



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 04:35 AM EDT

PDB ID : 8W1W / pdb_00008w1w
Title : 2.03 angstrom resolution crystal structure of as-isolated KatG from Mycobacterium tuberculosis with an MYW-OOH cofactor
Authors : Liu, A.; Li, J.
Deposited on : 2024-02-19
Resolution : 2.03 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

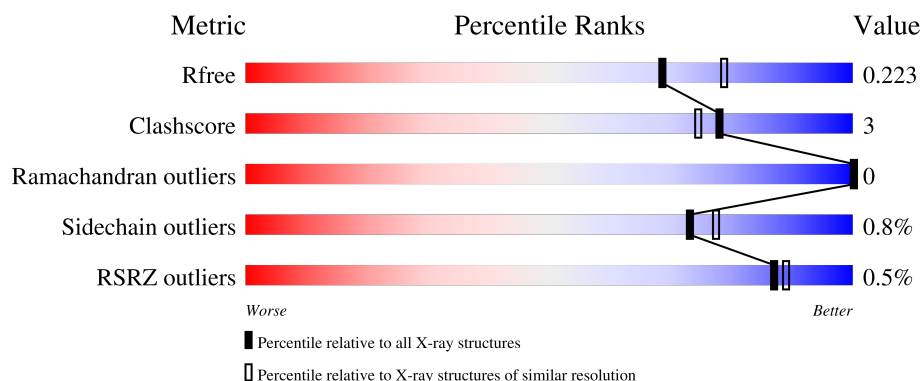
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	88% 8% • •
1	B	741	91% 6% •
1	C	741	91% 6% •
1	D	741	92% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	803	-	X	-	-
5	ACT	B	806	-	X	-	-
5	ACT	B	807	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25482 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.

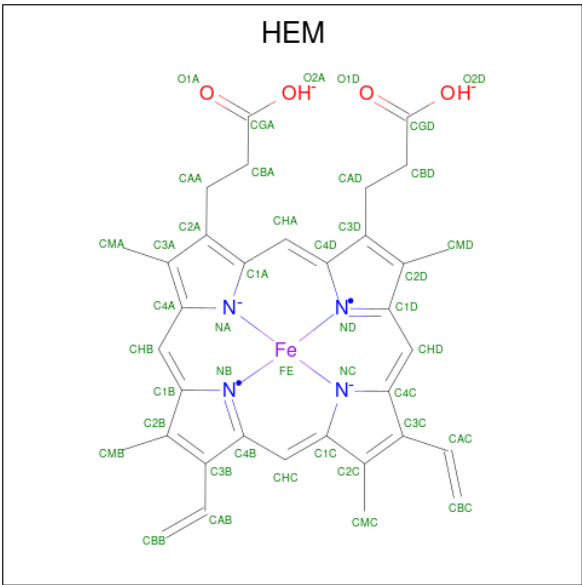
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	1	0
			5539	3520	956	1044	19			
1	B	717	Total	C	N	O	S	0	2	0
			5545	3524	956	1046	19			
1	C	717	Total	C	N	O	S	0	1	0
			5539	3520	956	1044	19			
1	D	717	Total	C	N	O	S	0	1	0
			5539	3520	956	1044	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).

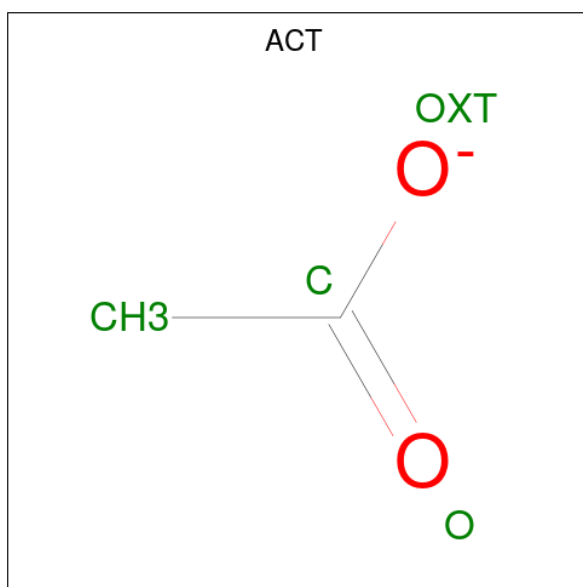
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

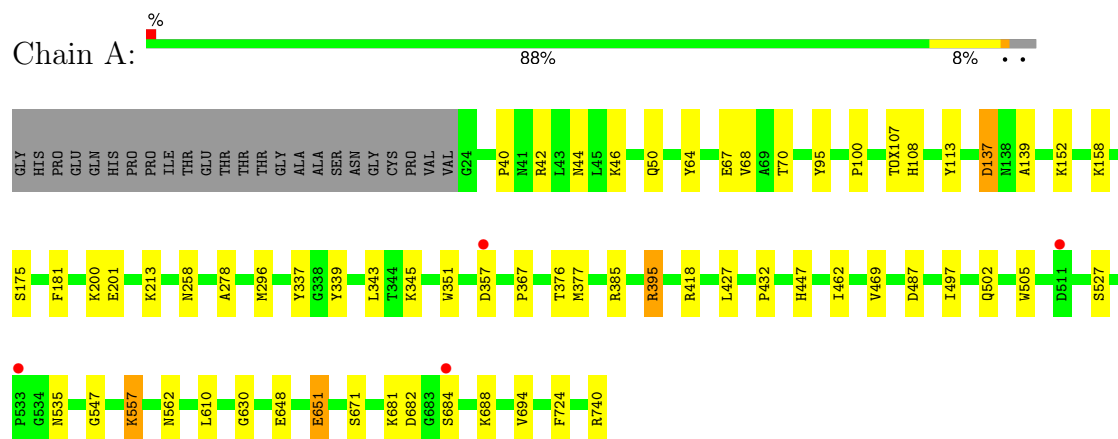
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	733	Total	O	0	0
			733	733		
6	B	762	Total	O	0	0
			762	762		
6	C	763	Total	O	0	0
			763	763		
6	D	810	Total	O	0	0
			810	810		

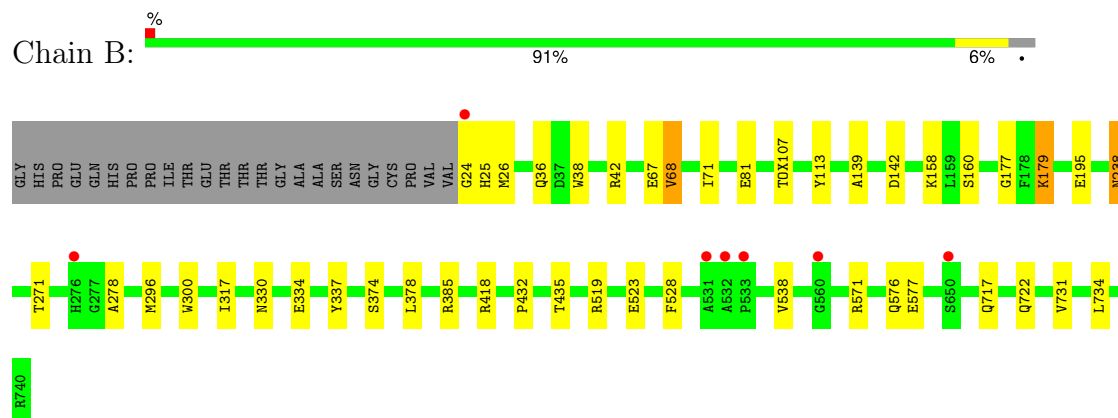
3 Residue-property plots

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.

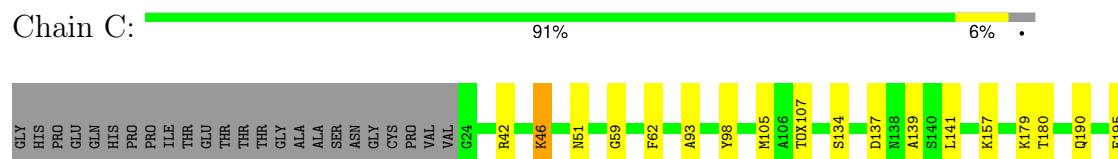
• Molecule 1: Catalase-peroxidase

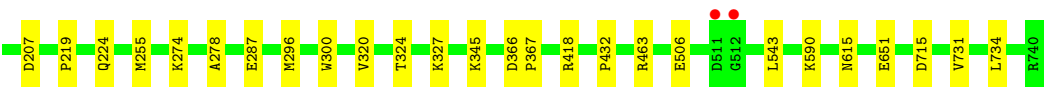


• Molecule 1: Catalase-peroxidase

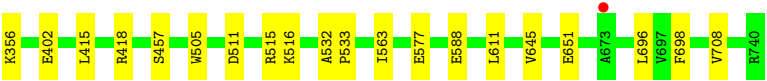
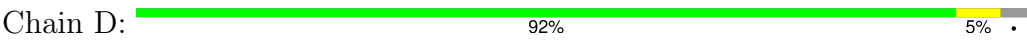


• Molecule 1: Catalase-peroxidase





● Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.67Å 150.67Å 311.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 2.03 47.99 – 2.03	Depositor EDS
% Data completeness (in resolution range)	90.3 (47.99-2.03) 83.3 (47.99-2.03)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, R_{free}	0.166 , 0.223 0.166 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25482	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6753e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, NA, TOX, ACT, 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	1.01	4/5674 (0.1%)	0.96	6/7720 (0.1%)
1	B	1.00	5/5683 (0.1%)	0.93	4/7732 (0.1%)
1	C	1.03	5/5674 (0.1%)	0.94	5/7720 (0.1%)
1	D	1.02	1/5674 (0.0%)	0.93	3/7720 (0.0%)
All	All	1.02	15/22705 (0.1%)	0.94	18/30892 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	PRO	N-CD	-9.70	1.34	1.47
1	B	577	GLU	C-O	-6.80	1.16	1.24
1	B	238	ASN	C-O	-6.44	1.16	1.24
1	C	278	ALA	C-O	-6.41	1.15	1.24
1	C	46	LYS	C-O	-6.09	1.16	1.24
1	B	68	VAL	CB-CG1	-5.97	1.32	1.52
1	D	278	ALA	C-O	-5.97	1.16	1.24
1	A	395	ARG	C-O	-5.96	1.17	1.24
1	B	296	MET	SD-CE	-5.83	1.65	1.79
1	A	139	ALA	C-O	-5.63	1.17	1.23
1	A	497	ILE	CG1-CD1	-5.31	1.31	1.51
1	C	195	GLU	CG-CD	5.17	1.65	1.52
1	B	278	ALA	C-O	-5.14	1.17	1.24
1	C	296	MET	SD-CE	-5.10	1.66	1.79
1	A	651	GLU	CD-OE2	5.01	1.34	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	A	40	PRO	CA-C-N	-7.16	111.20	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PRO	C-N-CA	-7.16	111.20	122.73
1	D	42	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	D	278	ALA	N-CA-C	6.26	119.77	111.75
1	D	296	MET	CG-SD-CE	-6.16	87.35	100.90
1	A	278	ALA	N-CA-C	5.99	119.69	112.38
1	C	195	GLU	CB-CG-CD	5.90	122.62	112.60
1	B	278	ALA	N-CA-C	5.65	119.89	112.89
1	C	278	ALA	N-CA-C	5.58	119.35	112.54
1	B	576	GLN	CA-C-N	5.48	127.89	120.38
1	B	576	GLN	C-N-CA	5.48	127.89	120.38
1	A	201	GLU	CB-CG-CD	5.46	121.89	112.60
1	A	42	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	571	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	C	432	PRO	CA-C-N	-5.13	113.08	122.38
1	C	432	PRO	C-N-CA	-5.13	113.08	122.38
1	C	42	ARG	NE-CZ-NH1	-5.07	116.43	121.50

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	5539	0	5367	43	0
1	B	5545	0	5373	28	0
1	C	5539	0	5367	25	0
1	D	5539	0	5367	27	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	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	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	0	23	1	0
4	C	18	0	24	1	0
4	D	12	0	15	1	0
5	A	4	0	3	0	0
5	B	8	0	6	2	0
5	D	4	0	3	1	0
6	A	733	0	0	11	1
6	B	762	0	0	10	1
6	C	763	0	0	6	0
6	D	810	0	0	5	0
All	All	25482	0	21684	123	2

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 3.

All (123) 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:D:326:THR:C	1:D:327:LYS:HD3	1.86	1.00
1:B:113:TYR:CD2	1:B:418[B]:ARG:HD3	2.18	0.78
1:A:64:TYR:CZ	1:A:68:VAL:CG1	2.69	0.74
1:A:70:THR:HG21	1:A:158:LYS:NZ	2.07	0.70
1:B:81:GLU:HG2	6:B:1420:HOH:O	1.92	0.68
1:A:64:TYR:O	1:A:68:VAL:HG22	1.95	0.67
1:A:181:PHE:CE2	1:A:432:PRO:HG3	2.32	0.65
1:D:26:MET:HE3	1:D:38:TRP:CE2	2.32	0.64
1:A:64:TYR:CE1	1:A:68:VAL:HG13	2.33	0.64
1:B:418[B]:ARG:NH2	6:B:902:HOH:O	2.22	0.63
1:A:64:TYR:CZ	1:A:68:VAL:HG13	2.34	0.63
1:A:345:LYS:HE2	1:A:351:TRP:CD2	2.35	0.62
1:A:345:LYS:HE2	1:A:351:TRP:CE3	2.37	0.60
1:A:557:LYS:HE3	1:A:562:ASN:HD21	1.68	0.58
1:A:610:LEU:HD22	1:A:694:VAL:HG13	1.87	0.55
1:D:326:THR:O	1:D:327:LYS:HD3	2.06	0.55
1:C:366:ASP:OD1	1:C:367:PRO:HD2	2.06	0.55
1:C:179:LYS:HE3	1:C:180:THR:O	2.05	0.55
1:B:418[B]:ARG:HD2	6:B:936:HOH:O	2.06	0.54
1:A:70:THR:HG21	1:A:158:LYS:HZ2	1.71	0.54
1:A:296:MET:HE1	1:D:696:LEU:HG	1.89	0.54
6:A:1007:HOH:O	5:D:805:ACT:H2	2.08	0.54
1:C:274:LYS:HB2	1:C:320:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HA	4:B:803:GOL:H12	1.90	0.53
1:B:519:ARG:O	1:B:523:GLU:HG3	2.09	0.53
1:C:51:ASN:ND2	1:C:190:GLN:HG2	2.23	0.53
1:C:731:VAL:HA	1:C:734:LEU:HG	1.91	0.52
1:A:682:ASP:OD1	1:A:684:SER:HB3	2.10	0.51
1:B:179:LYS:H	5:B:807:ACT:H1	1.76	0.51
1:D:326:THR:C	1:D:327:LYS:CD	2.75	0.51
1:B:330:ASN:O	1:B:334:GLU:HG3	2.10	0.51
1:A:447:HIS:HB3	1:A:535:ASN:O	2.11	0.51
1:B:717:GLN:HB3	6:B:1535:HOH:O	2.11	0.50
4:D:803:GOL:H12	6:D:1385:HOH:O	2.12	0.50
1:C:506:GLU:HG2	6:C:1500:HOH:O	2.12	0.48
1:D:505:TRP:CG	1:D:588:GLU:HG3	2.49	0.48
1:A:108:HIS:CE1	1:A:137:ASP:O	2.67	0.48
1:A:64:TYR:CZ	1:A:68:VAL:HG11	2.46	0.48
1:D:327:LYS:HD3	1:D:327:LYS:N	2.28	0.48
1:A:681:LYS:NZ	6:A:926:HOH:O	2.45	0.48
1:C:463:ARG:HD2	6:C:937:HOH:O	2.13	0.48
6:B:1485:HOH:O	1:C:715:ASP:HB3	2.14	0.47
1:C:93:ALA:HB2	1:C:98:TYR:CZ	2.49	0.47
1:C:255:MET:O	1:C:418[B]:ARG:NH1	2.48	0.47
1:A:462:ILE:HG21	1:A:547:GLY:HA2	1.97	0.47
1:B:238:ASN:ND2	6:B:924:HOH:O	2.42	0.47
1:B:722:GLN:NE2	6:B:928:HOH:O	2.44	0.47
1:C:345:LYS:HE3	6:C:1027:HOH:O	2.14	0.47
1:D:402:GLU:OE1	1:D:402:GLU:N	2.35	0.46
1:D:651:GLU:HG2	6:D:990:HOH:O	2.15	0.46
1:C:615:ASN:OD1	4:C:805:GOL:H32	2.15	0.46
1:B:432:PRO:HB2	6:B:1379:HOH:O	2.16	0.46
1:A:258:ASN:HB2	6:A:1117:HOH:O	2.16	0.46
1:C:62:PHE:CE1	1:C:157:LYS:HE3	2.51	0.46
1:D:645:VAL:O	1:D:645:VAL:HG12	2.16	0.45
1:D:515:ARG:HD3	6:D:1482:HOH:O	2.15	0.45
1:B:139:ALA:HA	1:B:300:TRP:CZ3	2.52	0.45
1:A:50:GLN:HG2	6:A:1400:HOH:O	2.16	0.45
1:B:337:TYR:CE1	1:B:385:ARG:HG3	2.51	0.45
1:D:340:GLU:HB3	1:D:356:LYS:HE2	1.98	0.45
1:A:557:LYS:HE3	1:A:562:ASN:ND2	2.32	0.45
1:B:731:VAL:HA	1:B:734:LEU:HG	1.99	0.45
1:D:179:LYS:HA	1:D:179:LYS:HD2	1.82	0.45
1:B:68:VAL:O	1:B:71:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:OD1	1:B:142:ASP:N	2.48	0.44
1:B:435:THR:HG21	6:B:1555:HOH:O	2.17	0.44
1:B:24:GLY:O	1:B:25:HIS:ND1	2.50	0.44
1:A:339:TYR:OH	6:A:901:HOH:O	2.20	0.44
1:A:648:GLU:OE1	1:A:688:LYS:NZ	2.39	0.44
1:C:139:ALA:HA	1:C:300:TRP:CZ3	2.52	0.44
1:D:415:LEU:HA	1:D:418[B]:ARG:HD3	2.00	0.44
1:A:213:LYS:HE3	6:A:1530:HOH:O	2.17	0.44
1:A:152:LYS:NZ	4:A:803:GOL:H2	2.33	0.44
1:C:179:LYS:HA	1:C:179:LYS:HD2	1.81	0.44
1:A:67:GLU:O	1:A:70:THR:HB	2.18	0.43
1:B:418[A]:ARG:HA	1:B:418[A]:ARG:HD2	1.87	0.43
1:D:698:PHE:HB3	1:D:708:VAL:HG21	2.00	0.43
1:B:177:GLY:O	5:B:807:ACT:H3	2.19	0.43
1:B:238:ASN:OD1	1:D:238:ASN:HB2	2.18	0.43
1:D:418[B]:ARG:H	1:D:418[B]:ARG:HG2	1.66	0.43
1:D:342:GLU:HB3	1:D:356:LYS:HG2	2.01	0.43
1:A:68:VAL:HG21	1:A:427:LEU:HD12	2.00	0.43
1:A:469:VAL:HB	1:A:651:GLU:CD	2.44	0.43
1:D:326:THR:H	1:D:327:LYS:NZ	2.16	0.43
1:B:26:MET:HE3	1:B:38:TRP:CE2	2.54	0.42
1:C:59:GLY:O	6:C:901:HOH:O	2.21	0.42
1:A:671:SER:HB3	6:A:1085:HOH:O	2.17	0.42
1:B:528:PHE:CE2	1:B:538:VAL:HG23	2.54	0.42
1:C:651:GLU:HG2	6:C:1091:HOH:O	2.20	0.42
1:A:64:TYR:CE2	1:A:68:VAL:HG11	2.54	0.42
1:A:376:THR:O	1:A:377:MET:HG2	2.18	0.42
1:D:415:LEU:O	1:D:418[B]:ARG:HG2	2.20	0.42
1:A:44:ASN:OD1	1:A:46:LYS:HG3	2.19	0.42
1:D:327:LYS:CD	1:D:327:LYS:N	2.83	0.42
1:B:271:THR:HG23	6:B:976:HOH:O	2.20	0.42
1:D:577:GLU:H	1:D:577:GLU:CD	2.26	0.41
1:A:113:TYR:HE1	1:A:487:ASP:HB3	1.85	0.41
1:A:357:ASP:N	6:A:947:HOH:O	2.53	0.41
1:C:651:GLU:HG2	6:C:931:HOH:O	2.19	0.41
1:D:239:PRO:HD3	1:D:351:TRP:CD1	2.55	0.41
1:D:516:LYS:HE2	6:D:1024:HOH:O	2.21	0.41
1:A:630:GLY:HA3	1:A:724:PHE:CE1	2.55	0.41
1:B:67:GLU:HB3	1:B:158:LYS:HA	2.03	0.41
1:C:139:ALA:HA	1:C:300:TRP:CH2	2.56	0.41
1:C:134:SER:HB3	1:C:287:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:CD1	1:A:367:PRO:HA	2.56	0.41
1:A:740:ARG:NE	6:A:921:HOH:O	2.43	0.41
1:B:36:GLN:NE2	1:B:42:ARG:HG2	2.36	0.41
1:B:317:ILE:HG21	1:B:378:LEU:CD2	2.50	0.41
1:D:532:ALA:HB1	1:D:533:PRO:HD2	2.02	0.41
1:A:418[B]:ARG:NE	6:A:906:HOH:O	2.34	0.41
1:C:207:ASP:HB2	1:C:224:GLN:HG2	2.02	0.41
1:C:324:THR:HB	1:C:327:LYS:HB3	2.03	0.41
1:C:366:ASP:CG	1:C:367:PRO:HD2	2.45	0.41
1:D:45:LEU:HD23	1:D:611:LEU:HD21	2.02	0.41
1:A:502:GLN:HG2	1:A:505:TRP:CH2	2.56	0.41
1:A:70:THR:HG21	1:A:158:LYS:HZ1	1.81	0.40
1:A:337:TYR:CE1	1:A:385:ARG:HG3	2.56	0.40
1:C:105:MET:HB2	1:C:141:LEU:HD22	2.04	0.40
1:A:100:PRO:HD2	6:A:1197:HOH:O	2.21	0.40
1:C:418[A]:ARG:HA	1:C:418[A]:ARG:HD2	1.91	0.40
1:A:343:LEU:HG	1:A:351:TRP:CE3	2.57	0.40
1:D:563:ILE:HG13	6:D:1375:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1149:HOH:O	6:B:1149:HOH:O[8_445]	2.18	0.02
6:A:1415:HOH:O	6:A:1575:HOH:O[6_445]	2.19	0.01

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	715/741 (96%)	698 (98%)	17 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	716/741 (97%)	700 (98%)	16 (2%)	0	100	100
1	C	715/741 (96%)	698 (98%)	17 (2%)	0	100	100
1	D	715/741 (96%)	697 (98%)	18 (2%)	0	100	100
All	All	2861/2964 (96%)	2793 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	565/583 (97%)	559 (99%)	6 (1%)	65	68
1	B	566/583 (97%)	563 (100%)	3 (0%)	81	85
1	C	565/583 (97%)	561 (99%)	4 (1%)	76	80
1	D	565/583 (97%)	561 (99%)	4 (1%)	76	80
All	All	2261/2332 (97%)	2244 (99%)	17 (1%)	73	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	175	SER
1	A	200	LYS
1	A	395	ARG
1	A	527	SER
1	A	557	LYS
1	B	179	LYS
1	B	195	GLU
1	B	374	SER
1	C	46	LYS
1	C	137	ASP
1	C	543	LEU
1	C	590	LYS

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Mol	Chain	Res	Type
1	D	137	ASP
1	D	194	ASP
1	D	457	SER
1	D	511	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	HIS
1	A	562	ASN
1	B	36	GLN
1	B	190	GLN
1	B	400	HIS
1	B	434	GLN
1	B	722	GLN
1	C	116	HIS
1	C	190	GLN
1	C	236	ASN
1	D	116	HIS
1	D	190	GLN
1	D	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	B	107	1,2	14,17,18	2.55	6 (42%)	12,23,25	1.88	5 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	A	107	1	14,17,18	2.43	4 (28%)	12,23,25	1.41	2 (16%)
1	TOX	D	107	1	14,17,18	3.09	5 (35%)	12,23,25	2.27	4 (33%)
1	TOX	C	107	1	14,17,18	2.80	5 (35%)	12,23,25	1.91	4 (33%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	TOX	O1-NE1	8.40	1.50	1.39
1	B	107	TOX	O1-NE1	6.46	1.47	1.39
1	A	107	TOX	O1-NE1	6.19	1.47	1.39
1	C	107	TOX	CD2-CE2	-6.09	1.33	1.41
1	C	107	TOX	O1-NE1	5.97	1.46	1.39
1	D	107	TOX	CD2-CE2	-5.34	1.33	1.41
1	A	107	TOX	CD2-CG	-4.58	1.36	1.44
1	D	107	TOX	CD2-CG	-4.48	1.36	1.44
1	C	107	TOX	CD2-CG	-3.66	1.38	1.44
1	B	107	TOX	CE2-NE1	-3.46	1.33	1.39
1	B	107	TOX	CD2-CG	-3.23	1.38	1.44
1	A	107	TOX	CE2-NE1	-3.11	1.34	1.39
1	B	107	TOX	CH2-CZ3	2.51	1.43	1.38
1	C	107	TOX	CE2-NE1	-2.35	1.35	1.39
1	D	107	TOX	CB-CA	2.33	1.58	1.53
1	A	107	TOX	CD2-CE2	-2.26	1.38	1.41
1	B	107	TOX	CB-CA	2.10	1.58	1.53
1	B	107	TOX	CE3-CD2	-2.10	1.36	1.39
1	D	107	TOX	CZ2-CE2	2.01	1.42	1.39
1	C	107	TOX	CB-CG	2.00	1.54	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	TOX	CZ3-CH2-CZ2	-4.83	114.28	120.24
1	D	107	TOX	CB-CG-CD1	-3.65	121.59	126.67
1	C	107	TOX	CB-CG-CD1	-3.29	122.09	126.67
1	C	107	TOX	CZ3-CH2-CZ2	-3.26	116.22	120.24
1	B	107	TOX	CB-CG-CD1	-3.21	122.20	126.67
1	D	107	TOX	CH2-CZ3-CE3	3.16	124.14	120.24
1	B	107	TOX	CZ3-CH2-CZ2	-3.05	116.48	120.24
1	C	107	TOX	CE2-CD2-CG	2.60	109.79	107.39
1	B	107	TOX	CB-CG-CD2	2.59	131.68	126.70
1	D	107	TOX	CD2-CG-CD1	2.54	108.65	106.34
1	A	107	TOX	CB-CG-CD1	-2.52	123.16	126.67
1	B	107	TOX	CE2-CD2-CG	2.26	109.47	107.39
1	A	107	TOX	CB-CG-CD2	2.17	130.87	126.70
1	B	107	TOX	CE3-CD2-CE2	-2.02	116.91	119.24
1	C	107	TOX	CB-CG-CD2	2.01	130.56	126.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	107	TOX	N-CA-CB-CG
1	A	107	TOX	C-CA-CB-CG
1	B	107	TOX	N-CA-CB-CG
1	B	107	TOX	C-CA-CB-CG
1	C	107	TOX	N-CA-CB-CG
1	C	107	TOX	C-CA-CB-CG
1	D	107	TOX	N-CA-CB-CG
1	D	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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
4	GOL	C	803	-	5,5,5	0.38	0	5,5,5	0.59	0
2	HEM	D	801	1	50,50,50	1.81	15 (30%)	67,82,82	1.14	5 (7%)
5	ACT	B	807	-	3,3,3	0.90	0	3,3,3	1.63	1 (33%)
4	GOL	D	803	-	5,5,5	1.49	1 (20%)	5,5,5	2.04	2 (40%)
5	ACT	D	805	-	3,3,3	1.30	1 (33%)	3,3,3	0.45	0
2	HEM	B	801	1	50,50,50	1.68	9 (18%)	67,82,82	1.10	4 (5%)
4	GOL	A	803	-	5,5,5	1.19	1 (20%)	5,5,5	2.09	4 (80%)
4	GOL	B	803	-	5,5,5	0.54	0	5,5,5	0.83	0
4	GOL	B	804	-	5,5,5	0.71	0	5,5,5	1.55	1 (20%)
2	HEM	C	801	1	50,50,50	1.88	14 (28%)	67,82,82	1.36	10 (14%)
4	GOL	C	805	-	5,5,5	0.75	0	5,5,5	1.14	0
4	GOL	B	805	-	5,5,5	0.82	0	5,5,5	0.99	0
2	HEM	A	801	1	50,50,50	1.79	12 (24%)	67,82,82	0.93	3 (4%)
4	GOL	A	804	-	5,5,5	0.43	0	5,5,5	0.69	0
4	GOL	D	804	-	5,5,5	0.52	0	5,5,5	0.40	0
5	ACT	A	805	-	3,3,3	1.22	0	3,3,3	1.94	2 (66%)
5	ACT	B	806	-	3,3,3	1.30	1 (33%)	3,3,3	2.02	2 (66%)
4	GOL	C	804	-	5,5,5	0.71	0	5,5,5	2.28	2 (40%)

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
4	GOL	C	803	-	-	0/4/4/4	-
2	HEM	D	801	1	-	3/14/54/54	-
4	GOL	D	803	-	-	2/4/4/4	-
2	HEM	B	801	1	-	3/14/54/54	-
4	GOL	A	803	-	-	2/4/4/4	-
4	GOL	B	803	-	-	1/4/4/4	-
4	GOL	B	804	-	-	3/4/4/4	-
2	HEM	C	801	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	805	-	-	4/4/4/4	-
4	GOL	B	805	-	-	1/4/4/4	-
2	HEM	A	801	1	-	3/14/54/54	-
4	GOL	A	804	-	-	1/4/4/4	-
4	GOL	D	804	-	-	1/4/4/4	-
4	GOL	C	804	-	-	1/4/4/4	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEM	FE-NC	5.14	2.12	1.95
2	D	801	HEM	FE-NA	5.02	2.11	1.95
2	B	801	HEM	C1C-NC	-4.53	1.31	1.39
2	A	801	HEM	CMD-C2D	4.48	1.59	1.50
2	B	801	HEM	FE-NC	4.21	2.09	1.95
2	D	801	HEM	FE-NB	3.65	2.06	1.94
2	C	801	HEM	FE-ND	3.55	2.05	1.94
2	B	801	HEM	CAB-C3B	3.48	1.56	1.47
2	A	801	HEM	C3B-C2B	-3.42	1.30	1.37
2	A	801	HEM	C4C-NC	-3.42	1.33	1.39
2	A	801	HEM	FE-NB	3.40	2.05	1.94
2	A	801	HEM	CAB-C3B	3.36	1.56	1.47
2	D	801	HEM	FE-ND	3.32	2.05	1.94
2	C	801	HEM	FE-NB	3.25	2.04	1.94
2	A	801	HEM	FE-NC	3.24	2.05	1.95
4	D	803	GOL	O2-C2	-3.24	1.34	1.43
2	C	801	HEM	C3B-C2B	-3.18	1.30	1.37
2	D	801	HEM	C3B-C2B	-3.15	1.30	1.37
2	C	801	HEM	C1B-NB	-3.12	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.03	1.31	1.37
2	D	801	HEM	C1A-NA	-2.92	1.34	1.39
2	D	801	HEM	C4C-NC	-2.90	1.34	1.39
2	B	801	HEM	C2A-C3A	-2.90	1.31	1.38
2	D	801	HEM	C4B-NB	-2.79	1.33	1.38
2	C	801	HEM	CMB-C2B	2.75	1.56	1.50
2	D	801	HEM	FE-NC	2.74	2.04	1.95
2	C	801	HEM	FE-NA	2.71	2.04	1.95
2	C	801	HEM	C2A-C3A	-2.71	1.31	1.38
2	C	801	HEM	C3D-C2D	-2.71	1.30	1.36
2	C	801	HEM	CAC-C3C	2.69	1.54	1.47
2	D	801	HEM	C4D-ND	-2.65	1.35	1.40
2	B	801	HEM	C3B-C2B	-2.65	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-ND	2.65	2.03	1.94
2	A	801	HEM	CMB-C2B	2.63	1.56	1.50
2	A	801	HEM	CMA-C3A	2.63	1.56	1.50
2	C	801	HEM	CAB-C3B	2.62	1.54	1.47
4	A	803	GOL	O3-C3	2.61	1.53	1.42
2	D	801	HEM	CAC-C3C	2.49	1.54	1.47
2	B	801	HEM	CMD-C2D	2.46	1.55	1.50
2	D	801	HEM	CMD-C2D	2.45	1.55	1.50
2	D	801	HEM	CAB-C3B	2.45	1.53	1.47
2	B	801	HEM	CMB-C2B	2.44	1.55	1.50
2	A	801	HEM	CHD-C4C	-2.30	1.33	1.38
2	B	801	HEM	C3C-C4C	-2.26	1.42	1.46
2	C	801	HEM	CMD-C2D	2.25	1.55	1.50
2	A	801	HEM	C1C-NC	-2.24	1.35	1.39
5	D	805	ACT	O-C	2.21	1.31	1.22
2	D	801	HEM	O2A-CGA	-2.19	1.23	1.30
2	C	801	HEM	C4D-ND	-2.17	1.36	1.40
5	B	806	ACT	O-C	2.12	1.31	1.22
2	D	801	HEM	CAD-C3D	2.11	1.56	1.51
2	C	801	HEM	O2A-CGA	-2.10	1.23	1.30
2	A	801	HEM	C4A-C3A	2.07	1.48	1.43
2	D	801	HEM	CAA-C2A	2.01	1.56	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	HEM	CAA-CBA-CGA	-4.15	102.65	113.67
2	B	801	HEM	CAA-CBA-CGA	-3.87	103.40	113.67
4	D	803	GOL	O3-C3-C2	-3.66	93.92	110.38
4	C	804	GOL	O2-C2-C3	-3.38	95.17	109.18
2	C	801	HEM	C3B-C4B-NB	-3.16	107.20	109.47
2	A	801	HEM	O2A-CGA-O1A	-2.96	115.72	123.33
2	C	801	HEM	CHC-C4B-NB	2.95	127.60	124.42
2	C	801	HEM	CAA-CBA-CGA	-2.93	105.89	113.67
2	A	801	HEM	CAA-CBA-CGA	-2.84	106.12	113.67
2	B	801	HEM	CHD-C4C-NC	2.79	127.49	124.45
4	C	804	GOL	C3-C2-C1	-2.68	101.97	111.80
2	C	801	HEM	C4C-NC-C1C	2.67	110.18	105.82
5	B	806	ACT	OXT-C-CH3	2.62	126.03	115.05
4	B	804	GOL	O2-C2-C1	2.61	120.00	109.18
2	D	801	HEM	C3A-C4A-NA	-2.56	106.04	110.14
4	A	803	GOL	O2-C2-C3	2.54	119.70	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	HEM	C4A-NA-C1A	2.54	109.96	105.82
2	C	801	HEM	CMC-C2C-C1C	-2.50	120.32	124.73
5	A	805	ACT	OXT-C-O	-2.47	112.86	122.03
2	C	801	HEM	O2D-CGD-CBD	2.31	121.31	114.00
5	B	806	ACT	O-C-CH3	-2.31	113.06	122.53
5	A	805	ACT	OXT-C-CH3	2.29	124.63	115.05
2	B	801	HEM	CHB-C1B-NB	2.21	127.11	124.37
2	D	801	HEM	CAA-C2A-C1A	2.20	129.25	124.94
4	A	803	GOL	O3-C3-C2	2.20	120.28	110.38
2	D	801	HEM	CHD-C4C-NC	2.20	126.85	124.45
4	D	803	GOL	C3-C2-C1	2.18	119.80	111.80
4	A	803	GOL	O2-C2-C1	2.15	118.07	109.18
2	C	801	HEM	C4C-CHD-C1D	2.14	130.58	126.02
2	C	801	HEM	CHC-C1C-C2C	2.12	129.90	125.49
4	A	803	GOL	C3-C2-C1	2.12	119.57	111.80
2	A	801	HEM	O2A-CGA-CBA	2.11	120.67	114.00
2	B	801	HEM	O2D-CGD-CBD	2.10	120.65	114.00
5	B	807	ACT	OXT-C-CH3	2.04	123.60	115.05
2	C	801	HEM	C4B-C3B-C2B	2.03	109.15	107.28
2	C	801	HEM	C3C-C2C-C1C	2.01	108.95	107.05

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	804	GOL	O1-C1-C2-C3
4	B	804	GOL	C1-C2-C3-O3
4	C	805	GOL	C1-C2-C3-O3
4	D	803	GOL	C1-C2-C3-O3
4	A	804	GOL	C1-C2-C3-O3
4	C	805	GOL	O1-C1-C2-C3
4	B	804	GOL	O1-C1-C2-O2
4	D	803	GOL	O2-C2-C3-O3
4	A	803	GOL	O2-C2-C3-O3
4	C	805	GOL	O2-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
4	C	804	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
4	C	805	GOL	O1-C1-C2-O2
4	B	803	GOL	C1-C2-C3-O3
2	B	801	HEM	CAA-CBA-CGA-O2A

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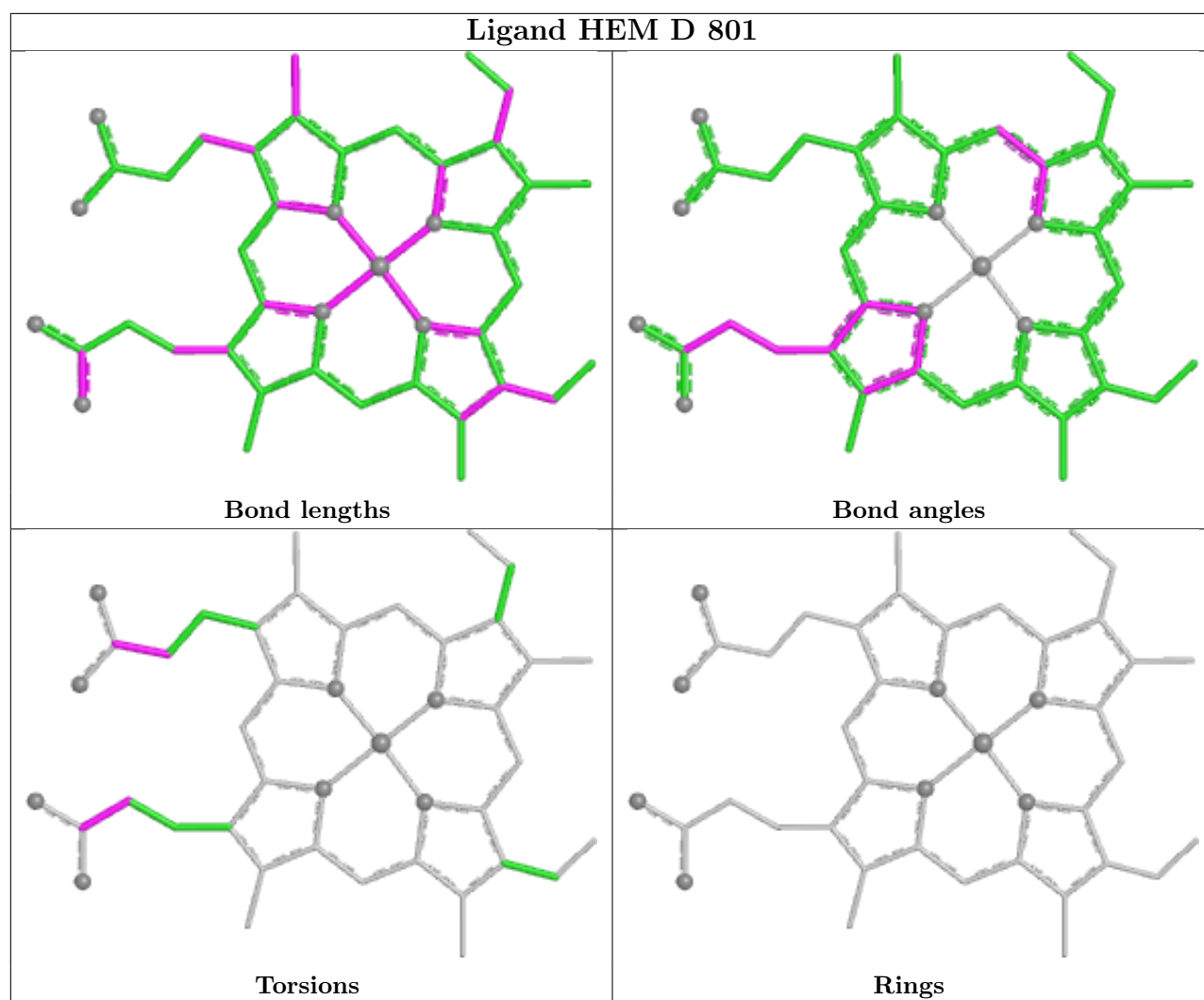
Mol	Chain	Res	Type	Atoms
2	B	801	HEM	CAA-CBA-CGA-O1A
2	C	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O1A
2	D	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	D	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAD-CBD-CGD-O2D
2	D	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O1D

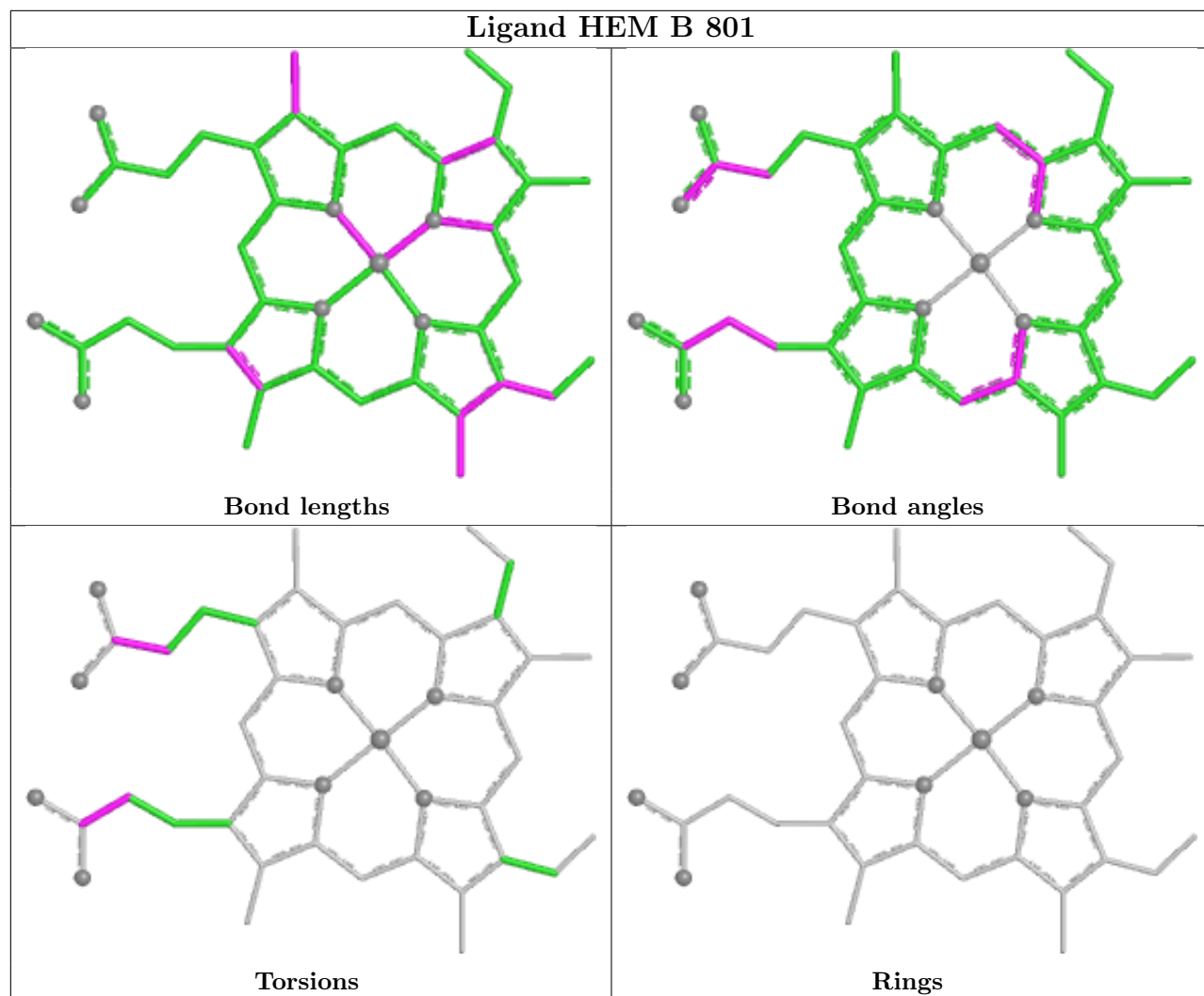
There are no ring outliers.

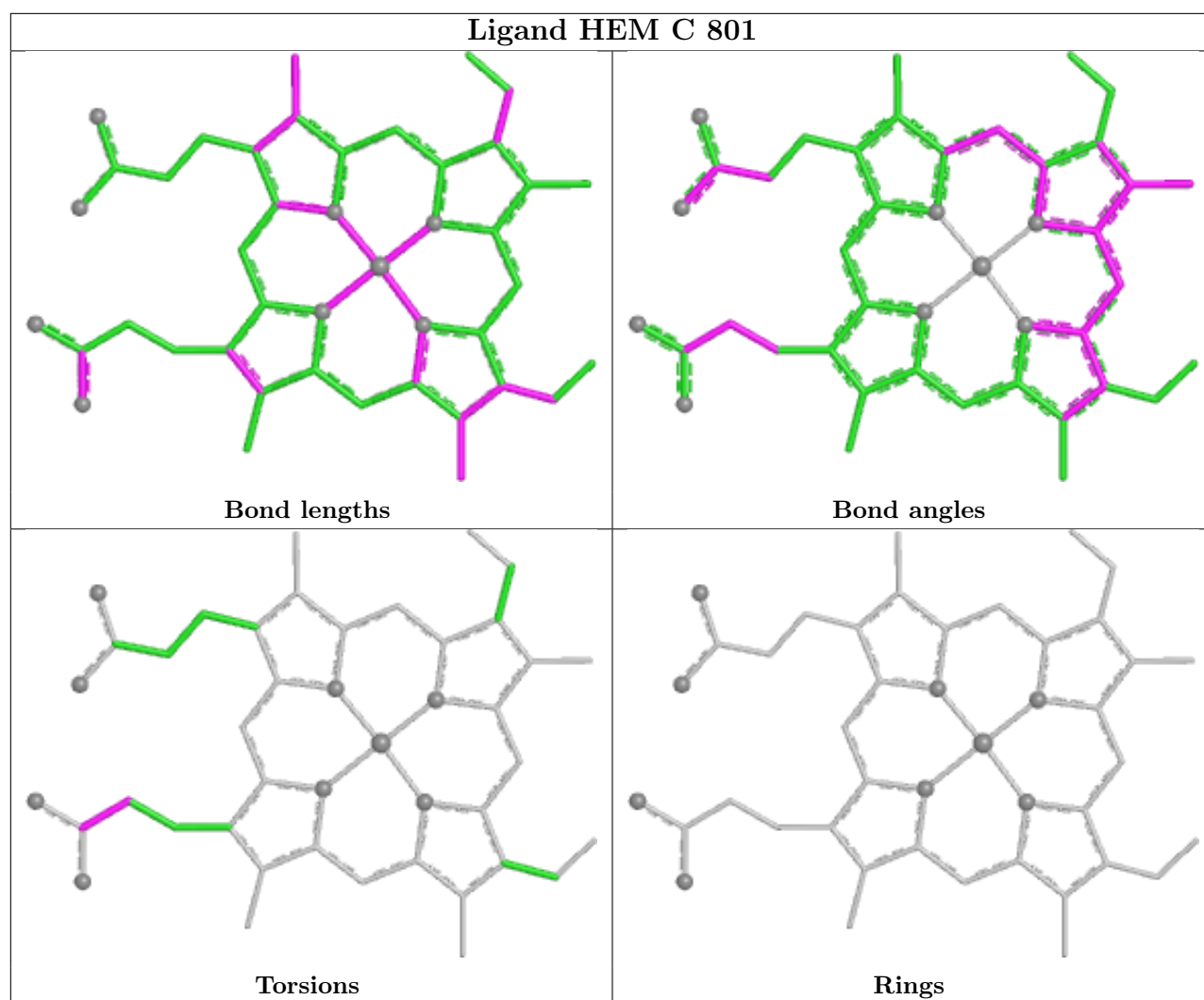
6 monomers are involved in 7 short contacts:

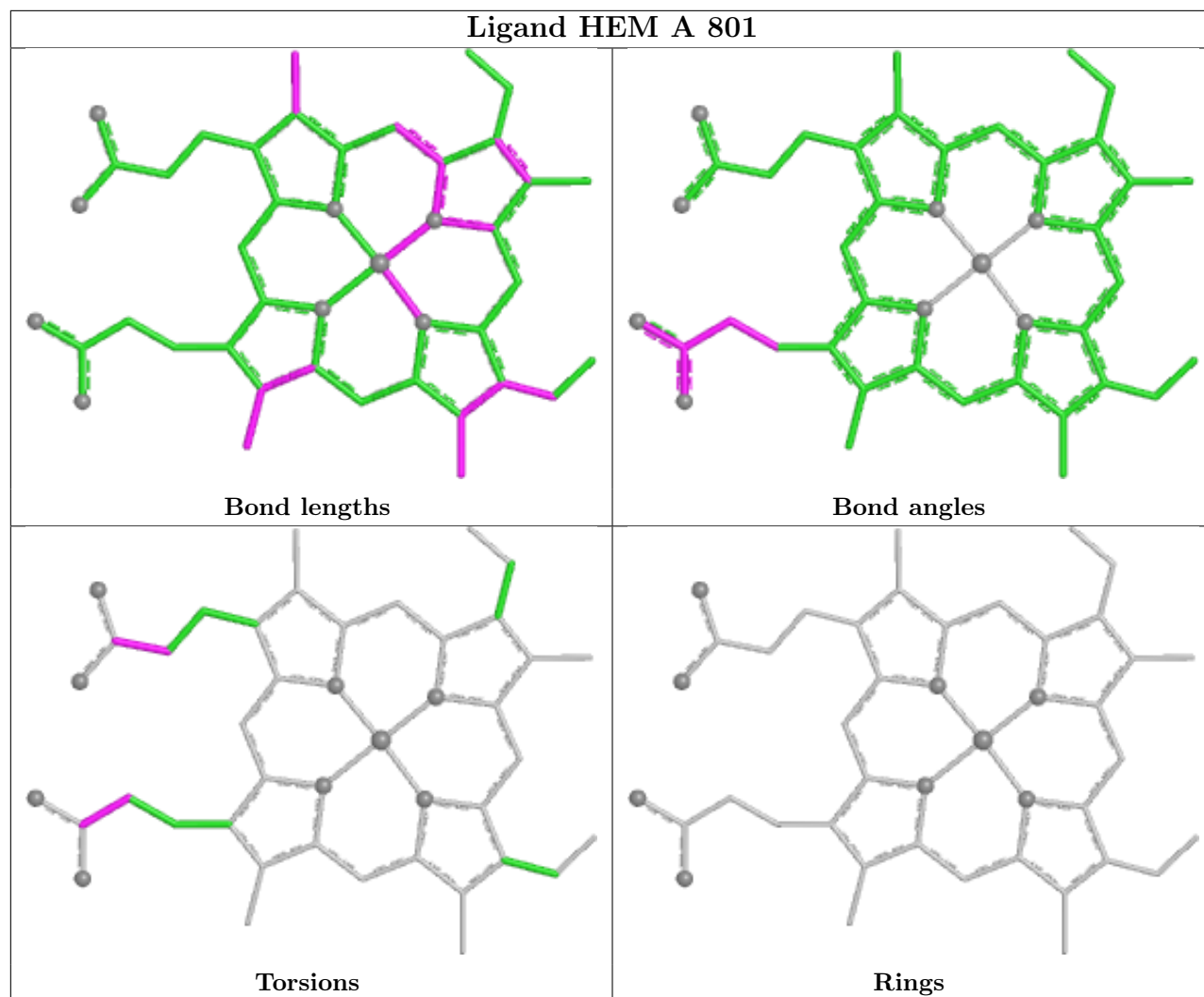
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	807	ACT	2	0
4	D	803	GOL	1	0
5	D	805	ACT	1	0
4	A	803	GOL	1	0
4	B	803	GOL	1	0
4	C	805	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å²)	Q<0.9	
1	A	716/741 (96%)	-0.47	4 (0%)	85	87	7, 16, 30, 46	1 (0%)
1	B	716/741 (96%)	-0.40	7 (0%)	79	81	7, 17, 31, 48	2 (0%)
1	C	716/741 (96%)	-0.55	2 (0%)	90	92	7, 14, 26, 41	1 (0%)
1	D	716/741 (96%)	-0.57	2 (0%)	90	92	7, 14, 27, 43	1 (0%)
All	All	2864/2964 (96%)	-0.50	15 (0%)	87	89	7, 15, 29, 48	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	PRO	3.1
1	B	531	ALA	3.1
1	B	532	ALA	3.1
1	D	673	ALA	2.4
1	D	59	GLY	2.4
1	C	512	GLY	2.3
1	A	533	PRO	2.3
1	C	511	ASP	2.3
1	A	684	SER	2.2
1	A	357	ASP	2.1
1	B	24	GLY	2.1
1	A	511	ASP	2.1
1	B	276	HIS	2.1
1	B	560	GLY	2.1
1	B	650	SER	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($\text{\AA}^2$)	Q<0.9
1	TOX	A	107	16/17	0.96	0.05	8,10,15,16	0
1	TOX	B	107	16/17	0.96	0.07	8,10,13,18	0
1	TOX	D	107	16/17	0.96	0.06	6,8,12,15	0
1	TOX	C	107	16/17	0.97	0.06	7,9,14,16	0

6.3 Carbohydrates [i](#)

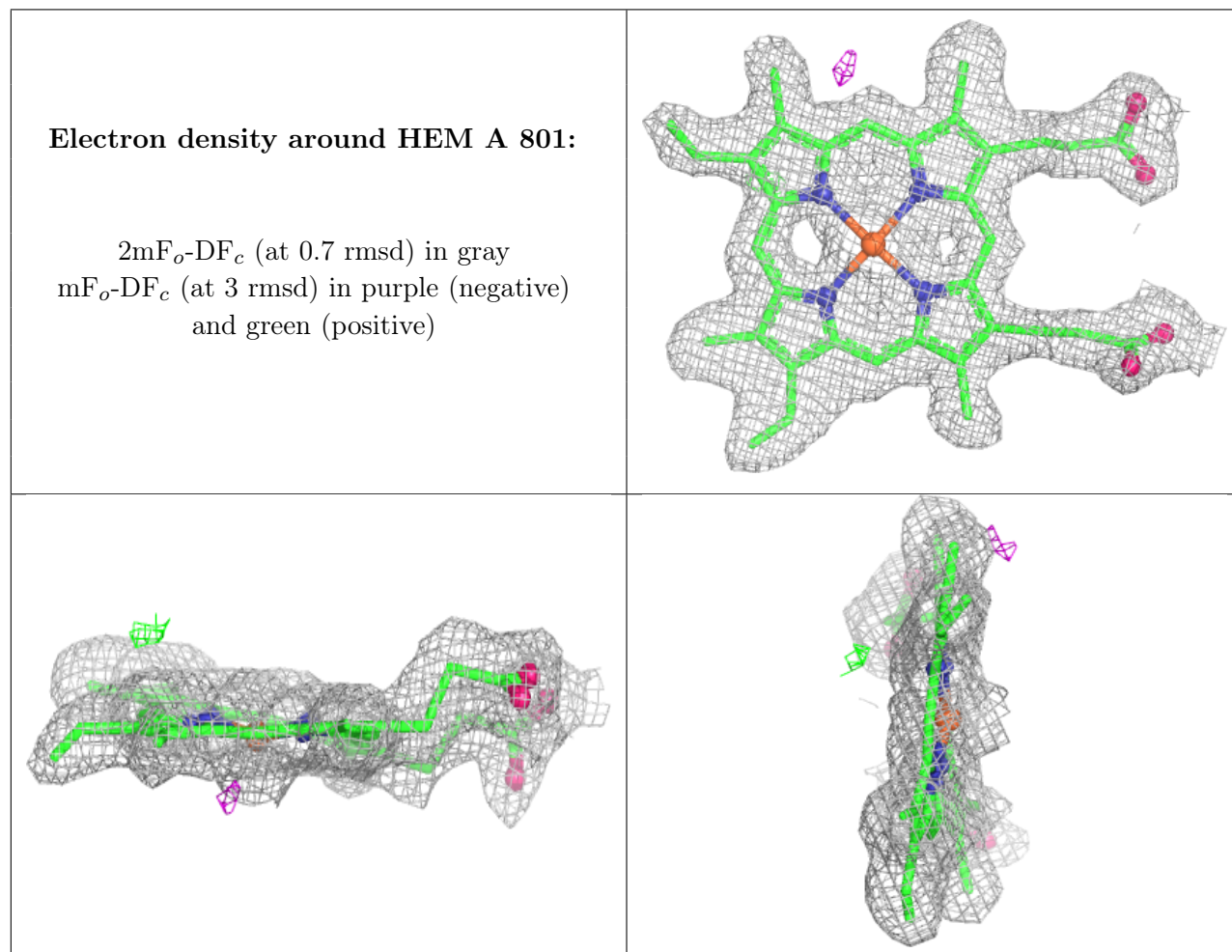
There are no oligosaccharides in this entry.

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.

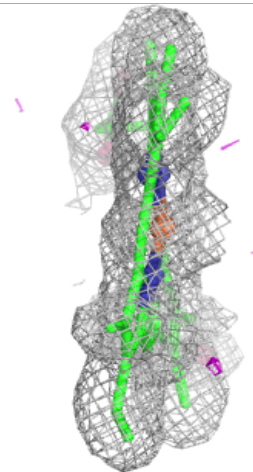
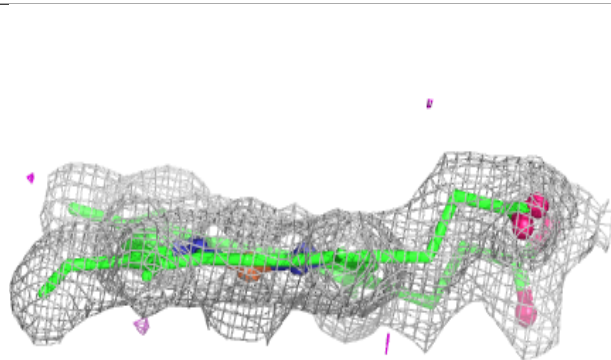
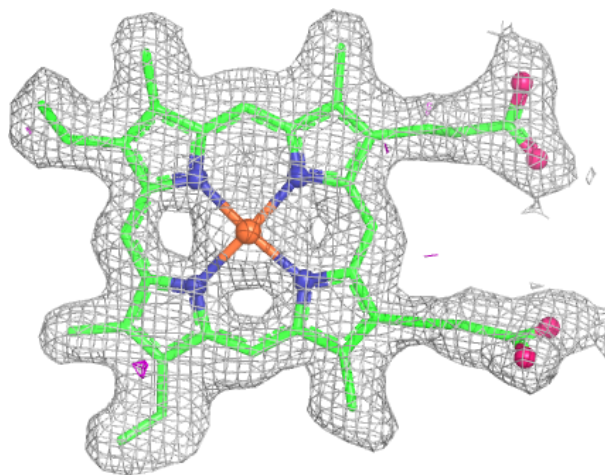
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	B	807	4/4	0.69	0.16	19,34,34,38	0
5	ACT	A	805	4/4	0.75	0.17	22,26,29,33	0
5	ACT	B	806	4/4	0.83	0.13	17,22,25,27	0
4	GOL	C	805	6/6	0.88	0.12	18,24,28,28	0
4	GOL	D	804	6/6	0.90	0.13	18,25,30,37	0
5	ACT	D	805	4/4	0.90	0.13	18,21,21,28	0
4	GOL	A	803	6/6	0.91	0.09	15,18,19,20	0
4	GOL	B	805	6/6	0.91	0.11	20,22,28,31	0
4	GOL	B	804	6/6	0.92	0.10	20,22,23,29	0
4	GOL	A	804	6/6	0.95	0.09	16,19,22,29	0
4	GOL	C	804	6/6	0.95	0.11	14,18,20,25	0
4	GOL	C	803	6/6	0.96	0.06	14,16,17,20	0
3	NA	D	802	1/1	0.96	0.04	15,15,15,15	0
4	GOL	D	803	6/6	0.97	0.07	14,15,16,17	0
4	GOL	B	803	6/6	0.97	0.06	15,15,17,19	0
3	NA	B	802	1/1	0.97	0.05	15,15,15,15	0
3	NA	C	802	1/1	0.98	0.04	19,19,19,19	0
2	HEM	A	801	43/43	0.98	0.06	9,12,14,16	0
2	HEM	C	801	43/43	0.99	0.04	7,10,12,15	0
2	HEM	D	801	43/43	0.99	0.04	6,10,12,12	0
3	NA	A	802	1/1	0.99	0.04	16,16,16,16	0
2	HEM	B	801	43/43	0.99	0.05	8,11,13,14	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.



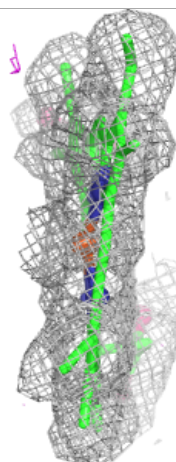
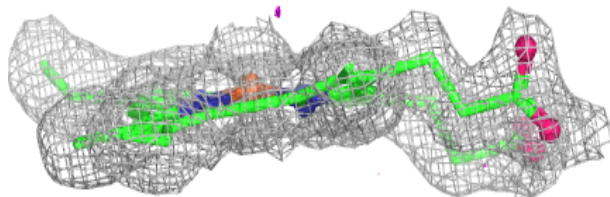
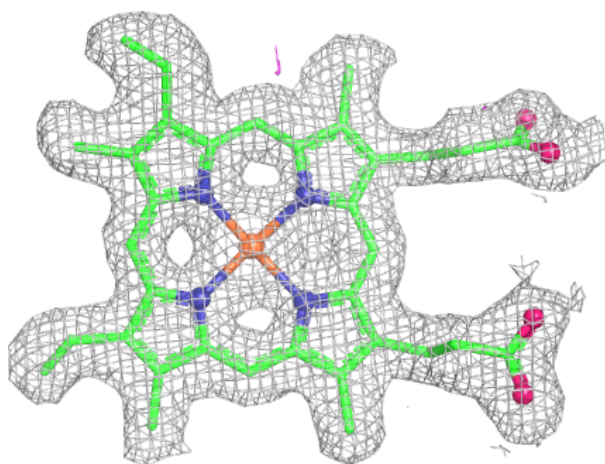
Electron density around HEM C 801:

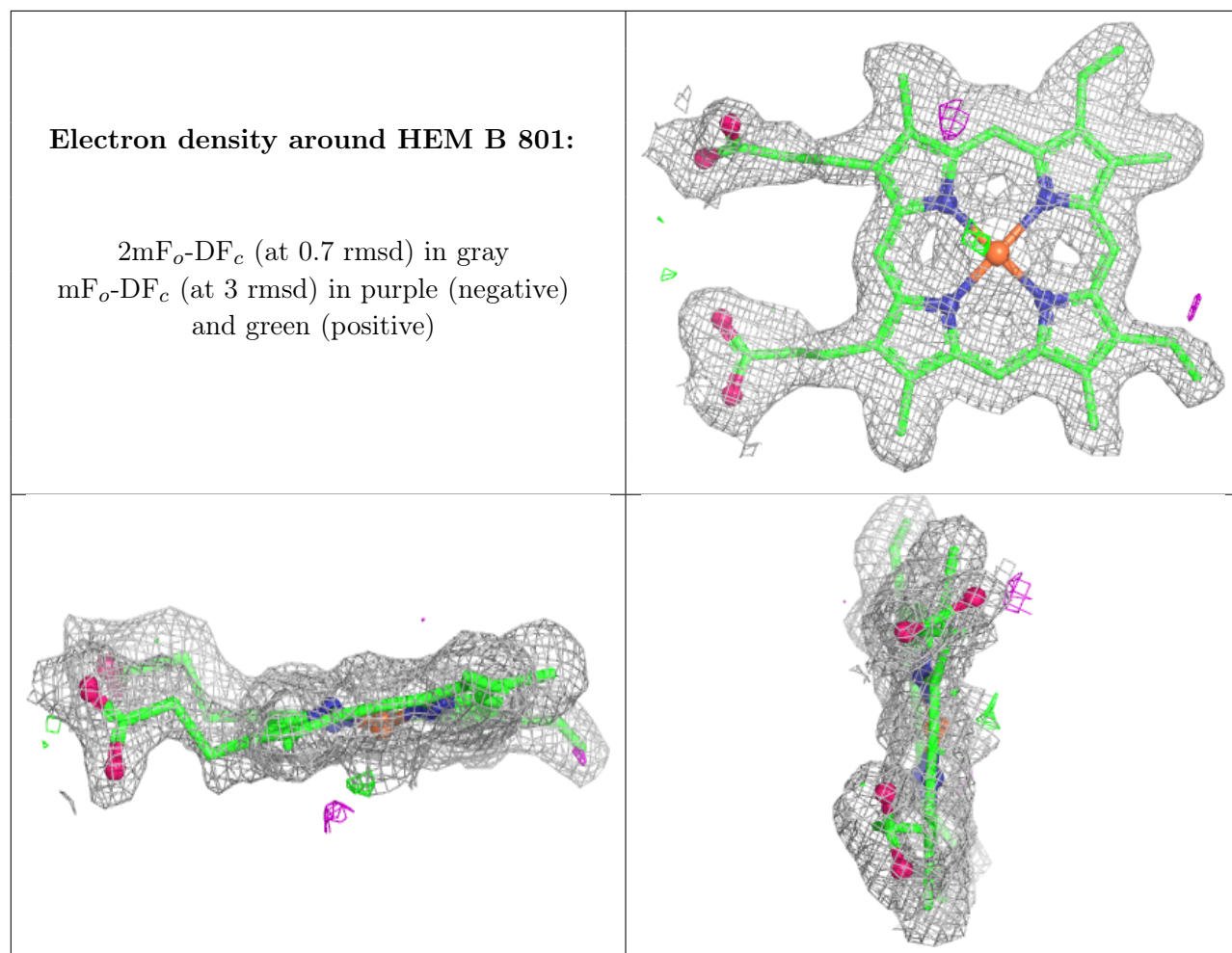
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.