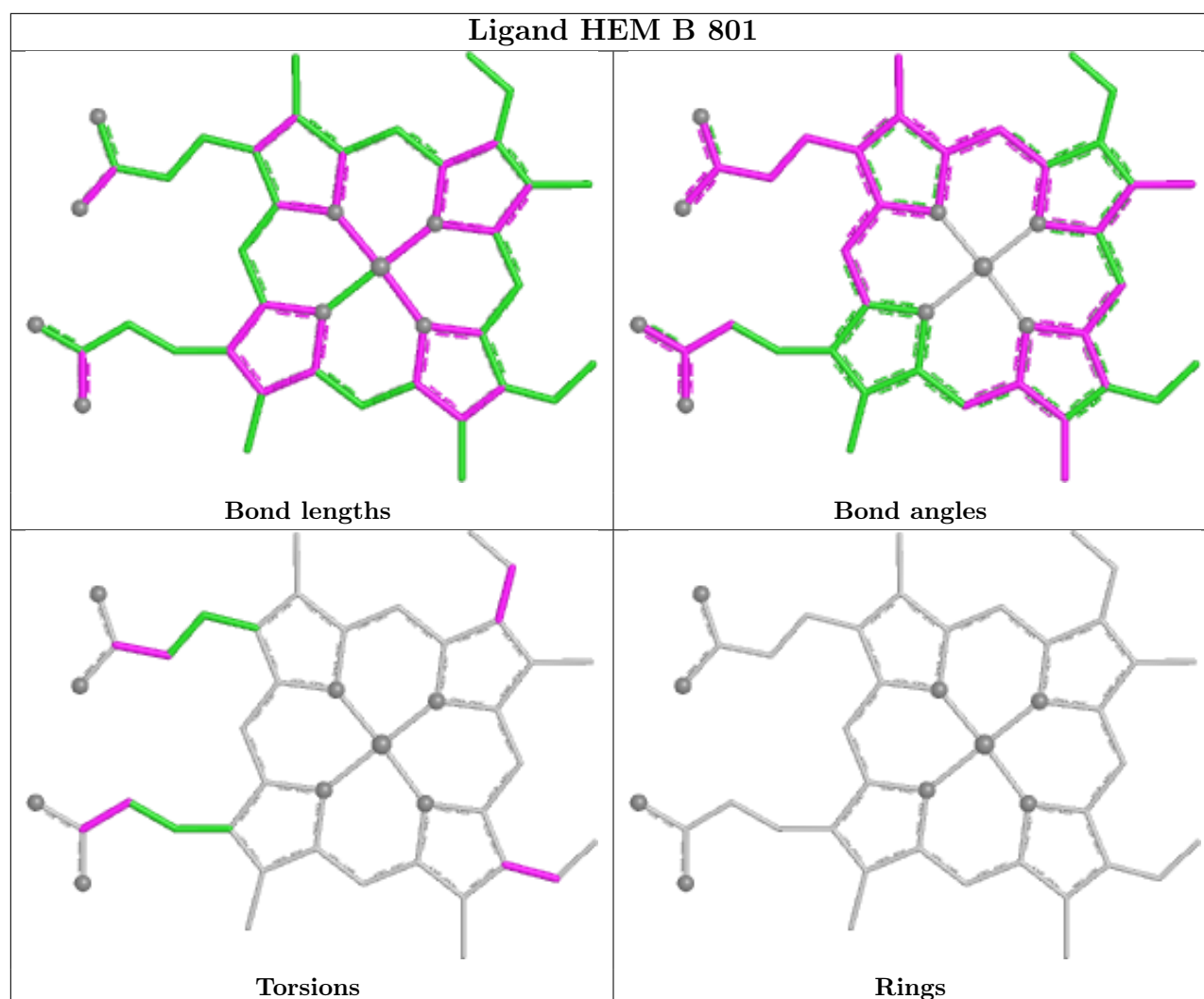
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	716/741 (96%)	-1.55	0 100 100	19, 34, 54, 77	0
1	B	716/741 (96%)	-1.64	0 100 100	17, 27, 42, 57	0
1	C	716/741 (96%)	-1.54	0 100 100	19, 34, 55, 74	0
1	D	716/741 (96%)	-1.65	0 100 100	17, 27, 42, 60	0
All	All	2864/2964 (96%)	-1.59	0 100 100	17, 30, 51, 77	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	TOX	B	107[A]	16/17	0.99	0.03	21,23,30,36	1
1	TOX	B	107[B]	16/17	0.99	0.03	21,23,30,36	1
1	TOX	D	107[A]	16/17	0.99	0.03	20,23,32,35	1
1	TOX	D	107[B]	16/17	0.99	0.03	20,23,32,35	1
1	TOX	C	107[A]	16/17	1.00	0.02	21,24,29,38	1
1	TOX	C	107[B]	16/17	1.00	0.02	21,24,30,38	1
1	TOX	A	107[A]	16/17	1.00	0.03	19,24,28,39	1
1	TOX	A	107[B]	16/17	1.00	0.03	19,24,28,39	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

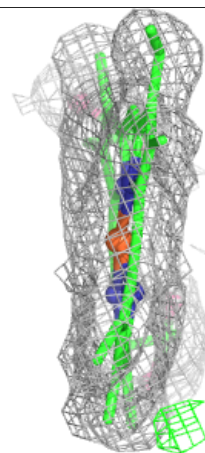
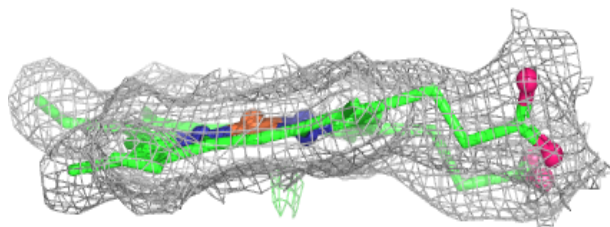
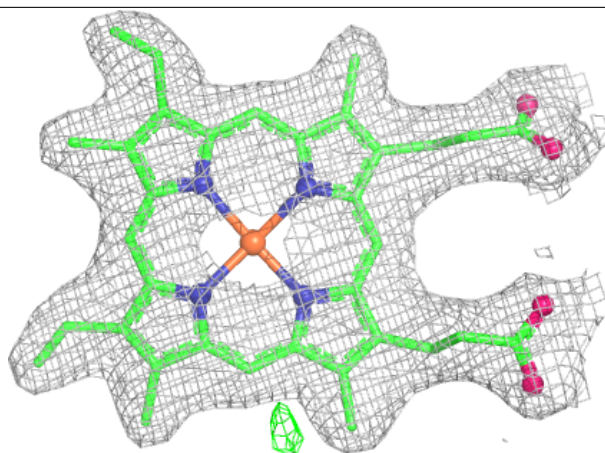
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	802	1/1	0.99	0.02	40,40,40,40	0
3	NA	B	802	1/1	0.99	0.02	43,43,43,43	0
3	NA	D	802	1/1	0.99	0.02	39,39,39,39	0
4	GOL	A	803	6/6	0.99	0.03	23,27,31,36	0
4	GOL	B	803	6/6	0.99	0.03	28,32,34,34	0
4	GOL	C	803	6/6	0.99	0.03	25,26,30,44	0
4	GOL	D	803	6/6	0.99	0.03	29,31,35,36	0
2	HEM	C	801	43/43	1.00	0.02	17,25,30,33	0
2	HEM	D	801	43/43	1.00	0.02	17,23,27,28	0
2	HEM	A	801	43/43	1.00	0.02	21,26,31,34	0
2	HEM	B	801	43/43	1.00	0.02	19,24,29,31	0
3	NA	C	802	1/1	1.00	0.01	38,38,38,38	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.

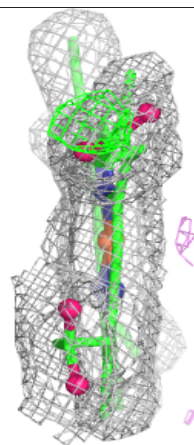
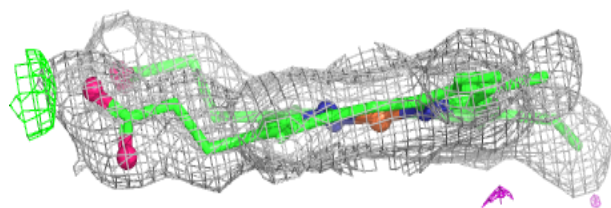
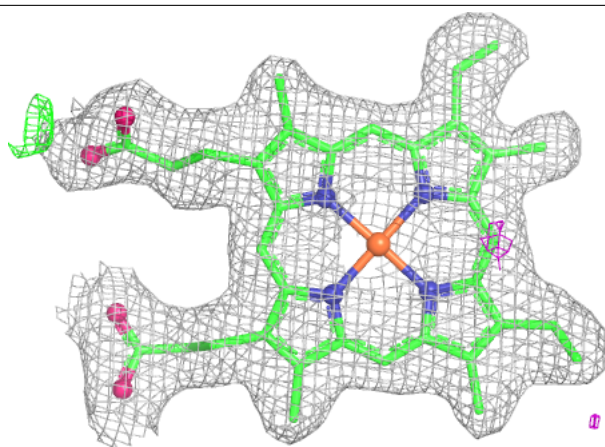
Electron density around HEM C 801:

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



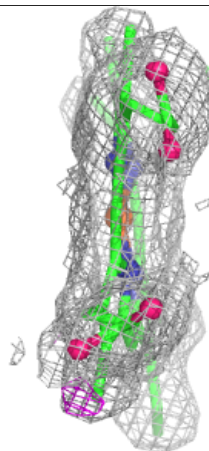
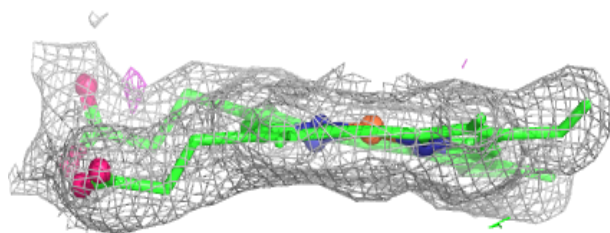
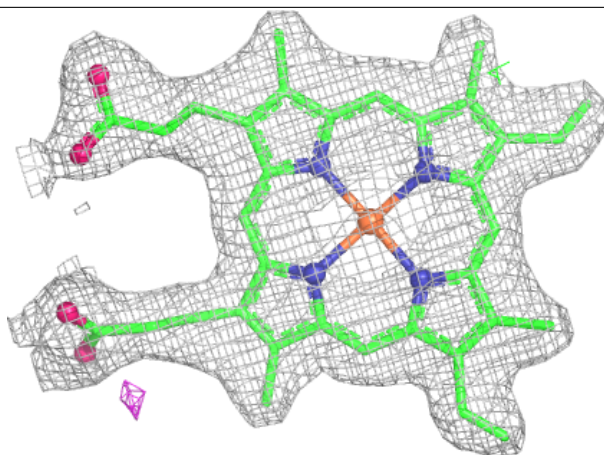
Electron density around HEM D 801:

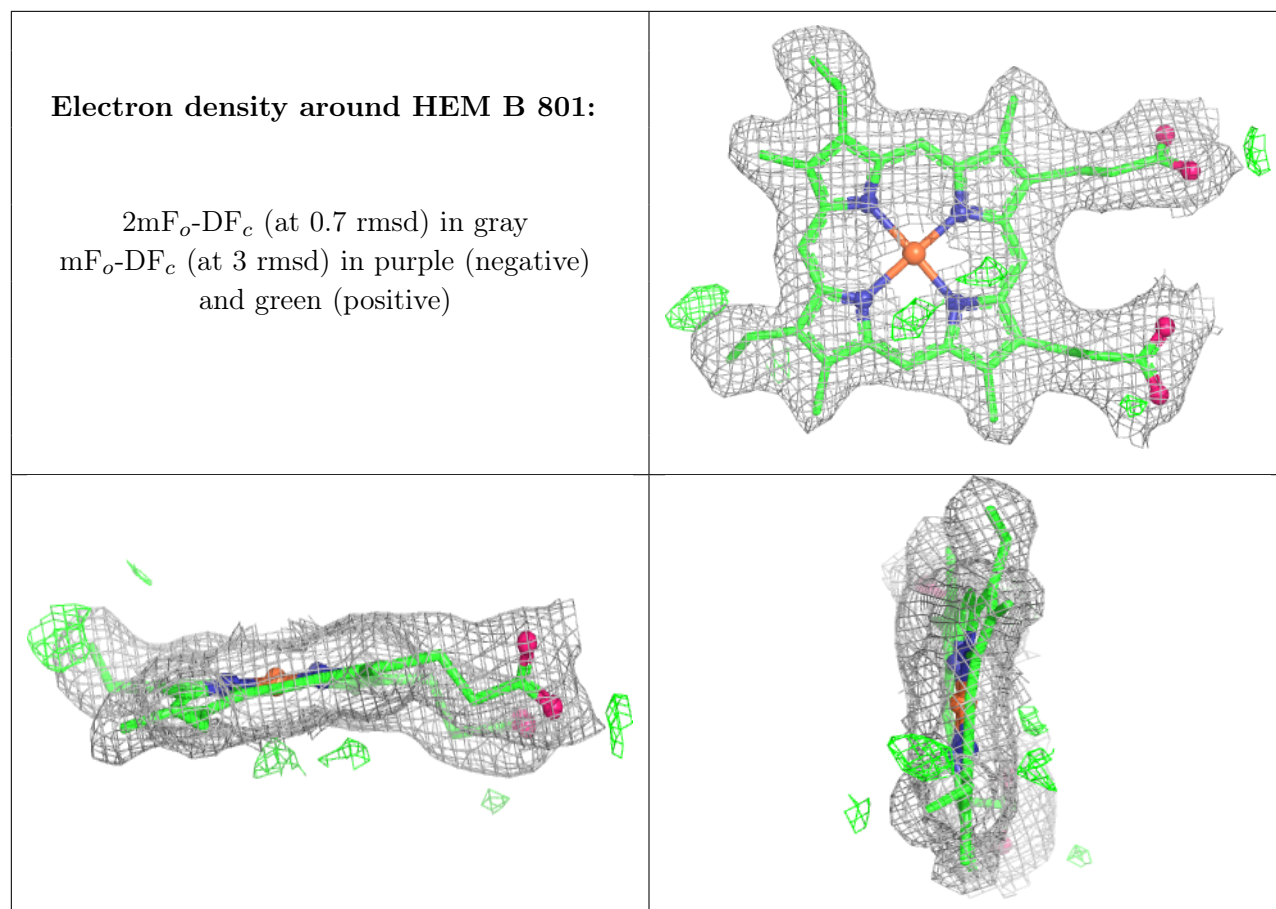
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 801:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.