



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 08:35 PM EST

PDB ID : 1DF1  
Title : MURINE INOSOXOXY DIMER WITH ISOTHIOUREA BOUND IN THE ACTIVE SITE  
Authors : Crane, B.R.; Rosenfeld, R.J.; Arvai, A.S.; Ghosh, D.K.; Ghosh, S.; Tainer, J.A.; Stuehr, D.J.; Getzoff, E.D.  
Deposited on : 1999-11-16  
Resolution : 2.35 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : rb-20030736  
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) : rb-20030736

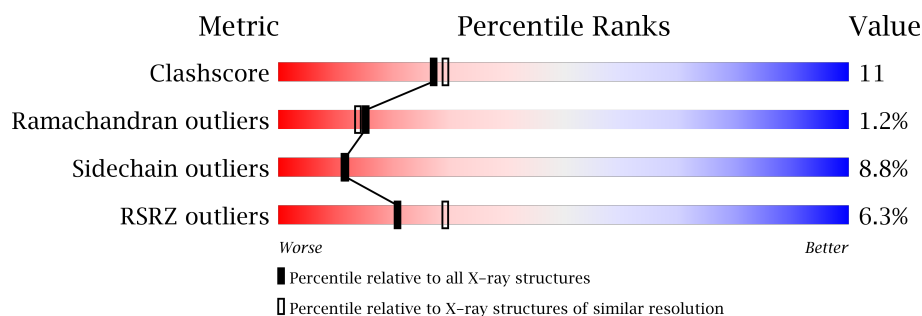
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	423	
1	B	423	

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
5	ITU	B	1899	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7198 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.

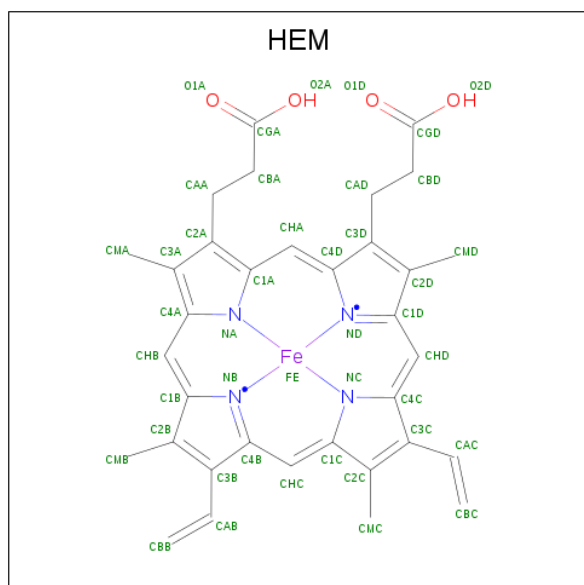
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3423	2194	590	618	21			
1	B	420	Total	C	N	O	S	0	0	0
			3423	2194	590	618	21			

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

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

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



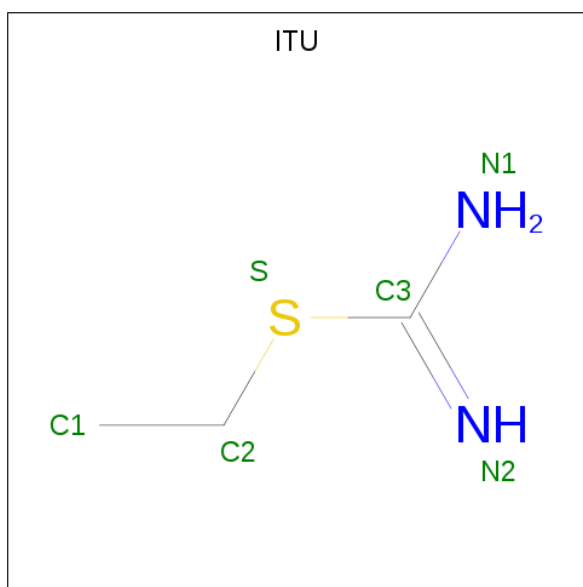
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- 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		
			17	9	5	3		
4	B	1	Total	C	N	O		
			17	9	5	3		

- Molecule 5 is ETHYLISOTHIOUREA (three-letter code: ITU) (formula:  $C_3H_8N_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			6	3	2	1		
5	B	1	Total	C	N	S	0	0
			6	3	2	1		

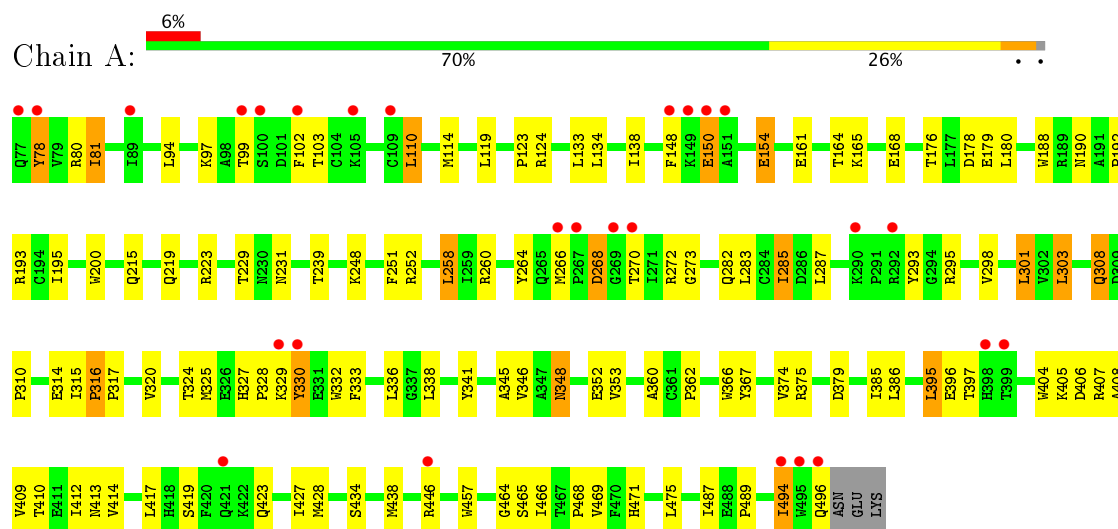
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	0
			107	107		
6	B	111	Total	O	0	0
			111	111		

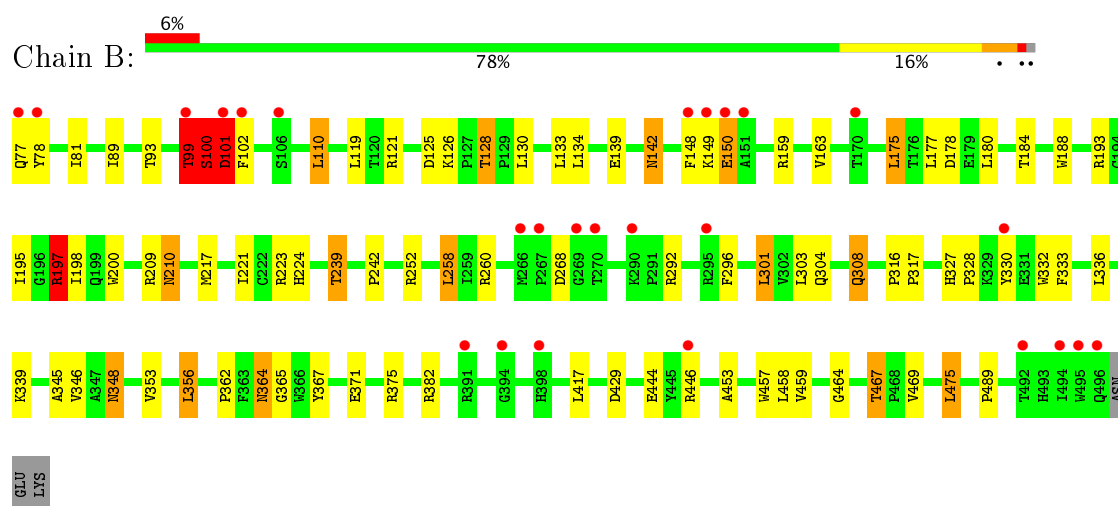
### 3 Residue-property plots

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: NITRIC OXIDE SYNTHASE



#### • Molecule 1: NITRIC OXIDE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.46 Å   214.46 Å   112.75 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.35 19.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.35) 92.4 (19.98-2.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.35 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.223 ,   0.298 0.238 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: HEM, ZN, ITU, 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	0.60	0/3523	0.81	1/4789 (0.0%)
1	B	0.59	0/3523	0.82	5/4789 (0.1%)
All	All	0.59	0/7046	0.82	6/9578 (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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	197	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	110	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	101	ASP	CA-C-N	-5.40	105.31	117.20
1	B	99	THR	N-CA-C	-5.30	96.68	111.00
1	B	175	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	110	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	ASP	Mainchain



## 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	3423	0	3320	85	0
1	B	3423	0	3320	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
4	A	17	0	14	0	0
4	B	17	0	14	0	0
5	A	6	0	7	1	0
5	B	6	0	7	7	0
6	A	107	0	0	20	1
6	B	111	0	0	28	0
All	All	7198	0	6742	156	1

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 11.

All (156) 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)
5:B:1899:ITU:S	6:B:1125:HOH:O	2.30	0.89
1:B:364:ASN:HA	6:B:1124:HOH:O	1.74	0.86
1:A:195:ILE:HG13	6:A:1031:HOH:O	1.83	0.79
1:A:404:TRP:HE3	6:A:1063:HOH:O	1.67	0.76
1:B:217:MET:HB3	1:B:303:LEU:HD23	1.68	0.74
1:A:239:THR:HB	6:A:909:HOH:O	1.88	0.72
3:B:901:HEM:HHC	6:B:1090:HOH:O	1.90	0.72
5:B:1899:ITU:H12	6:B:1124:HOH:O	1.89	0.70
1:B:301:LEU:HB3	1:B:303:LEU:HD11	1.73	0.70
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.78	0.66
1:A:457:TRP:CE3	6:A:1131:HOH:O	2.49	0.66
1:A:80:ARG:NH2	6:A:1121:HOH:O	2.29	0.65
1:B:239:THR:HG23	1:B:362:PRO:HG2	1.78	0.65
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.11	0.65
3:B:901:HEM:HMC2	6:B:1090:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1899:ITU:H13	6:B:1123:HOH:O	1.98	0.64
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.45	0.63
1:A:405:LYS:O	1:A:409:VAL:HG23	1.99	0.63
1:A:348:ASN:H	1:A:348:ASN:HD22	1.47	0.62
1:A:408:ALA:HB2	6:A:1063:HOH:O	1.99	0.62
1:B:303:LEU:HD12	1:B:303:LEU:N	2.15	0.62
1:A:348:ASN:ND2	1:A:348:ASN:H	1.97	0.61
1:A:266:MET:SD	1:A:272:ARG:HD3	2.41	0.61
1:A:457:TRP:HE3	6:A:1131:HOH:O	1.83	0.60
3:A:901:HEM:HH A	6:A:1131:HOH:O	2.01	0.60
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.16	0.60
1:A:223:ARG:HD3	6:A:993:HOH:O	2.01	0.60
1:B:195:ILE:HG13	6:B:1002:HOH:O	2.02	0.60
1:B:346:VAL:HB	6:B:945:HOH:O	2.01	0.59
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.85	0.58
1:A:154:GLU:CD	1:A:154:GLU:H	2.06	0.58
1:A:465:SER:O	1:A:471:HIS:HE1	1.87	0.58
1:B:345:ALA:HA	6:B:1124:HOH:O	2.03	0.58
1:A:348:ASN:HD22	1:A:348:ASN:N	2.00	0.57
1:B:239:THR:HB	6:B:1105:HOH:O	2.05	0.57
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.71	0.56
1:B:99:THR:O	1:B:100:SER:O	2.24	0.56
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.88	0.55
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.88	0.55
1:B:365:GLY:HA3	6:B:1090:HOH:O	2.08	0.54
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.88	0.54
1:B:89:ILE:HD11	6:B:1122:HOH:O	2.07	0.54
1:A:301:LEU:HD22	1:A:315:ILE:HG12	1.90	0.54
5:B:1899:ITU:H11	6:B:1000:HOH:O	2.06	0.54
1:B:195:ILE:HD13	6:B:1137:HOH:O	2.08	0.54
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.89	0.54
1:A:494:ILE:H	1:A:494:ILE:HD12	1.73	0.53
1:B:149:LYS:O	1:B:150:GLU:HG2	2.08	0.53
5:B:1899:ITU:C1	6:B:1123:HOH:O	2.54	0.53
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.90	0.53
1:B:128:THR:HG23	6:B:1080:HOH:O	2.09	0.53
1:A:239:THR:HG23	1:A:362:PRO:HG2	1.91	0.53
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.45	0.53
1:B:209:ARG:O	1:B:242:PRO:HG3	2.09	0.52
1:B:346:VAL:HG21	6:B:1000:HOH:O	2.09	0.52
5:B:1899:ITU:H21	6:B:999:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:HB2	6:A:995:HOH:O	2.11	0.51
1:B:159:ARG:O	1:B:163:VAL:HG23	2.10	0.51
1:A:102:PHE:CG	1:A:103:THR:N	2.78	0.51
1:A:410:THR:O	1:A:414:VAL:HG23	2.11	0.51
1:B:365:GLY:N	6:B:1125:HOH:O	2.42	0.51
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.46	0.51
1:B:348:ASN:H	1:B:348:ASN:ND2	2.08	0.50
1:B:356:LEU:HG	6:B:1106:HOH:O	2.10	0.50
1:A:124:ARG:NH1	1:A:124:ARG:HG3	2.26	0.50
1:B:304:GLN:HG3	1:B:308:GLN:O	2.11	0.50
1:A:348:ASN:ND2	1:A:348:ASN:N	2.59	0.49
1:B:382:ARG:NH2	6:B:1126:HOH:O	2.45	0.49
1:A:134:LEU:O	1:A:138:ILE:HG12	2.13	0.49
1:A:272:ARG:HG2	1:A:295:ARG:HE	1.78	0.49
1:B:467:THR:HG23	1:B:469:VAL:HG22	1.94	0.49
1:A:150:GLU:HG2	1:A:150:GLU:O	2.14	0.47
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.29	0.47
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.96	0.47
1:B:348:ASN:H	1:B:348:ASN:HD22	1.63	0.47
1:A:366:TRP:HB2	6:A:907:HOH:O	2.14	0.47
1:A:438:MET:CE	1:A:469:VAL:HG12	2.44	0.47
1:B:210:ASN:ND2	1:B:210:ASN:H	2.11	0.47
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.97	0.47
1:A:330:TYR:HB3	1:A:332:TRP:NE1	2.29	0.47
1:B:210:ASN:N	1:B:210:ASN:HD22	2.12	0.47
1:B:195:ILE:N	6:B:1002:HOH:O	2.49	0.46
1:A:324:THR:H	1:A:423:GLN:HE22	1.63	0.46
1:B:180:LEU:O	1:B:184:THR:HG23	2.16	0.46
1:B:356:LEU:HD13	1:B:356:LEU:HA	1.74	0.46
1:B:464:GLY:O	1:B:467:THR:HG22	2.16	0.46
1:A:367:TYR:HD2	6:A:1071:HOH:O	1.99	0.45
1:A:413:ASN:O	1:A:417:LEU:HD13	2.17	0.45
1:B:371:GLU:OE2	5:B:1899:ITU:N2	2.49	0.45
1:B:367:TYR:HD2	6:B:1053:HOH:O	1.99	0.45
1:A:248:LYS:HB2	6:A:990:HOH:O	2.16	0.45
1:B:417:LEU:HD21	1:B:429:ASP:HB3	1.97	0.45
1:A:346:VAL:HG23	5:A:899:ITU:H11	1.99	0.45
1:B:197:ARG:H	1:B:197:ARG:HG2	1.61	0.45
1:B:210:ASN:HD22	1:B:210:ASN:H	1.65	0.45
1:A:374:VAL:CG2	1:A:413:ASN:HD21	2.29	0.44
1:A:272:ARG:HG2	1:A:295:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.98	0.44
1:A:303:LEU:O	1:A:310:PRO:HA	2.16	0.44
1:B:371:GLU:HB3	6:B:1021:HOH:O	2.16	0.44
1:A:466:ILE:HG22	1:A:466:ILE:O	2.18	0.44
1:B:348:ASN:N	1:B:348:ASN:HD22	2.14	0.44
1:A:283:LEU:O	1:A:287:LEU:HG	2.16	0.44
1:A:78:TYR:C	1:A:78:TYR:CD1	2.90	0.44
3:A:901:HEM:HAA1	6:A:1131:HOH:O	2.18	0.44
1:B:77:GLN:HG3	1:B:78:TYR:H	1.83	0.44
1:B:224:HIS:HB2	6:B:1105:HOH:O	2.17	0.43
1:B:193:ARG:HB3	1:B:457:TRP:CE3	2.52	0.43
1:A:215:GLN:HE21	1:A:219:GLN:NE2	2.14	0.43
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.82	0.43
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.18	0.43
1:A:408:ALA:CB	6:A:1063:HOH:O	2.62	0.43
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.78	0.43
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.53	0.43
1:A:190:ASN:O	1:A:192:PRO:HD3	2.19	0.43
1:A:407:ARG:HH11	1:A:407:ARG:HG3	1.83	0.43
1:A:438:MET:HE2	1:A:469:VAL:HG12	2.01	0.43
1:B:258:LEU:HA	1:B:258:LEU:HD12	1.90	0.43
1:A:333:PHE:O	1:A:336:LEU:HB2	2.19	0.43
1:A:397:THR:HG22	1:A:397:THR:O	2.18	0.43
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.34	0.43
1:A:272:ARG:HE	1:A:295:ARG:HG3	1.84	0.43
1:A:329:LYS:HB3	1:A:330:TYR:HD1	1.84	0.43
1:B:333:PHE:O	1:B:336:LEU:HB2	2.19	0.43
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.53	0.42
1:B:296:PHE:HB2	1:B:339:LYS:HE3	2.01	0.42
1:A:193:ARG:HD2	6:A:1033:HOH:O	2.19	0.42
1:A:341:TYR:HB2	6:A:1070:HOH:O	2.20	0.42
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.35	0.42
1:A:325:MET:HA	1:A:419:SER:OG	2.19	0.42
1:A:386:LEU:HD21	1:A:409:VAL:HG22	2.02	0.42
1:A:94:LEU:HD12	1:A:97:LYS:HD2	2.01	0.42
1:B:330:TYR:HD2	1:B:332:TRP:HE1	1.66	0.42
1:A:165:LYS:HE3	1:A:165:LYS:HB2	1.88	0.41
1:A:248:LYS:HD2	6:A:990:HOH:O	2.20	0.41
1:A:164:THR:O	1:A:168:GLU:HG2	2.20	0.41
1:A:251:PHE:O	1:A:360:ALA:HB2	2.21	0.41
1:A:273:GLY:HA3	6:A:1060:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:HB2	6:B:1055:HOH:O	2.20	0.41
1:A:154:GLU:N	1:A:154:GLU:CD	2.74	0.41
1:A:366:TRP:H	3:A:901:HEM:HAB	1.85	0.41
1:A:316:PRO:HA	1:A:317:PRO:HD3	1.89	0.41
1:B:195:ILE:HG22	1:B:195:ILE:O	2.20	0.41
1:B:198:ILE:HG22	6:B:953:HOH:O	2.20	0.41
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.51	0.41
1:A:282:GLN:O	1:A:285:ILE:HG22	2.21	0.41
1:B:142:ASN:HD22	1:B:142:ASN:N	2.18	0.41
1:A:123:PRO:HD3	1:A:487:ILE:HD12	2.02	0.40
1:A:229:THR:HG22	1:A:231:ASN:H	1.86	0.40
1:A:272:ARG:NE	1:A:295:ARG:HG3	2.36	0.40
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.87	0.40
1:A:352:GLU:HG3	1:A:353:VAL:N	2.36	0.40
1:B:102:PHE:HB2	6:B:1135:HOH:O	2.22	0.40
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.84	0.40
1:A:195:ILE:HB	6:A:975:HOH:O	2.22	0.40
1:A:427:ILE:HG13	1:A:428:MET:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1101:HOH:O	6:A:1101:HOH:O[11_655]	0.33	1.87

## 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	418/423 (99%)	381 (91%)	30 (7%)	7 (2%)	<b>11</b> <b>8</b>
1	B	418/423 (99%)	385 (92%)	30 (7%)	3 (1%)	<b>25</b> <b>27</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	836/846 (99%)	766 (92%)	60 (7%)	10 (1%)	15	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	293	TYR
1	A	308	GLN
1	A	395	LEU
1	B	100	SER
1	B	308	GLN
1	A	464	GLY
1	A	270	THR
1	A	268	ASP
1	B	150	GLU

### 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	368/371 (99%)	338 (92%)	30 (8%)	13	14
1	B	368/371 (99%)	333 (90%)	35 (10%)	10	9
All	All	736/742 (99%)	671 (91%)	65 (9%)	12	11

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	81	ILE
1	A	110	LEU
1	A	114	MET
1	A	119	LEU
1	A	133	LEU
1	A	150	GLU
1	A	154	GLU

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Mol	Chain	Res	Type
1	A	161	GLU
1	A	178	ASP
1	A	180	LEU
1	A	258	LEU
1	A	260	ARG
1	A	264	TYR
1	A	268	ASP
1	A	285	ILE
1	A	301	LEU
1	A	303	LEU
1	A	308	GLN
1	A	314	GLU
1	A	316	PRO
1	A	330	TYR
1	A	338	LEU
1	A	348	ASN
1	A	395	LEU
1	A	396	GLU
1	A	406	ASP
1	A	446	ARG
1	A	494	ILE
1	A	496	GLN
1	B	93	THR
1	B	99	THR
1	B	100	SER
1	B	101	ASP
1	B	110	LEU
1	B	119	LEU
1	B	125	ASP
1	B	126	LYS
1	B	128	THR
1	B	130	LEU
1	B	133	LEU
1	B	134	LEU
1	B	139	GLU
1	B	142	ASN
1	B	148	PHE
1	B	175	LEU
1	B	177	LEU
1	B	178	ASP
1	B	197	ARG
1	B	210	ASN

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Mol	Chain	Res	Type
1	B	223	ARG
1	B	239	THR
1	B	258	LEU
1	B	260	ARG
1	B	268	ASP
1	B	292	ARG
1	B	301	LEU
1	B	348	ASN
1	B	353	VAL
1	B	356	LEU
1	B	364	ASN
1	B	444	GLU
1	B	446	ARG
1	B	467	THR
1	B	475	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	348	ASN
1	A	413	ASN
1	A	443	ASN
1	A	471	HIS
1	B	95	HIS
1	B	142	ASN
1	B	156	HIS
1	B	210	ASN
1	B	220	HIS
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	493	HIS

### 5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
5	ITU	A	899	-	4,5,5	1.01	0	3,5,5	1.95	1 (33%)
3	HEM	A	901	1	28,50,50	1.95	7 (25%)	17,82,82	1.99	4 (23%)
4	H4B	A	902	-	14,18,18	0.60	0	12,26,26	2.29	6 (50%)
5	ITU	B	1899	-	4,5,5	1.26	0	3,5,5	5.13	1 (33%)
4	H4B	B	1902	-	14,18,18	0.67	0	12,26,26	2.34	6 (50%)
3	HEM	B	901	1	28,50,50	2.07	8 (28%)	17,82,82	2.00	4 (23%)

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
5	ITU	A	899	-	-	0/3/3/3	0/0/0/0
3	HEM	A	901	1	-	0/6/54/54	0/0/8/8
4	H4B	A	902	-	-	0/8/17/17	0/2/2/2
5	ITU	B	1899	-	-	0/3/3/3	0/0/0/0
4	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
3	HEM	B	901	1	-	0/6/54/54	0/0/8/8

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	C3B-CAB	-4.95	1.38	1.47
3	B	901	HEM	C3B-CAB	-4.63	1.38	1.47
3	B	901	HEM	C3B-C2B	-3.89	1.35	1.40
3	B	901	HEM	C3C-CAC	-3.64	1.40	1.47
3	A	901	HEM	C3C-CAC	-2.59	1.42	1.47
3	B	901	HEM	CAD-C3D	-2.05	1.48	1.52
3	A	901	HEM	C1A-NA	2.53	1.41	1.36
3	A	901	HEM	C1D-ND	2.61	1.41	1.36
3	B	901	HEM	C1D-ND	3.08	1.42	1.36
3	A	901	HEM	C4A-NA	3.20	1.43	1.36
3	B	901	HEM	C4A-NA	3.22	1.43	1.36
3	B	901	HEM	C1B-NB	3.27	1.40	1.36
3	A	901	HEM	C1B-NB	3.91	1.41	1.36
3	B	901	HEM	C4C-NC	4.16	1.41	1.36
3	A	901	HEM	C4C-NC	4.19	1.41	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1899	ITU	C2-S-C3	-8.80	93.88	103.16
3	B	901	HEM	C1D-C2D-C3D	-5.29	103.31	107.00
3	A	901	HEM	C4C-C3C-C2C	-5.17	103.28	106.90
3	B	901	HEM	C4C-C3C-C2C	-4.11	104.03	106.90
5	A	899	ITU	C2-S-C3	-3.34	99.64	103.16
3	A	901	HEM	C1D-C2D-C3D	-2.87	105.00	107.00
4	B	1902	H4B	N3-C2-N1	-2.48	121.43	125.45
3	A	901	HEM	CMA-C3A-C4A	-2.48	124.66	128.46
3	B	901	HEM	CAD-C3D-C2D	-2.45	122.01	129.00
4	A	902	H4B	N3-C2-N1	-2.40	121.56	125.45
3	B	901	HEM	CMC-C2C-C3C	2.60	129.71	124.89
4	A	902	H4B	C2-N1-C8A	2.86	120.96	114.51
4	A	902	H4B	C4-C4A-C8A	2.93	117.21	114.56
4	A	902	H4B	C4-N3-C2	2.96	120.31	116.06
4	B	1902	H4B	C2-N1-C8A	3.03	121.33	114.51
4	B	1902	H4B	C4-C4A-C8A	3.11	117.38	114.56
4	B	1902	H4B	C4-N3-C2	3.15	120.59	116.06
3	A	901	HEM	CMC-C2C-C3C	3.29	131.00	124.89
4	A	902	H4B	C6-C7-N8	3.45	116.48	111.01
4	B	1902	H4B	C7-C6-N5	3.49	117.48	110.31
4	B	1902	H4B	C6-C7-N8	3.59	116.72	111.01
4	A	902	H4B	C7-C6-N5	3.79	118.09	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	899	ITU	1	0
3	A	901	HEM	3	0
5	B	1899	ITU	7	0
3	B	901	HEM	2	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	420/423 (99%)	0.24	27 (6%) 20 29	18, 45, 78, 91	9 (2%)
1	B	420/423 (99%)	0.26	26 (6%) 21 30	25, 45, 76, 98	9 (2%)
All	All	840/846 (99%)	0.25	53 (6%) 21 29	18, 45, 77, 98	18 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	TRP	4.9
1	B	290	LYS	4.4
1	B	267	PRO	4.3
1	B	270	THR	4.2
1	B	106	SER	4.1
1	B	494	ILE	3.8
1	A	330	TYR	3.7
1	A	77	GLN	3.6
1	A	148	PHE	3.5
1	B	77	GLN	3.4
1	B	99	THR	3.4
1	B	269	GLY	3.4
1	A	149	LYS	3.2
1	A	495	TRP	3.2
1	B	149	LYS	3.2
1	A	105	LYS	3.2
1	B	150	GLU	3.2
1	B	78	TYR	3.2
1	B	492	THR	3.1
1	A	99	THR	3.0
1	A	267	PRO	3.0
1	A	290	LYS	2.9
1	B	394	GLY	2.9
1	B	151	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	151	ALA	2.9
1	B	496	GLN	2.8
1	A	269	GLY	2.6
1	A	496	GLN	2.6
1	A	292	ARG	2.6
1	A	329	LYS	2.6
1	B	295	ARG	2.6
1	A	494	ILE	2.6
1	A	78	TYR	2.5
1	B	101	ASP	2.5
1	B	102	PHE	2.5
1	B	148	PHE	2.5
1	B	330	TYR	2.4
1	A	89	ILE	2.4
1	A	446	ARG	2.4
1	A	398	HIS	2.3
1	B	446	ARG	2.3
1	B	170	THR	2.3
1	A	150	GLU	2.3
1	A	109	CYS	2.3
1	B	398	HIS	2.3
1	A	266	MET	2.2
1	B	391	ARG	2.1
1	A	102	PHE	2.1
1	A	270	THR	2.1
1	B	266	MET	2.1
1	A	421	GLN	2.1
1	A	100	SER	2.0
1	A	399	THR	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
5	ITU	B	1899	6/6	0.97	0.12	-0.48	19,29,35,39	0
5	ITU	A	899	6/6	0.98	0.11	-1.00	22,24,27,34	0
3	HEM	A	901	43/43	0.98	0.09	-1.13	17,24,30,34	0
4	H4B	B	1902	17/17	0.97	0.09	-1.23	20,24,33,34	0
3	HEM	B	901	43/43	0.98	0.09	-1.26	18,24,30,36	0
4	H4B	A	902	17/17	0.97	0.07	-2.15	19,23,31,31	0
2	ZN	A	900	1/1	0.79	0.11	-	78,78,78,78	1
2	ZN	B	900	1/1	0.81	0.11	-	52,52,52,52	1

## 6.5 Other polymers

There are no such residues in this entry.