



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:15 pm GMT

PDB ID : 4IG5  
Title : Crystal Structure of Methimazole Inhibited Dimeric Goat Lactoperoxidase at 1.97Å Resolution  
Authors : Singh, R.P.; Singh, N.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2012-12-16  
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

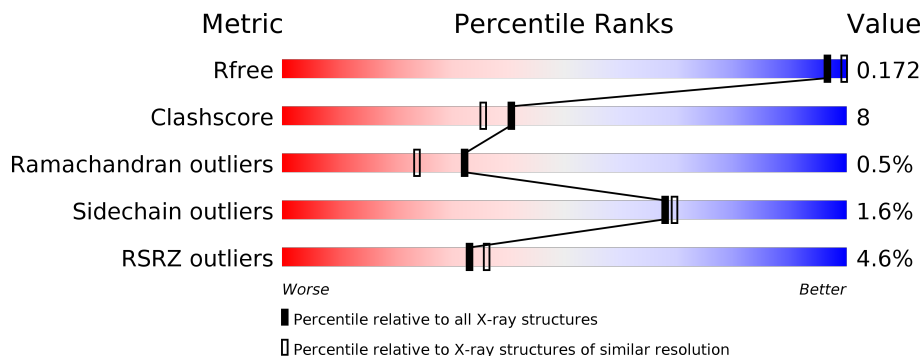
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	595	<div> <div>4%</div> <div>86%</div> <div>12%</div> </div>
1	B	595	<div> <div>5%</div> <div>84%</div> <div>14%</div> </div>

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
3	NAG	A	603	-	-	-	X
5	NO3	A	607	-	-	-	X
5	NO3	A	608	-	-	-	X
5	NO3	A	610	-	-	-	X
5	NO3	A	611	-	-	-	X
5	NO3	B	609	-	-	-	X
5	NO3	B	610	-	-	-	X
5	NO3	B	611	-	-	-	X
6	GOL	A	613	-	-	-	X
6	GOL	A	614	-	-	-	X
6	GOL	A	615	-	-	-	X
6	GOL	B	616	-	-	-	X
7	MMZ	A	616	-	X	X	X
7	MMZ	B	617	-	X	X	X
8	NAG	B	604	-	-	-	X

## 2 Entry composition [i](#)

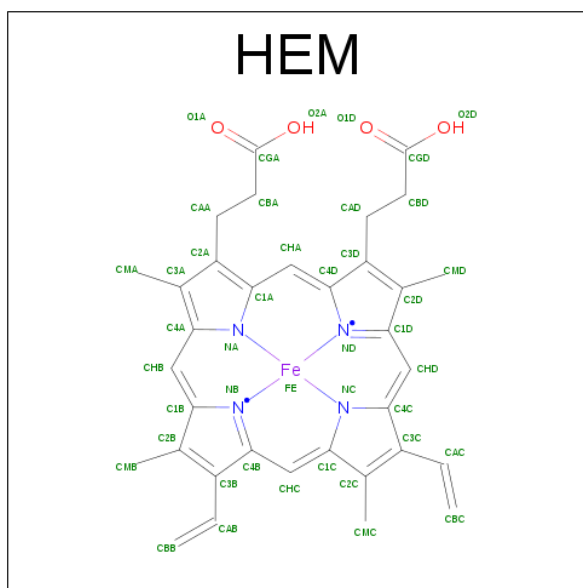
There are 9 unique types of molecules in this entry. The entry contains 10659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactoperoxidase.

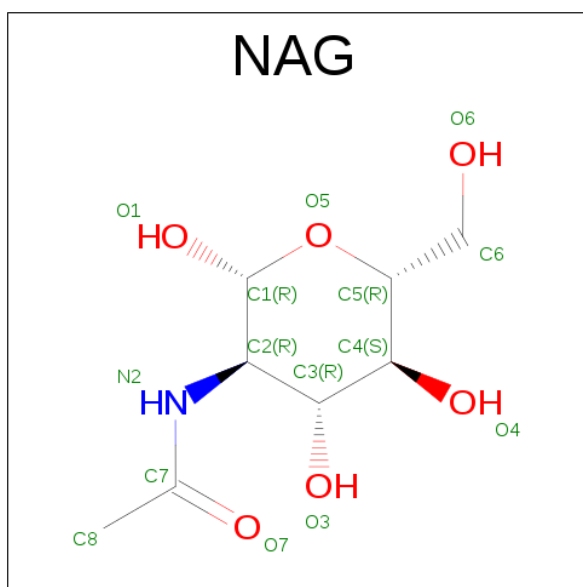
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4754	3021	844	863	26			
1	B	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

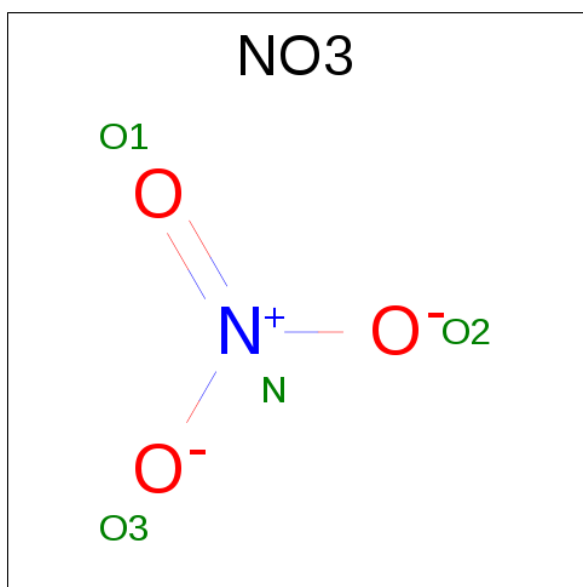


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

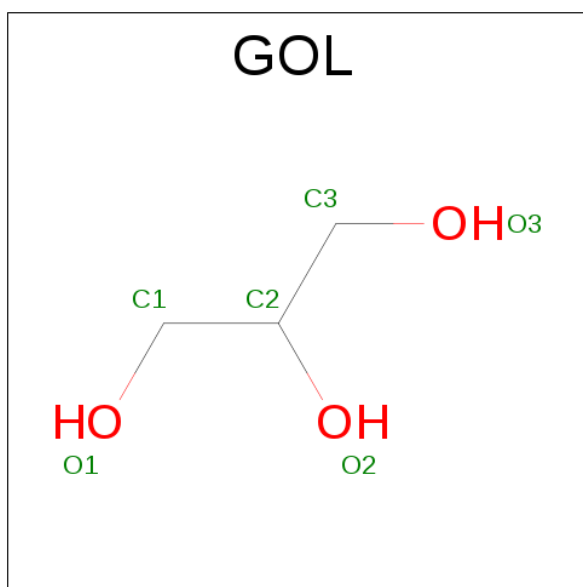
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



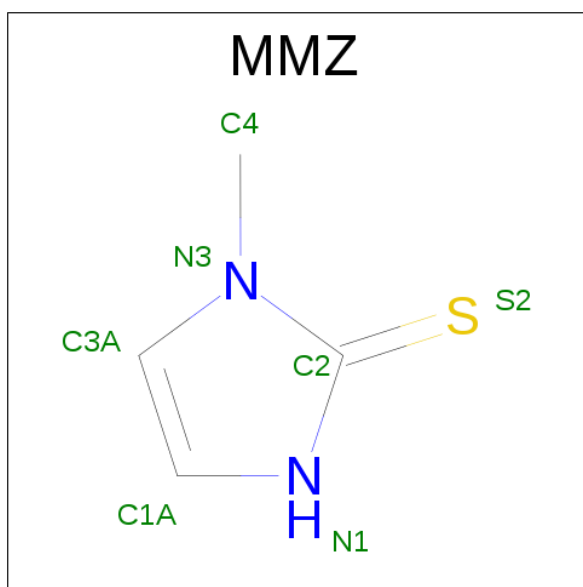
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is 1-METHYL-1,3-DIHYDRO-2H-IMIDAZOLE-2-THIONE (three-letter code: MMZ) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			7	4	2	1		
7	B	1	Total	C	N	S	0	0
			7	4	2	1		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	2	Total	C	N	O	0	0
			28	16	2	10		
8	B	2	Total	C	N	O	0	0
			28	16	2	10		

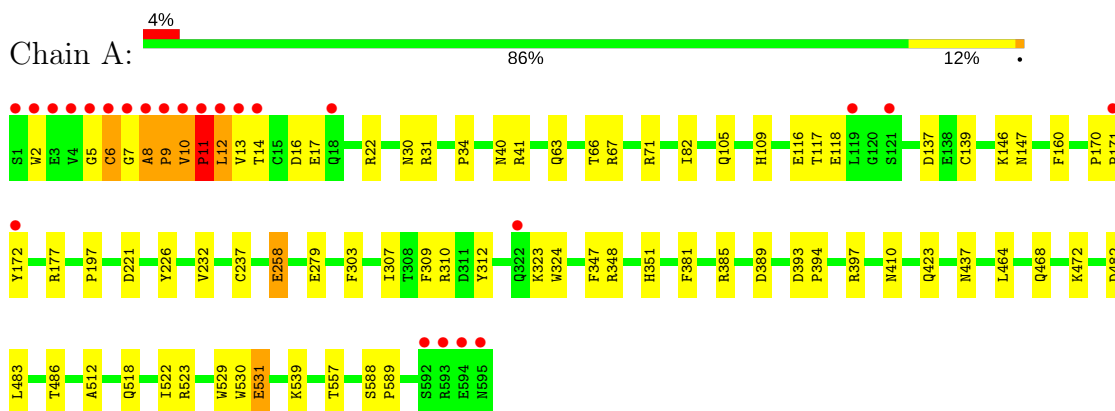
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	444	Total	O	0	0
			444	444		
9	B	382	Total	O	0	0
			382	382		

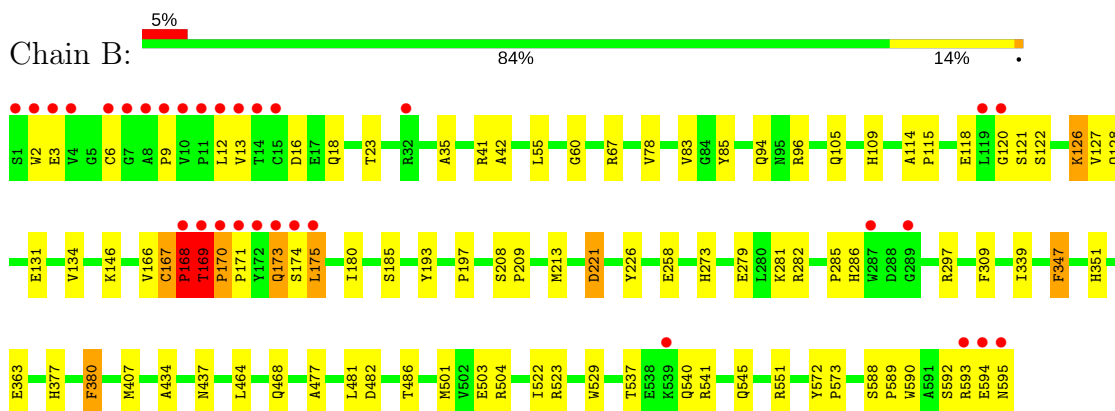
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Lactoperoxidase



#### • Molecule 1: Lactoperoxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.31Å 93.02Å 81.53Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	40.40 – 1.97 40.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.40-1.97) 94.9 (40.40-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.162 , 0.209 0.174 , 0.172	Depositor DCC
$R_{free}$ test set	2412 reflections (3.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -l,k,h 0.176 for h,-k,-l 0.028 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, MMZ, CA, HEM, NO3

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	1.15	6/4883 (0.1%)	0.99	18/6632 (0.3%)
1	B	1.10	8/4882 (0.2%)	0.96	9/6632 (0.1%)
All	All	1.12	14/9765 (0.1%)	0.97	27/13264 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	593	ARG	CD-NE	9.16	1.62	1.46
1	B	593	ARG	CG-CD	6.73	1.68	1.51
1	B	380	PHE	CD1-CE1	5.55	1.50	1.39
1	A	258	GLU	CG-CD	5.50	1.60	1.51
1	A	312	TYR	CE1-CZ	5.47	1.45	1.38
1	A	512	ALA	CA-CB	5.47	1.64	1.52
1	A	309	PHE	CD2-CE2	5.37	1.50	1.39
1	B	593	ARG	CB-CG	5.37	1.67	1.52
1	B	347	PHE	CE1-CZ	5.35	1.47	1.37
1	B	78	VAL	CB-CG2	5.32	1.64	1.52
1	A	160	PHE	CE1-CZ	5.28	1.47	1.37
1	A	139	CYS	CB-SG	-5.18	1.73	1.81
1	B	590	TRP	NE1-CE2	-5.17	1.30	1.37
1	B	85	TYR	CG-CD2	5.01	1.45	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	B	173	GLN	N-CA-C	12.23	144.03	111.00
1	B	173	GLN	CB-CA-C	-9.13	92.14	110.40
1	B	593	ARG	CB-CA-C	8.31	127.03	110.40
1	A	177	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	67	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	397	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	96	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	593	ARG	CG-CD-NE	6.83	126.14	111.80
1	A	10	VAL	N-CA-C	6.42	128.32	111.00
1	A	10	VAL	C-N-CD	-6.40	106.51	120.60
1	A	22	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	397	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	67	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	221	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	482	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	169	THR	C-N-CD	-5.84	107.76	120.60
1	A	177	ARG	CB-CG-CD	-5.70	96.79	111.60
1	A	11	PRO	N-CA-C	5.69	126.89	112.10
1	A	2	TRP	CA-CB-CG	-5.56	103.14	113.70
1	A	12	LEU	N-CA-C	5.53	125.92	111.00
1	A	310	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	348	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	67	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	348	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	8	ALA	C-N-CD	-5.07	109.44	120.60
1	A	482	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	PRO	Peptide
1	B	167	CYS	Peptide
1	B	168	PRO	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4754	0	4646	75	0
1	B	4753	0	4646	86	0
2	A	43	0	30	7	0
2	B	43	0	30	1	0
3	A	56	0	52	0	0
3	B	28	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	0	0	0
5	B	16	0	0	0	0
6	A	24	0	32	3	0
6	B	24	0	32	2	0
7	A	7	0	6	9	0
7	B	7	0	6	10	0
8	B	56	0	50	2	0
9	A	444	0	0	1	0
9	B	382	0	0	1	0
All	All	10659	0	9556	158	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 (158) 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:B:169:THR:CB	1:B:170:PRO:HD2	1.38	1.39
1:B:169:THR:CG2	1:B:170:PRO:HD2	1.53	1.37
1:B:169:THR:HB	1:B:170:PRO:HD2	1.20	1.16
1:B:169:THR:HG22	1:B:170:PRO:CD	1.80	1.11
1:B:169:THR:CB	1:B:170:PRO:CD	2.29	1.09
1:A:197:PRO:HG2	1:B:170:PRO:HG2	1.11	1.06
1:B:169:THR:HG22	1:B:170:PRO:HD2	1.33	1.06
1:B:169:THR:CG2	1:B:170:PRO:CD	2.36	1.02
1:B:594:GLU:O	1:B:595:ASN:HB2	1.59	1.01
1:A:12:LEU:HD12	1:A:13:VAL:H	1.25	1.01
1:B:594:GLU:OE2	1:B:595:ASN:N	1.93	0.99
1:A:258:GLU:OE2	2:A:601:HEM:HMB1	0.80	0.97
1:B:169:THR:HB	1:B:170:PRO:CD	1.89	0.97
1:B:170:PRO:HB3	1:B:171:PRO:HD3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:CB	7:B:617:MMZ:H41	1.99	0.93
1:B:170:PRO:CB	1:B:171:PRO:CD	2.48	0.90
1:A:197:PRO:CG	1:B:170:PRO:HG2	2.00	0.89
1:B:173:GLN:HG2	1:B:174:SER:N	1.86	0.87
1:A:258:GLU:HB3	7:A:616:MMZ:H41	1.54	0.87
1:A:109:HIS:HE1	7:A:616:MMZ:H42	1.38	0.86
1:A:12:LEU:CD1	1:A:13:VAL:H	1.92	0.83
1:A:258:GLU:CD	2:A:601:HEM:HMB1	1.98	0.83
1:B:258:GLU:HB3	7:B:617:MMZ:H41	1.59	0.82
1:B:169:THR:HG22	1:B:170:PRO:HD3	1.60	0.82
1:B:170:PRO:HB3	1:B:171:PRO:CD	2.08	0.79
1:B:55:LEU:HD22	1:B:175:LEU:O	1.82	0.79
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.31	0.78
1:A:109:HIS:CE1	7:A:616:MMZ:H42	2.18	0.78
1:B:170:PRO:CB	1:B:171:PRO:HD3	2.14	0.78
1:B:351:HIS:HD1	1:B:437:ASN:HD21	1.31	0.76
1:B:594:GLU:CD	1:B:595:ASN:H	1.90	0.75
1:A:116:GLU:HG2	1:A:117:THR:N	2.00	0.74
1:B:109:HIS:HE1	7:B:617:MMZ:H42	1.53	0.73
1:A:170:PRO:HG2	1:B:134:VAL:HG21	1.71	0.72
1:A:258:GLU:CB	7:A:616:MMZ:H41	2.18	0.72
1:A:464:LEU:O	1:A:468:GLN:HG3	1.91	0.71
1:A:171:PRO:O	1:A:172:TYR:HB2	1.92	0.70
8:B:604:NAG:H61	8:B:605:NAG:C1	2.22	0.70
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.75	0.68
1:A:258:GLU:HG3	7:A:616:MMZ:C3A	2.24	0.67
1:A:17:GLU:HA	1:A:31:ARG:HH22	1.61	0.66
1:A:5:GLY:O	1:A:6:CYS:SG	2.52	0.66
1:B:594:GLU:O	1:B:595:ASN:CB	2.37	0.65
1:A:63:GLN:OE1	1:A:71:ARG:NH1	2.28	0.65
1:B:286:HIS:HE2	1:B:592:SER:HB3	1.62	0.65
1:B:169:THR:HB	1:B:170:PRO:CG	2.28	0.64
1:A:258:GLU:CD	2:A:601:HEM:CMB	2.63	0.64
1:B:60:GLY:H	6:B:614:GOL:H2	1.62	0.63
1:B:551:ARG:O	1:B:551:ARG:HD3	1.99	0.63
1:B:109:HIS:CE1	7:B:617:MMZ:H42	2.33	0.62
1:A:197:PRO:HG2	1:B:170:PRO:CG	2.06	0.61
2:A:601:HEM:HBC2	2:A:601:HEM:HMC1	1.84	0.60
1:A:530:TRP:CE2	1:A:531:GLU:HG2	2.37	0.59
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.84	0.59
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:HG2	1:A:589:PRO:HG3	1.85	0.58
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.38	0.58
1:A:12:LEU:HD12	1:A:13:VAL:N	2.08	0.57
1:B:258:GLU:HG3	7:B:617:MMZ:C3A	2.34	0.56
1:B:105:GLN:HE21	7:B:617:MMZ:H43	1.69	0.56
1:A:105:GLN:HE21	7:A:616:MMZ:H43	1.69	0.56
1:B:170:PRO:CB	1:B:171:PRO:HD2	2.34	0.55
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.04	0.55
1:A:116:GLU:CG	1:A:117:THR:N	2.68	0.55
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.41	0.55
1:B:468:GLN:HG2	1:B:477:ALA:HB3	1.89	0.55
1:B:12:LEU:HG	1:B:197:PRO:HG2	1.90	0.54
1:B:169:THR:HB	1:B:170:PRO:HG2	1.90	0.54
1:A:16:ASP:OD1	1:A:17:GLU:N	2.42	0.53
1:A:518:GLN:O	1:A:522:ILE:HG23	2.08	0.53
1:A:522:ILE:HB	9:A:1107:HOH:O	2.09	0.53
1:A:12:LEU:CG	1:A:13:VAL:N	2.71	0.53
1:A:12:LEU:HG	1:A:13:VAL:N	2.24	0.53
1:A:258:GLU:HG3	7:A:616:MMZ:H3A	1.90	0.53
1:A:109:HIS:NE2	7:A:616:MMZ:S2	2.72	0.52
1:B:594:GLU:CG	1:B:595:ASN:N	2.72	0.52
1:A:171:PRO:O	1:A:172:TYR:CB	2.57	0.52
1:B:127:VAL:HG13	1:B:131:GLU:HG3	1.92	0.52
1:B:170:PRO:HB2	1:B:171:PRO:HD2	1.91	0.52
1:B:185:SER:HB3	1:B:339:ILE:HG12	1.92	0.51
1:B:537:THR:OG1	1:B:540:GLN:HG3	2.11	0.51
1:B:55:LEU:CD2	1:B:175:LEU:O	2.56	0.51
1:A:13:VAL:CG1	1:A:14:THR:N	2.74	0.50
1:A:170:PRO:O	1:B:128:GLN:NE2	2.44	0.50
1:B:258:GLU:CG	7:B:617:MMZ:H41	2.41	0.50
1:B:13:VAL:HG11	1:B:23:THR:HG21	1.94	0.50
1:A:232:VAL:O	1:A:232:VAL:HG23	2.11	0.49
1:A:393:ASP:OD1	1:A:557:THR:HB	2.13	0.49
1:B:279:GLU:OE1	1:B:279:GLU:HA	2.13	0.49
1:B:170:PRO:HB2	1:B:171:PRO:CD	2.36	0.49
1:B:2:TRP:CE3	1:B:3:GLU:HG3	2.47	0.49
1:A:116:GLU:CG	1:A:117:THR:H	2.26	0.49
1:A:146:LYS:O	1:A:147:ASN:HB2	2.13	0.48
1:A:303:PHE:O	1:A:307:ILE:HG12	2.13	0.48
1:B:258:GLU:HB2	7:B:617:MMZ:H41	1.92	0.48
1:B:105:GLN:NE2	7:B:617:MMZ:H43	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:TYR:CE1	1:B:297:ARG:HG3	2.48	0.48
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.49	0.48
1:B:588:SER:OG	1:B:589:PRO:HD3	2.14	0.48
1:A:12:LEU:CG	1:A:13:VAL:H	2.27	0.47
1:B:503:GLU:HG2	1:B:504:ARG:HG3	1.95	0.47
1:B:541:ARG:O	1:B:545:GLN:HG3	2.15	0.47
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.95	0.47
1:A:11:PRO:HG3	1:A:41:ARG:HD3	1.96	0.47
1:A:529:TRP:NE1	1:A:531:GLU:HG3	2.30	0.46
1:A:170:PRO:HB2	1:B:128:GLN:HE22	1.80	0.46
1:A:116:GLU:HG2	1:A:118:GLU:H	1.80	0.46
1:A:12:LEU:CD1	1:A:13:VAL:N	2.71	0.46
1:A:116:GLU:HG2	1:A:117:THR:H	1.76	0.46
1:A:14:THR:HB	1:B:120:GLY:HA3	1.98	0.46
1:A:30:ASN:O	1:A:34:PRO:HA	2.16	0.46
1:B:94:GLN:HG2	9:B:812:HOH:O	2.16	0.46
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.51	0.45
2:B:602:HEM:HMC2	2:B:602:HEM:HBC2	1.97	0.45
1:B:118:GLU:O	1:B:121:SER:HB2	2.16	0.45
1:B:522:ILE:HD13	1:B:522:ILE:HG21	1.81	0.45
1:B:523:ARG:HG3	1:B:529:TRP:CE2	2.51	0.45
1:A:105:GLN:NE2	7:A:616:MMZ:H43	2.32	0.45
1:B:42:ALA:HB2	1:B:166:VAL:HG21	1.98	0.45
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.46	0.44
1:B:35:ALA:HB1	1:B:41:ARG:NE	2.32	0.44
1:B:281:LYS:HE3	1:B:285:PRO:HA	1.99	0.44
1:B:122:SER:O	1:B:126:LYS:HD3	2.18	0.44
1:B:83:VAL:HG11	1:B:434:ALA:CB	2.48	0.44
1:B:363:GLU:HG2	1:B:363:GLU:H	1.29	0.43
1:B:60:GLY:N	6:B:614:GOL:H2	2.32	0.43
1:A:468:GLN:O	1:A:472:LYS:N	2.51	0.43
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.47	0.43
1:B:109:HIS:NE2	7:B:617:MMZ:S2	2.78	0.43
1:A:137:ASP:HA	6:A:614:GOL:H12	2.00	0.43
1:A:6:CYS:SG	1:A:7:GLY:N	2.92	0.43
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.67	0.43
8:B:607:NAG:H62	8:B:608:NAG:C1	2.50	0.42
1:A:237:CYS:HA	1:A:381:PHE:O	2.19	0.42
1:A:82:ILE:CD1	1:A:483:LEU:HD12	2.48	0.42
1:A:9:PRO:C	1:A:11:PRO:HD2	2.40	0.42
1:B:594:GLU:CD	1:B:595:ASN:N	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:O	1:A:31:ARG:NH1	2.52	0.42
1:A:258:GLU:OE2	2:A:601:HEM:HMB2	1.96	0.42
1:A:10:VAL:N	1:A:11:PRO:HD2	2.33	0.42
1:A:66:THR:O	6:A:613:GOL:H11	2.20	0.42
1:B:286:HIS:HE2	1:B:592:SER:CB	2.29	0.42
1:B:309:PHE:CD1	1:B:529:TRP:HH2	2.37	0.42
1:B:208:SER:HA	1:B:209:PRO:HD2	1.89	0.41
1:A:323:LYS:HE2	1:A:324:TRP:CZ2	2.55	0.41
1:B:464:LEU:HA	1:B:481:LEU:HD12	2.02	0.41
1:B:114:ALA:HA	1:B:115:PRO:HD2	1.93	0.41
1:B:166:VAL:HG12	1:B:180:ILE:HG12	2.01	0.41
1:A:10:VAL:HG22	1:B:171:PRO:HG3	2.03	0.41
1:A:12:LEU:HD23	1:B:122:SER:N	2.36	0.40
1:A:423:GLN:OE1	6:A:615:GOL:H11	2.21	0.40
1:B:173:GLN:CG	1:B:174:SER:N	2.63	0.40
1:B:572:TYR:CD1	1:B:573:PRO:HA	2.56	0.40
1:A:9:PRO:HB2	1:A:40:ASN:HB3	2.02	0.40
1:B:193:TYR:CD1	1:B:297:ARG:HG3	2.57	0.40
1:A:385:ARG:O	1:A:389:ASP:HB3	2.22	0.40
1:A:529:TRP:CD1	1:A:531:GLU:HG3	2.57	0.40
1:B:407:MET:HB3	1:B:501:MET:CE	2.51	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	593/595 (100%)	573 (97%)	18 (3%)	2 (0%)	44	38
1	B	593/595 (100%)	563 (95%)	26 (4%)	4 (1%)	25	17
All	All	1186/1190 (100%)	1136 (96%)	44 (4%)	6 (0%)	32	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	11	PRO
1	B	170	PRO
1	B	9	PRO
1	B	168	PRO
1	B	169	THR

### 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	517/517 (100%)	512 (99%)	5 (1%)	80	83
1	B	517/517 (100%)	505 (98%)	12 (2%)	56	55
All	All	1034/1034 (100%)	1017 (98%)	17 (2%)	68	69

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

Mol	Chain	Res	Type
1	A	6	CYS
1	A	347	PHE
1	A	410	ASN
1	A	486	THR
1	A	531	GLU
1	B	6	CYS
1	B	16	ASP
1	B	18	GLN
1	B	126	LYS
1	B	146	LYS
1	B	167	CYS
1	B	168	PRO
1	B	169	THR
1	B	175	LEU
1	B	282	ARG
1	B	347	PHE
1	B	486	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	521	GLN
1	A	574	HIS
1	B	128	GLN
1	B	558	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

4 carbohydrates 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$
8	NAG	B	604	1,8	14,14,15	0.29	0	15,19,21	0.57	0
8	NAG	B	605	8	14,14,15	0.65	0	15,19,21	3.04	5 (33%)
8	NAG	B	607	1,8	14,14,15	1.05	1 (7%)	15,19,21	2.08	3 (20%)
8	NAG	B	608	8	14,14,15	1.45	2 (14%)	15,19,21	1.39	2 (13%)

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
8	NAG	B	604	1,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	605	8	-	0/6/23/26	0/1/1/1
8	NAG	B	607	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	608	8	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	608	NAG	O5-C1	-3.74	1.37	1.43
8	B	608	NAG	C2-N2	-2.67	1.41	1.46
8	B	607	NAG	O7-C7	-2.41	1.17	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	605	NAG	C2-N2-C7	-5.81	114.47	122.94
8	B	607	NAG	C6-C5-C4	-3.72	104.29	113.00
8	B	605	NAG	C4-C3-C2	-3.71	105.58	111.02
8	B	605	NAG	O3-C3-C4	-3.22	103.36	110.36
8	B	605	NAG	O4-C4-C3	-3.18	103.44	110.36
8	B	607	NAG	C1-C2-N2	-2.31	106.55	110.49
8	B	608	NAG	O5-C1-C2	-2.30	108.27	111.47
8	B	608	NAG	O4-C4-C5	2.58	115.80	109.28
8	B	607	NAG	C1-O5-C5	5.51	119.75	112.17
8	B	605	NAG	C1-O5-C5	7.84	122.97	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	604	NAG	1	0
8	B	605	NAG	1	0
8	B	607	NAG	1	0
8	B	608	NAG	1	0

## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	A	601	1,7	28,50,50	2.05	6 (21%)	17,82,82	1.99	4 (23%)
3	NAG	A	602	1	14,14,15	1.68	2 (14%)	15,19,21	2.62	6 (40%)
3	NAG	A	603	1	14,14,15	0.77	0	15,19,21	2.61	7 (46%)
3	NAG	A	604	1	14,14,15	0.56	0	15,19,21	2.14	4 (26%)
3	NAG	A	605	1	14,14,15	0.99	1 (7%)	15,19,21	1.96	3 (20%)
5	NO3	A	607	-	1,3,3	2.07	1 (100%)	0,3,3	0.00	-
5	NO3	A	608	-	1,3,3	4.08	1 (100%)	0,3,3	0.00	-
5	NO3	A	609	-	1,3,3	4.30	1 (100%)	0,3,3	0.00	-
5	NO3	A	610	-	1,3,3	4.59	1 (100%)	0,3,3	0.00	-
5	NO3	A	611	-	1,3,3	4.50	1 (100%)	0,3,3	0.00	-
6	GOL	A	612	-	5,5,5	0.38	0	5,5,5	1.07	0
6	GOL	A	613	-	5,5,5	0.48	0	5,5,5	1.11	0
6	GOL	A	614	-	5,5,5	0.55	0	5,5,5	1.77	2 (40%)
6	GOL	A	615	-	5,5,5	0.55	0	5,5,5	1.33	1 (20%)
7	MMZ	A	616	2	5,7,7	5.45	4 (80%)	6,9,9	4.62	6 (100%)
2	HEM	B	602	1,7	28,50,50	2.11	9 (32%)	17,82,82	2.22	4 (23%)
3	NAG	B	603	1	14,14,15	1.15	1 (7%)	15,19,21	1.88	4 (26%)
3	NAG	B	606	1	14,14,15	0.43	0	15,19,21	1.02	2 (13%)
5	NO3	B	609	-	1,3,3	3.69	1 (100%)	0,3,3	0.00	-
5	NO3	B	610	-	1,3,3	3.37	1 (100%)	0,3,3	0.00	-
5	NO3	B	611	-	1,3,3	4.73	1 (100%)	0,3,3	0.00	-
5	NO3	B	612	-	1,3,3	4.60	1 (100%)	0,3,3	0.00	-
6	GOL	B	613	-	5,5,5	0.38	0	5,5,5	0.67	0
6	GOL	B	614	-	5,5,5	0.21	0	5,5,5	1.45	1 (20%)
6	GOL	B	615	-	5,5,5	0.47	0	5,5,5	1.10	1 (20%)
6	GOL	B	616	-	5,5,5	0.29	0	5,5,5	0.47	0
7	MMZ	B	617	2	5,7,7	5.75	4 (80%)	6,9,9	4.95	4 (66%)

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	A	601	1,7	-	0/6/54/54	0/0/8/8
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	NO3	A	607	-	-	0/0/0/0	0/0/0/0
5	NO3	A	608	-	-	0/0/0/0	0/0/0/0
5	NO3	A	609	-	-	0/0/0/0	0/0/0/0
5	NO3	A	610	-	-	0/0/0/0	0/0/0/0
5	NO3	A	611	-	-	0/0/0/0	0/0/0/0
6	GOL	A	612	-	-	0/4/4/4	0/0/0/0
6	GOL	A	613	-	-	0/4/4/4	0/0/0/0
6	GOL	A	614	-	-	0/4/4/4	0/0/0/0
6	GOL	A	615	-	-	0/4/4/4	0/0/0/0
7	MMZ	A	616	2	-	0/0/0/0	0/1/1/1
2	HEM	B	602	1,7	-	0/6/54/54	0/0/8/8
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	606	1	-	0/6/23/26	0/1/1/1
5	NO3	B	609	-	-	0/0/0/0	0/0/0/0
5	NO3	B	610	-	-	0/0/0/0	0/0/0/0
5	NO3	B	611	-	-	0/0/0/0	0/0/0/0
5	NO3	B	612	-	-	0/0/0/0	0/0/0/0
6	GOL	B	613	-	-	0/4/4/4	0/0/0/0
6	GOL	B	614	-	-	0/4/4/4	0/0/0/0
6	GOL	B	615	-	-	0/4/4/4	0/0/0/0
6	GOL	B	616	-	-	0/4/4/4	0/0/0/0
7	MMZ	B	617	2	-	0/0/0/0	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	617	MMZ	C3A-C1A	-9.04	1.36	1.52
7	A	616	MMZ	C3A-C1A	-8.98	1.36	1.52
2	A	601	HEM	C3B-C2B	-5.63	1.32	1.40
2	A	601	HEM	C3C-C2C	-4.35	1.34	1.40
3	A	602	NAG	O5-C1	-4.29	1.36	1.43
7	B	617	MMZ	C1A-N1	-4.27	1.37	1.46
7	A	616	MMZ	C1A-N1	-3.94	1.37	1.46
7	B	617	MMZ	C3A-N3	-3.64	1.34	1.46
2	B	602	HEM	C3B-C2B	-3.52	1.35	1.40
7	A	616	MMZ	C3A-N3	-3.24	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAG	C2-N2	-3.06	1.40	1.46
3	B	603	NAG	O5-C1	-2.94	1.38	1.43
2	B	602	HEM	C3C-C2C	-2.92	1.36	1.40
3	A	605	NAG	O5-C1	-2.82	1.39	1.43
2	B	602	HEM	C1A-NA	-2.27	1.31	1.36
5	A	607	NO3	O1-N	2.07	1.31	1.23
2	A	601	HEM	CAA-C2A	2.16	1.55	1.52
2	B	602	HEM	CAA-C2A	2.38	1.56	1.52
2	B	602	HEM	CMD-C2D	2.69	1.57	1.51
2	B	602	HEM	CMA-C3A	2.74	1.57	1.51
2	A	601	HEM	C3B-CAB	3.21	1.54	1.47
5	B	610	NO3	O1-N	3.37	1.36	1.23
2	A	601	HEM	C3C-CAC	3.56	1.54	1.47
2	B	602	HEM	C3B-CAB	3.58	1.55	1.47
5	B	609	NO3	O1-N	3.69	1.37	1.23
2	A	601	HEM	C3D-C2D	3.94	1.49	1.37
5	A	608	NO3	O1-N	4.08	1.39	1.23
2	B	602	HEM	C3C-CAC	4.21	1.56	1.47
5	A	609	NO3	O1-N	4.30	1.39	1.23
5	A	611	NO3	O1-N	4.50	1.40	1.23
5	A	610	NO3	O1-N	4.59	1.41	1.23
5	B	612	NO3	O1-N	4.60	1.41	1.23
5	B	611	NO3	O1-N	4.73	1.41	1.23
2	B	602	HEM	C3D-C2D	4.73	1.51	1.37
7	A	616	MMZ	C2-S2	6.47	1.78	1.67
7	B	617	MMZ	C2-S2	7.21	1.79	1.67

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	617	MMZ	C4-N3-C2	-7.02	120.61	126.51
7	B	617	MMZ	C1A-N1-C2	-6.88	103.90	113.17
7	A	616	MMZ	C4-N3-C2	-6.60	120.96	126.51
3	A	602	NAG	C3-C4-C5	-6.56	98.66	110.22
2	B	602	HEM	CBA-CAA-C2A	-5.15	102.64	112.48
2	A	601	HEM	CAD-CBD-CGD	-5.09	103.96	112.66
7	A	616	MMZ	C1A-N1-C2	-4.80	106.71	113.17
7	A	616	MMZ	C3A-N3-C2	-4.15	108.25	111.14
2	B	602	HEM	CAD-CBD-CGD	-4.07	105.70	112.66
2	B	602	HEM	CBD-CAD-C3D	-3.99	104.85	112.47
3	A	603	NAG	O3-C3-C4	-3.52	102.70	110.36
3	B	603	NAG	C1-C2-N2	-3.47	104.57	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C1-C2-N2	-3.42	104.65	110.49
3	A	602	NAG	O5-C1-C2	-3.40	106.74	111.47
3	A	603	NAG	O7-C7-C8	-3.20	116.23	122.06
2	A	601	HEM	CBD-CAD-C3D	-3.15	106.46	112.47
3	A	605	NAG	C6-C5-C4	-3.04	105.89	113.00
3	A	602	NAG	C1-O5-C5	-2.63	108.54	112.17
2	A	601	HEM	CBA-CAA-C2A	-2.63	107.46	112.48
3	B	603	NAG	O3-C3-C4	-2.61	104.67	110.36
3	B	606	NAG	O5-C1-C2	-2.50	108.00	111.47
3	A	603	NAG	O6-C6-C5	-2.47	103.03	111.34
6	B	615	GOL	O3-C3-C2	-2.42	97.86	110.07
3	A	602	NAG	C2-N2-C7	-2.41	119.43	122.94
3	A	605	NAG	C1-C2-N2	-2.29	106.58	110.49
6	A	615	GOL	C3-C2-C1	-2.17	102.89	111.52
3	B	603	NAG	C1-O5-C5	-2.14	109.22	112.17
3	A	603	NAG	C4-C3-C2	2.00	113.95	111.02
3	B	606	NAG	C1-O5-C5	2.00	114.93	112.17
2	B	602	HEM	CMD-C2D-C1D	2.26	131.94	128.46
6	A	614	GOL	O2-C2-C1	2.27	119.56	108.84
6	A	614	GOL	O2-C2-C3	2.27	119.58	108.84
3	A	604	NAG	O5-C1-C2	2.30	114.67	111.47
6	B	614	GOL	O2-C2-C3	2.47	120.51	108.84
2	A	601	HEM	CMC-C2C-C3C	2.57	129.66	124.89
7	B	617	MMZ	C4-N3-C3A	2.65	129.41	120.30
3	A	604	NAG	C2-N2-C7	2.78	127.00	122.94
7	A	616	MMZ	C3A-C1A-N1	2.84	105.94	102.61
7	A	616	MMZ	C4-N3-C3A	2.98	130.57	120.30
3	A	604	NAG	C4-C3-C2	3.09	115.54	111.02
3	A	603	NAG	C1-C2-N2	3.37	116.25	110.49
3	A	602	NAG	O4-C4-C3	3.77	118.56	110.36
3	B	603	NAG	C4-C3-C2	4.16	117.11	111.02
3	A	603	NAG	C2-N2-C7	4.19	129.06	122.94
3	A	603	NAG	C1-O5-C5	4.93	118.96	112.17
7	A	616	MMZ	C1A-C3A-N3	5.24	107.06	103.02
3	A	605	NAG	C1-O5-C5	5.55	119.81	112.17
3	A	604	NAG	C1-O5-C5	5.91	120.31	112.17
7	B	617	MMZ	C3A-C1A-N1	6.22	109.90	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	7	0
6	A	613	GOL	1	0
6	A	614	GOL	1	0
6	A	615	GOL	1	0
7	A	616	MMZ	9	0
2	B	602	HEM	1	0
6	B	614	GOL	2	0
7	B	617	MMZ	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	595/595 (100%)	-0.13	24 (4%)	39	42	12, 25, 56, 103	0
1	B	595/595 (100%)	0.13	31 (5%)	28	31	12, 29, 71, 117	0
All	All	1190/1190 (100%)	0.00	55 (4%)	33	36	12, 27, 65, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	TRP	19.2
1	A	2	TRP	16.0
1	A	8	ALA	15.7
1	B	13	VAL	13.8
1	B	174	SER	13.5
1	B	9	PRO	13.2
1	B	12	LEU	13.2
1	B	1	SER	12.2
1	B	10	VAL	12.1
1	A	13	VAL	11.5
1	A	12	LEU	11.0
1	B	11	PRO	10.9
1	B	172	TYR	10.7
1	A	9	PRO	10.0
1	B	170	PRO	9.9
1	B	171	PRO	9.6
1	A	10	VAL	9.2
1	A	4	VAL	8.7
1	B	3	GLU	8.5
1	A	6	CYS	8.0
1	A	11	PRO	7.2
1	A	119	LEU	7.2
1	B	8	ALA	7.1
1	B	175	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	119	LEU	6.8
1	B	593	ARG	6.8
1	B	173	GLN	6.7
1	A	3	GLU	6.4
1	B	595	ASN	6.2
1	B	7	GLY	6.1
1	B	14	THR	6.0
1	B	4	VAL	5.9
1	B	594	GLU	5.8
1	A	1	SER	5.6
1	A	172	TYR	5.5
1	A	14	THR	4.8
1	A	594	GLU	4.7
1	A	593	ARG	4.6
1	A	595	ASN	4.3
1	A	18	GLN	3.5
1	B	289	GLY	3.4
1	B	168	PRO	3.3
1	B	120	GLY	3.2
1	B	287	TRP	3.1
1	A	5	GLY	3.0
1	B	6	CYS	2.9
1	B	32	ARG	2.7
1	B	169	THR	2.6
1	B	539	LYS	2.4
1	A	322	GLN	2.4
1	A	121	SER	2.4
1	A	7	GLY	2.3
1	B	15	CYS	2.2
1	A	592	SER	2.1
1	A	171	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	B	604	14/15	0.90	0.14	2.14	22,32,44,44	0
8	NAG	B	607	14/15	0.90	0.12	0.14	49,52,55,61	0
8	NAG	B	605	14/15	0.84	0.23	-	50,56,58,58	0
8	NAG	B	608	14/15	0.84	0.17	-	70,79,86,88	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	613	6/6	0.90	0.23	20.65	47,48,48,51	0
5	NO3	A	608	4/4	0.78	0.21	11.19	61,63,63,64	0
7	MMZ	A	616	7/7	0.94	0.19	8.37	33,37,38,45	0
5	NO3	A	607	4/4	0.98	0.11	4.91	21,23,23,24	0
7	MMZ	B	617	7/7	0.92	0.18	4.91	31,33,38,45	0
6	GOL	A	614	6/6	0.95	0.15	4.87	27,30,40,43	0
5	NO3	B	611	4/4	0.82	0.19	4.67	66,67,68,70	0
3	NAG	A	603	14/15	0.79	0.19	4.54	48,56,60,62	0
5	NO3	B	609	4/4	0.98	0.13	4.15	31,31,34,36	0
5	NO3	A	611	4/4	0.81	0.21	3.64	79,79,80,81	0
5	NO3	B	610	4/4	0.97	0.10	3.40	30,30,31,33	0
6	GOL	B	616	6/6	0.81	0.17	3.39	75,81,82,85	0
6	GOL	A	615	6/6	0.81	0.18	2.86	43,46,50,57	0
5	NO3	A	610	4/4	0.89	0.14	2.01	50,52,53,54	0
6	GOL	A	612	6/6	0.97	0.13	0.67	30,37,38,39	0
6	GOL	B	615	6/6	0.96	0.12	0.52	42,46,48,48	0
3	NAG	A	602	14/15	0.92	0.11	0.38	25,37,48,49	0
3	NAG	B	603	14/15	0.87	0.13	0.37	58,64,69,74	0
2	HEM	A	601	43/43	0.98	0.09	0.29	11,14,18,19	0
2	HEM	B	602	43/43	0.99	0.09	0.20	8,14,17,22	0
6	GOL	B	614	6/6	0.97	0.10	0.11	33,35,36,39	0
3	NAG	A	605	14/15	0.97	0.09	-0.17	27,33,40,44	0
6	GOL	B	613	6/6	0.96	0.12	-0.17	34,38,43,46	0
4	CA	A	606	1/1	0.99	0.08	-0.47	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	601	1/1	0.99	0.03	-6.24	18,18,18,18	0
5	NO3	A	609	4/4	0.92	0.13	-	41,42,44,47	0
3	NAG	A	604	14/15	0.82	0.15	-	54,62,66,67	0
5	NO3	B	612	4/4	0.97	0.12	-	37,41,42,43	0
3	NAG	B	606	14/15	0.81	0.19	-	54,58,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.