



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:43 AM EDT

PDB ID : 8W1X / pdb_00008w1x
Title : 2.35-angstrom resolution intermediate crystal structure of KatG from Mycobacterium tuberculosis with an MYW-OOH cofactor soaked with peroxide for 5 minutes
Authors : Liu, A.; Li, J.
Deposited on : 2024-02-19
Resolution : 2.35 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

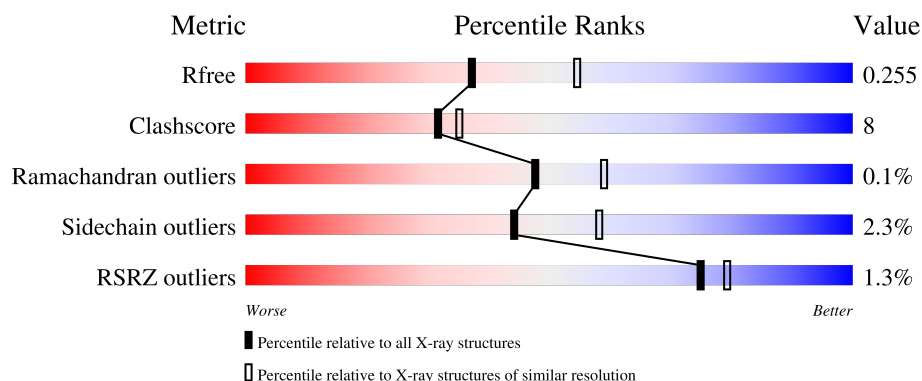
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

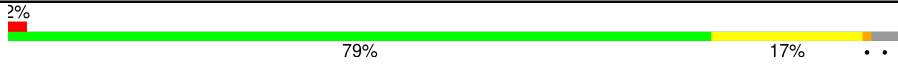
The reported resolution of this entry is 2.35 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
2	B	741	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11790 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	0	0
			5529	3515	953	1042	19			

There are 2 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

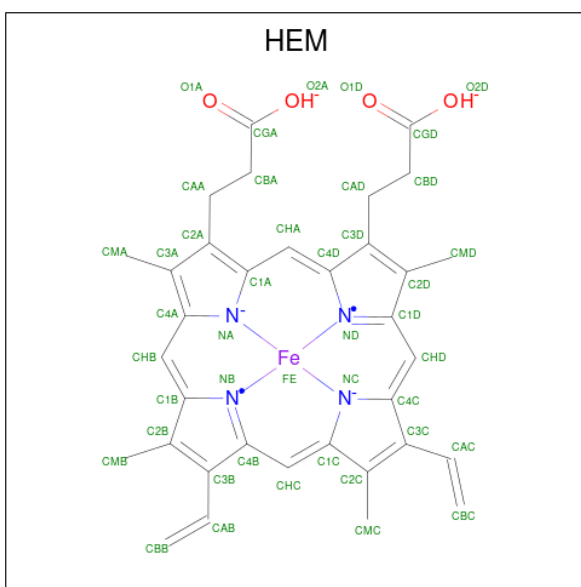
- Molecule 2 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	717	Total	C	N	O	S	0	0	0
			5531	3515	953	1044	19			

There are 2 discrepancies between the modelled and reference sequences:

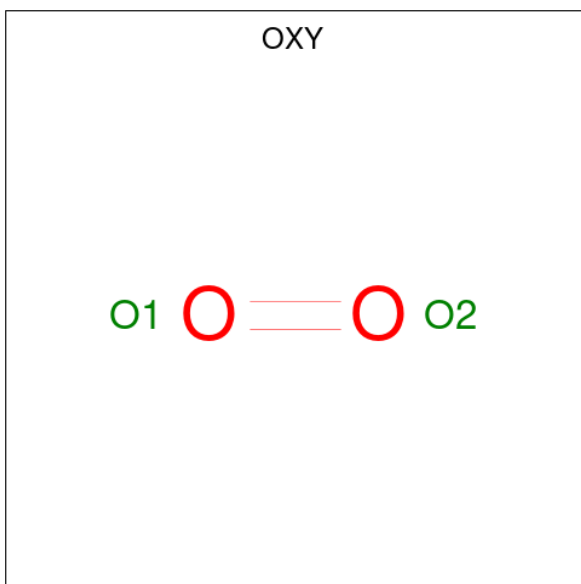
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A0D5ZBI4
B	1	HIS	-	expression tag	UNP A0A0D5ZBI4

- Molecule 3 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
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).

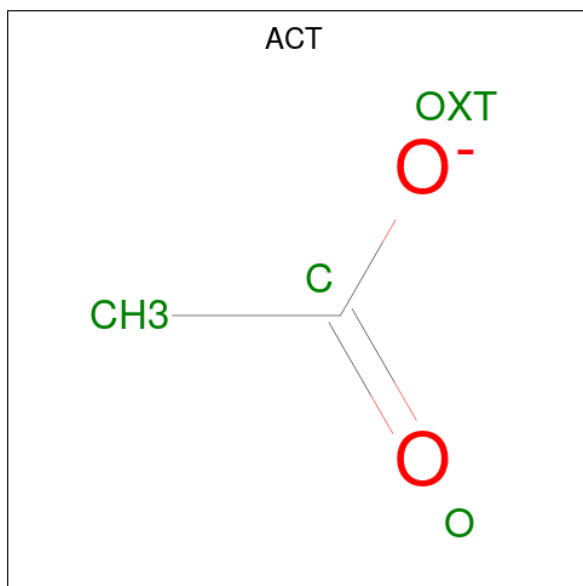


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

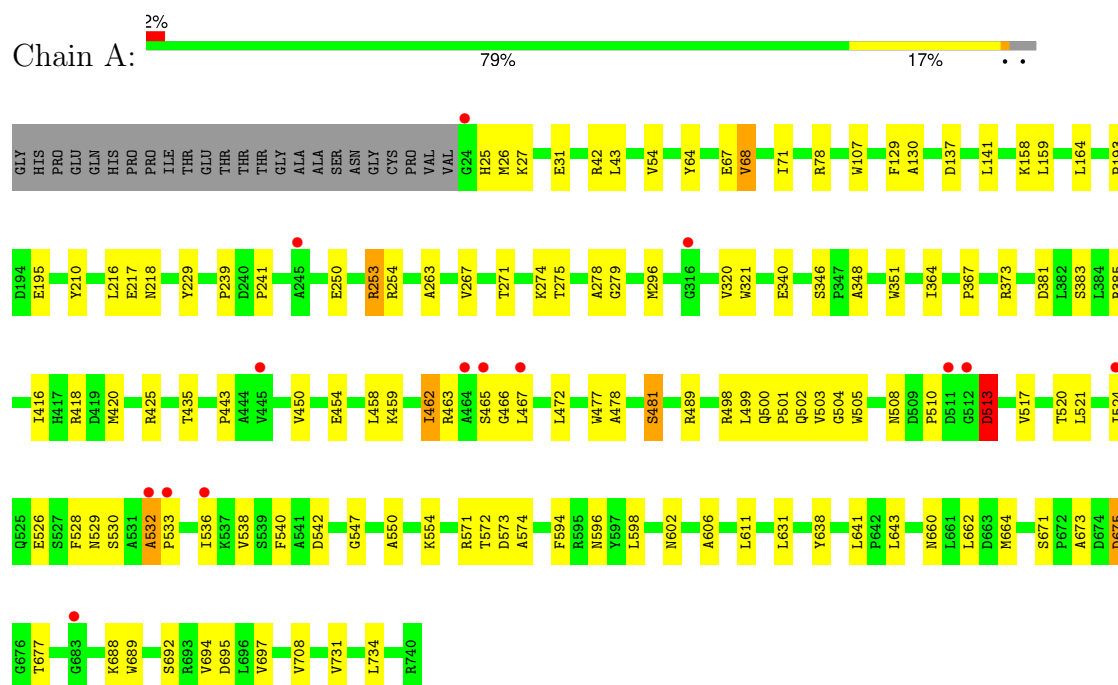
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	245	Total	O	0	0
			245	245		
8	B	376	Total	O	0	0
			376	376		

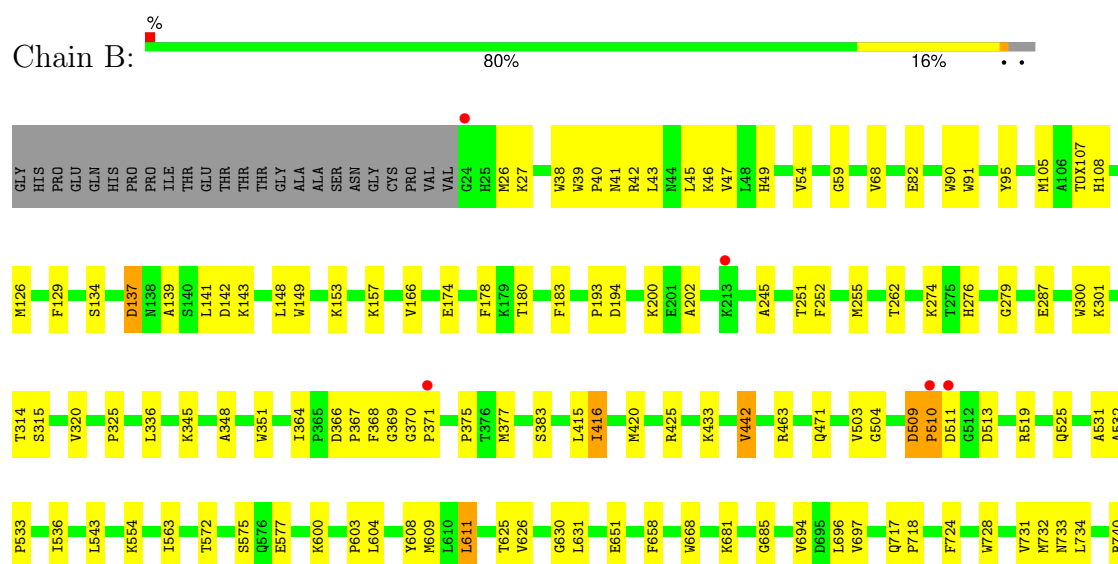
3 Residue-property plots

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 2: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.46Å 150.46Å 155.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.35 47.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	90.3 (47.72-2.35) 82.9 (47.72-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.191 , 0.256 0.191 , 0.255	Depositor DCC
R_{free} test set	2027 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k 0.018 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11790	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	1/5680 (0.0%)	0.62	9/7732 (0.1%)
2	B	0.46	1/5663 (0.0%)	0.60	1/7706 (0.0%)
All	All	0.47	2/11343 (0.0%)	0.61	10/15438 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	LEU	C-O	-5.46	1.16	1.24
2	B	531	ALA	C-O	-5.29	1.16	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	GLY	N-CA-C	-8.45	102.97	115.72
1	A	532	ALA	CA-C-N	7.93	128.01	119.28
1	A	532	ALA	C-N-CA	7.93	128.01	119.28
1	A	278	ALA	N-CA-C	6.51	120.48	112.54
1	A	466	GLY	CA-C-N	-6.09	114.32	122.72
1	A	466	GLY	C-N-CA	-6.09	114.32	122.72
2	B	509	ASP	N-CA-C	5.67	122.35	109.81
1	A	513	ASP	N-CA-C	5.46	118.94	112.72
1	A	279	GLY	CA-C-N	5.33	125.50	119.90
1	A	279	GLY	C-N-CA	5.33	125.50	119.90

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	5529	0	5355	90	0
2	B	5531	0	5354	91	0
3	A	43	0	30	3	0
3	B	43	0	30	3	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
7	B	12	0	16	2	0
8	A	245	0	0	5	0
8	B	376	0	0	7	0
All	All	11790	0	10791	177	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 8.

All (177) 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)
2:B:45:LEU:HD23	2:B:611:LEU:HD21	1.56	0.87
2:B:604:LEU:HB2	2:B:609:MET:HE3	1.62	0.80
1:A:274:LYS:HG3	1:A:320:VAL:HG22	1.62	0.80
1:A:458:LEU:O	1:A:462:ILE:HG13	1.82	0.79
1:A:467:LEU:HD22	1:A:517:VAL:HG22	1.65	0.77
1:A:296:MET:HE3	2:B:668:TRP:CD1	2.21	0.76
1:A:478:ALA:HB1	1:A:508:ASN:ND2	2.03	0.73
1:A:340:GLU:OE2	1:A:385:ARG:NH2	2.24	0.71
1:A:454:GLU:O	1:A:458:LEU:HD12	1.91	0.70
2:B:519:ARG:NH1	8:B:903:HOH:O	2.24	0.70
1:A:513:ASP:N	1:A:513:ASP:OD1	2.25	0.69
2:B:157:LYS:HA	7:B:802:GOL:H32	1.74	0.68
1:A:463:ARG:HE	1:A:554:LYS:HD3	1.59	0.67
1:A:274:LYS:HD2	1:A:275:THR:O	1.95	0.67
1:A:478:ALA:HB1	1:A:508:ASN:HD21	1.58	0.67
1:A:129:PHE:HB3	1:A:193:PRO:HG3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:MET:HE1	2:B:696:LEU:HG	1.76	0.65
2:B:503:VAL:O	2:B:510:PRO:CG	2.45	0.65
1:A:503:VAL:O	1:A:510:PRO:HB3	1.97	0.64
1:A:68:VAL:O	1:A:71:ILE:HG22	1.98	0.63
1:A:443:PRO:HB2	1:A:572:THR:HG21	1.81	0.63
2:B:129:PHE:HB3	2:B:193:PRO:HG3	1.80	0.63
1:A:274:LYS:CG	1:A:320:VAL:HG22	2.30	0.62
2:B:26:MET:HE3	2:B:38:TRP:CE2	2.35	0.62
2:B:126:MET:HE3	2:B:194:ASP:HB2	1.83	0.61
1:A:526:GLU:O	1:A:530:SER:N	2.29	0.61
2:B:345:LYS:HE3	2:B:351:TRP:CE3	2.36	0.61
1:A:463:ARG:NE	1:A:554:LYS:HD3	2.16	0.60
2:B:39:TRP:HB2	2:B:42:ARG:HD2	1.85	0.59
2:B:577:GLU:H	2:B:577:GLU:CD	2.11	0.58
2:B:504:GLY:HA2	2:B:510:PRO:HG2	1.87	0.57
1:A:477:TRP:O	1:A:481:SER:HB3	2.05	0.57
1:A:675:ASP:N	1:A:675:ASP:OD1	2.38	0.56
1:A:688:LYS:HE3	1:A:689:TRP:CZ2	2.41	0.56
2:B:301:LYS:NZ	8:B:911:HOH:O	2.39	0.55
2:B:366:ASP:HB3	2:B:369:GLY:O	2.06	0.55
1:A:250:GLU:OE2	1:A:253:ARG:NH1	2.40	0.55
2:B:274:LYS:HB2	2:B:320:VAL:HG22	1.89	0.55
2:B:503:VAL:O	2:B:510:PRO:HG3	2.06	0.54
3:A:801:HEM:HMB2	3:A:801:HEM:HBB2	1.88	0.54
1:A:271:THR:HG23	8:A:927:HOH:O	2.07	0.54
2:B:733:ASN:O	2:B:740:ARG:NH2	2.41	0.54
2:B:366:ASP:HB3	2:B:370:GLY:HA3	1.90	0.53
1:A:107:TRP:HZ3	1:A:229:TYR:HH	1.54	0.53
1:A:498:ARG:HD3	1:A:540:PHE:CD2	2.44	0.53
2:B:509:ASP:CG	2:B:509:ASP:O	2.50	0.53
1:A:420:MET:O	1:A:425:ARG:HD3	2.09	0.52
2:B:46:LYS:HG2	2:B:49:HIS:CE1	2.44	0.52
1:A:239:PRO:O	1:A:241:PRO:HD3	2.10	0.52
1:A:504:GLY:HA2	1:A:510:PRO:HG3	1.92	0.52
1:A:43:LEU:HG	1:A:611:LEU:HD11	1.90	0.51
1:A:458:LEU:O	1:A:462:ILE:CG1	2.55	0.51
1:A:692:SER:N	1:A:695:ASP:OD2	2.37	0.51
1:A:459:LYS:HG2	1:A:550:ALA:HB2	1.93	0.51
2:B:533:PRO:HG2	2:B:536:ILE:HD12	1.93	0.51
1:A:694:VAL:O	1:A:697:VAL:HG12	2.11	0.51
1:A:450:VAL:CG1	1:A:538:VAL:HG12	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLN:HG2	1:A:505:TRP:CZ3	2.46	0.50
1:A:598:LEU:HD22	1:A:606:ALA:HB2	1.94	0.50
2:B:366:ASP:HB2	8:B:1126:HOH:O	2.10	0.50
2:B:46:LYS:HG2	2:B:49:HIS:NE2	2.27	0.50
1:A:27:LYS:NZ	2:B:40:PRO:O	2.42	0.50
2:B:463:ARG:HD3	2:B:554:LYS:HB2	1.94	0.50
2:B:41:ASN:O	2:B:608:TYR:OH	2.28	0.49
1:A:195:GLU:HA	1:A:195:GLU:OE2	2.12	0.49
1:A:463:ARG:HH21	1:A:554:LYS:HD2	1.76	0.49
1:A:78:ARG:NH1	8:A:907:HOH:O	2.35	0.49
2:B:274:LYS:CB	2:B:320:VAL:HG22	2.43	0.48
2:B:174:GLU:HA	2:B:178:PHE:O	2.13	0.48
1:A:450:VAL:HG11	1:A:538:VAL:HG12	1.94	0.48
1:A:239:PRO:HG3	1:A:351:TRP:CG	2.48	0.48
2:B:364:ILE:HD12	2:B:375:PRO:HA	1.96	0.48
1:A:498:ARG:HG3	1:A:499:LEU:HD23	1.95	0.48
2:B:139:ALA:HA	2:B:300:TRP:CH2	2.48	0.48
1:A:542:ASP:OD1	1:A:571:ARG:HB2	2.14	0.48
2:B:532:ALA:HB1	2:B:533:PRO:HD2	1.95	0.47
2:B:139:ALA:HA	2:B:300:TRP:CZ3	2.49	0.47
2:B:694:VAL:O	2:B:697:VAL:HG12	2.14	0.47
1:A:443:PRO:HB2	1:A:572:THR:CG2	2.44	0.47
1:A:673:ALA:HB3	1:A:675:ASP:OD1	2.15	0.47
2:B:731:VAL:HA	2:B:734:LEU:HG	1.96	0.47
2:B:279:GLY:O	2:B:348:ALA:HB2	2.15	0.47
2:B:525:GLN:HB2	2:B:543:LEU:HD12	1.97	0.47
2:B:442:VAL:HG13	2:B:572:THR:OG1	2.15	0.47
2:B:59:GLY:O	8:B:901:HOH:O	2.20	0.46
2:B:366:ASP:OD1	2:B:367:PRO:HD2	2.15	0.46
1:A:64:TYR:O	1:A:68:VAL:HG13	2.14	0.46
1:A:498:ARG:HD3	1:A:540:PHE:CE2	2.50	0.46
1:A:662:LEU:HD11	1:A:708:VAL:HG12	1.96	0.46
1:A:529:ASN:O	1:A:532:ALA:HB2	2.15	0.46
1:A:418:ARG:HA	1:A:418:ARG:HD2	1.71	0.46
1:A:463:ARG:HH21	1:A:554:LYS:HA	1.80	0.46
2:B:251:THR:O	2:B:255:MET:HG3	2.16	0.46
1:A:210:TYR:CZ	1:A:216:LEU:HD13	2.50	0.46
2:B:142:ASP:OD2	2:B:143:LYS:HE3	2.16	0.46
1:A:532:ALA:HA	1:A:533:PRO:HD3	1.59	0.45
2:B:471:GLN:HE21	2:B:513:ASP:CG	2.24	0.45
3:A:801:HEM:HMC1	3:A:801:HEM:HBC2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ILE:HG13	8:B:1094:HOH:O	2.17	0.45
2:B:509:ASP:N	2:B:510:PRO:HD3	2.31	0.45
1:A:25:HIS:CD2	2:B:200:LYS:HG3	2.51	0.45
2:B:603:PRO:HD2	2:B:609:MET:SD	2.57	0.45
1:A:731:VAL:HA	1:A:734:LEU:HG	1.99	0.45
1:A:462:ILE:HG21	1:A:547:GLY:HA2	1.99	0.45
1:A:130:ALA:O	1:A:193:PRO:HB3	2.17	0.44
1:A:458:LEU:HD11	1:A:528:PHE:CE2	2.52	0.44
2:B:252:PHE:CD2	2:B:262:THR:HG23	2.52	0.44
2:B:625:THR:HG22	2:B:658:PHE:HE2	1.82	0.44
1:A:671:SER:HB2	1:A:677:THR:HG22	1.99	0.44
2:B:366:ASP:CG	2:B:367:PRO:HD2	2.41	0.44
1:A:275:THR:HG22	3:A:801:HEM:HAA1	1.99	0.44
2:B:46:LYS:HA	2:B:49:HIS:CE1	2.53	0.44
2:B:315:SER:HB3	3:B:801:HEM:HBA1	2.00	0.44
2:B:336:LEU:HD13	2:B:377:MET:HE3	1.99	0.44
2:B:503:VAL:O	2:B:510:PRO:HG2	2.17	0.44
1:A:489:ARG:NH1	8:A:925:HOH:O	2.50	0.43
2:B:134:SER:HB3	2:B:287:GLU:HG3	2.00	0.43
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.70	0.43
1:A:321:TRP:NE1	1:A:381:ASP:OD2	2.50	0.43
1:A:274:LYS:NZ	1:A:367:PRO:HG3	2.34	0.43
2:B:575:SER:HB2	2:B:577:GLU:OE1	2.18	0.43
1:A:31:GLU:HG2	2:B:608:TYR:CE2	2.53	0.43
2:B:630:GLY:HA3	2:B:724:PHE:CE2	2.53	0.43
2:B:95:TYR:CZ	2:B:325:PRO:HG2	2.53	0.43
2:B:740:ARG:HD2	8:B:1251:HOH:O	2.19	0.43
1:A:520:THR:O	1:A:524:ILE:HD12	2.19	0.43
2:B:728:TRP:O	2:B:732:MET:HG2	2.19	0.43
3:B:801:HEM:HMD2	3:B:801:HEM:HAD1	1.84	0.43
1:A:638:TYR:O	1:A:641:LEU:HG	2.19	0.43
2:B:141:LEU:HD23	2:B:141:LEU:HA	1.75	0.43
2:B:95:TYR:CE2	2:B:325:PRO:HG2	2.54	0.43
2:B:142:ASP:N	2:B:142:ASP:OD1	2.52	0.43
1:A:521:LEU:HA	1:A:524:ILE:HD12	1.99	0.42
2:B:681:LYS:HD3	2:B:685:GLY:O	2.18	0.42
1:A:373:ARG:HB2	8:A:1018:HOH:O	2.19	0.42
1:A:660:ASN:HD22	1:A:660:ASN:HA	1.70	0.42
2:B:91:TRP:CE3	2:B:143:LYS:HD3	2.54	0.42
2:B:366:ASP:CB	2:B:370:GLY:HA3	2.49	0.42
2:B:717:GLN:N	2:B:718:PRO:HD2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LEU:HG	2:B:416:ILE:HD13	2.00	0.42
2:B:27:LYS:HD3	2:B:27:LYS:HA	1.46	0.42
2:B:631:LEU:HD23	2:B:631:LEU:HA	1.86	0.42
2:B:314:THR:HB	3:B:801:HEM:O1A	2.19	0.42
2:B:433:LYS:HD3	2:B:433:LYS:HA	1.84	0.42
2:B:577:GLU:CD	2:B:577:GLU:N	2.76	0.42
1:A:263:ALA:O	1:A:267:VAL:HG23	2.20	0.42
2:B:245:ALA:HB2	2:B:383:SER:HB3	2.02	0.42
2:B:105:MET:HE1	2:B:148:LEU:HD11	2.01	0.42
1:A:26:MET:HE3	2:B:202:ALA:HB2	2.02	0.41
1:A:594:PHE:HB3	1:A:631:LEU:HD12	2.02	0.41
1:A:67:GLU:HB3	1:A:158:LYS:HA	2.03	0.41
2:B:166:VAL:HG13	2:B:183:PHE:HE1	1.85	0.41
2:B:174:GLU:OE2	2:B:180:THR:N	2.52	0.41
1:A:499:LEU:HD11	1:A:574:ALA:O	2.20	0.41
1:A:521:LEU:HA	1:A:521:LEU:HD23	1.71	0.41
2:B:108:HIS:CE1	2:B:137:ASP:O	2.73	0.41
2:B:420:MET:O	2:B:425:ARG:HD3	2.19	0.41
2:B:157:LYS:HA	7:B:802:GOL:C3	2.47	0.41
1:A:602:ASN:HB2	8:A:1102:HOH:O	2.21	0.41
1:A:502:GLN:HG2	1:A:505:TRP:CH2	2.56	0.41
1:A:596:ASN:ND2	1:A:643:LEU:HB2	2.36	0.41
2:B:370:GLY:HA2	2:B:371:PRO:HD3	1.84	0.41
1:A:217:GLU:HG2	1:A:218:ASN:O	2.20	0.41
2:B:651:GLU:HG2	8:B:1051:HOH:O	2.21	0.41
1:A:443:PRO:HD2	1:A:573:ASP:O	2.21	0.41
1:A:664:MET:HG2	2:B:90:TRP:CE2	2.55	0.41
2:B:276:HIS:HB2	2:B:314:THR:H	1.86	0.41
2:B:367:PRO:HB2	2:B:368:PHE:CE1	2.57	0.41
1:A:159:LEU:HD21	1:A:164:LEU:HD13	2.03	0.40
1:A:500:GLN:HG3	1:A:501:PRO:HA	2.03	0.40
1:A:529:ASN:O	1:A:532:ALA:CB	2.69	0.40
2:B:149:TRP:NE1	2:B:153:LYS:HD2	2.35	0.40
1:A:216:LEU:HB3	1:A:254:ARG:CZ	2.51	0.40
1:A:320:VAL:HB	1:A:364:ILE:HG21	2.03	0.40
2:B:724:PHE:CD1	2:B:724:PHE:C	3.00	0.40
1:A:346:SER:C	1:A:348:ALA:H	2.29	0.40
2:B:174:GLU:HG2	2:B:178:PHE:O	2.21	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	715/741 (96%)	688 (96%)	27 (4%)	0	100	100
2	B	714/741 (96%)	691 (97%)	22 (3%)	1 (0%)	48	59
All	All	1429/1482 (96%)	1379 (96%)	49 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	510	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	565/584 (97%)	551 (98%)	14 (2%)	42	55
2	B	564/583 (97%)	552 (98%)	12 (2%)	47	61
All	All	1129/1167 (97%)	1103 (98%)	26 (2%)	44	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	54	VAL
1	A	68	VAL
1	A	137	ASP
1	A	253	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	383	SER
1	A	416	ILE
1	A	435	THR
1	A	462	ILE
1	A	465	SER
1	A	481	SER
1	A	513	ASP
1	A	536	ILE
1	A	675	ASP
2	B	43	LEU
2	B	47	VAL
2	B	54	VAL
2	B	68	VAL
2	B	82	GLU
2	B	137	ASP
2	B	416	ILE
2	B	442	VAL
2	B	511	ASP
2	B	600	LYS
2	B	611	LEU
2	B	626	VAL

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

Mol	Chain	Res	Type
1	A	36	GLN
1	A	190	GLN
1	A	561	HIS
1	A	660	ASN
2	B	36	GLN
2	B	49	HIS
2	B	578	GLN
2	B	722	GLN
2	B	733	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TOX	B	107	2	14,17,18	2.48	4 (28%)	12,23,25	2.14	5 (41%)

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	TOX	B	107	2	-	2/5/8/10	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	TOX	O1-NE1	7.44	1.48	1.39
2	B	107	TOX	CD2-CG	-3.35	1.38	1.44
2	B	107	TOX	CD2-CE2	-2.53	1.37	1.41
2	B	107	TOX	CZ2-CE2	2.14	1.42	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	TOX	CZ3-CH2-CZ2	-3.56	115.84	120.24
2	B	107	TOX	CZ2-CE2-NE1	3.29	134.61	129.37
2	B	107	TOX	CB-CG-CD1	-2.67	122.95	126.67
2	B	107	TOX	CZ2-CE2-CD2	-2.41	119.26	121.95
2	B	107	TOX	CH2-CZ2-CE2	2.10	122.52	118.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	107	TOX	N-CA-CB-CG
2	B	107	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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z > 2$
7	GOL	B	802	-	5,5,5	0.51	0	5,5,5	1.35	0
3	HEM	A	801	8,1	50,50,50	1.63	9 (18%)	67,82,82	1.25	8 (11%)
6	ACT	B	804	-	3,3,3	0.64	0	3,3,3	1.22	0
7	GOL	B	803	-	5,5,5	0.47	0	5,5,5	0.80	0
3	HEM	B	801	2	50,50,50	2.19	21 (42%)	67,82,82	2.03	15 (22%)
6	ACT	A	804	-	3,3,3	0.66	0	3,3,3	0.99	0
4	OXY	A	802	-	1,1,1	0.09	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
3	HEM	B	801	2	-	3/14/54/54	-
7	GOL	B	803	-	-	4/4/4/4	-
3	HEM	A	801	8,1	-	2/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	802	-	-	4/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	FE-NB	5.13	2.10	1.94
3	A	801	HEM	FE-ND	5.02	2.10	1.94
3	B	801	HEM	C4B-NB	-4.94	1.29	1.38
3	B	801	HEM	FE-NB	4.76	2.09	1.94
3	B	801	HEM	C1B-NB	-4.66	1.32	1.40
3	B	801	HEM	C3C-C4C	-4.20	1.38	1.46
3	B	801	HEM	C1A-C2A	-4.01	1.36	1.44
3	B	801	HEM	O2A-CGA	-3.69	1.18	1.30
3	B	801	HEM	C1C-C2C	-3.44	1.38	1.45
3	A	801	HEM	CAC-C3C	3.27	1.56	1.47
3	B	801	HEM	C1C-NC	-3.17	1.33	1.39
3	B	801	HEM	FE-NC	3.01	2.05	1.95
3	A	801	HEM	CAB-C3B	2.99	1.55	1.47
3	B	801	HEM	C2A-C3A	-2.99	1.31	1.38
3	A	801	HEM	FE-NC	2.96	2.04	1.95
3	B	801	HEM	C1B-C2B	-2.90	1.38	1.44
3	B	801	HEM	C4A-NA	-2.87	1.34	1.39
3	A	801	HEM	FE-NA	2.82	2.04	1.95
3	B	801	HEM	C1D-ND	-2.79	1.33	1.38
3	B	801	HEM	C4A-C3A	-2.67	1.36	1.43
3	B	801	HEM	C3D-C2D	-2.48	1.31	1.36
3	B	801	HEM	C4C-NC	-2.47	1.35	1.39
3	B	801	HEM	C1A-NA	-2.43	1.35	1.39
3	B	801	HEM	C4D-ND	-2.42	1.36	1.40
3	B	801	HEM	FE-ND	-2.37	1.87	1.94
3	A	801	HEM	CMB-C2B	2.31	1.55	1.50
3	B	801	HEM	O2D-CGD	-2.17	1.23	1.30
3	A	801	HEM	CMD-C2D	2.14	1.55	1.50
3	B	801	HEM	C3B-C2B	-2.09	1.32	1.37
3	A	801	HEM	C2A-C3A	-2.07	1.33	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	HEM	CAD-C3D-C4D	5.69	134.62	124.70
3	B	801	HEM	C1B-NB-C4B	5.42	111.63	105.21
3	B	801	HEM	C3B-C4B-NB	-4.91	105.94	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	HEM	CHC-C4B-NB	4.52	129.29	124.42
3	B	801	HEM	CAD-C3D-C2D	-4.05	120.29	127.87
3	B	801	HEM	CBD-CAD-C3D	4.01	123.62	112.53
3	B	801	HEM	CHD-C1D-ND	3.92	128.64	124.42
3	B	801	HEM	CHB-C1B-NB	3.31	128.46	124.37
3	B	801	HEM	O2D-CGD-CBD	2.88	123.09	114.00
3	A	801	HEM	C4D-ND-C1D	2.80	108.53	105.21
3	B	801	HEM	O2A-CGA-O1A	-2.70	116.38	123.33
3	B	801	HEM	CHD-C1D-C2D	-2.70	120.77	125.03
3	B	801	HEM	O2D-CGD-O1D	-2.50	116.91	123.33
3	B	801	HEM	C4C-NC-C1C	2.43	109.78	105.82
3	A	801	HEM	C2A-C1A-NA	-2.43	107.45	110.15
3	A	801	HEM	CHB-C4A-NA	2.41	128.23	123.86
3	A	801	HEM	C2D-C1D-ND	-2.40	107.13	109.90
3	A	801	HEM	CAA-CBA-CGA	-2.29	107.60	113.67
3	B	801	HEM	CHA-C1A-NA	2.28	127.99	123.86
3	A	801	HEM	C3D-C4D-ND	-2.19	107.77	110.17
3	B	801	HEM	CHD-C4C-NC	2.14	126.79	124.45
3	A	801	HEM	C4A-C3A-C2A	2.12	109.25	106.82
3	A	801	HEM	CHC-C1C-NC	2.04	126.67	124.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

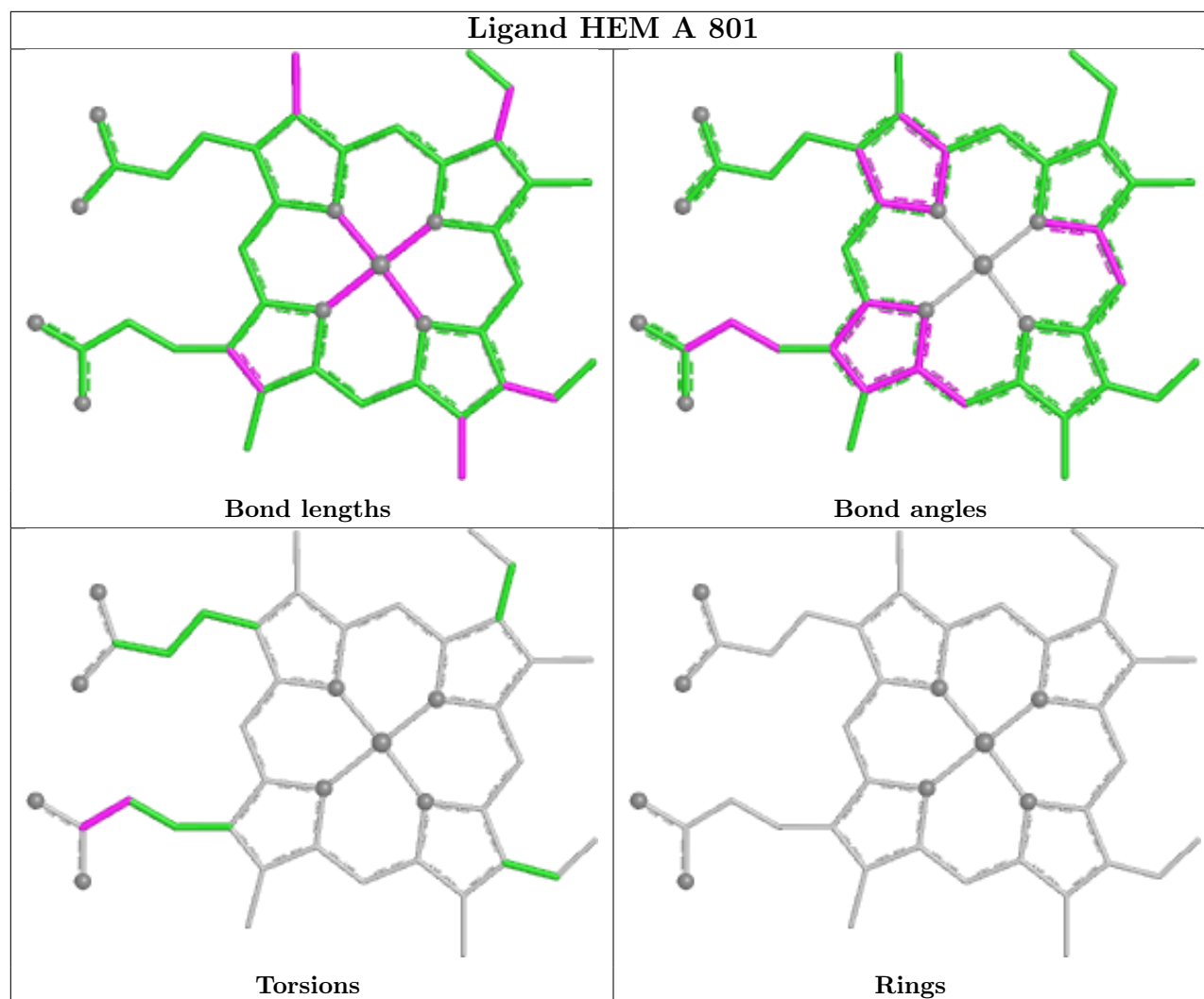
Mol	Chain	Res	Type	Atoms
7	B	802	GOL	O1-C1-C2-C3
7	B	802	GOL	C1-C2-C3-O3
7	B	803	GOL	C1-C2-C3-O3
7	B	802	GOL	O1-C1-C2-O2
7	B	802	GOL	O2-C2-C3-O3
7	B	803	GOL	O1-C1-C2-C3
7	B	803	GOL	O2-C2-C3-O3
7	B	803	GOL	O1-C1-C2-O2
3	A	801	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAA-CBA-CGA-O2A
3	A	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	C2B-C3B-CAB-CBB

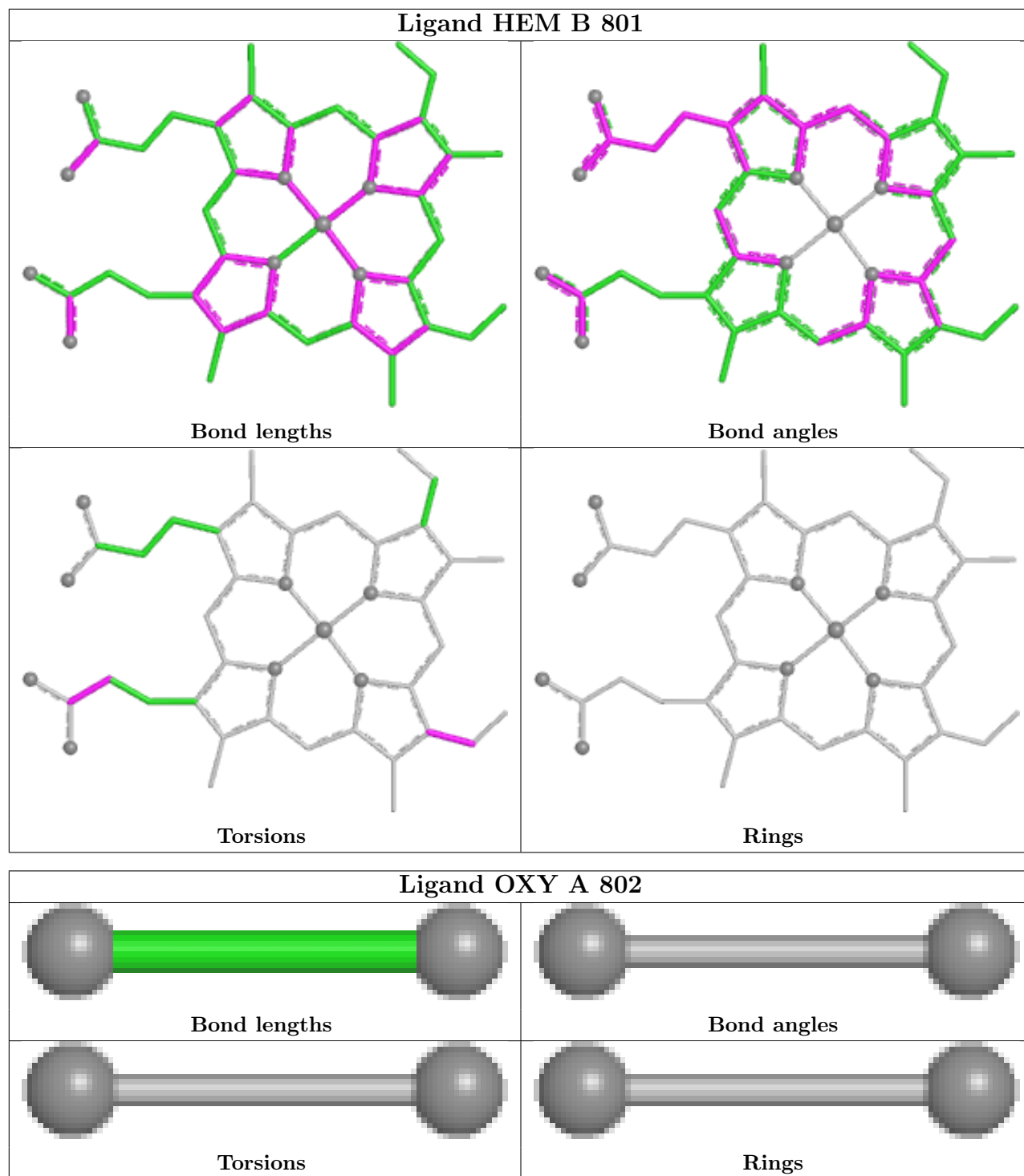
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	802	GOL	2	0
3	A	801	HEM	3	0
3	B	801	HEM	3	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 ⓘ

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	717/741 (96%)	0.20	14 (1%) 65 70	16, 33, 57, 79	0
2	B	716/741 (96%)	-0.19	5 (0%) 84 87	14, 26, 43, 69	0
All	All	1433/1482 (96%)	0.01	19 (1%) 75 79	14, 30, 52, 79	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	510	PRO	4.7
1	A	467	LEU	3.5
1	A	465	SER	3.1
1	A	464	ALA	3.0
1	A	524	ILE	2.9
2	B	511	ASP	2.8
1	A	24	GLY	2.8
1	A	533	PRO	2.7
2	B	24	GLY	2.6
1	A	512	GLY	2.6
1	A	536	ILE	2.4
2	B	371	PRO	2.3
1	A	511	ASP	2.3
2	B	213	LYS	2.2
1	A	316	GLY	2.1
1	A	445	VAL	2.1
1	A	245	ALA	2.1
1	A	532	ALA	2.1
1	A	683	GLY	2.1

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
2	TOX	B	107	16/17	0.95	0.08	18,21,29,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

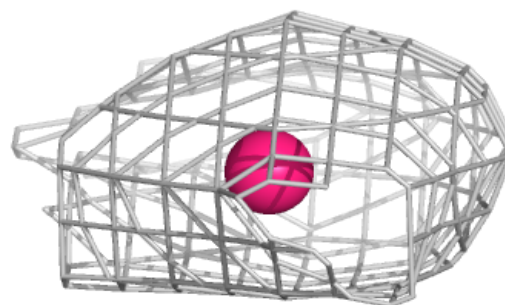
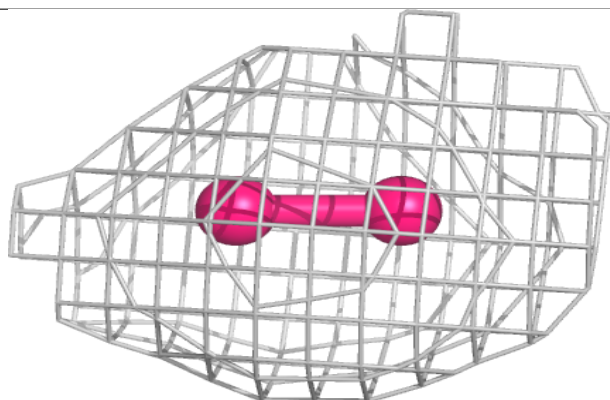
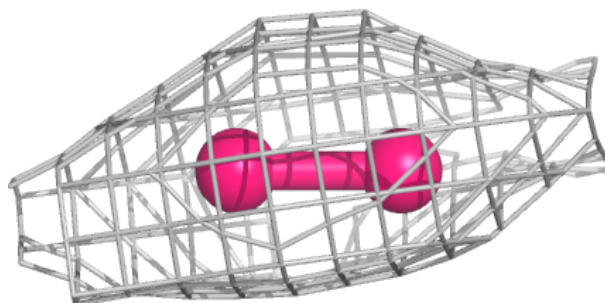
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	803	6/6	0.89	0.13	25,26,34,36	0
6	ACT	B	804	4/4	0.90	0.11	20,26,34,40	0
6	ACT	A	804	4/4	0.90	0.10	22,29,34,37	0
7	GOL	B	802	6/6	0.91	0.10	22,27,32,34	0
4	OXY	A	802	2/2	0.92	0.11	34,34,34,39	0
5	NA	A	803	1/1	0.95	0.05	23,23,23,23	0
3	HEM	B	801	43/43	0.96	0.09	17,22,29,40	0
3	HEM	A	801	43/43	0.97	0.07	19,25,30,36	0

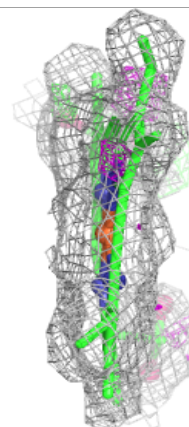
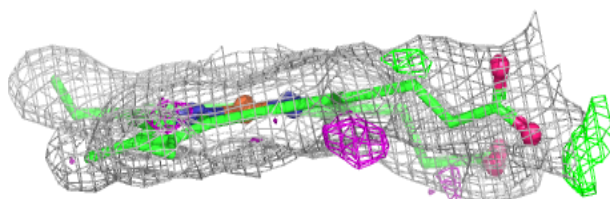
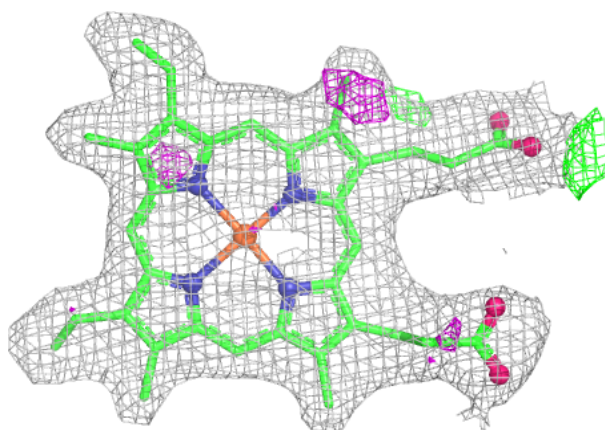
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

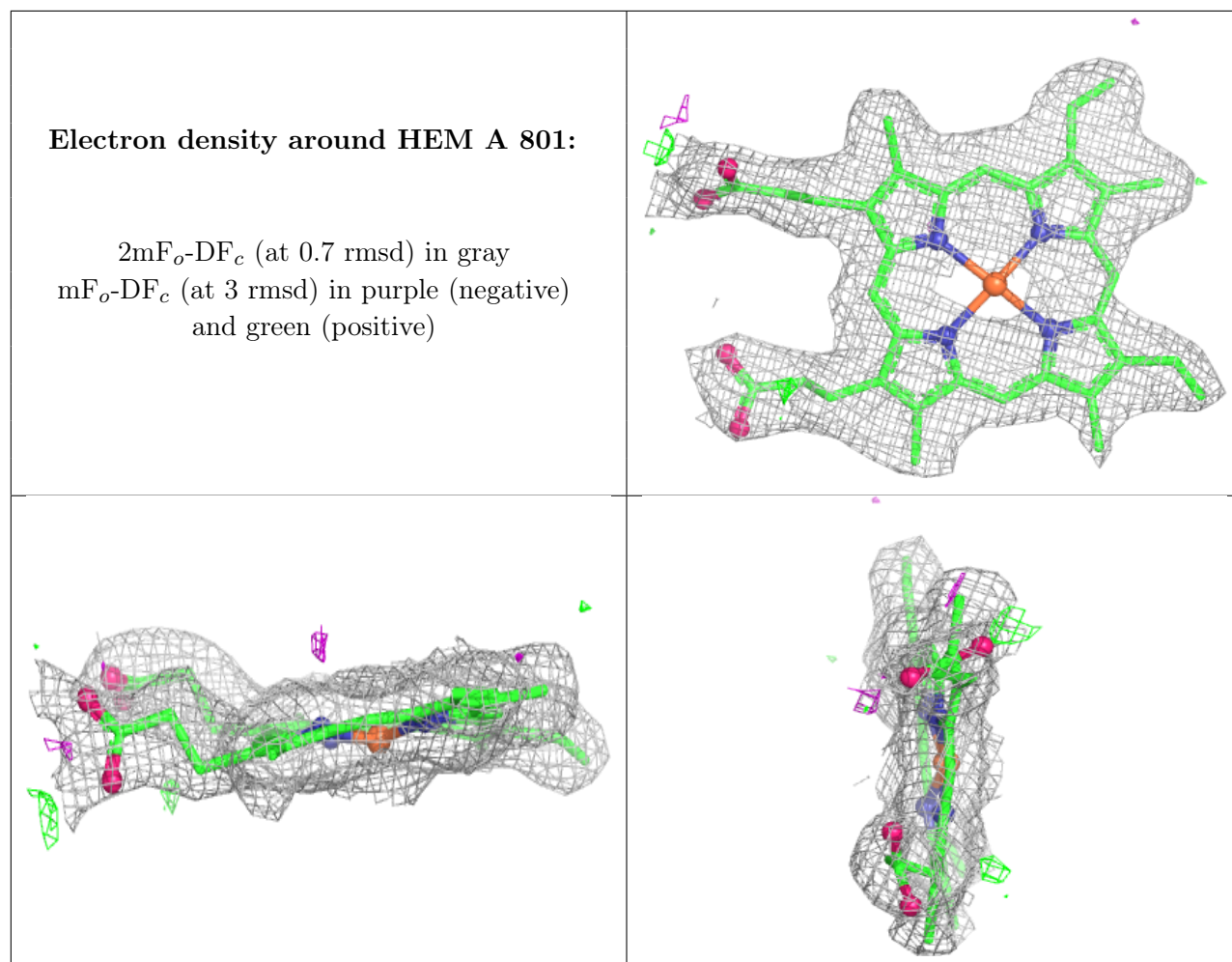
Electron density around OXY A 802:

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

**Electron density around HEM B 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.