



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2016 – 04:53 AM EDT

PDB ID : 5FF1  
Title : Two way mode of binding of antithyroid drug methimazole to mammalian heme peroxidases: Structure of the complex of lactoperoxidase with methimazole at 1.97 Angstrom resolution  
Authors : Singh, R.P.; Singh, A.; Sirohi, H.; Singh, A.K.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2015-12-17  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027790

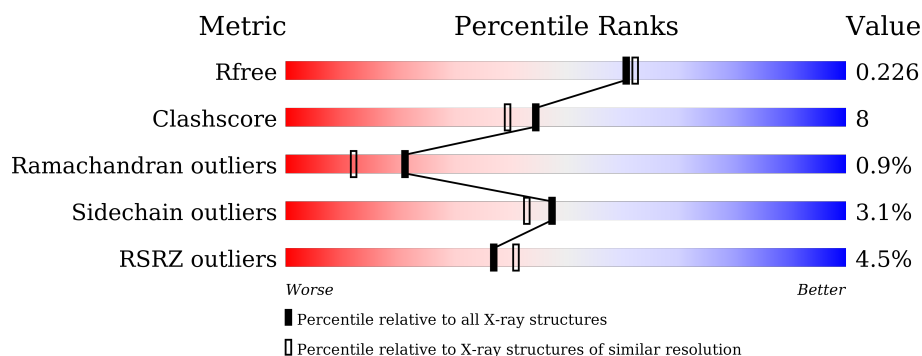
# 1 Overall quality at a glance

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))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (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>3%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	B	595	<div> <div>6%</div> <div>88%</div> <div>10%</div> <div>..</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
2	MMZ	A	601	-	X	X	X
2	MMZ	A	602	-	X	X	X
2	MMZ	B	601	-	X	X	X
2	MMZ	B	613	-	X	X	X
6	NO3	A	610	-	-	-	X
6	NO3	A	612	-	-	-	X
6	NO3	A	613	-	-	-	X
6	NO3	B	610	-	-	-	X
6	NO3	B	611	-	-	-	X
7	GOL	A	615	-	-	-	X
7	GOL	A	617	-	-	-	X
7	GOL	B	616	-	-	-	X

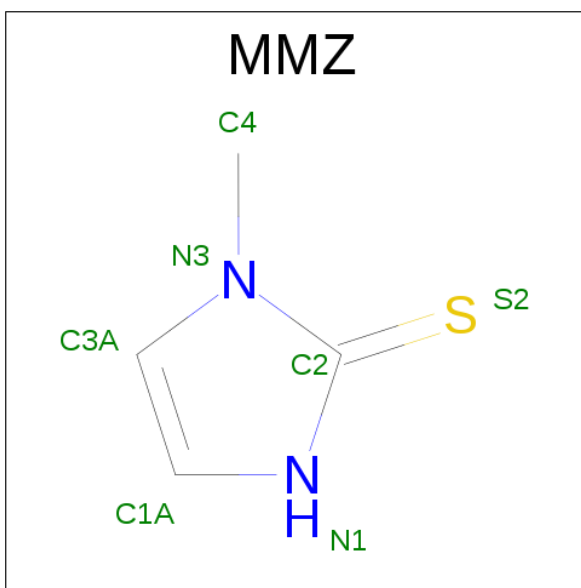


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

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

- Molecule 2 is 1-METHYL-1,3-DIHYDRO-2H-IMIDAZOLE-2-THIONE (three-letter code: MMZ) (formula:  $C_4H_6N_2S$ ).



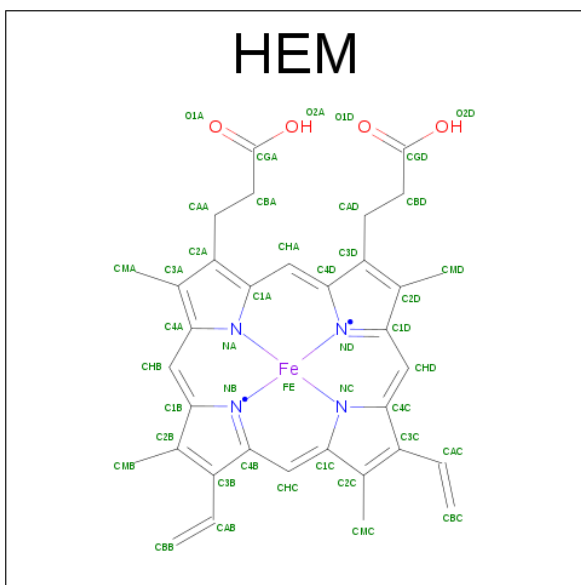
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 7	C 4	N 2	S 1	0	0
2	A	1	Total 7	C 4	N 2	S 1	0	0
2	B	1	Total 7	C 4	N 2	S 1	0	0
2	B	1	Total 7	C 4	N 2	S 1	0	0

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

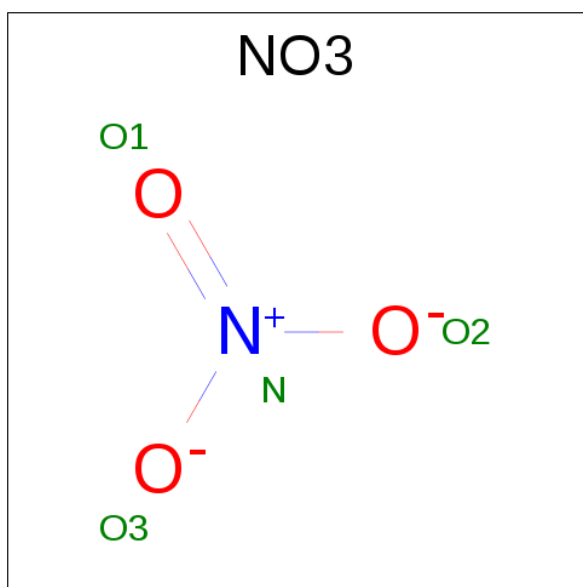


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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

- Molecule 7 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
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
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.

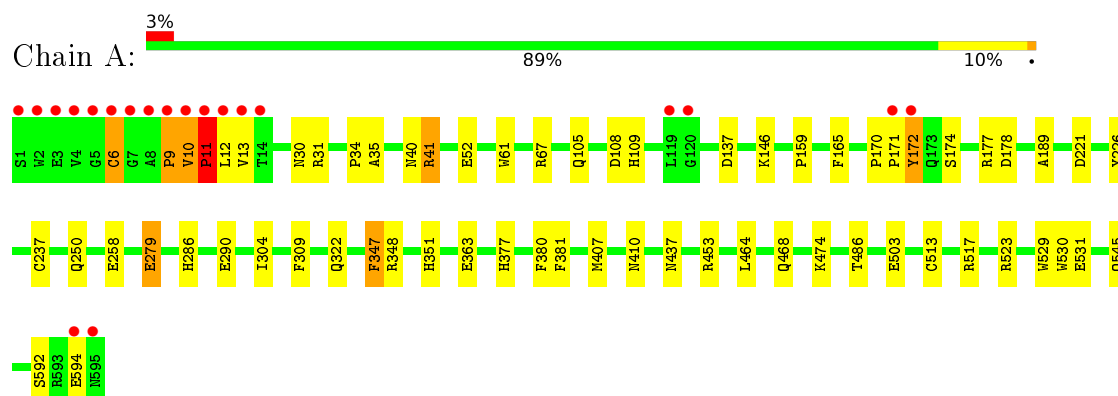
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	415	Total	O	0	0
			415	415		
8	B	360	Total	O	0	0
			360	360		



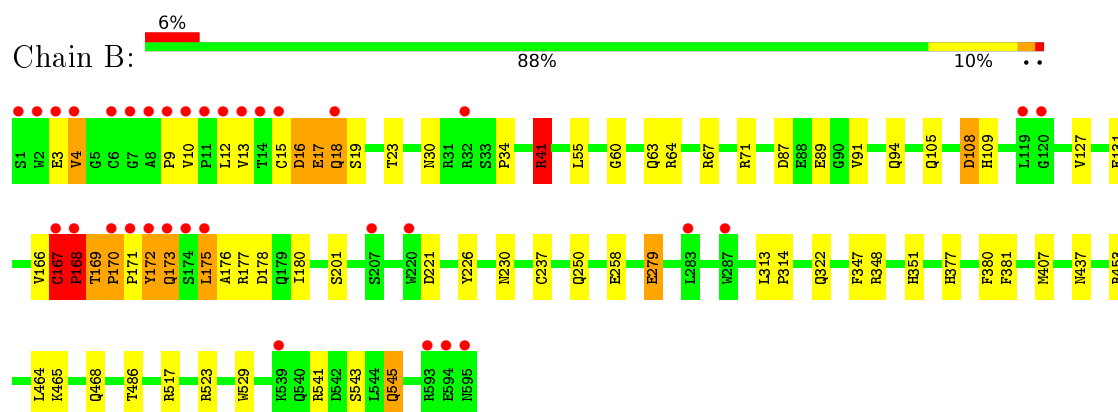
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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)	40.43 – 1.97 40.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.43-1.97) 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 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.226 0.183 , 0.226	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 , 38.5	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	0.95	EDS
Total number of atoms	10608	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	0.90	2/4883 (0.0%)	0.92	9/6632 (0.1%)
1	B	0.86	1/4882 (0.0%)	0.90	10/6632 (0.2%)
All	All	0.88	3/9765 (0.0%)	0.91	19/13264 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	ASP	CA-CB	-7.42	1.37	1.53
1	A	177	ARG	CD-NE	-5.78	1.36	1.46
1	A	137	ASP	C-N	-5.03	1.22	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	A	177	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	177	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	B	177	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	B	178	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	67	ARG	NE-CZ-NH1	6.17	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	167	CYS	N-CA-C	-5.88	95.13	111.00
1	A	347	PHE	CB-CG-CD1	5.76	124.83	120.80
1	A	178	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	453	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	348	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	67	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	541	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	453	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	11	PRO	N-CA-C	5.53	126.47	112.10
1	A	67	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	41	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	348	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	4644	64	0
1	B	4753	0	4645	83	0
2	A	14	0	6	21	0
2	B	14	0	7	26	0
3	A	56	0	52	0	0
3	B	70	0	64	0	0
4	A	43	0	30	14	0
4	B	43	0	30	12	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	16	0	0	0	0
7	A	24	0	32	3	0
7	B	24	0	32	1	0
8	A	415	0	0	5	0
8	B	360	0	0	3	0
All	All	10608	0	9542	153	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 (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	4:A:607:HEM:CMD	1.64	1.45
1:B:108:ASP:OD2	4:B:607:HEM:CMD	1.67	1.42
1:B:258:GLU:OE2	4:B:607:HEM:CMB	1.68	1.41
1:A:258:GLU:OE2	4:A:607:HEM:CMB	1.76	1.32
1:A:258:GLU:OE2	4:A:607:HEM:HMB1	0.93	1.11
1:B:169:THR:HG22	1:B:170:PRO:HD2	1.36	1.07
1:B:108:ASP:OD2	4:B:607:HEM:HMD1	0.83	1.00
1:B:258:GLU:OE2	4:B:607:HEM:HMB1	0.82	0.99
1:B:169:THR:HG22	1:B:170:PRO:CD	1.92	0.98
1:A:258:GLU:CG	2:A:601:MMZ:H42	1.94	0.98
1:A:108:ASP:CG	4:A:607:HEM:HMD1	1.88	0.94
1:A:250:GLN:HG3	8:A:1039:HOH:O	1.71	0.90
1:A:108:ASP:OD2	4:A:607:HEM:HMD1	0.73	0.90
1:B:258:GLU:CG	2:B:613:MMZ:H42	2.03	0.88
1:B:258:GLU:CD	2:B:613:MMZ:H42	1.93	0.88
1:B:230:ASN:HB2	1:B:250:GLN:HG2	1.57	0.83
1:B:258:GLU:CD	4:B:607:HEM:HMB1	2.01	0.81
1:A:258:GLU:CD	2:A:601:MMZ:H42	2.02	0.80
1:B:258:GLU:HB3	2:B:601:MMZ:H41	1.63	0.80
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.26	0.80
1:B:105:GLN:NE2	2:B:613:MMZ:H41	2.02	0.75
1:B:351:HIS:HD1	1:B:437:ASN:HD21	1.31	0.74
1:B:41:ARG:HH21	1:B:41:ARG:HG3	1.51	0.73
1:B:105:GLN:NE2	2:B:601:MMZ:H43	2.03	0.73
1:A:258:GLU:HG3	2:A:601:MMZ:H42	1.71	0.71
4:A:607:HEM:HBC2	4:A:607:HEM:HMC2	1.71	0.71
1:B:105:GLN:NE2	2:B:601:MMZ:C4	2.53	0.70
1:B:175:LEU:HD12	1:B:176:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:CG	4:A:607:HEM:CMD	2.57	0.68
1:B:279:GLU:HA	1:B:279:GLU:OE1	1.93	0.68
1:B:109:HIS:HE2	2:B:613:MMZ:C3A	2.07	0.68
1:A:279:GLU:HA	1:A:279:GLU:OE1	1.93	0.67
1:B:258:GLU:CB	2:B:601:MMZ:H41	2.24	0.67
1:B:169:THR:HG22	1:B:170:PRO:HD3	1.77	0.66
1:B:13:VAL:HG11	1:B:23:THR:HG21	1.78	0.65
1:B:41:ARG:HH21	1:B:41:ARG:CG	2.10	0.65
1:A:464:LEU:O	1:A:468:GLN:HG3	1.97	0.65
1:A:105:GLN:NE2	2:A:602:MMZ:C4	2.60	0.64
1:B:94:GLN:HG2	8:B:982:HOH:O	1.96	0.64
1:B:169:THR:CG2	1:B:170:PRO:HD2	2.23	0.64
1:A:52:GLU:OE2	7:A:614:GOL:O1	2.16	0.63
1:B:258:GLU:CD	4:B:607:HEM:CMB	2.64	0.63
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.34	0.63
1:A:105:GLN:NE2	2:A:602:MMZ:H43	2.14	0.63
1:A:11:PRO:HB3	1:A:41:ARG:CZ	2.29	0.63
1:A:109:HIS:HE2	2:A:601:MMZ:C3A	2.13	0.61
1:B:169:THR:HG23	8:B:860:HOH:O	2.00	0.61
1:A:258:GLU:CB	2:A:601:MMZ:H42	2.32	0.60
1:A:258:GLU:CB	2:A:601:MMZ:C4	2.79	0.60
1:A:109:HIS:HE1	2:A:602:MMZ:H42	1.68	0.59
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.85	0.59
1:B:523:ARG:HG3	1:B:529:TRP:CE2	2.38	0.58
1:A:171:PRO:O	1:A:172:TYR:HB2	2.03	0.58
1:A:258:GLU:HB3	2:A:602:MMZ:H41	1.84	0.58
1:B:3:GLU:O	1:B:4:VAL:O	2.21	0.57
1:B:109:HIS:NE2	2:B:613:MMZ:C3A	2.67	0.57
1:B:87:ASP:OD1	1:B:89:GLU:HB2	2.05	0.57
1:B:464:LEU:O	1:B:468:GLN:HG3	2.04	0.57
1:A:105:GLN:NE2	2:A:601:MMZ:H41	2.18	0.57
1:B:258:GLU:CB	2:B:613:MMZ:C4	2.81	0.57
4:A:607:HEM:HBB2	4:A:607:HEM:HMB2	1.86	0.56
1:B:258:GLU:HB3	2:B:613:MMZ:H43	1.87	0.56
1:A:290:GLU:HG2	1:B:10:VAL:HG13	1.86	0.56
1:A:12:LEU:HD13	1:A:35:ALA:HB2	1.88	0.56
1:A:258:GLU:HB3	2:A:601:MMZ:C4	2.35	0.55
2:A:601:MMZ:C1A	4:A:607:HEM:C1A	2.89	0.55
1:B:258:GLU:OE1	2:B:613:MMZ:H42	2.05	0.54
4:A:607:HEM:CMC	4:A:607:HEM:HBC2	2.38	0.54
1:B:109:HIS:HE1	2:B:601:MMZ:H42	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:CB	2:B:613:MMZ:H42	2.38	0.53
1:A:109:HIS:CE1	2:A:602:MMZ:H42	2.43	0.53
1:B:169:THR:CG2	1:B:170:PRO:CD	2.77	0.53
1:B:166:VAL:HG13	1:B:180:ILE:HG12	1.89	0.53
1:A:170:PRO:HA	1:A:171:PRO:C	2.29	0.53
1:A:170:PRO:HA	1:A:172:TYR:N	2.24	0.53
1:A:9:PRO:HB2	1:A:40:ASN:HB3	1.91	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
1:B:166:VAL:CG1	1:B:180:ILE:HG12	2.38	0.53
1:B:16:ASP:O	1:B:17:GLU:C	2.47	0.53
1:B:105:GLN:NE2	2:B:601:MMZ:H42	2.23	0.51
1:B:16:ASP:OD1	1:B:19:SER:HB2	2.09	0.51
1:B:258:GLU:CB	2:B:613:MMZ:H43	2.40	0.51
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.45	0.51
1:A:12:LEU:HD12	1:A:13:VAL:H	1.75	0.51
1:B:105:GLN:HE21	2:B:601:MMZ:C4	2.22	0.50
1:A:468:GLN:OE1	1:A:474:LYS:HG3	2.10	0.50
1:B:230:ASN:CB	1:B:250:GLN:HG2	2.35	0.50
1:B:109:HIS:CE1	2:B:613:MMZ:C3A	2.95	0.50
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.46	0.49
1:A:468:GLN:NE2	1:A:474:LYS:HD2	2.27	0.49
1:A:108:ASP:OD2	4:A:607:HEM:C2D	2.54	0.49
1:A:105:GLN:NE2	2:A:602:MMZ:H42	2.28	0.49
1:A:30:ASN:O	1:A:34:PRO:HA	2.13	0.48
1:A:258:GLU:CG	2:A:601:MMZ:C4	2.81	0.48
1:A:109:HIS:NE2	2:A:601:MMZ:C3A	2.76	0.48
1:B:108:ASP:OD2	4:B:607:HEM:C2D	2.58	0.48
4:B:607:HEM:HMB2	4:B:607:HEM:HBB2	1.94	0.48
1:A:159:PRO:O	7:A:617:GOL:H12	2.14	0.48
1:A:258:GLU:OE2	4:A:607:HEM:HMB2	1.99	0.48
1:B:170:PRO:HB2	1:B:171:PRO:CD	2.44	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.14	0.47
1:B:60:GLY:H	7:B:615:GOL:H2	1.78	0.47
1:A:105:GLN:HE21	2:A:602:MMZ:C4	2.28	0.47
1:B:175:LEU:HD12	1:B:176:ALA:N	2.26	0.47
1:A:10:VAL:HG23	1:B:171:PRO:HD3	1.96	0.47
1:B:105:GLN:HE21	2:B:601:MMZ:H43	1.77	0.47
1:B:172:TYR:HA	8:B:776:HOH:O	2.15	0.47
1:B:545:GLN:HE21	1:B:545:GLN:HB2	1.52	0.46
4:A:607:HEM:HBB2	4:A:607:HEM:CMB	2.45	0.46
1:B:30:ASN:O	1:B:34:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:CB	2:A:601:MMZ:H43	2.46	0.46
1:A:530:TRP:CE2	1:A:531:GLU:HG2	2.51	0.46
1:B:3:GLU:O	1:B:4:VAL:C	2.53	0.46
1:A:279:GLU:HG2	8:A:1083:HOH:O	2.14	0.46
1:B:63:GLN:O	1:B:71:ARG:CZ	2.63	0.46
4:B:607:HEM:HBC2	4:B:607:HEM:HMC2	1.97	0.46
1:A:61:TRP:CH2	7:A:616:GOL:H2	2.51	0.45
1:A:286:HIS:NE2	1:A:592:SER:O	2.48	0.45
4:B:607:HEM:CMB	4:B:607:HEM:HBB2	2.46	0.45
1:A:9:PRO:CB	1:A:40:ASN:HB3	2.46	0.45
1:B:258:GLU:HG3	2:B:613:MMZ:H42	1.90	0.45
1:B:258:GLU:HG3	2:B:613:MMZ:S2	2.57	0.45
1:B:237:CYS:HA	1:B:381:PHE:O	2.16	0.45
1:B:407:MET:C	1:B:407:MET:SD	2.96	0.44
1:A:258:GLU:CD	4:A:607:HEM:CMB	2.72	0.44
1:B:258:GLU:OE2	4:B:607:HEM:C2B	2.61	0.44
1:B:41:ARG:CZ	1:B:41:ARG:HB3	2.48	0.44
8:A:1071:HOH:O	1:B:171:PRO:HD3	2.18	0.44
1:B:105:GLN:HE22	2:B:601:MMZ:H43	1.82	0.44
1:B:15:CYS:O	1:B:16:ASP:C	2.55	0.44
1:B:170:PRO:CB	1:B:171:PRO:HD3	2.47	0.43
1:A:6:CYS:HB3	1:A:165:PHE:CE2	2.53	0.43
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.53	0.43
1:A:468:GLN:HB3	8:A:1075:HOH:O	2.17	0.43
1:A:6:CYS:HB3	1:A:165:PHE:CZ	2.53	0.43
1:B:41:ARG:NH2	1:B:41:ARG:CB	2.82	0.43
1:B:127:VAL:HG13	1:B:131:GLU:HG3	2.00	0.42
1:A:407:MET:SD	1:A:407:MET:C	2.97	0.42
1:A:513:CYS:O	1:A:517:ARG:HG3	2.19	0.42
1:B:109:HIS:NE2	2:B:601:MMZ:S2	2.86	0.42
1:B:109:HIS:CE1	2:B:601:MMZ:H42	2.53	0.42
1:A:545:GLN:HG3	8:A:911:HOH:O	2.19	0.42
1:B:258:GLU:CG	2:B:613:MMZ:C4	2.86	0.41
1:B:18:GLN:O	1:B:19:SER:C	2.59	0.41
1:A:309:PHE:CD1	1:A:529:TRP:HH2	2.37	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:B:313:LEU:N	1:B:314:PRO:CD	2.83	0.41
1:B:41:ARG:NH2	1:B:41:ARG:CG	2.74	0.41
1:A:258:GLU:HB3	2:A:601:MMZ:H43	2.02	0.40
1:A:258:GLU:OE1	2:A:601:MMZ:H42	2.19	0.40
1:B:258:GLU:OE1	2:B:613:MMZ:C4	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:HD13	1:B:173:GLN:O	2.22	0.40
1:B:258:GLU:OE2	4:B:607:HEM:HMB2	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/595 (100%)	572 (96%)	19 (3%)	2 (0%)	46	39
1	B	593/595 (100%)	561 (95%)	23 (4%)	9 (2%)	13	5
All	All	1186/1190 (100%)	1133 (96%)	42 (4%)	11 (1%)	21	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	B	168	PRO
1	B	170	PRO
1	B	175	LEU
1	B	9	PRO
1	A	9	PRO
1	B	4	VAL
1	B	173	GLN
1	B	17	GLU
1	B	169	THR
1	B	167	CYS

### 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%)	502 (97%)	15 (3%)	50	46
1	B	517/517 (100%)	500 (97%)	17 (3%)	45	40
All	All	1034/1034 (100%)	1002 (97%)	32 (3%)	47	43

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	10	VAL
1	A	31	ARG
1	A	41	ARG
1	A	146	LYS
1	A	172	TYR
1	A	174	SER
1	A	279	GLU
1	A	322	GLN
1	A	347	PHE
1	A	363	GLU
1	A	410	ASN
1	A	486	THR
1	A	503	GLU
1	A	594	GLU
1	B	12	LEU
1	B	16	ASP
1	B	18	GLN
1	B	41	ARG
1	B	64	ARG
1	B	91	VAL
1	B	168	PRO
1	B	172	TYR
1	B	201	SER
1	B	279	GLU
1	B	322	GLN
1	B	347	PHE

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Mol	Chain	Res	Type
1	B	465	LYS
1	B	486	THR
1	B	517	ARG
1	B	543	SER
1	B	545	GLN

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

Mol	Chain	Res	Type
1	A	250	GLN
1	A	329	GLN
1	A	568	GLN
1	B	128	GLN
1	B	329	GLN
1	B	364	ASN
1	B	423	GLN
1	B	545	GLN
1	B	558	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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	MMZ	A	601	2	5,7,7	5.06	3 (60%)	6,9,9	2.76	4 (66%)
2	MMZ	A	602	2,4	5,7,7	4.73	3 (60%)	6,9,9	4.76	4 (66%)
3	NAG	A	603	1	14,14,15	1.28	1 (7%)	15,19,21	1.76	2 (13%)
3	NAG	A	604	1	14,14,15	0.72	0	15,19,21	1.92	6 (40%)
3	NAG	A	605	1	14,14,15	0.63	0	15,19,21	2.46	6 (40%)
3	NAG	A	606	1	14,14,15	0.90	1 (7%)	15,19,21	2.05	3 (20%)
4	HEM	A	607	1,2	24,50,50	1.49	4 (16%)	16,82,82	1.60	3 (18%)
6	NO3	A	609	-	1,3,3	1.91	0	0,3,3	0.00	-
6	NO3	A	610	-	1,3,3	0.63	0	0,3,3	0.00	-
6	NO3	A	611	-	1,3,3	0.12	0	0,3,3	0.00	-
6	NO3	A	612	-	1,3,3	0.06	0	0,3,3	0.00	-
6	NO3	A	613	-	1,3,3	0.17	0	0,3,3	0.00	-
7	GOL	A	614	-	5,5,5	0.52	0	5,5,5	1.45	2 (40%)
7	GOL	A	615	-	5,5,5	0.21	0	5,5,5	1.18	0
7	GOL	A	616	-	5,5,5	0.50	0	5,5,5	0.72	0
7	GOL	A	617	-	5,5,5	1.12	1 (20%)	5,5,5	1.57	1 (20%)
2	MMZ	B	601	2,4	5,7,7	4.78	3 (60%)	6,9,9	5.94	6 (100%)
3	NAG	B	602	1	14,14,15	1.05	1 (7%)	15,19,21	2.17	5 (33%)
3	NAG	B	603	1	14,14,15	0.68	0	15,19,21	1.46	2 (13%)
3	NAG	B	604	1	14,14,15	0.49	0	15,19,21	1.72	2 (13%)
3	NAG	B	605	1,3	14,14,15	0.55	0	15,19,21	2.67	4 (26%)
3	NAG	B	606	3	14,14,15	0.99	1 (7%)	15,19,21	0.99	1 (6%)
4	HEM	B	607	1,2	24,50,50	1.76	5 (20%)	16,82,82	1.35	2 (12%)
6	NO3	B	609	-	1,3,3	0.18	0	0,3,3	0.00	-
6	NO3	B	610	-	1,3,3	0.47	0	0,3,3	0.00	-
6	NO3	B	611	-	1,3,3	0.29	0	0,3,3	0.00	-
6	NO3	B	612	-	1,3,3	0.05	0	0,3,3	0.00	-
2	MMZ	B	613	2	5,7,7	4.92	3 (60%)	6,9,9	2.68	4 (66%)
7	GOL	B	614	-	5,5,5	0.47	0	5,5,5	0.56	0
7	GOL	B	615	-	5,5,5	0.71	0	5,5,5	0.78	0
7	GOL	B	616	-	5,5,5	0.48	0	5,5,5	0.93	0
7	GOL	B	617	-	5,5,5	0.74	0	5,5,5	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMZ	A	601	2	-	0/0/0/0	0/1/1/1
2	MMZ	A	602	2,4	-	0/0/0/0	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
3	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	HEM	A	607	1,2	-	0/6/54/54	0/0/8/8
6	NO3	A	609	-	-	0/0/0/0	0/0/0/0
6	NO3	A	610	-	-	0/0/0/0	0/0/0/0
6	NO3	A	611	-	-	0/0/0/0	0/0/0/0
6	NO3	A	612	-	-	0/0/0/0	0/0/0/0
6	NO3	A	613	-	-	0/0/0/0	0/0/0/0
7	GOL	A	614	-	-	0/4/4/4	0/0/0/0
7	GOL	A	615	-	-	0/4/4/4	0/0/0/0
7	GOL	A	616	-	-	0/4/4/4	0/0/0/0
7	GOL	A	617	-	-	0/4/4/4	0/0/0/0
2	MMZ	B	601	2,4	-	0/0/0/0	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	606	3	-	0/6/23/26	0/1/1/1
4	HEM	B	607	1,2	-	0/6/54/54	0/0/8/8
6	NO3	B	609	-	-	0/0/0/0	0/0/0/0
6	NO3	B	610	-	-	0/0/0/0	0/0/0/0
6	NO3	B	611	-	-	0/0/0/0	0/0/0/0
6	NO3	B	612	-	-	0/0/0/0	0/0/0/0
2	MMZ	B	613	2	-	0/0/0/0	0/1/1/1
7	GOL	B	614	-	-	0/4/4/4	0/0/0/0
7	GOL	B	615	-	-	0/4/4/4	0/0/0/0
7	GOL	B	616	-	-	0/4/4/4	0/0/0/0
7	GOL	B	617	-	-	0/4/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MMZ	C3A-C1A	-9.15	1.35	1.52
2	B	601	MMZ	C3A-C1A	-8.94	1.35	1.52
2	B	613	MMZ	C3A-C1A	-8.93	1.35	1.52
2	A	602	MMZ	C3A-C1A	-8.88	1.35	1.52
4	B	607	HEM	C1B-NB	-4.83	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MMZ	C1A-N1	-4.80	1.35	1.46
2	B	613	MMZ	C3A-N3	-4.53	1.30	1.46
2	A	602	MMZ	C1A-N1	-4.47	1.36	1.46
2	A	601	MMZ	C3A-N3	-4.46	1.30	1.46
2	B	613	MMZ	C1A-N1	-4.45	1.36	1.46
2	B	601	MMZ	C1A-N1	-4.38	1.36	1.46
2	B	601	MMZ	C3A-N3	-3.84	1.32	1.46
4	B	607	HEM	C4D-ND	-3.79	1.31	1.36
3	A	603	NAG	O5-C1	-3.66	1.37	1.43
2	A	602	MMZ	C3A-N3	-3.57	1.33	1.46
4	B	607	HEM	C1C-NC	-3.50	1.32	1.36
4	A	607	HEM	C1B-NB	-3.22	1.32	1.36
4	A	607	HEM	C3B-C2B	-2.90	1.36	1.40
4	A	607	HEM	C4D-ND	-2.79	1.33	1.36
3	B	606	NAG	O5-C1	-2.74	1.39	1.43
4	B	607	HEM	C3B-C2B	-2.66	1.37	1.40
3	A	606	NAG	O5-C1	-2.58	1.39	1.43
3	B	602	NAG	O5-C1	-2.48	1.39	1.43
4	A	607	HEM	C3D-C2D	-2.09	1.31	1.37
4	B	607	HEM	C4C-NC	2.03	1.39	1.36
7	A	617	GOL	O2-C2	2.35	1.50	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	MMZ	C4-N3-C2	-12.64	115.09	126.44
2	A	602	MMZ	C4-N3-C2	-9.74	117.70	126.44
3	B	602	NAG	O3-C3-C4	-4.40	100.44	110.36
3	A	603	NAG	C3-C4-C5	-3.93	103.22	110.23
3	B	605	NAG	O7-C7-C8	-3.80	115.07	122.07
3	A	604	NAG	C4-C3-C2	-3.44	106.00	111.34
4	B	607	HEM	CBA-CAA-C2A	-3.40	106.52	112.49
2	A	601	MMZ	C1A-N1-C2	-3.17	109.30	113.16
3	A	603	NAG	O5-C5-C4	-3.02	105.13	110.13
3	A	604	NAG	O6-C6-C5	-2.95	101.46	111.30
4	A	607	HEM	CBA-CAA-C2A	-2.92	107.35	112.49
4	A	607	HEM	CBD-CAD-C3D	-2.91	107.36	112.47
3	A	604	NAG	O7-C7-C8	-2.85	116.83	122.07
3	A	604	NAG	C3-C4-C5	-2.82	105.19	110.23
2	B	613	MMZ	C1A-N1-C2	-2.82	109.73	113.16
3	B	605	NAG	C6-C5-C4	-2.75	106.09	112.99
2	B	601	MMZ	C1A-N1-C2	-2.71	109.86	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	617	GOL	C3-C2-C1	-2.69	99.72	111.06
3	A	605	NAG	O3-C3-C4	-2.61	104.46	110.36
3	B	603	NAG	O5-C5-C4	-2.60	105.83	110.13
3	B	602	NAG	O7-C7-C8	-2.58	117.32	122.07
7	A	614	GOL	C3-C2-C1	-2.39	100.98	111.06
4	B	607	HEM	CBD-CAD-C3D	-2.38	108.28	112.47
3	A	606	NAG	O7-C7-C8	-2.37	117.71	122.07
3	B	603	NAG	O4-C4-C3	-2.36	105.03	110.36
3	A	605	NAG	O3-C3-C2	-2.31	104.44	109.37
3	B	602	NAG	O5-C5-C4	-2.30	106.32	110.13
3	B	602	NAG	C1-O5-C5	-2.20	108.91	112.14
4	A	607	HEM	CAD-C3D-C2D	-2.01	123.27	129.00
7	A	614	GOL	O2-C2-C1	2.05	118.32	108.47
3	A	604	NAG	C8-C7-N2	2.06	120.04	116.10
2	A	602	MMZ	C4-N3-C3A	2.06	127.98	120.33
2	B	601	MMZ	C1A-C3A-N3	2.07	104.83	103.07
3	B	606	NAG	O4-C4-C5	2.16	114.91	109.23
3	B	605	NAG	O5-C5-C4	2.30	113.94	110.13
3	A	605	NAG	O4-C4-C5	2.35	115.42	109.23
3	A	606	NAG	O5-C5-C4	2.39	114.10	110.13
3	A	605	NAG	O5-C5-C4	2.50	114.27	110.13
3	B	604	NAG	O5-C5-C4	2.51	114.29	110.13
2	A	602	MMZ	C3A-C1A-N1	2.54	105.86	102.62
3	A	605	NAG	C4-C3-C2	2.66	115.47	111.34
2	B	601	MMZ	C4-N3-C3A	2.77	130.61	120.33
2	B	613	MMZ	C3A-C1A-N1	2.77	106.16	102.62
2	A	601	MMZ	C1A-C3A-N3	2.79	105.44	103.07
2	B	601	MMZ	C3A-C1A-N1	2.80	106.19	102.62
2	B	613	MMZ	C3A-N3-C2	2.90	113.00	111.23
3	A	604	NAG	O3-C3-C2	3.12	116.06	109.37
2	A	601	MMZ	C3A-N3-C2	3.32	113.26	111.23
2	A	601	MMZ	C3A-C1A-N1	3.67	107.31	102.62
2	B	613	MMZ	C1A-C3A-N3	4.17	106.60	103.07
3	B	602	NAG	C4-C3-C2	4.39	118.16	111.34
2	B	601	MMZ	C3A-N3-C2	4.99	114.28	111.23
2	A	602	MMZ	C3A-N3-C2	4.99	114.28	111.23
3	B	604	NAG	C1-O5-C5	5.29	119.92	112.14
3	A	606	NAG	C1-O5-C5	5.97	120.92	112.14
3	A	605	NAG	C1-O5-C5	7.36	122.96	112.14
3	B	605	NAG	C1-O5-C5	7.87	123.71	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MMZ	14	0
2	A	602	MMZ	7	0
4	A	607	HEM	14	0
7	A	614	GOL	1	0
7	A	616	GOL	1	0
7	A	617	GOL	1	0
2	B	601	MMZ	11	0
4	B	607	HEM	12	0
2	B	613	MMZ	15	0
7	B	615	GOL	1	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%)	-0.17	20 (3%)	49	53	13, 24, 59, 137	0
1	B	595/595 (100%)	0.18	34 (5%)	27	31	13, 28, 70, 163	0
All	All	1190/1190 (100%)	0.01	54 (4%)	37	41	13, 26, 66, 163	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	TRP	19.4
1	B	1	SER	17.0
1	A	2	TRP	16.7
1	B	12	LEU	15.7
1	B	11	PRO	14.3
1	B	172	TYR	13.9
1	B	9	PRO	13.7
1	A	10	VAL	11.5
1	B	10	VAL	11.4
1	A	8	ALA	11.3
1	B	174	SER	11.2
1	B	13	VAL	10.8
1	A	12	LEU	10.3
1	B	7	GLY	10.1
1	A	9	PRO	10.1
1	B	171	PRO	9.7
1	A	13	VAL	9.2
1	B	8	ALA	8.7
1	A	1	SER	8.6
1	A	11	PRO	8.6
1	B	170	PRO	8.2
1	B	3	GLU	7.5
1	B	594	GLU	7.4
1	B	595	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	14	THR	6.4
1	A	14	THR	6.3
1	B	4	VAL	6.1
1	A	5	GLY	6.1
1	A	4	VAL	5.9
1	A	3	GLU	5.6
1	B	173	GLN	5.6
1	A	594	GLU	4.9
1	B	6	CYS	4.9
1	B	119	LEU	4.8
1	A	119	LEU	4.4
1	A	7	GLY	3.9
1	B	593	ARG	3.6
1	A	171	PRO	3.6
1	A	172	TYR	3.4
1	B	15	CYS	3.3
1	A	6	CYS	3.2
1	A	595	ASN	3.0
1	B	287	TRP	2.8
1	A	120	GLY	2.5
1	B	539	LYS	2.5
1	B	120	GLY	2.5
1	B	32	ARG	2.4
1	B	283	LEU	2.4
1	B	220	TRP	2.3
1	B	167	CYS	2.2
1	B	168	PRO	2.1
1	B	18	GLN	2.1
1	B	207	SER	2.0
1	B	175	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	MMZ	A	601	7/7	0.96	0.19	14.00	34,35,37,41	7
2	MMZ	A	602	7/7	0.95	0.17	11.69	28,29,31,31	7
7	GOL	A	615	6/6	0.92	0.20	11.35	35,39,42,47	0
6	NO3	A	610	4/4	0.90	0.15	5.76	51,51,52,54	0
6	NO3	A	613	4/4	0.81	0.26	5.73	65,70,72,74	0
2	MMZ	B	613	7/7	0.95	0.16	5.51	25,27,29,31	7
7	GOL	A	617	6/6	0.80	0.30	5.37	36,47,54,58	0
2	MMZ	B	601	7/7	0.95	0.15	5.30	27,28,30,31	7
6	NO3	B	610	4/4	0.98	0.10	3.37	24,25,29,31	0
7	GOL	B	616	6/6	0.94	0.18	3.06	31,34,35,37	0
6	NO3	B	611	4/4	0.83	0.18	2.98	55,61,62,69	0
6	NO3	A	612	4/4	0.91	0.19	2.77	40,45,47,53	0
3	NAG	A	604	14/15	0.87	0.17	1.66	53,59,62,62	0
6	NO3	B	609	4/4	0.98	0.09	1.24	24,29,32,32	0
7	GOL	A	616	6/6	0.96	0.11	0.94	22,24,31,38	0
7	GOL	B	617	6/6	0.83	0.13	0.71	51,56,58,59	0
6	NO3	A	609	4/4	0.99	0.07	0.55	18,18,19,22	0
4	HEM	B	607	43/43	0.99	0.09	0.42	12,14,16,19	0
4	HEM	A	607	43/43	0.98	0.09	0.40	14,16,17,19	0
3	NAG	A	606	14/15	0.94	0.10	0.37	27,32,40,45	0
3	NAG	B	603	14/15	0.93	0.10	0.16	22,31,41,48	0
7	GOL	B	615	6/6	0.96	0.10	0.15	24,26,27,28	0
3	NAG	A	603	14/15	0.95	0.09	0.06	27,36,43,49	0
3	NAG	B	602	14/15	0.88	0.13	0.02	47,60,68,73	0
7	GOL	A	614	6/6	0.95	0.09	-0.11	25,30,31,32	0
5	CA	B	608	1/1	0.99	0.08	-0.17	25,25,25,25	0
7	GOL	B	614	6/6	0.95	0.11	-0.25	26,28,34,39	0
3	NAG	B	605	14/15	0.92	0.10	-0.85	41,54,56,56	0
5	CA	A	608	1/1	1.00	0.06	-2.78	19,19,19,19	0
3	NAG	B	606	14/15	0.83	0.17	-	49,57,66,67	0
6	NO3	A	611	4/4	0.93	0.14	-	36,36,40,44	0
3	NAG	B	604	14/15	0.77	0.17	-	57,67,69,72	0
6	NO3	B	612	4/4	0.96	0.12	-	30,36,37,42	0
3	NAG	A	605	14/15	0.73	0.18	-	54,60,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.