Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E6T
Title	:	Structure of murine INOS oxygenase domain with inhibitor AR-C118901
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	:	2008-08-15
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

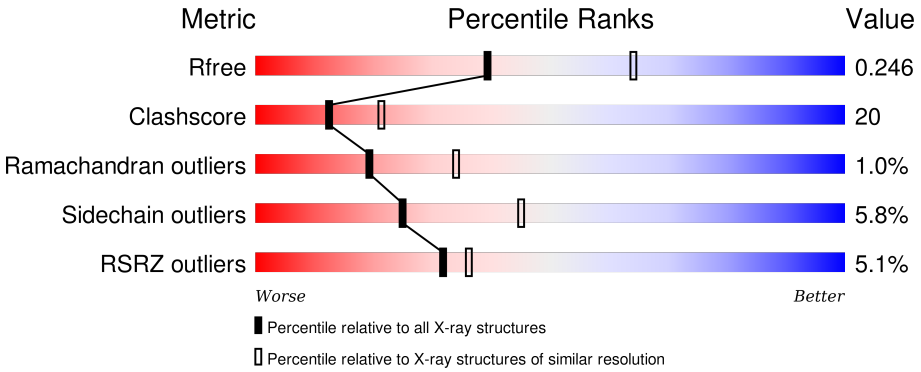
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 >=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 <=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	433	6%, 61%, 31%
1	B	433	4%, 64%, 27%, 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	A	902	X	-	-	-

2 Entry composition

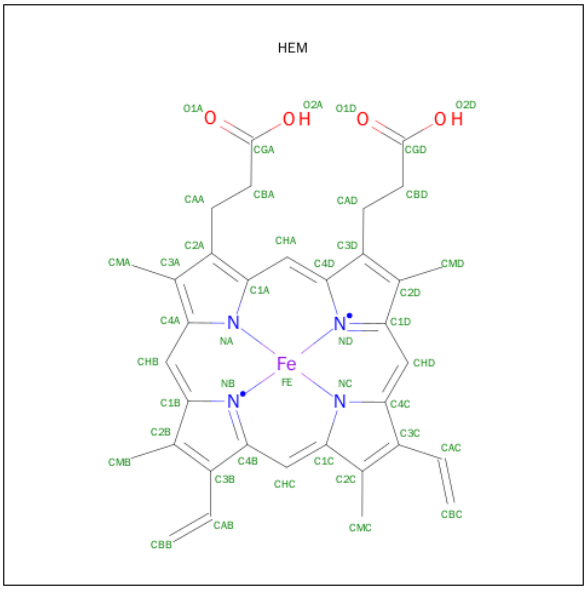
There are 5 unique types of molecules in this entry. The entry contains 7161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

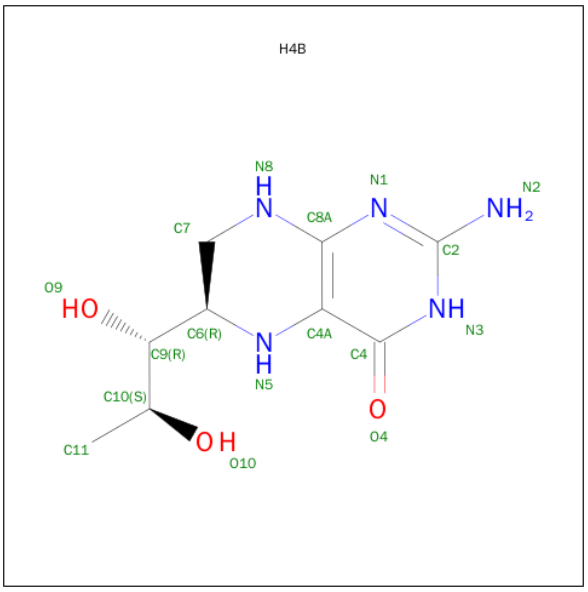
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3385	2171	582	612	20			
1	B	410	Total	C	N	O	S	0	0	0
			3347	2148	577	602	20			

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



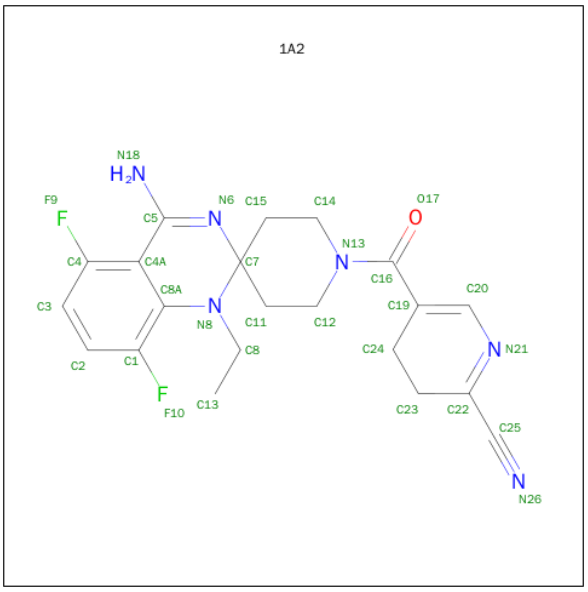
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is 5-(4'-AMINO-1'-ETHYL-5',8'-DIFLUORO-1'H-SPIRO[PIPERIDINE-4,2'-QUINAZOLINE]-1-YLCARBONYL)PICOLINONITRILE (three-letter code: 1A2) (formula: $C_{21}H_{22}F_2N_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			30	21	2	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			30	21	2	6	1		

- Molecule 5 is water.

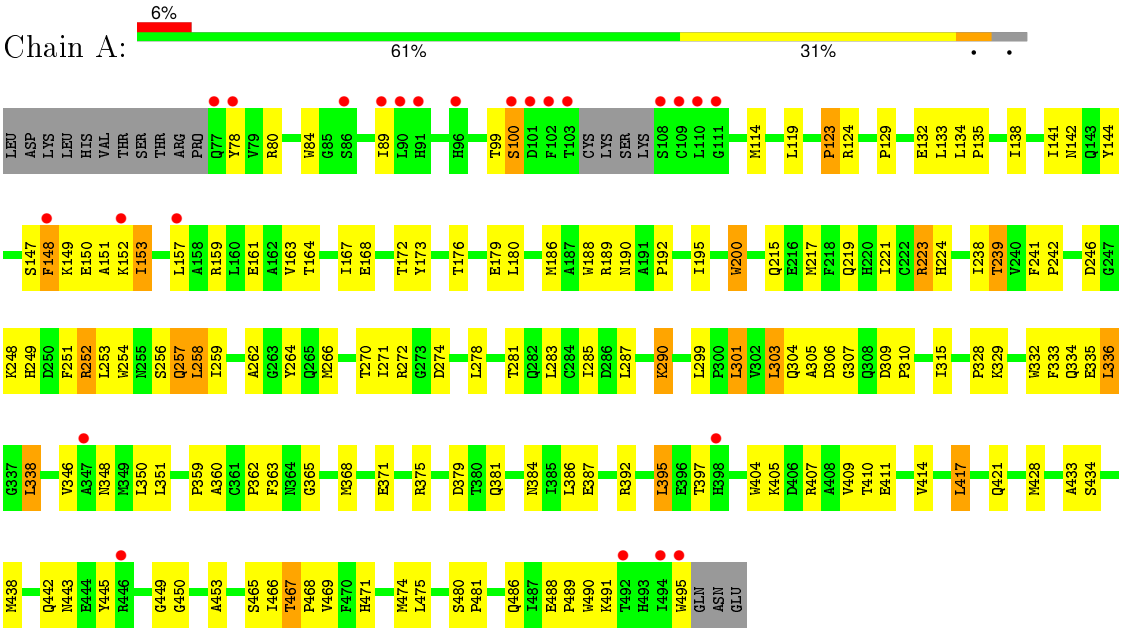
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	137	Total	O	0	0
			137	137		

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.

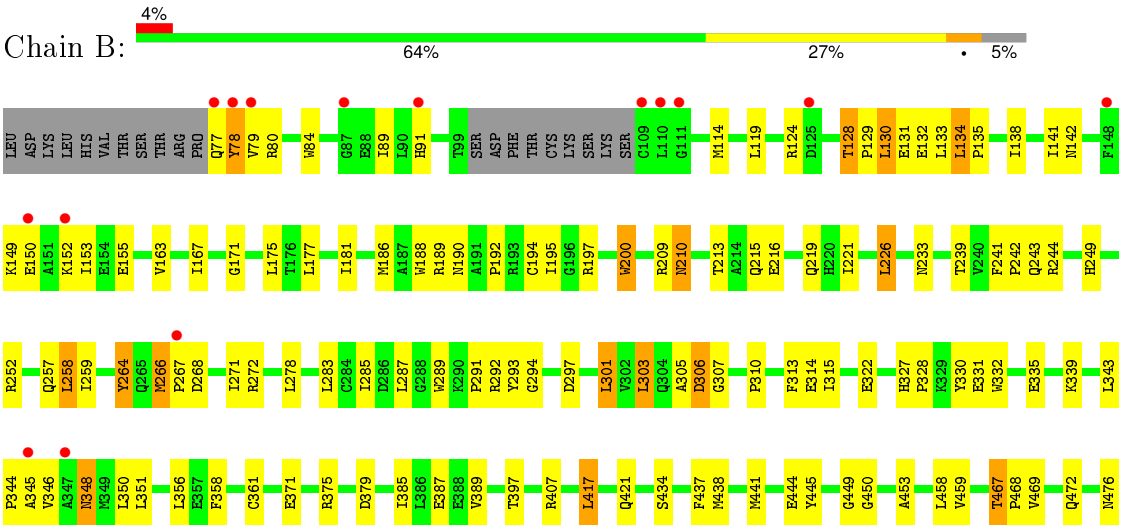
- Molecule 1: Nitric oxide synthase, inducible

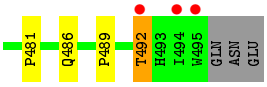
Chain A:



- Molecule 1: Nitric oxide synthase, inducible

Chain B:




P481
Q486
P489
T492
H493
I494
W495
GLN
ASN
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	213.99Å 213.99Å 116.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 2.50 29.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (19.98-2.50) 88.8 (29.86-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.267 0.226 , 0.246	Depositor DCC
R_{free} test set	2649 reflections (5.76%)	DCC
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 52558 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7161	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, H4B, 1A2

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	0.38	0/3484	0.63	1/4737 (0.0%)
1	B	0.37	0/3445	0.63	0/4684
All	All	0.38	0/6929	0.63	1/9421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	GLY	N-CA-C	-5.28	99.89	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3385	0	3278	150	0
1	B	3347	0	3248	111	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	14	0	0
3	B	17	0	14	0	0
4	A	30	0	22	3	0
4	B	30	0	22	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	112	0	0	16	0
5	B	137	0	0	4	0
All	All	7161	0	6658	265	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 20.

All (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HB	5:B:2039:HOH:O	1.32	1.30
1:A:153:ILE:HD12	1:A:153:ILE:H	1.22	1.00
2:A:901:HEM:HBA2	4:A:905:1A2:H82	1.42	1.00
1:A:99:THR:HG22	1:A:100:SER:H	1.31	0.93
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.51	0.90
2:B:901:HEM:HBA2	4:B:905:1A2:H82	1.56	0.87
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.44	0.81
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.66	0.78
1:A:99:THR:HG22	1:A:100:SER:N	1.98	0.77
1:A:134:LEU:O	1:A:138:ILE:HG12	1.83	0.77
1:A:251:PHE:O	1:A:252:ARG:HG2	1.84	0.77
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.66	0.77
1:A:195:ILE:HG21	1:A:368:MET:HE3	1.66	0.77
1:A:132:GLU:O	1:A:135:PRO:HD2	1.87	0.74
1:A:224:HIS:ND1	1:A:239:THR:HG22	2.03	0.72
1:A:239:THR:HG23	1:A:362:PRO:HG2	1.72	0.71
1:B:152:LYS:HD2	1:B:155:GLU:OE2	1.90	0.71
1:A:124:ARG:HD3	5:A:1018:HOH:O	1.90	0.71
1:A:336:LEU:HB3	1:A:338:LEU:HD22	1.73	0.70
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.22	0.70
1:A:153:ILE:HD12	1:A:153:ILE:N	2.02	0.69
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.75	0.68
1:B:343:LEU:O	5:B:2073:HOH:O	2.12	0.68
1:B:195:ILE:CG2	1:B:437:PHE:HB2	2.24	0.68
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.76	0.67
1:A:405:LYS:O	1:A:409:VAL:HG23	1.95	0.66
1:B:186:MET:HE1	1:B:189:ARG:HH11	1.60	0.66
1:A:89:ILE:HD12	1:A:89:ILE:N	2.11	0.66
1:A:290:LYS:CD	1:A:290:LYS:H	2.08	0.65
1:B:417:LEU:O	1:B:421:GLN:HG3	1.95	0.65
1:B:215:GLN:O	1:B:219:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:C	1:B:306:ASP:O	2.36	0.64
1:A:290:LYS:CE	1:A:290:LYS:H	2.10	0.64
1:A:215:GLN:O	1:A:219:GLN:HG3	1.97	0.64
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.33	0.64
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.80	0.63
1:A:195:ILE:HD13	1:A:368:MET:HE1	1.80	0.63
1:B:385:ILE:O	1:B:389:VAL:HG23	1.99	0.63
1:A:266:MET:SD	1:A:272:ARG:HD3	2.39	0.63
1:A:163:VAL:O	1:A:167:ILE:HG13	1.99	0.63
1:A:283:LEU:O	1:A:287:LEU:HG	1.99	0.63
1:A:159:ARG:O	1:A:163:VAL:HG23	1.98	0.63
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.99	0.63
1:A:407:ARG:HD3	5:A:1115:HOH:O	1.97	0.62
2:B:901:HEM:HBA2	4:B:905:1A2:C8	2.28	0.62
1:B:177:LEU:O	1:B:181:ILE:HD13	1.99	0.62
1:B:78:TYR:CZ	1:B:91:HIS:HD2	2.18	0.61
1:A:217:MET:CE	1:A:303:LEU:HB3	2.29	0.61
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.31	0.61
1:A:153:ILE:H	1:A:153:ILE:CD1	1.92	0.61
1:A:438:MET:CE	1:A:469:VAL:HG12	2.30	0.61
1:B:195:ILE:HG22	1:B:437:PHE:HB2	1.81	0.60
1:B:239:THR:O	1:B:361:CYS:HA	2.01	0.60
1:B:303:LEU:HD23	1:B:313:PHE:CD2	2.36	0.60
1:A:290:LYS:H	1:A:290:LYS:HD2	1.66	0.60
1:A:304:GLN:O	1:A:304:GLN:HG3	2.02	0.60
1:A:141:ILE:HD13	1:A:163:VAL:HG21	1.83	0.60
1:A:281:THR:O	1:A:285:ILE:HG12	2.02	0.60
1:B:301:LEU:HB3	1:B:303:LEU:HD21	1.84	0.59
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.85	0.59
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.85	0.59
1:B:195:ILE:HG22	1:B:195:ILE:O	2.03	0.58
1:A:290:LYS:HE3	1:A:290:LYS:H	1.67	0.58
1:B:303:LEU:O	1:B:310:PRO:HA	2.03	0.58
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.34	0.58
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.68	0.58
1:A:445:TYR:HA	1:A:450:GLY:H	1.68	0.58
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.34	0.58
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.34	0.58
1:B:303:LEU:HD22	1:B:303:LEU:N	2.19	0.57
1:A:411:GLU:O	1:A:414:VAL:HG22	2.03	0.57
1:A:410:THR:O	1:A:414:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:MET:HB3	1:B:481:PRO:HG2	1.86	0.57
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.35	0.57
1:B:190:ASN:O	1:B:192:PRO:HD3	2.05	0.57
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.86	0.57
1:B:149:LYS:HG2	1:B:150:GLU:N	2.20	0.56
2:A:901:HEM:HBA2	4:A:905:1A2:C8	2.28	0.56
1:B:167:ILE:HG23	1:B:171:GLY:O	2.05	0.56
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.86	0.56
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.71	0.56
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.87	0.56
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.88	0.56
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.35	0.56
1:A:333:PHE:HB3	5:A:1097:HOH:O	2.04	0.56
1:B:289:TRP:NE1	1:B:314:GLU:OE1	2.37	0.55
1:A:153:ILE:O	1:A:157:LEU:HD13	2.06	0.55
1:B:492:THR:OG1	1:B:492:THR:O	2.22	0.55
1:B:331:GLU:HA	1:B:331:GLU:OE1	2.06	0.55
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.89	0.54
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.89	0.54
1:A:350:LEU:HD23	1:A:351:LEU:N	2.22	0.54
1:A:217:MET:HE1	1:A:303:LEU:HB3	1.88	0.54
1:A:238:ILE:HG13	1:A:363:PHE:HB3	1.89	0.54
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.43	0.54
1:B:301:LEU:CD1	1:B:315:ILE:HD11	2.33	0.54
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.22	0.54
1:A:466:ILE:O	1:A:466:ILE:HG22	2.08	0.54
1:B:133:LEU:C	1:B:133:LEU:HD13	2.28	0.53
1:B:186:MET:HE1	1:B:189:ARG:NH1	2.22	0.53
1:A:465:SER:O	1:A:471:HIS:HE1	1.90	0.53
1:A:264:TYR:HB2	1:A:266:MET:HE2	1.89	0.53
1:A:215:GLN:NE2	5:A:1058:HOH:O	2.36	0.52
1:B:129:PRO:HG2	1:B:132:GLU:HG2	1.91	0.52
1:B:175:LEU:HD13	1:B:356:LEU:HD12	1.91	0.52
1:B:195:ILE:HD11	1:B:458:LEU:O	2.09	0.52
1:A:249:HIS:C	1:A:306:ASP:O	2.48	0.52
1:A:274:ASP:OD2	5:A:1079:HOH:O	2.18	0.52
1:A:149:LYS:HG2	1:A:150:GLU:N	2.24	0.52
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.92	0.52
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.92	0.52
1:B:194:CYS:O	1:B:197:ARG:NH1	2.42	0.52
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HG23	1:B:437:PHE:HB2	1.91	0.52
1:A:350:LEU:HD23	1:A:350:LEU:C	2.31	0.51
1:B:346:VAL:HG22	4:B:905:1A2:H133	1.91	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.44	0.51
1:B:80:ARG:NH2	1:B:89:ILE:HD13	2.26	0.51
1:B:258:LEU:HB3	1:B:259:ILE:HD12	1.92	0.51
1:A:80:ARG:NH1	1:A:89:ILE:HG21	2.26	0.51
1:B:259:ILE:HD12	1:B:259:ILE:N	2.26	0.51
1:B:209:ARG:O	1:B:242:PRO:HG3	2.11	0.50
1:A:328:PRO:O	1:A:329:LYS:HD2	2.11	0.50
1:A:488:GLU:OE1	1:A:491:LYS:HE2	2.11	0.50
1:B:77:GLN:NE2	1:B:77:GLN:HA	2.27	0.50
1:A:189:ARG:O	5:A:1036:HOH:O	2.18	0.50
1:A:480:SER:HA	1:A:481:PRO:C	2.32	0.50
1:A:186:MET:HE1	1:A:189:ARG:HH11	1.77	0.50
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.94	0.49
1:A:346:VAL:HG22	4:A:905:1A2:H133	1.94	0.49
1:B:283:LEU:O	1:B:287:LEU:HG	2.11	0.49
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.93	0.49
1:B:397:THR:HG22	1:B:397:THR:O	2.12	0.49
1:A:190:ASN:O	1:A:192:PRO:HD3	2.12	0.49
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.77	0.49
1:A:251:PHE:C	1:A:252:ARG:HG2	2.32	0.49
1:A:368:MET:HE1	1:A:433:ALA:HB1	1.94	0.49
1:B:186:MET:HE3	1:B:189:ARG:HD3	1.94	0.49
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.93	0.49
1:B:438:MET:HE3	1:B:469:VAL:HA	1.95	0.49
1:A:252:ARG:HH21	1:A:489:PRO:HD3	1.76	0.49
1:A:239:THR:CG2	1:A:362:PRO:HG2	2.41	0.48
1:B:78:TYR:CD1	1:B:78:TYR:C	2.86	0.48
1:B:407:ARG:HG3	5:B:2109:HOH:O	2.11	0.48
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.48	0.48
1:A:290:LYS:N	1:A:290:LYS:HD2	2.28	0.48
1:A:303:LEU:O	1:A:310:PRO:HA	2.13	0.48
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.48	0.48
1:B:186:MET:CE	1:B:189:ARG:HD3	2.43	0.48
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.96	0.48
1:A:149:LYS:HG2	1:A:150:GLU:HG3	1.95	0.48
1:A:442:GLN:HG3	1:A:443:ASN:N	2.29	0.48
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.14	0.47
1:B:346:VAL:CG2	4:B:905:1A2:H133	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:TYR:HA	1:B:450:GLY:H	1.80	0.47
1:B:371:GLU:OE1	4:B:905:1A2:N6	2.48	0.47
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.44	0.47
1:A:129:PRO:HG3	5:A:1019:HOH:O	2.14	0.47
1:B:305:ALA:O	1:B:307:GLY:N	2.47	0.47
1:A:148:PHE:CE2	1:A:152:LYS:HE2	2.50	0.47
1:A:144:TYR:O	1:A:147:SER:HB3	2.15	0.47
1:A:264:TYR:HB2	1:A:266:MET:CE	2.45	0.47
1:A:186:MET:CE	1:A:189:ARG:HH11	2.28	0.47
1:B:195:ILE:HG23	1:B:437:PHE:CB	2.45	0.47
1:A:438:MET:HE2	1:A:469:VAL:HG12	1.94	0.47
1:B:124:ARG:HH21	1:B:128:THR:HB	1.79	0.47
1:A:417:LEU:O	1:A:421:GLN:HG3	2.16	0.46
1:B:445:TYR:O	1:B:449:GLY:HA2	2.14	0.46
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.45	0.46
1:A:301:LEU:HD13	1:A:315:ILE:HD11	1.97	0.46
1:B:129:PRO:HB2	1:B:131:GLU:CD	2.36	0.46
1:A:488:GLU:HG3	5:A:1122:HOH:O	2.14	0.46
1:A:246:ASP:CG	1:A:248:LYS:H	2.18	0.46
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.31	0.46
1:B:332:TRP:O	1:B:335:GLU:HB2	2.15	0.46
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.23	0.46
1:A:99:THR:CG2	1:A:100:SER:H	2.03	0.46
1:A:395:LEU:HD23	1:A:404:TRP:HB2	1.98	0.46
1:A:259:ILE:N	1:A:259:ILE:HD12	2.31	0.46
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.30	0.45
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.46	0.45
1:A:428:MET:HB3	5:A:1048:HOH:O	2.16	0.45
1:A:78:TYR:CD1	1:A:78:TYR:C	2.90	0.45
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.45	0.45
1:A:262:ALA:HB2	1:A:299:LEU:HG	1.99	0.45
1:A:332:TRP:O	1:A:335:GLU:HB2	2.16	0.45
1:A:368:MET:CE	1:A:433:ALA:HB1	2.46	0.45
1:B:266:MET:CE	1:B:272:ARG:HE	2.30	0.45
1:A:301:LEU:HB3	1:A:303:LEU:HD13	1.98	0.45
1:A:124:ARG:CD	5:A:1018:HOH:O	2.56	0.44
1:B:84:TRP:NE1	1:B:114:MET:HG3	2.32	0.44
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.98	0.44
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.98	0.44
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.52	0.44
1:B:453:ALA:O	1:B:476:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLY:N	1:B:297:ASP:OD2	2.50	0.44
1:A:151:ALA:HB1	5:A:1022:HOH:O	2.17	0.44
1:A:141:ILE:HD11	1:A:163:VAL:HG11	1.99	0.44
1:A:266:MET:HB2	1:A:270:THR:O	2.17	0.44
1:B:350:LEU:HD23	1:B:350:LEU:C	2.38	0.44
1:B:375:ARG:O	1:B:379:ASP:HB2	2.18	0.44
1:A:241:PHE:HB3	1:A:242:PRO:HD2	2.00	0.44
1:B:438:MET:HE2	1:B:469:VAL:HG12	1.99	0.44
1:A:84:TRP:CE2	1:A:114:MET:HG3	2.53	0.44
1:A:371:GLU:O	1:A:375:ARG:HB2	2.18	0.44
1:A:133:LEU:C	1:A:133:LEU:HD23	2.39	0.44
1:B:441:MET:HE1	1:B:472:GLN:HG2	2.01	0.43
1:B:434:SER:HB3	1:B:468:PRO:HD2	2.00	0.43
1:A:334:GLN:HA	5:A:1096:HOH:O	2.17	0.43
1:A:434:SER:OG	1:A:468:PRO:HD2	2.19	0.43
1:A:333:PHE:O	1:A:336:LEU:HB2	2.18	0.43
1:A:172:THR:OG1	1:A:173:TYR:N	2.50	0.43
1:B:186:MET:HB3	1:B:481:PRO:CG	2.49	0.43
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.01	0.43
1:B:138:ILE:HG22	1:B:142:ASN:ND2	2.33	0.43
1:A:238:ILE:CG1	1:A:363:PHE:HB3	2.48	0.43
1:B:226:LEU:O	1:B:226:LEU:HD23	2.18	0.43
1:A:290:LYS:N	1:A:290:LYS:HE3	2.34	0.43
1:A:465:SER:C	1:A:467:THR:H	2.21	0.43
1:B:438:MET:CE	1:B:469:VAL:HG12	2.48	0.43
1:A:164:THR:O	1:A:168:GLU:HG2	2.19	0.43
1:A:445:TYR:O	1:A:449:GLY:HA2	2.19	0.43
1:A:397:THR:O	1:A:397:THR:HG22	2.18	0.43
1:B:194:CYS:HB2	2:B:901:HEM:ND	2.34	0.42
1:B:124:ARG:HD2	1:B:244:ARG:HD3	2.01	0.42
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.54	0.42
1:A:253:LEU:HD12	1:A:253:LEU:N	2.34	0.42
1:A:309:ASP:OD1	1:A:495:TRP:HA	2.19	0.42
1:A:223:ARG:HD2	5:A:1059:HOH:O	2.19	0.42
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.32	0.42
1:B:348:ASN:ND2	1:B:348:ASN:H	2.18	0.42
1:B:322:GLU:OE2	1:B:339:LYS:HE3	2.19	0.42
1:A:453:ALA:HB3	1:A:474:MET:HB2	2.01	0.42
1:A:195:ILE:HG21	1:A:368:MET:CE	2.43	0.42
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.55	0.42
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:O	1:A:124:ARG:HG3	2.20	0.41
1:A:467:THR:HG21	1:A:469:VAL:HG22	2.01	0.41
1:B:351:LEU:HB3	1:B:358:PHE:HB2	2.02	0.41
1:B:210:ASN:N	1:B:210:ASN:HD22	2.17	0.41
1:A:306:ASP:HB3	1:A:307:GLY:H	1.72	0.41
1:A:149:LYS:HE2	1:A:150:GLU:HG3	2.03	0.41
1:B:348:ASN:H	1:B:348:ASN:HD22	1.68	0.41
1:B:78:TYR:HD1	1:B:79:VAL:N	2.19	0.41
1:A:434:SER:OG	1:A:467:THR:HG23	2.20	0.41
1:A:368:MET:HE1	1:A:433:ALA:CB	2.51	0.41
1:A:445:TYR:O	1:A:449:GLY:N	2.54	0.41
1:A:303:LEU:N	1:A:303:LEU:CD1	2.83	0.41
1:B:80:ARG:NH2	1:B:89:ILE:CD1	2.84	0.41
1:A:252:ARG:HH12	1:A:486:GLN:HB3	1.86	0.41
1:A:360:ALA:HA	5:A:1073:HOH:O	2.20	0.41
1:A:258:LEU:HB3	1:A:259:ILE:HD12	2.01	0.41
1:B:153:ILE:HG13	1:B:153:ILE:H	1.67	0.41
1:A:384:ASN:HA	5:A:1104:HOH:O	2.21	0.41
1:A:251:PHE:O	1:A:360:ALA:HB2	2.21	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.89	0.40
1:B:195:ILE:HG13	5:B:2038:HOH:O	2.22	0.40
1:A:368:MET:CE	1:A:433:ALA:CB	2.99	0.40
1:A:89:ILE:CD1	1:A:89:ILE:N	2.81	0.40
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.55	0.40
1:A:256:SER:HB2	1:A:257:GLN:OE1	2.22	0.40
1:A:242:PRO:HB2	1:A:251:PHE:CE1	2.56	0.40
1:A:249:HIS:C	5:A:1068:HOH:O	2.60	0.40
1:A:379:ASP:HB3	1:A:381:GLN:OE1	2.20	0.40
1:A:138:ILE:O	1:A:142:ASN:ND2	2.54	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	411/433 (95%)	370 (90%)	38 (9%)	3 (1%)	26 46
1	B	406/433 (94%)	362 (89%)	39 (10%)	5 (1%)	16 29
All	All	817/866 (94%)	732 (90%)	77 (9%)	8 (1%)	19 34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	B	306	ASP
1	A	123	PRO
1	A	200	TRP
1	B	200	TRP
1	B	268	ASP
1	B	344	PRO
1	B	266	MET

5.3.2 Protein sidechains (i)

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	363/381 (95%)	341 (94%)	22 (6%)	23 42
1	B	358/381 (94%)	338 (94%)	20 (6%)	26 47
All	All	721/762 (95%)	679 (94%)	42 (6%)	25 45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	148	PHE
1	A	153	ILE
1	A	161	GLU
1	A	180	LEU
1	A	223	ARG
1	A	239	THR
1	A	252	ARG

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Mol	Chain	Res	Type
1	A	257	GLN
1	A	258	LEU
1	A	290	LYS
1	A	301	LEU
1	A	303	LEU
1	A	336	LEU
1	A	338	LEU
1	A	348	ASN
1	A	386	LEU
1	A	387	GLU
1	A	395	LEU
1	A	417	LEU
1	A	467	THR
1	A	475	LEU
1	B	78	TYR
1	B	119	LEU
1	B	128	THR
1	B	130	LEU
1	B	134	LEU
1	B	210	ASN
1	B	226	LEU
1	B	233	ASN
1	B	257	GLN
1	B	258	LEU
1	B	264	TYR
1	B	292	ARG
1	B	301	LEU
1	B	303	LEU
1	B	348	ASN
1	B	417	LEU
1	B	444	GLU
1	B	467	THR
1	B	486	GLN
1	B	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	91	HIS
1	A	142	ASN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	348	ASN
1	A	471	HIS
1	B	77	GLN
1	B	91	HIS
1	B	210	ASN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	901	-	30,50,50	2.81	11 (36%)	24,82,82	2.34	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	H4B	A	902	-	13,18,18	1.71	2 (15%)	11,26,26	2.02	5 (45%)
4	1A2	A	905	-	26,33,33	3.67	14 (53%)	26,49,49	2.40	11 (42%)
2	HEM	B	901	-	30,50,50	2.45	9 (30%)	24,82,82	2.17	9 (37%)
3	H4B	B	902	-	13,18,18	1.82	2 (15%)	11,26,26	2.02	5 (45%)
4	1A2	B	905	-	26,33,33	3.86	15 (57%)	26,49,49	2.42	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	901	-	-	0/10/54/54	0/0/8/8
3	H4B	A	902	-	1/1/3/5	0/8/17/17	0/2/2/2
4	1A2	A	905	-	-	0/10/53/53	0/3/4/4
2	HEM	B	901	-	-	0/10/54/54	0/0/8/8
3	H4B	B	902	-	-	0/8/17/17	0/2/2/2
4	1A2	B	905	-	-	0/10/53/53	0/3/4/4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C2D-C3D	-7.13	1.33	1.54
2	A	901	HEM	C2D-C3D	-6.69	1.34	1.54
2	A	901	HEM	C3C-CAC	-6.50	1.39	1.51
4	B	905	1A2	C25-C22	-6.45	1.36	1.44
3	B	902	H4B	C7-N8	-6.03	1.38	1.46
2	B	901	HEM	C3C-CAC	-5.99	1.40	1.51
2	A	901	HEM	C3B-CAB	-5.95	1.40	1.51
4	A	905	1A2	C25-C22	-5.84	1.37	1.44
2	A	901	HEM	C3D-C4D	-5.62	1.44	1.51
3	A	902	H4B	C7-N8	-5.56	1.38	1.46
4	A	905	1A2	C23-C22	-5.19	1.39	1.49
4	B	905	1A2	C23-C22	-5.09	1.39	1.49
4	B	905	1A2	C4A-C5	-4.64	1.40	1.46
2	B	901	HEM	C3B-CAB	-4.63	1.42	1.51
2	B	901	HEM	C3D-C4D	-3.87	1.46	1.51
4	A	905	1A2	C4A-C5	-3.80	1.41	1.46
2	A	901	HEM	C2C-C1C	-3.73	1.45	1.52
4	B	905	1A2	C24-C19	-3.69	1.43	1.50
4	A	905	1A2	C24-C23	-3.49	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C3B-C4B	-3.40	1.48	1.51
4	A	905	1A2	C24-C19	-3.21	1.44	1.50
4	B	905	1A2	C24-C23	-2.96	1.40	1.52
4	A	905	1A2	F10-C1	-2.74	1.29	1.35
4	A	905	1A2	C16-C19	-2.72	1.45	1.49
2	A	901	HEM	C2B-C1B	-2.42	1.43	1.51
4	B	905	1A2	F10-C1	-2.41	1.29	1.35
4	B	905	1A2	C16-C19	-2.40	1.45	1.49
2	B	901	HEM	C3B-C4B	-2.32	1.49	1.51
2	A	901	HEM	CAD-C3D	-2.16	1.49	1.54
2	B	901	HEM	C2B-C1B	-2.15	1.44	1.51
3	A	902	H4B	C4A-N5	-2.11	1.33	1.38
3	B	902	H4B	C4A-N5	-2.04	1.33	1.38
4	B	905	1A2	C14-N13	2.11	1.50	1.47
2	B	901	HEM	FE-NB	2.35	2.09	1.97
4	A	905	1A2	O17-C16	2.35	1.28	1.23
2	A	901	HEM	C1C-NC	2.37	1.38	1.36
4	A	905	1A2	C8-N8	2.46	1.49	1.46
4	B	905	1A2	C4A-C4	2.46	1.42	1.39
2	B	901	HEM	FE-NC	2.47	2.05	1.95
4	A	905	1A2	C20-N21	2.54	1.42	1.36
4	B	905	1A2	O17-C16	2.57	1.28	1.23
2	B	901	HEM	C4C-NC	2.68	1.39	1.36
2	A	901	HEM	FE-NC	2.94	2.07	1.95
4	A	905	1A2	C16-N13	3.29	1.40	1.34
4	B	905	1A2	C20-N21	3.35	1.44	1.36
4	A	905	1A2	C4A-C4	3.49	1.44	1.39
2	A	901	HEM	C4C-NC	3.63	1.40	1.36
4	B	905	1A2	C8-N8	3.66	1.51	1.46
4	B	905	1A2	C16-N13	4.27	1.42	1.34
4	A	905	1A2	C5-N6	7.33	1.37	1.28
4	B	905	1A2	C5-N6	7.57	1.37	1.28
4	A	905	1A2	C25-N26	11.35	1.34	1.14
4	B	905	1A2	C25-N26	11.51	1.34	1.14

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	905	1A2	C14-C15-C7	-6.77	106.88	113.11
4	A	905	1A2	C14-C15-C7	-6.70	106.94	113.11
4	B	905	1A2	C14-N13-C12	-5.27	102.79	112.56
4	A	905	1A2	C14-N13-C12	-4.58	104.05	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	905	1A2	C12-C11-C7	-4.15	109.29	113.11
4	B	905	1A2	C4A-C8A-C1	-3.74	115.79	118.80
4	A	905	1A2	C4A-C8A-C1	-3.30	116.14	118.80
4	B	905	1A2	C15-C14-N13	-3.21	103.82	111.11
4	A	905	1A2	C15-C14-N13	-3.16	103.94	111.11
4	B	905	1A2	C12-C11-C7	-2.91	110.43	113.11
2	A	901	HEM	CBD-CAD-C3D	-2.66	105.82	113.55
4	B	905	1A2	C23-C22-N21	-2.46	120.62	123.83
4	A	905	1A2	C11-C12-N13	-2.40	105.66	111.11
3	B	902	H4B	N3-C2-N1	-2.24	121.86	125.53
4	A	905	1A2	C23-C22-N21	-2.17	120.99	123.83
3	A	902	H4B	N3-C2-N1	-2.17	121.98	125.53
4	A	905	1A2	C3-C4-C4A	-2.07	119.84	123.42
2	B	901	HEM	CAA-C2A-C3A	-2.06	123.11	129.00
2	B	901	HEM	CMD-C2D-C3D	2.03	123.32	114.35
2	A	901	HEM	C3B-C4B-CHC	2.12	126.14	123.16
4	B	905	1A2	F9-C4-C4A	2.17	121.36	118.09
2	A	901	HEM	CMD-C2D-C3D	2.38	124.87	114.35
3	A	902	H4B	C2-N1-C8A	2.47	120.10	114.54
4	A	905	1A2	C24-C23-C22	2.50	119.13	111.71
3	B	902	H4B	C7-C6-N5	2.52	115.67	110.45
4	A	905	1A2	F9-C4-C4A	2.56	121.94	118.09
4	B	905	1A2	C23-C24-C19	2.57	121.77	114.02
4	A	905	1A2	C23-C24-C19	2.58	121.79	114.02
3	A	902	H4B	C7-C6-N5	2.59	115.83	110.45
3	B	902	H4B	C2-N1-C8A	2.59	120.37	114.54
4	B	905	1A2	C24-C23-C22	2.74	119.83	111.71
3	B	902	H4B	C4-C4A-C8A	2.88	117.17	114.56
3	A	902	H4B	C4-C4A-C8A	2.90	117.19	114.56
2	A	901	HEM	CMB-C2B-C3B	2.96	123.93	116.53
3	B	902	H4B	C4-N3-C2	3.01	120.12	115.94
2	A	901	HEM	CAA-C2A-C1A	3.07	130.34	127.01
2	A	901	HEM	C3B-CAB-CBB	3.08	129.19	124.46
2	B	901	HEM	CMB-C2B-C3B	3.15	124.39	116.53
2	B	901	HEM	C3B-CAB-CBB	3.16	129.31	124.46
3	A	902	H4B	C4-N3-C2	3.22	120.41	115.94
2	B	901	HEM	C3B-C4B-CHC	3.28	127.78	123.16
2	B	901	HEM	CAD-C3D-C2D	3.42	123.04	113.22
2	A	901	HEM	CAD-C3D-C4D	3.55	124.98	112.47
2	B	901	HEM	C2D-C3D-C4D	3.75	107.85	101.50
2	A	901	HEM	CAD-C3D-C2D	3.88	124.36	113.22
2	B	901	HEM	CMC-C2C-C3C	4.06	126.67	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	HEM	CAD-C3D-C4D	4.57	128.59	112.47
2	A	901	HEM	CMC-C2C-C3C	4.81	128.54	116.53
2	A	901	HEM	C2D-C3D-C4D	5.26	110.42	101.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	2	0
4	A	905	1A2	3	0
2	B	901	HEM	3	0
4	B	905	1A2	5	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^{th} 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^2)	Q<0.9
1	A	415/433 (95%)	0.20	24 (5%)	26	30	29, 51, 85, 123	0
1	B	410/433 (94%)	0.11	18 (4%)	38	43	30, 50, 77, 95	0
All	All	825/866 (95%)	0.16	42 (5%)	32	36	29, 50, 81, 123	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	11.0
1	A	102	PHE	10.4
1	A	101	ASP	6.8
1	B	110	LEU	6.0
1	A	110	LEU	5.6
1	B	494	ILE	5.3
1	A	495	TRP	4.5
1	A	108	SER	4.3
1	A	78	TYR	3.6
1	B	495	TRP	3.6
1	B	77	GLN	3.5
1	A	494	ILE	3.3
1	B	148	PHE	3.2
1	A	109	CYS	3.2
1	A	152	LYS	3.1
1	B	152	LYS	3.1
1	A	100	SER	3.1
1	A	90	LEU	3.0
1	A	111	GLY	3.0
1	B	87	GLY	2.9
1	A	148	PHE	2.9
1	A	89	ILE	2.8
1	A	77	GLN	2.7
1	B	78	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	2.6
1	B	109	CYS	2.6
1	A	398	HIS	2.5
1	B	267	PRO	2.4
1	A	96	HIS	2.4
1	B	111	GLY	2.4
1	A	492	THR	2.4
1	B	79	VAL	2.4
1	A	446	ARG	2.3
1	B	150	GLU	2.3
1	B	125	ASP	2.2
1	A	91	HIS	2.2
1	B	347	ALA	2.2
1	A	86	SER	2.1
1	B	492	THR	2.1
1	A	347	ALA	2.1
1	B	345	ALA	2.0
1	B	91	HIS	2.0

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

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

6.3 Carbohydrates (i)

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^{th} 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^2)	Q<0.9
4	1A2	A	905	30/30	0.91	0.22	1.77	45,50,58,59	0
4	1A2	B	905	30/30	0.92	0.22	1.05	48,52,55,60	0
2	HEM	A	901	43/43	0.97	0.18	0.35	27,30,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	H4B	B	902	17/17	0.97	0.18	0.24	40,41,46,47	0
2	HEM	B	901	43/43	0.97	0.18	0.23	29,31,40,47	0
3	H4B	A	902	17/17	0.96	0.14	-0.40	46,48,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.