



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3E7G  
Title : Structure of human INOSOX with inhibitor AR-C95791  
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 2008-08-18  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

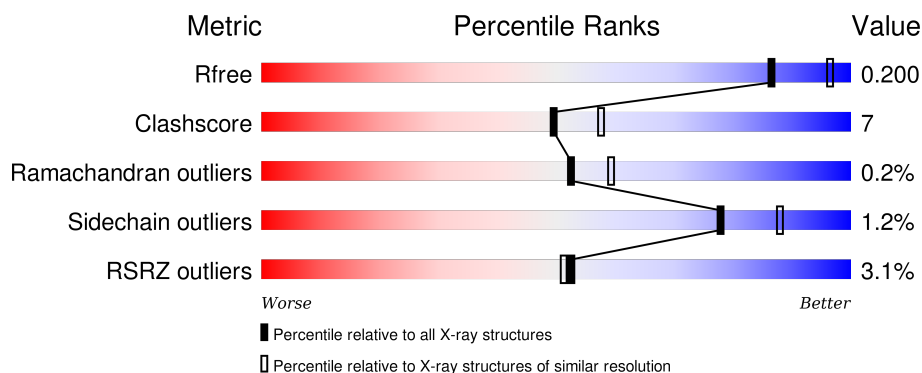
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	424	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>..</div> </div>
1	B	424	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	424	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div></div> </div>
1	D	424	<div> <div>4%</div> <div>79%</div> <div>20%</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
4	H4B	A	902	X	-	-	-
4	H4B	D	3902	X	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14516 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 Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	B	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	C	423	Total	C	N	O	S	0	0	0
			3440	2198	600	620	22			
1	D	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

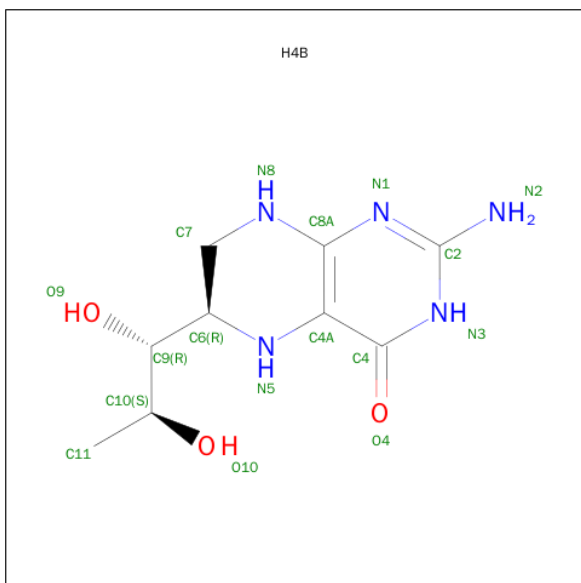
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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



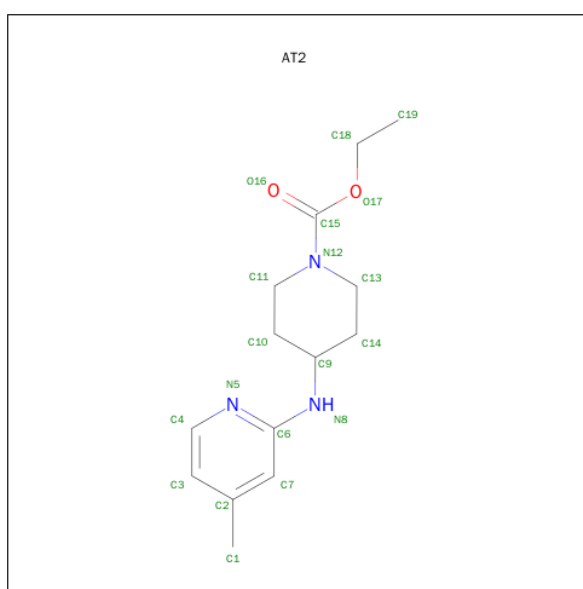
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		
4	C	1	Total	C	N	O	0	0
			17	9	5	3		
4	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is ETHYL 4-[(4-METHYLPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (three-letter code: AT2) (formula:  $C_{14}H_{21}N_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	3	2		
5	B	1	Total	C	N	O	0	0
			19	14	3	2		
5	C	1	Total	C	N	O	0	0
			19	14	3	2		
5	D	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		

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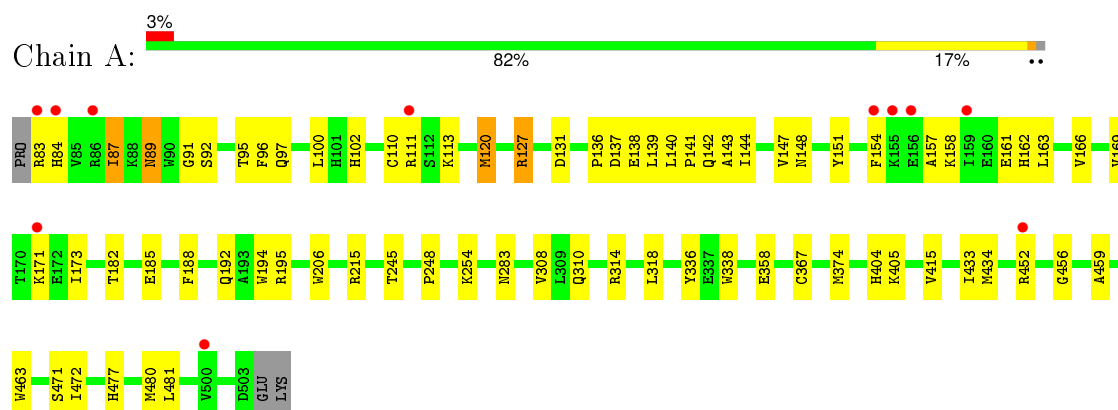
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	110	Total 110	O 110	0	0
6	C	137	Total 137	O 137	0	0
6	D	136	Total 136	O 136	0	0

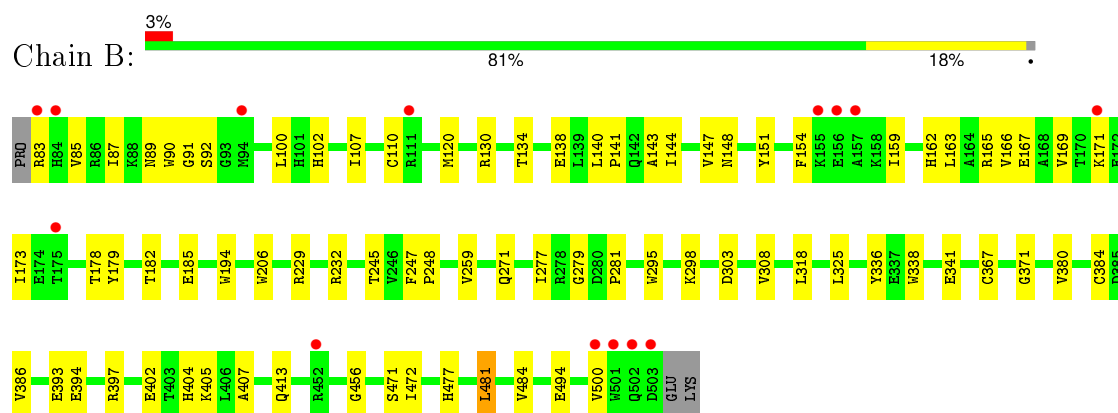
### 3 Residue-property plots [i](#)

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.

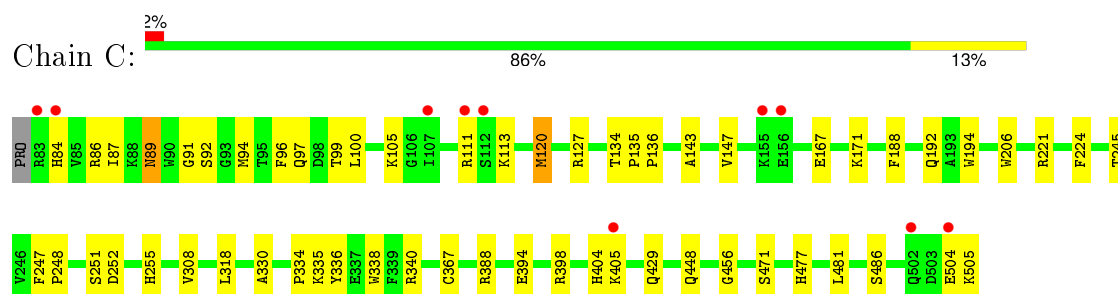
- Molecule 1: Nitric oxide synthase, inducible



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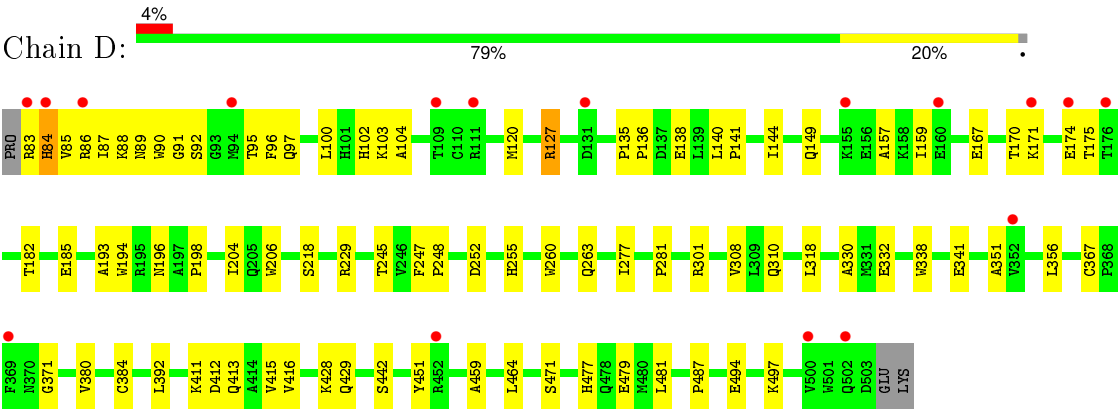


- Molecule 1: Nitric oxide synthase, inducible





● Molecule 1: Nitric oxide synthase, inducible



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.21Å 158.67Å 191.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.20 39.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.2 (39.51-2.20) 84.8 (39.50-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.182 , 0.213 0.174 , 0.200	Depositor DCC
$R_{free}$ test set	6628 reflections (5.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 141475 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HEM, ZN, AT2, H4B

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	0.44	0/3517	0.65	1/4774 (0.0%)
1	B	0.43	0/3517	0.64	1/4774 (0.0%)
1	C	0.45	0/3539	0.66	0/4801
1	D	0.45	0/3517	0.64	1/4774 (0.0%)
All	All	0.44	0/14090	0.65	3/19123 (0.0%)

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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	MET	N-CA-C	-5.66	95.72	111.00
1	D	371	GLY	N-CA-C	-5.14	100.25	113.10
1	B	371	GLY	N-CA-C	-5.06	100.45	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	451	TYR	Sidechain

## 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	3418	0	3318	50	0
1	B	3418	0	3317	51	0
1	C	3440	0	3339	44	0
1	D	3418	0	3317	58	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
3	D	43	0	30	0	0
4	A	17	0	14	1	0
4	B	17	0	14	2	0
4	C	17	0	15	1	0
4	D	17	0	14	0	0
5	A	19	0	21	0	0
5	B	19	0	21	0	0
5	C	19	0	21	0	0
5	D	19	0	21	0	0
6	A	121	0	0	0	0
6	B	110	0	0	1	0
6	C	137	0	0	1	0
6	D	136	0	0	5	0
All	All	14516	0	13552	196	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 7.

All (196) 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:260:TRP:HE1	1:D:310:GLN:HE21	1.07	1.00
1:D:260:TRP:HE1	1:D:310:GLN:NE2	1.65	0.93
1:A:192:GLN:HE22	1:A:195:ARG:HH11	1.22	0.86
1:C:505:LYS:HG2	1:C:505:LYS:O	1.79	0.82
1:C:505:LYS:CG	1:C:505:LYS:O	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HD12	1:B:166:VAL:HG13	1.69	0.75
1:A:89:ASN:HD22	1:A:92:SER:H	1.33	0.75
1:D:89:ASN:ND2	1:D:92:SER:H	1.86	0.73
1:A:140:LEU:O	1:A:144:ILE:HG12	1.89	0.72
1:D:167:GLU:O	1:D:171:LYS:HD3	1.89	0.71
1:D:170:THR:O	1:D:174:GLU:HG3	1.90	0.70
1:C:94:MET:HE1	1:C:448:GLN:HG2	1.72	0.70
1:A:89:ASN:ND2	1:A:92:SER:H	1.89	0.70
1:D:89:ASN:HD22	1:D:92:SER:H	1.40	0.69
1:C:167:GLU:O	1:C:171:LYS:HD3	1.93	0.69
1:D:135:PRO:HB2	1:D:138:GLU:HG3	1.77	0.67
1:B:405:LYS:HE2	1:B:407:ALA:HB3	1.75	0.67
1:D:140:LEU:O	1:D:144:ILE:HG12	1.95	0.67
1:D:140:LEU:HB3	1:D:141:PRO:HD3	1.78	0.65
1:D:83:ARG:O	1:D:84:HIS:HB3	1.95	0.65
1:A:83:ARG:O	1:A:102:HIS:HE1	1.80	0.64
1:C:221:ARG:HG3	1:C:221:ARG:NH2	2.14	0.62
1:C:221:ARG:HG3	1:C:221:ARG:HH21	1.65	0.62
1:A:89:ASN:ND2	1:A:91:GLY:H	1.99	0.61
1:D:87:ILE:HG21	1:D:481:LEU:HD13	1.83	0.61
1:A:404:HIS:CD2	1:A:405:LYS:HG3	2.35	0.60
1:D:196:ASN:O	1:D:198:PRO:HD3	2.01	0.60
1:B:89:ASN:HD22	1:B:92:SER:H	1.49	0.60
1:B:182:THR:OG1	1:B:185:GLU:HG3	2.02	0.60
1:A:215:ARG:O	1:A:248:PRO:HG3	2.02	0.60
1:D:89:ASN:ND2	1:D:91:GLY:H	2.00	0.59
1:B:159:ILE:O	1:B:163:LEU:HD23	2.01	0.59
1:B:87:ILE:HD11	1:B:481:LEU:HD13	1.84	0.59
1:C:471:SER:O	1:C:477:HIS:HE1	1.87	0.58
1:C:221:ARG:HD2	6:C:6120:HOH:O	2.02	0.58
1:D:330:ALA:H	1:D:429:GLN:HE22	1.49	0.58
1:A:87:ILE:HD11	1:A:481:LEU:CD1	2.34	0.57
1:D:301:ARG:HD3	6:D:7132:HOH:O	2.03	0.57
1:A:308:VAL:HG22	1:A:318:LEU:CD2	2.35	0.57
1:B:232:ARG:NH1	1:B:325:LEU:HD21	2.20	0.57
1:B:308:VAL:HG22	1:B:318:LEU:CD2	2.35	0.57
1:A:158:LYS:HD2	1:A:161:GLU:OE2	2.04	0.57
1:B:338:TRP:O	1:B:341:GLU:HB2	2.04	0.56
1:C:340:ARG:HH21	1:C:340:ARG:HG3	1.70	0.56
1:B:143:ALA:O	1:B:147:VAL:HG23	2.06	0.56
1:C:143:ALA:O	1:C:147:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:HG22	1:C:318:LEU:CD2	2.35	0.55
1:D:471:SER:O	1:D:477:HIS:HE1	1.90	0.55
1:A:182:THR:OG1	1:A:185:GLU:HG3	2.07	0.55
1:B:295:TRP:CZ2	1:B:298:LYS:HE2	2.41	0.55
1:B:295:TRP:HZ2	1:B:298:LYS:HE2	1.71	0.55
1:A:169:VAL:O	1:A:173:ILE:HG13	2.07	0.54
1:C:86:ARG:HH21	1:C:97:GLN:NE2	2.05	0.54
1:B:471:SER:O	1:B:477:HIS:HE1	1.90	0.54
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.42	0.54
1:C:87:ILE:HG21	1:C:481:LEU:HD13	1.91	0.53
1:A:188:PHE:CZ	1:A:192:GLN:HG3	2.44	0.53
1:C:84:HIS:CE1	1:C:97:GLN:HE21	2.26	0.53
1:B:130:ARG:NH2	1:B:134:THR:OG1	2.42	0.53
1:D:413:GLN:NE2	6:D:7134:HOH:O	2.42	0.53
1:A:131:ASP:O	1:A:254:LYS:HE3	2.10	0.52
1:C:504:GLU:CD	1:C:504:GLU:O	2.47	0.52
1:A:100:LEU:HB3	1:A:456:GLY:HA3	1.92	0.52
1:B:83:ARG:O	1:B:102:HIS:HE1	1.91	0.52
1:C:334:PRO:O	1:C:335:LYS:HD3	2.09	0.52
1:A:162:HIS:O	1:A:166:VAL:HG23	2.10	0.52
1:B:89:ASN:ND2	1:B:91:GLY:H	2.06	0.52
1:D:182:THR:OG1	1:D:185:GLU:HG3	2.09	0.52
1:B:162:HIS:O	1:B:166:VAL:HG23	2.10	0.52
1:B:165:ARG:O	1:B:169:VAL:HG23	2.09	0.52
1:B:500:VAL:O	1:B:500:VAL:HG23	2.09	0.51
1:D:204:ILE:HG21	1:D:442:SER:OG	2.10	0.51
1:B:336:TYR:HB3	1:B:338:TRP:CE2	2.45	0.51
1:D:252:ASP:OD1	1:D:255:HIS:HD2	1.93	0.51
1:C:100:LEU:HB3	1:C:456:GLY:HA3	1.92	0.51
1:D:277:ILE:HG21	1:D:281:PRO:HB3	1.93	0.51
1:A:84:HIS:CD2	1:A:97:GLN:NE2	2.80	0.50
1:B:386:VAL:HG22	6:B:5090:HOH:O	2.10	0.50
1:D:356:LEU:C	1:D:356:LEU:HD23	2.32	0.50
1:B:138:GLU:O	1:B:141:PRO:HD2	2.12	0.50
1:C:188:PHE:CZ	1:C:192:GLN:HG3	2.47	0.50
1:B:402:GLU:HB3	1:B:404:HIS:CE1	2.47	0.50
1:A:136:PRO:HA	1:A:139:LEU:HB3	1.94	0.49
1:C:84:HIS:HB3	1:C:99:THR:HG22	1.94	0.49
1:B:140:LEU:O	1:B:144:ILE:HG12	2.13	0.49
1:C:94:MET:HE1	1:C:96:PHE:CZ	2.47	0.49
1:A:111:ARG:NH2	1:A:113:LYS:HE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ARG:HG3	1:C:388:ARG:HH11	1.78	0.49
1:C:120:MET:CG	4:C:2902:H4B:H9	2.43	0.49
1:C:89:ASN:HD22	1:C:92:SER:H	1.60	0.49
1:D:84:HIS:CE1	1:D:97:GLN:HE21	2.31	0.49
1:A:84:HIS:CD2	1:A:97:GLN:HE22	2.31	0.48
1:A:452:ARG:HH21	1:A:452:ARG:HG2	1.78	0.48
1:B:169:VAL:O	1:B:173:ILE:HG13	2.14	0.48
1:A:95:THR:HG22	1:A:96:PHE:N	2.29	0.48
1:A:245:THR:O	1:A:367:CYS:HA	2.14	0.48
1:D:171:LYS:O	1:D:175:THR:HG23	2.14	0.47
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.49	0.47
1:D:85:VAL:HB	1:D:481:LEU:HD21	1.96	0.47
1:B:298:LYS:HE3	1:B:303:ASP:HB3	1.97	0.47
1:B:247:PHE:HB3	1:B:248:PRO:CD	2.44	0.47
1:D:412:ASP:O	1:D:416:VAL:HG23	2.14	0.47
1:A:415:VAL:HG11	1:B:472:ILE:HG13	1.97	0.47
1:B:151:TYR:HA	1:B:154:PHE:CD2	2.50	0.47
1:A:113:LYS:NZ	1:B:102:HIS:O	2.47	0.47
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.49	0.46
1:D:392:LEU:HB2	6:D:7131:HOH:O	2.16	0.46
1:D:308:VAL:HG22	1:D:318:LEU:CD2	2.45	0.46
1:B:120:MET:HG2	4:B:1902:H4B:H9	1.98	0.46
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.46	0.46
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.98	0.46
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.51	0.46
1:A:143:ALA:O	1:A:147:VAL:HG23	2.16	0.46
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.51	0.46
1:C:245:THR:O	1:C:367:CYS:HA	2.15	0.46
1:B:245:THR:O	1:B:367:CYS:HA	2.16	0.46
1:B:159:ILE:HG22	1:B:163:LEU:HD23	1.98	0.45
1:D:88:LYS:O	1:D:479:GLU:HG3	2.16	0.45
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.51	0.45
1:D:229:ARG:HD3	6:D:7064:HOH:O	2.16	0.45
1:D:86:ARG:CZ	1:D:95:THR:HG21	2.46	0.45
1:A:138:GLU:O	1:A:142:GLN:HG3	2.16	0.45
1:D:135:PRO:HA	1:D:136:PRO:HD3	1.90	0.45
1:B:271:GLN:HA	1:B:277:ILE:HD13	1.99	0.45
1:B:229:ARG:HG2	1:B:229:ARG:HH21	1.82	0.45
1:C:113:LYS:HZ1	1:D:102:HIS:HA	1.80	0.45
1:B:144:ILE:HG22	1:B:148:ASN:HD21	1.82	0.45
1:C:221:ARG:HH22	1:C:224:PHE:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:PHE:HB3	1:D:248:PRO:CD	2.47	0.45
1:B:85:VAL:HB	1:B:481:LEU:HD21	1.99	0.44
1:D:411:LYS:O	1:D:415:VAL:HG23	2.17	0.44
1:A:144:ILE:HG22	1:A:148:ASN:ND2	2.32	0.44
1:A:144:ILE:HG22	1:A:148:ASN:HD21	1.83	0.44
1:C:87:ILE:HG21	1:C:481:LEU:CD1	2.46	0.44
1:C:120:MET:HE2	1:D:90:TRP:CZ2	2.52	0.44
1:B:107:ILE:HD11	1:B:484:VAL:HG11	1.97	0.44
1:C:394:GLU:O	1:C:398:ARG:HG3	2.16	0.44
1:B:167:GLU:O	1:B:171:LYS:HD3	2.18	0.44
1:B:178:THR:OG1	1:B:179:TYR:N	2.51	0.44
1:D:332:GLU:OE1	1:D:428:LYS:NZ	2.37	0.44
3:C:2901:HEM:HMC1	3:C:2901:HEM:HBC2	1.98	0.44
1:A:120:MET:HG3	1:B:90:TRP:NE1	2.33	0.44
1:C:89:ASN:ND2	1:C:91:GLY:H	2.16	0.44
1:D:247:PHE:HB3	1:D:248:PRO:HD2	2.00	0.43
1:A:137:ASP:N	1:A:137:ASP:OD2	2.51	0.43
1:D:86:ARG:HG3	1:D:95:THR:HG23	1.99	0.43
1:D:88:LYS:HE3	1:D:90:TRP:CE2	2.53	0.43
1:A:471:SER:O	1:A:477:HIS:HE1	2.01	0.43
1:A:140:LEU:CD1	1:A:173:ILE:HD12	2.48	0.43
1:C:87:ILE:HG13	1:C:96:PHE:HB2	2.01	0.43
1:B:279:GLY:O	1:B:281:PRO:HD3	2.19	0.43
1:C:330:ALA:H	1:C:429:GLN:HE22	1.66	0.43
1:B:394:GLU:HA	1:B:397:ARG:NH1	2.33	0.43
1:A:336:TYR:HB3	1:A:338:TRP:CE2	2.54	0.43
1:A:310:GLN:HG3	1:A:314:ARG:O	2.19	0.43
1:A:127:ARG:NH1	1:A:358:GLU:HG3	2.34	0.43
1:D:245:THR:O	1:D:367:CYS:HA	2.18	0.43
1:C:252:ASP:OD1	1:C:255:HIS:HD2	2.01	0.43
1:B:380:VAL:O	1:B:384:CYS:HB2	2.19	0.43
1:D:127:ARG:HA	1:D:127:ARG:HD3	1.76	0.43
1:C:404:HIS:CE1	1:C:405:LYS:HE3	2.54	0.43
1:C:336:TYR:HB3	1:C:338:TRP:CE2	2.54	0.43
1:C:251:SER:OG	1:C:252:ASP:N	2.53	0.42
1:D:494:GLU:HG3	1:D:497:LYS:HE3	2.00	0.42
1:D:89:ASN:HD22	1:D:92:SER:N	2.13	0.42
1:A:138:GLU:O	1:A:141:PRO:HD2	2.18	0.42
1:A:472:ILE:O	1:A:472:ILE:HG22	2.20	0.42
1:B:393:GLU:OE2	1:B:397:ARG:NH2	2.52	0.42
1:D:149:GLN:NE2	6:D:7068:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:MET:CG	4:B:1902:H4B:H9	2.50	0.41
1:A:87:ILE:HD13	1:A:87:ILE:HA	1.71	0.41
1:C:340:ARG:NH2	1:C:340:ARG:HG3	2.35	0.41
1:D:95:THR:CG2	1:D:96:PHE:N	2.83	0.41
1:B:87:ILE:HD11	1:B:481:LEU:CD1	2.50	0.41
1:D:159:ILE:H	1:D:159:ILE:HG13	1.67	0.41
1:D:263:GLN:HA	1:D:351:ALA:O	2.21	0.41
1:D:193:ALA:HB2	1:D:487:PRO:HB2	2.03	0.41
1:A:171:LYS:HD2	1:A:171:LYS:N	2.35	0.41
1:D:86:ARG:NE	1:D:95:THR:HG21	2.36	0.41
1:D:338:TRP:O	1:D:341:GLU:HB2	2.20	0.41
1:D:100:LEU:CD1	1:D:103:LYS:HD2	2.51	0.41
1:C:134:THR:HA	1:C:135:PRO:HD3	1.86	0.41
1:A:83:ARG:C	1:A:102:HIS:HE1	2.23	0.41
1:C:113:LYS:NZ	1:D:102:HIS:O	2.54	0.41
1:D:380:VAL:O	1:D:384:CYS:HB2	2.21	0.41
1:A:463:TRP:HA	4:A:902:H4B:N1	2.36	0.41
1:C:127:ARG:HD3	1:C:127:ARG:HA	1.92	0.41
1:A:110:CYS:HB3	1:B:110:CYS:HB3	2.02	0.41
1:C:113:LYS:NZ	1:D:102:HIS:HA	2.36	0.41
1:A:89:ASN:ND2	1:A:91:GLY:N	2.67	0.40
1:C:105:LYS:HE2	1:C:486:SER:HB2	2.04	0.40
1:B:87:ILE:HD13	1:B:87:ILE:HA	1.76	0.40
1:A:459:ALA:HB3	1:A:480:MET:HB3	2.04	0.40
1:A:151:TYR:HA	1:A:154:PHE:CD2	2.56	0.40
1:A:433:ILE:HG13	1:A:434:MET:N	2.36	0.40
1:D:459:ALA:HB1	1:D:464:LEU:CD1	2.52	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	419/424 (99%)	402 (96%)	16 (4%)	1 (0%)	52	59
1	B	419/424 (99%)	398 (95%)	21 (5%)	0	100	100
1	C	421/424 (99%)	400 (95%)	21 (5%)	0	100	100
1	D	419/424 (99%)	401 (96%)	15 (4%)	3 (1%)	26	25
All	All	1678/1696 (99%)	1601 (95%)	73 (4%)	4 (0%)	52	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	HIS
1	D	104	ALA
1	D	157	ALA
1	A	157	ALA

### 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	365/370 (99%)	359 (98%)	6 (2%)	70	82
1	B	365/370 (99%)	361 (99%)	4 (1%)	80	89
1	C	368/370 (100%)	364 (99%)	4 (1%)	80	89
1	D	365/370 (99%)	362 (99%)	3 (1%)	86	93
All	All	1463/1480 (99%)	1446 (99%)	17 (1%)	78	88

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

Mol	Chain	Res	Type
1	A	87	ILE
1	A	89	ASN
1	A	120	MET
1	A	127	ARG
1	A	163	LEU
1	A	283	ASN
1	B	259	VAL

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Mol	Chain	Res	Type
1	B	413	GLN
1	B	481	LEU
1	B	494	GLU
1	C	89	ASN
1	C	111	ARG
1	C	120	MET
1	C	136	PRO
1	D	120	MET
1	D	127	ARG
1	D	218	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	97	GLN
1	A	102	HIS
1	A	148	ASN
1	A	192	GLN
1	A	239	ASN
1	A	255	HIS
1	A	283	ASN
1	A	404	HIS
1	A	427	GLN
1	A	429	GLN
1	A	477	HIS
1	A	502	GLN
1	B	89	ASN
1	B	97	GLN
1	B	102	HIS
1	B	148	ASN
1	B	271	GLN
1	B	288	GLN
1	B	413	GLN
1	B	427	GLN
1	B	477	HIS
1	C	89	ASN
1	C	97	GLN
1	C	102	HIS
1	C	255	HIS
1	C	288	GLN
1	C	404	HIS

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Mol	Chain	Res	Type
1	C	427	GLN
1	C	429	GLN
1	C	477	HIS
1	D	89	ASN
1	D	97	GLN
1	D	239	ASN
1	D	255	HIS
1	D	283	ASN
1	D	310	GLN
1	D	413	GLN
1	D	429	GLN
1	D	448	GLN
1	D	477	HIS
1	D	502	GLN

### 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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
3	HEM	A	901	1	30,50,50	2.66	10 (33%)	24,82,82	2.55	11 (45%)
4	H4B	A	902	-	13,18,18	1.69	2 (15%)	11,26,26	2.06	5 (45%)
5	AT2	A	906	-	20,20,20	1.75	4 (20%)	26,26,26	1.68	5 (19%)
3	HEM	B	1901	1	30,50,50	2.70	12 (40%)	24,82,82	2.28	9 (37%)
4	H4B	B	1902	-	13,18,18	1.67	2 (15%)	11,26,26	2.10	5 (45%)
5	AT2	B	1906	-	20,20,20	1.74	5 (25%)	26,26,26	1.66	5 (19%)
3	HEM	C	2901	1	30,50,50	2.49	8 (26%)	24,82,82	2.35	9 (37%)
4	H4B	C	2902	-	13,18,18	1.63	2 (15%)	11,26,26	2.06	4 (36%)
5	AT2	C	2906	-	20,20,20	1.86	6 (30%)	26,26,26	1.53	5 (19%)
3	HEM	D	3901	1	30,50,50	2.85	10 (33%)	24,82,82	2.32	8 (33%)
4	H4B	D	3902	-	13,18,18	1.82	2 (15%)	11,26,26	2.22	5 (45%)
5	AT2	D	3906	-	20,20,20	1.82	5 (25%)	26,26,26	1.68	5 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	901	1	-	0/10/54/54	0/0/8/8
4	H4B	A	902	-	1/1/3/5	0/8/17/17	0/2/2/2
5	AT2	A	906	-	-	0/11/21/21	0/2/2/2
3	HEM	B	1901	1	-	0/10/54/54	0/0/8/8
4	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
5	AT2	B	1906	-	-	0/11/21/21	0/2/2/2
3	HEM	C	2901	1	-	0/10/54/54	0/0/8/8
4	H4B	C	2902	-	-	0/8/17/17	0/2/2/2
5	AT2	C	2906	-	-	0/11/21/21	0/2/2/2
3	HEM	D	3901	1	-	0/10/54/54	0/0/8/8
4	H4B	D	3902	-	1/1/3/5	0/8/17/17	0/2/2/2
5	AT2	D	3906	-	-	0/11/21/21	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	C2D-C3D	-6.57	1.34	1.54
3	A	901	HEM	C3B-CAB	-6.48	1.39	1.51
3	D	3901	HEM	C3B-C4B	-6.08	1.46	1.51
3	A	901	HEM	C3D-C4D	-6.04	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3901	HEM	C3C-CAC	-6.03	1.40	1.51
3	D	3901	HEM	C2D-C3D	-6.02	1.36	1.54
4	D	3902	H4B	C7-N8	-6.02	1.38	1.46
3	C	2901	HEM	C2D-C3D	-5.88	1.36	1.54
3	C	2901	HEM	C3B-CAB	-5.71	1.40	1.51
3	B	1901	HEM	C3B-CAB	-5.70	1.40	1.51
3	D	3901	HEM	C3D-C4D	-5.64	1.44	1.51
3	B	1901	HEM	C2D-C3D	-5.50	1.38	1.54
4	B	1902	H4B	C7-N8	-5.40	1.39	1.46
4	A	902	H4B	C7-N8	-5.39	1.39	1.46
3	C	2901	HEM	C3C-CAC	-5.34	1.41	1.51
3	B	1901	HEM	C3C-CAC	-5.29	1.41	1.51
4	C	2902	H4B	C7-N8	-5.24	1.39	1.46
3	B	1901	HEM	C3D-C4D	-5.22	1.44	1.51
3	D	3901	HEM	C3B-CAB	-5.18	1.41	1.51
3	C	2901	HEM	C2C-C1C	-5.15	1.42	1.52
3	B	1901	HEM	C3B-C4B	-4.98	1.47	1.51
3	A	901	HEM	C2C-C1C	-4.60	1.43	1.52
3	A	901	HEM	C3C-CAC	-4.57	1.42	1.51
3	B	1901	HEM	C2C-C1C	-4.17	1.44	1.52
3	D	3901	HEM	C2C-C1C	-3.99	1.45	1.52
3	A	901	HEM	C3B-C4B	-3.02	1.49	1.51
3	C	2901	HEM	C2B-C1B	-2.86	1.42	1.51
3	C	2901	HEM	C3B-C4B	-2.64	1.49	1.51
3	D	3901	HEM	C2B-C1B	-2.42	1.43	1.51
4	A	902	H4B	C4A-N5	-2.25	1.32	1.38
3	A	901	HEM	C2D-C1D	-2.21	1.44	1.51
4	C	2902	H4B	C4A-N5	-2.09	1.33	1.38
4	D	3902	H4B	C4A-N5	-2.09	1.33	1.38
3	B	1901	HEM	C2B-C1B	-2.04	1.45	1.51
4	B	1902	H4B	C4A-N5	-2.03	1.33	1.38
5	C	2906	AT2	C3-C4	2.01	1.42	1.38
3	A	901	HEM	CHC-C1C	2.07	1.41	1.36
5	B	1906	AT2	C3-C4	2.11	1.42	1.38
3	B	1901	HEM	CHD-C4C	2.12	1.41	1.36
5	C	2906	AT2	C7-C6	2.14	1.44	1.39
5	C	2906	AT2	C10-C9	2.15	1.57	1.51
5	D	3906	AT2	C3-C4	2.18	1.43	1.38
3	A	901	HEM	C1C-NC	2.20	1.38	1.36
3	B	1901	HEM	C4C-NC	2.23	1.38	1.36
5	A	906	AT2	C3-C4	2.27	1.43	1.38
3	B	1901	HEM	FE-NB	2.32	2.09	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3906	AT2	C10-C9	2.33	1.57	1.51
5	A	906	AT2	C4-N5	2.42	1.39	1.34
3	C	2901	HEM	FE-NB	2.66	2.11	1.97
3	B	1901	HEM	FE-NC	2.72	2.06	1.95
3	A	901	HEM	FE-NC	2.73	2.06	1.95
5	B	1906	AT2	C4-N5	2.74	1.40	1.34
5	C	2906	AT2	C4-N5	2.76	1.40	1.34
3	D	3901	HEM	FE-NC	2.76	2.06	1.95
5	D	3906	AT2	C4-N5	2.79	1.40	1.34
3	D	3901	HEM	CHC-C1C	2.83	1.43	1.36
5	B	1906	AT2	C10-C9	2.99	1.59	1.51
5	B	1906	AT2	C6-N5	3.35	1.40	1.34
3	D	3901	HEM	C1C-NC	3.63	1.40	1.36
3	B	1901	HEM	C1C-NC	3.74	1.40	1.36
3	C	2901	HEM	C1C-NC	3.76	1.40	1.36
5	B	1906	AT2	O16-C15	3.83	1.27	1.21
5	A	906	AT2	C6-N5	3.96	1.41	1.34
5	D	3906	AT2	C6-N5	4.06	1.41	1.34
5	D	3906	AT2	O16-C15	4.23	1.27	1.21
5	A	906	AT2	O16-C15	4.29	1.27	1.21
5	C	2906	AT2	C6-N5	4.40	1.42	1.34
5	C	2906	AT2	O16-C15	4.55	1.28	1.21

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1906	AT2	C7-C6-N5	-3.52	119.12	123.06
5	A	906	AT2	C7-C6-N5	-3.27	119.40	123.06
5	D	3906	AT2	C7-C6-N5	-3.24	119.44	123.06
5	A	906	AT2	C3-C4-N5	-3.09	120.37	123.90
5	C	2906	AT2	C7-C6-N5	-3.08	119.61	123.06
5	B	1906	AT2	C3-C4-N5	-3.05	120.42	123.90
5	D	3906	AT2	C3-C4-N5	-2.98	120.50	123.90
3	D	3901	HEM	CBA-CAA-C2A	-2.83	107.46	112.53
5	C	2906	AT2	C3-C4-N5	-2.79	120.72	123.90
3	C	2901	HEM	CBD-CAD-C3D	-2.74	105.57	113.55
3	A	901	HEM	CBD-CAD-C3D	-2.71	105.66	113.55
3	B	1901	HEM	CBA-CAA-C2A	-2.56	107.94	112.53
4	D	3902	H4B	N3-C2-N1	-2.49	121.45	125.53
4	A	902	H4B	N3-C2-N1	-2.45	121.51	125.53
4	B	1902	H4B	N3-C2-N1	-2.43	121.55	125.53
5	D	3906	AT2	O16-C15-N12	-2.37	119.82	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2902	H4B	N3-C2-N1	-2.33	121.71	125.53
5	A	906	AT2	O16-C15-N12	-2.33	119.89	124.32
5	C	2906	AT2	O16-C15-N12	-2.22	120.10	124.32
5	B	1906	AT2	O16-C15-N12	-2.22	120.10	124.32
3	A	901	HEM	CBA-CAA-C2A	-2.13	108.71	112.53
3	A	901	HEM	CMA-C3A-C4A	-2.09	124.91	128.36
5	C	2906	AT2	C10-C11-N12	-2.06	108.08	111.07
3	A	901	HEM	CMA-C3A-C2A	2.00	129.42	125.24
5	A	906	AT2	C13-C14-C9	2.02	113.61	110.37
5	D	3906	AT2	C18-O17-C15	2.06	119.05	115.63
5	B	1906	AT2	C4-N5-C6	2.12	120.20	117.28
3	B	1901	HEM	C3B-C4B-CHC	2.20	126.25	123.16
4	A	902	H4B	C2-N1-C8A	2.32	119.75	114.54
3	C	2901	HEM	C3B-CAB-CBB	2.37	128.09	124.46
4	B	1902	H4B	C7-C6-N5	2.51	115.66	110.45
3	B	1901	HEM	C3C-CAC-CBC	2.58	128.41	124.46
3	D	3901	HEM	C3B-C4B-CHC	2.72	127.00	123.16
4	C	2902	H4B	C2-N1-C8A	2.74	120.71	114.54
4	A	902	H4B	C7-C6-N5	2.79	116.25	110.45
4	D	3902	H4B	C2-N1-C8A	2.84	120.92	114.54
3	A	901	HEM	CMD-C2D-C3D	2.84	126.92	114.35
4	B	1902	H4B	C2-N1-C8A	2.85	120.95	114.54
4	B	1902	H4B	C4-C4A-C8A	2.86	117.16	114.56
4	D	3902	H4B	C7-C6-N5	2.90	116.46	110.45
4	A	902	H4B	C4-C4A-C8A	2.90	117.19	114.56
4	D	3902	H4B	C4-C4A-C8A	2.96	117.24	114.56
3	D	3901	HEM	C2D-C3D-C4D	2.98	106.55	101.50
4	C	2902	H4B	C4-C4A-C8A	3.01	117.29	114.56
3	B	1901	HEM	CMD-C2D-C3D	3.16	128.34	114.35
3	D	3901	HEM	CMD-C2D-C3D	3.17	128.38	114.35
4	A	902	H4B	C4-N3-C2	3.18	120.35	115.94
4	B	1902	H4B	C4-N3-C2	3.36	120.60	115.94
3	C	2901	HEM	CMD-C2D-C3D	3.45	129.60	114.35
3	C	2901	HEM	CMB-C2B-C3B	3.46	125.17	116.53
5	B	1906	AT2	O17-C15-N12	3.48	114.39	111.59
3	C	2901	HEM	C3B-C4B-CHC	3.48	128.07	123.16
3	C	2901	HEM	C2D-C3D-C4D	3.51	107.44	101.50
3	C	2901	HEM	CAD-C3D-C4D	3.52	124.88	112.47
3	B	1901	HEM	CAD-C3D-C4D	3.63	125.26	112.47
3	A	901	HEM	C3B-C4B-CHC	3.66	128.32	123.16
4	C	2902	H4B	C4-N3-C2	3.66	121.03	115.94
4	D	3902	H4B	C4-N3-C2	3.77	121.18	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1901	HEM	C2D-C3D-C4D	3.83	108.00	101.50
5	C	2906	AT2	O17-C15-N12	3.84	114.68	111.59
3	B	1901	HEM	CMB-C2B-C3B	3.85	126.15	116.53
3	A	901	HEM	CMB-C2B-C3B	4.05	126.64	116.53
3	A	901	HEM	CAD-C3D-C4D	4.09	126.89	112.47
3	D	3901	HEM	CAD-C3D-C4D	4.20	127.27	112.47
5	D	3906	AT2	O17-C15-N12	4.22	114.99	111.59
3	C	2901	HEM	CMC-C2C-C3C	4.24	127.12	116.53
3	A	901	HEM	CMC-C2C-C3C	4.24	127.13	116.53
3	D	3901	HEM	CMB-C2B-C3B	4.32	127.31	116.53
5	A	906	AT2	O17-C15-N12	4.42	115.15	111.59
3	D	3901	HEM	CAD-C3D-C2D	4.49	126.13	113.22
3	A	901	HEM	C3C-CAC-CBC	4.67	131.61	124.46
3	B	1901	HEM	CAD-C3D-C2D	4.70	126.73	113.22
3	B	1901	HEM	CMC-C2C-C3C	4.78	128.47	116.53
3	C	2901	HEM	CAD-C3D-C2D	5.02	127.65	113.22
3	D	3901	HEM	CMC-C2C-C3C	5.17	129.42	116.53
3	A	901	HEM	CAD-C3D-C2D	5.26	128.34	113.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	3902	H4B	C6
4	A	902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	H4B	1	0
4	B	1902	H4B	2	0
3	C	2901	HEM	1	0
4	C	2902	H4B	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	421/424 (99%)	-0.16	11 (2%) 59 58	29, 46, 79, 95	0
1	B	421/424 (99%)	-0.13	14 (3%) 50 49	30, 48, 80, 101	0
1	C	423/424 (99%)	-0.31	10 (2%) 62 61	25, 43, 73, 92	0
1	D	421/424 (99%)	-0.10	17 (4%) 42 41	29, 45, 75, 93	0
All	All	1686/1696 (99%)	-0.17	52 (3%) 52 51	25, 45, 77, 101	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	ARG	4.5
1	C	155	LYS	4.2
1	B	155	LYS	4.1
1	C	504	GLU	4.0
1	B	156	GLU	3.8
1	B	502	GLN	3.5
1	B	500	VAL	3.5
1	A	111	ARG	3.5
1	D	155	LYS	3.4
1	B	84	HIS	3.4
1	B	175	THR	3.3
1	A	500	VAL	3.3
1	C	83	ARG	3.3
1	D	111	ARG	3.2
1	A	155	LYS	3.2
1	A	156	GLU	3.0
1	A	86	ARG	3.0
1	A	452	ARG	3.0
1	C	156	GLU	2.9
1	D	452	ARG	2.9
1	B	171	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	111	ARG	2.8
1	D	94	MET	2.8
1	D	84	HIS	2.8
1	B	452	ARG	2.7
1	C	84	HIS	2.7
1	B	83	ARG	2.7
1	D	352	VAL	2.7
1	B	501	TRP	2.5
1	C	112	SER	2.5
1	B	157	ALA	2.5
1	C	107	ILE	2.5
1	D	369	PHE	2.4
1	A	84	HIS	2.4
1	D	86	ARG	2.4
1	A	83	ARG	2.4
1	D	176	THR	2.3
1	A	171	LYS	2.3
1	D	500	VAL	2.2
1	D	160	GLU	2.2
1	D	109	THR	2.2
1	D	174	GLU	2.1
1	C	502	GLN	2.1
1	D	171	LYS	2.1
1	D	502	GLN	2.1
1	D	83	ARG	2.1
1	D	131	ASP	2.1
1	A	159	ILE	2.1
1	C	405	LYS	2.1
1	A	154	PHE	2.0
1	B	94	MET	2.0
1	B	503	ASP	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 [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
4	H4B	D	3902	17/17	0.91	0.23	2.15	57,59,65,66	0
5	AT2	C	2906	19/19	0.98	0.17	1.65	24,27,34,34	0
5	AT2	A	906	19/19	0.98	0.19	1.38	27,29,31,31	0
4	H4B	A	902	17/17	0.94	0.20	1.35	53,55,62,63	0
5	AT2	D	3906	19/19	0.98	0.23	1.24	27,31,37,38	0
3	HEM	D	3901	43/43	0.98	0.23	1.18	30,32,39,43	0
3	HEM	A	901	43/43	0.98	0.19	1.14	29,31,34,39	0
5	AT2	B	1906	19/19	0.97	0.16	1.02	27,30,37,37	0
4	H4B	B	1902	17/17	0.92	0.19	0.97	58,59,65,65	0
3	HEM	B	1901	43/43	0.98	0.17	0.97	32,34,37,39	0
3	HEM	C	2901	43/43	0.99	0.15	0.63	25,29,34,38	0
4	H4B	C	2902	17/17	0.92	0.15	0.59	61,63,67,67	0
2	ZN	C	3002	1/1	0.98	0.07	-1.57	73,73,73,73	0
2	ZN	A	3001	1/1	0.99	0.10	-2.31	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.