WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EBD
Title	:	Structure of inhibited murine iNOS oxygenase domain
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.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on	:	2008-08-27
Resolution	:	2.40 Å(reported)

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

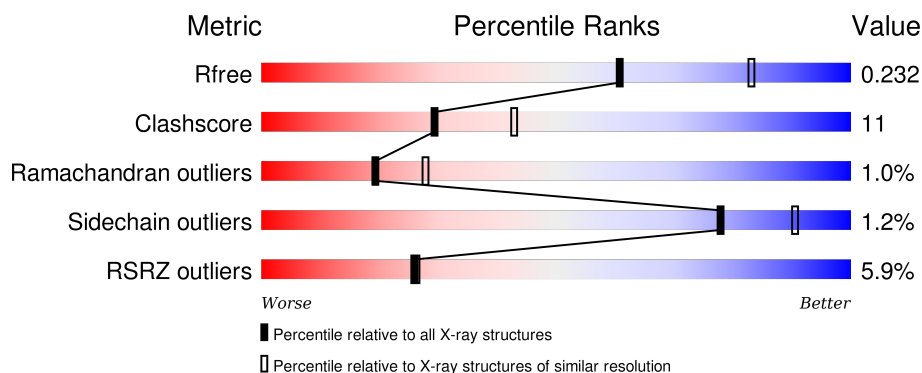|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		11
Ramachandran outliers		1.0%
Sidechain outliers		1.2%
RSRZ outliers		5.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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% — 72% — 24% · ·
1	B	433	5% — 74% — 22% · ·

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	-	-	-
3	H4B	B	2902	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7806 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 3425	C 2195	N 590	O 619	S 21	0	0	0
1	B	421	Total 3421	C 2193	N 589	O 618	S 21	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
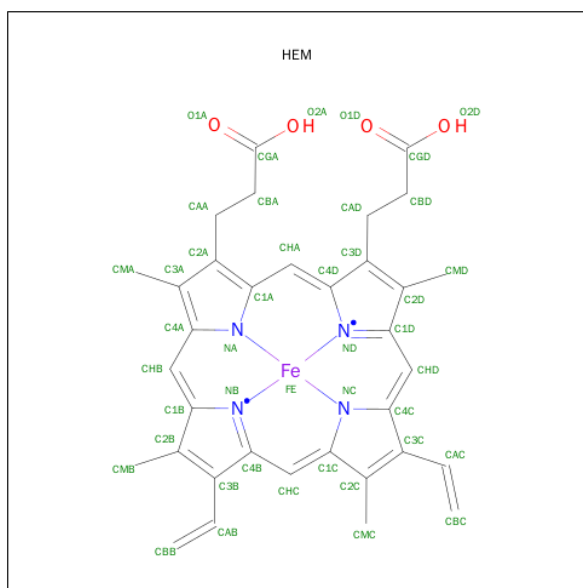
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
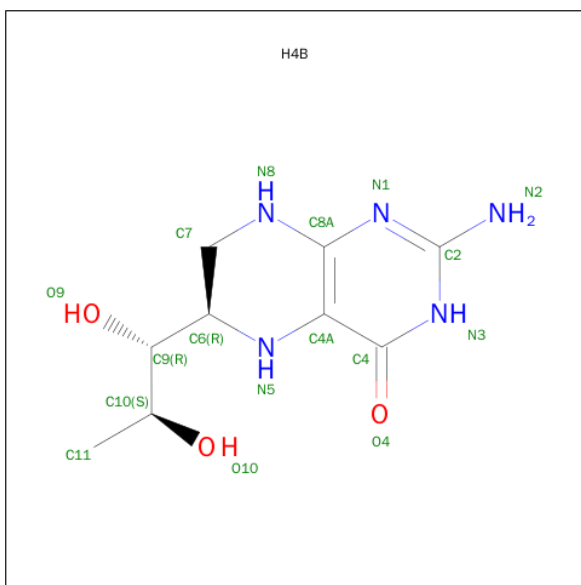
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (2S)-2-METHYL-2,3-DIHYDROTHIENO[2,3-F][1,4]OXAZEPIN-5-AMINE (three-letter code: 329) (formula: $C_8H_{10}N_2OS$).
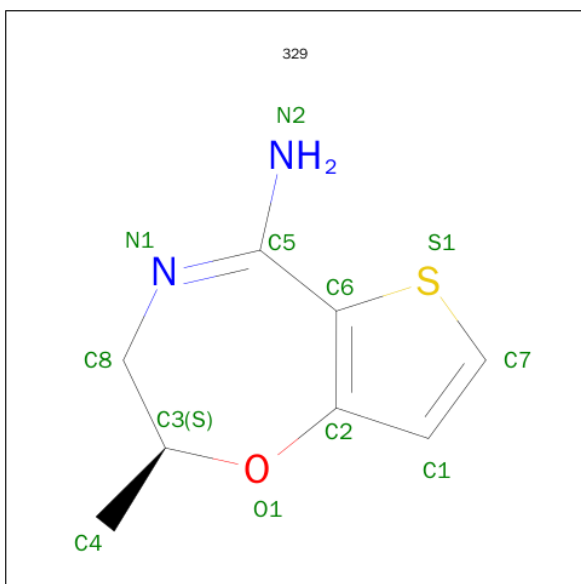
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	8	2	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	8	2	1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
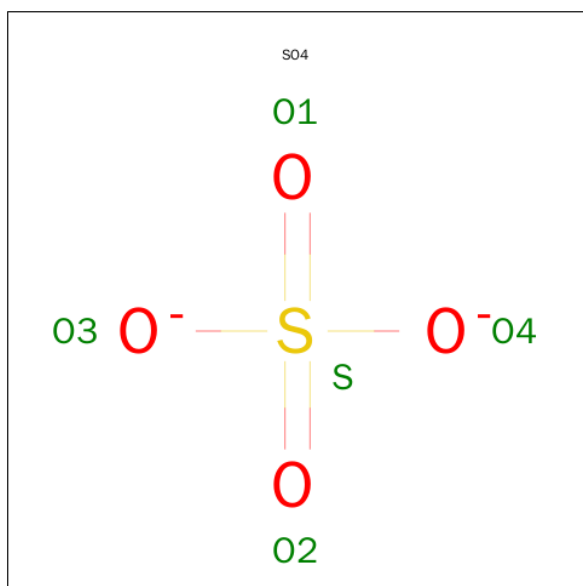
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total	O	0	0
			395	395		
6	B	401	Total	O	0	0
			401	401		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitric oxide synthase, inducible
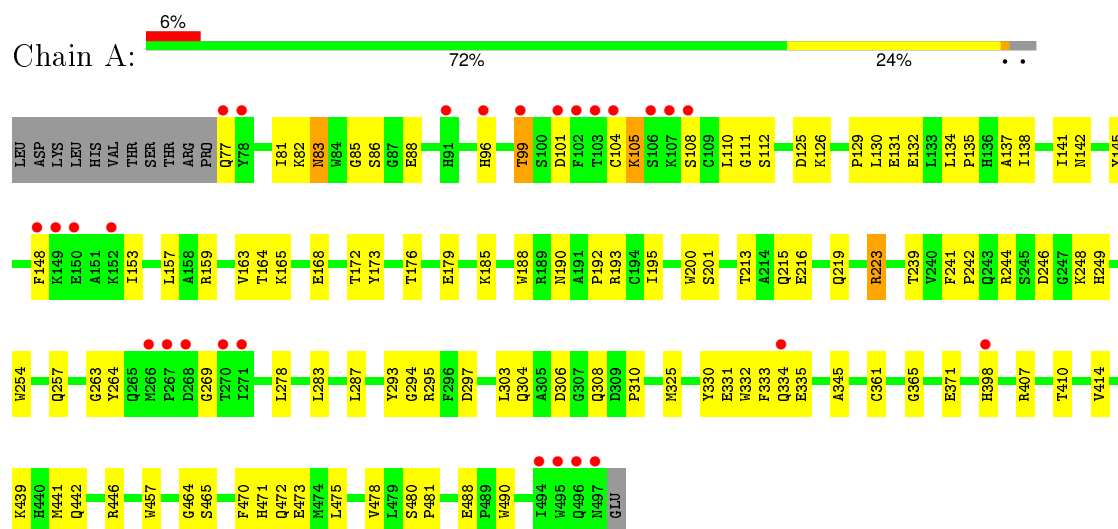
• Molecule 1: Nitric oxide synthase, inducible
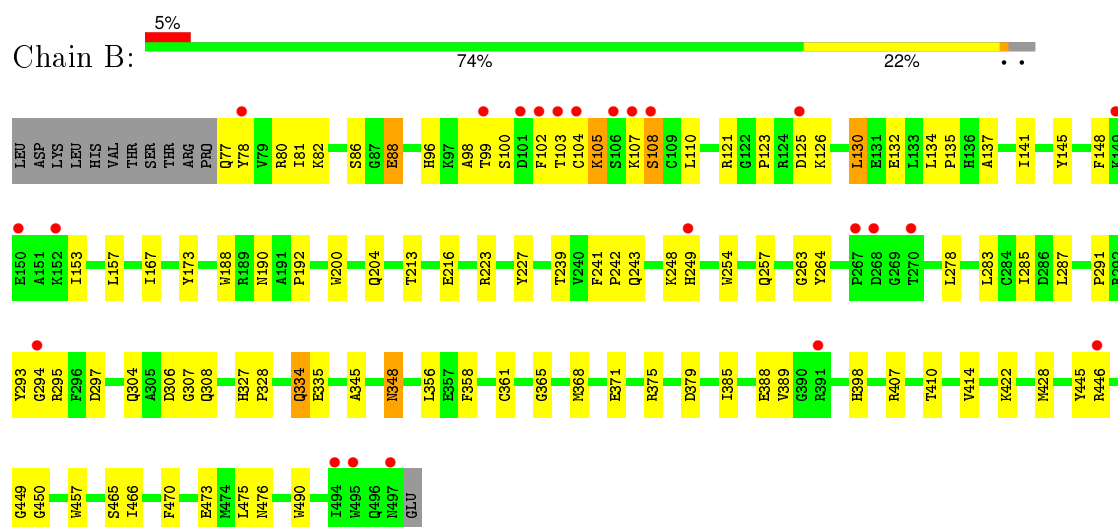
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	213.44Å 213.44Å 116.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 2.40 44.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.9 (44.65-2.40) 90.0 (44.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.24 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.248 0.203 , 0.232	Depositor DCC
R_{free} test set	2801 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	1 of 54828 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 329, H4B, SO4

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	0.34	0/3525	0.61	1/4792 (0.0%)
1	B	0.35	0/3521	0.61	1/4787 (0.0%)
All	All	0.34	0/7046	0.61	2/9579 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	GLY	N-CA-C	-5.23	100.03	113.10
1	B	365	GLY	N-CA-C	-5.15	100.22	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3425	0	3318	80	0
1	B	3421	0	3312	73	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	17	0	14	0	0
3	B	17	0	14	1	0
4	A	12	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	10	1	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	395	0	0	7	3
6	B	401	0	0	10	0
All	All	7806	0	6738	155	3

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 (155) 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:81:ILE:HD11	1:B:475:LEU:HD13	1.49	0.93
1:B:107:LYS:O	1:B:108:SER:HB3	1.77	0.82
1:B:388:GLU:HG2	6:B:4779:HOH:O	1.84	0.77
1:A:442:GLN:HE21	1:A:446:ARG:NH1	1.84	0.75
1:A:104:CYS:HA	1:A:110:LEU:HD13	1.70	0.72
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.71	0.71
1:A:83:ASN:HD22	1:A:86:SER:H	1.40	0.70
1:A:83:ASN:ND2	1:A:86:SER:H	1.89	0.69
1:B:98:ALA:O	1:B:100:SER:N	2.23	0.67
1:B:249:HIS:HB3	1:B:306:ASP:OD2	1.95	0.67
2:A:901:HEM:HBC2	2:A:901:HEM:HMC2	1.76	0.66
1:A:105:LYS:HD2	1:A:108:SER:HB3	1.78	0.65
1:A:442:GLN:HE21	1:A:446:ARG:HH12	1.40	0.65
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.97	0.64
1:B:263:GLY:O	1:B:278:LEU:HD23	1.97	0.64
1:A:134:LEU:O	1:A:138:ILE:HG12	1.99	0.63
1:B:77:GLN:O	1:B:96:HIS:HE1	1.81	0.63
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.98	0.62
1:A:82:LYS:O	1:A:473:GLU:HG3	1.99	0.62
1:B:153:ILE:O	1:B:157:LEU:HG	2.00	0.61
1:A:153:ILE:HG22	1:A:157:LEU:HD23	1.83	0.61
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.16	0.61
1:B:398:HIS:HB2	6:B:4580:HOH:O	2.01	0.61
1:A:215:GLN:HG3	1:A:219:GLN:HE21	1.66	0.60
1:B:107:LYS:O	1:B:108:SER:CB	2.49	0.60
1:B:304:GLN:HG3	1:B:308:GLN:O	2.03	0.59
1:B:385:ILE:O	1:B:389:VAL:HG23	2.02	0.59
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:HE1	1:A:472:GLN:HG2	1.85	0.58
1:A:137:ALA:O	1:A:141:ILE:HG12	2.03	0.57
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.40	0.57
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.39	0.57
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.20	0.56
1:A:407:ARG:HD2	6:A:4140:HOH:O	2.04	0.56
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.36	0.56
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.41	0.56
1:B:446:ARG:HH21	1:B:446:ARG:HG2	1.70	0.56
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.87	0.56
1:A:110:LEU:O	1:A:112:SER:N	2.31	0.55
1:A:110:LEU:HD12	1:A:110:LEU:N	2.21	0.55
1:A:86:SER:OG	1:A:88:GLU:HG2	2.06	0.55
1:A:331:GLU:O	1:A:334:GLN:HG2	2.07	0.55
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.08	0.54
1:A:465:SER:O	1:A:471:HIS:HE1	1.91	0.54
1:A:223:ARG:HD2	6:A:4190:HOH:O	2.07	0.53
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.91	0.53
1:A:239:THR:O	1:A:361:CYS:HA	2.07	0.53
1:B:375:ARG:O	1:B:379:ASP:HB2	2.07	0.53
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.23	0.53
1:A:132:GLU:O	1:A:135:PRO:HD2	2.08	0.53
1:B:132:GLU:O	1:B:135:PRO:HD2	2.08	0.53
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.43	0.53
1:A:441:MET:CE	1:A:472:GLN:HG2	2.39	0.52
1:A:165:LYS:HD2	1:A:165:LYS:N	2.24	0.52
1:B:145:TYR:HA	1:B:148:PHE:CE1	2.45	0.52
1:B:78:TYR:CD1	1:B:78:TYR:C	2.83	0.51
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.32	0.51
1:A:263:GLY:O	1:A:278:LEU:HD23	2.10	0.51
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.92	0.50
1:B:137:ALA:O	1:B:141:ILE:HG12	2.12	0.50
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.47	0.49
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.95	0.49
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.94	0.49
1:A:249:HIS:HB3	1:A:306:ASP:OD1	2.13	0.49
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.48	0.49
1:A:164:THR:O	1:A:168:GLU:HG3	2.13	0.49
1:A:246:ASP:OD1	1:A:248:LYS:HB2	2.13	0.49
1:A:283:LEU:O	1:A:287:LEU:HG	2.13	0.49
1:B:110:LEU:N	1:B:110:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.47	0.48
1:B:445:TYR:HA	1:B:450:GLY:H	1.77	0.48
1:A:294:GLY:N	1:A:297:ASP:OD2	2.33	0.48
1:A:83:ASN:ND2	1:A:85:GLY:H	2.12	0.48
1:A:131:GLU:O	1:A:135:PRO:HG2	2.14	0.48
1:A:295:ARG:HG3	6:A:4299:HOH:O	2.13	0.48
1:A:159:ARG:O	1:A:163:VAL:HG23	2.14	0.48
1:A:480:SER:HA	1:A:481:PRO:C	2.35	0.47
1:A:132:GLU:C	1:A:135:PRO:HD2	2.35	0.47
1:B:334:GLN:OE1	1:B:335:GLU:HG3	2.13	0.47
1:B:254:TRP:CE3	1:B:283:LEU:HD21	2.49	0.47
1:A:398:HIS:HB2	6:A:4216:HOH:O	2.15	0.47
1:B:257:GLN:HA	1:B:345:ALA:O	2.15	0.47
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.49	0.46
1:B:80:ARG:NH1	6:B:4605:HOH:O	2.48	0.46
1:A:172:THR:HG23	1:A:173:TYR:N	2.30	0.46
1:B:294:GLY:N	1:B:297:ASP:OD2	2.43	0.46
1:B:103:THR:HA	6:B:4501:HOH:O	2.15	0.46
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.81	0.46
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.45	0.46
1:B:283:LEU:O	1:B:287:LEU:HG	2.15	0.46
1:A:130:LEU:HD12	1:A:130:LEU:N	2.30	0.46
1:B:104:CYS:HA	1:B:110:LEU:HD13	1.97	0.46
1:A:213:THR:OG1	1:A:216:GLU:HG3	2.16	0.46
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.51	0.46
1:A:190:ASN:O	1:A:192:PRO:HD3	2.16	0.46
1:B:239:THR:O	1:B:361:CYS:HA	2.16	0.46
1:B:125:ASP:OD2	1:B:126:LYS:HG2	2.16	0.46
1:A:371:GLU:OE1	4:A:903:329:N1	2.48	0.46
1:B:102:PHE:HZ	1:B:476:ASN:ND2	2.14	0.45
1:B:107:LYS:HB2	6:B:4570:HOH:O	2.16	0.45
1:B:105:LYS:HB2	6:B:4719:HOH:O	2.16	0.45
1:A:334:GLN:HG3	1:A:335:GLU:N	2.31	0.45
1:A:244:ARG:HA	6:A:4079:HOH:O	2.16	0.45
1:A:410:THR:O	1:A:414:VAL:HG23	2.16	0.45
1:B:295:ARG:HD2	6:B:4564:HOH:O	2.16	0.45
1:B:466:ILE:O	1:B:466:ILE:HG22	2.16	0.45
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.51	0.44
1:A:83:ASN:C	1:A:83:ASN:HD22	2.20	0.44
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.76	0.44
1:A:99:THR:HG23	1:A:478:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.44
1:B:190:ASN:O	1:B:192:PRO:HD3	2.18	0.44
1:B:86:SER:OG	1:B:88:GLU:HB2	2.18	0.43
1:B:327:HIS:ND1	1:B:328:PRO:CD	2.81	0.43
1:A:110:LEU:N	1:A:110:LEU:CD1	2.81	0.43
1:B:82:LYS:O	1:B:473:GLU:HG3	2.18	0.43
1:B:334:GLN:OE1	1:B:335:GLU:N	2.52	0.43
1:B:125:ASP:O	1:B:248:LYS:HE3	2.19	0.43
2:B:2901:HEM:HHC	2:B:2901:HEM:HBB2	2.00	0.43
1:A:257:GLN:HA	1:A:345:ALA:O	2.19	0.43
1:A:333:PHE:HB3	6:A:4056:HOH:O	2.18	0.43
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.53	0.43
1:B:249:HIS:O	1:B:306:ASP:HA	2.19	0.43
1:A:439:LYS:HG2	6:A:4316:HOH:O	2.18	0.43
1:B:465:SER:HA	1:B:470:PHE:CG	2.53	0.43
1:A:330:TYR:CD1	1:A:332:TRP:CZ2	3.06	0.43
1:A:153:ILE:O	1:A:157:LEU:HD23	2.19	0.42
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.66	0.42
1:A:488:GLU:OE1	1:A:488:GLU:HA	2.19	0.42
1:B:407:ARG:HD2	6:B:4483:HOH:O	2.20	0.42
1:B:410:THR:O	1:B:414:VAL:HG23	2.19	0.42
1:A:304:GLN:HG3	1:A:308:GLN:O	2.19	0.42
1:A:195:ILE:HG12	1:A:195:ILE:O	2.19	0.42
1:B:368:MET:HA	1:B:428:MET:O	2.20	0.42
1:B:145:TYR:HA	1:B:148:PHE:CD1	2.54	0.41
1:A:442:GLN:HG2	1:A:446:ARG:NH1	2.34	0.41
1:A:77:GLN:O	1:A:96:HIS:HE1	2.03	0.41
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.51	0.41
1:B:445:TYR:O	1:B:449:GLY:HA2	2.20	0.41
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.56	0.41
1:B:371:GLU:OE1	4:B:2903:329:N1	2.53	0.41
1:B:457:TRP:HA	3:B:2902:H4B:N1	2.35	0.41
1:B:98:ALA:C	1:B:100:SER:H	2.18	0.41
1:B:348:ASN:H	1:B:348:ASN:ND2	2.19	0.41
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.56	0.41
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.03	0.41
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.03	0.40
1:B:123:PRO:HD3	6:B:4456:HOH:O	2.20	0.40
1:B:204:GLN:HG2	1:B:227:TYR:CZ	2.56	0.40
1:B:173:TYR:CE1	1:B:356:LEU:HD21	2.56	0.40
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:C	1:A:470:PHE:CD1	2.95	0.40
1:A:83:ASN:ND2	1:A:83:ASN:C	2.75	0.40
1:B:422:LYS:HG2	6:B:4766:HOH:O	2.21	0.40
1:A:185:LYS:HD3	1:A:201:SER:HA	2.03	0.40

All (3) 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:4177:HOH:O	6:A:4227:HOH:O[11_655]	1.97	0.23
6:A:4145:HOH:O	6:A:4177:HOH:O[11_655]	2.19	0.01
6:A:4261:HOH:O	6:A:4261:HOH:O[11_655]	2.19	0.01

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	419/433 (97%)	378 (90%)	36 (9%)	5 (1%)	16	23
1	B	419/433 (97%)	385 (92%)	31 (7%)	3 (1%)	26	38
All	All	838/866 (97%)	763 (91%)	67 (8%)	8 (1%)	19	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	THR
1	A	99	THR
1	A	111	GLY
1	A	464	GLY
1	A	105	LYS
1	B	108	SER
1	B	307	GLY

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Mol	Chain	Res	Type
1	A	269	GLY

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	367/381 (96%)	364 (99%)	3 (1%)	86	94
1	B	366/381 (96%)	360 (98%)	6 (2%)	70	86
All	All	733/762 (96%)	724 (99%)	9 (1%)	78	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	101	ASP
1	A	223	ARG
1	B	88	GLU
1	B	105	LYS
1	B	130	LEU
1	B	223	ARG
1	B	334	GLN
1	B	348	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	142	ASN
1	A	219	GLN
1	A	257	GLN
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS

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Mol	Chain	Res	Type
1	B	96	HIS
1	B	143	GLN
1	B	215	GLN
1	B	257	GLN
1	B	348	ASN
1	B	421	GLN
1	B	493	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 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	$\#|Z| > 2$
5	SO4	A	3003	-	4,4,4	0.26	0	6,6,6	0.09	0
5	SO4	A	3004	-	4,4,4	0.26	0	6,6,6	0.09	0
2	HEM	A	901	1	30,50,50	2.43	11 (36%)	24,82,82	2.29	9 (37%)
3	H4B	A	902	-	13,18,18	1.78	1 (7%)	11,26,26	9.89	7 (63%)
4	329	A	903	-	7,13,13	1.32	1 (14%)	1,18,18	1.64	0
2	HEM	B	2901	1	30,50,50	2.53	8 (26%)	24,82,82	2.33	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
3	H4B	B	2902	-	13,18,18	1.90	2 (15%)	11,26,26	7.23	9 (81%)
4	329	B	2903	-	7,13,13	1.38	1 (14%)	1,18,18	2.33	1 (100%)
5	SO4	B	3003	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	3004	-	4,4,4	0.26	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	3003	-	-	0/0/0/0	0/0/0/0
5	SO4	A	3004	-	-	0/0/0/0	0/0/0/0
2	HEM	A	901	1	-	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	329	A	903	-	-	0/0/13/13	0/1/2/2
2	HEM	B	2901	1	-	0/10/54/54	0/0/8/8
3	H4B	B	2902	-	1/1/3/5	0/8/17/17	0/2/2/2
4	329	B	2903	-	-	0/0/13/13	0/1/2/2
5	SO4	B	3003	-	-	0/0/0/0	0/0/0/0
5	SO4	B	3004	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2901	HEM	C2D-C3D	-6.38	1.35	1.54
3	B	2902	H4B	C7-N8	-6.23	1.38	1.46
2	A	901	HEM	C2D-C3D	-5.95	1.36	1.54
2	B	2901	HEM	C3C-CAC	-5.90	1.40	1.51
3	A	902	H4B	C7-N8	-5.82	1.38	1.46
2	B	2901	HEM	C3B-CAB	-5.66	1.40	1.51
2	A	901	HEM	C3B-CAB	-5.43	1.41	1.51
2	A	901	HEM	C3B-C4B	-5.33	1.47	1.51
2	B	2901	HEM	C3B-C4B	-4.97	1.47	1.51
2	A	901	HEM	C3C-CAC	-4.95	1.42	1.51
2	A	901	HEM	C2C-C1C	-3.66	1.45	1.52
2	B	2901	HEM	C2C-C1C	-3.60	1.45	1.52
2	A	901	HEM	C3D-C4D	-3.11	1.47	1.51
2	B	2901	HEM	C3D-C4D	-3.02	1.47	1.51
2	A	901	HEM	C2B-C1B	-2.51	1.43	1.51
2	B	2901	HEM	C2B-C1B	-2.45	1.43	1.51
2	A	901	HEM	C2D-C1D	-2.08	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2902	H4B	C4A-N5	-2.03	1.33	1.38
2	A	901	HEM	CBC-CAC	2.01	1.40	1.29
2	B	2901	HEM	CBB-CAB	2.03	1.41	1.29
4	A	903	329	C5-N1	2.03	1.33	1.29
2	A	901	HEM	FE-NC	2.15	2.04	1.95
4	B	2903	329	C5-N1	2.27	1.34	1.29
2	A	901	HEM	C4C-NC	2.43	1.39	1.36

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	H4B	C4-C4A-C8A	-27.89	89.33	114.56
3	B	2902	H4B	C4-C4A-C8A	-19.74	96.71	114.56
3	A	902	H4B	C4-N3-C2	-10.09	101.93	115.94
3	B	2902	H4B	C4-N3-C2	-7.77	105.15	115.94
3	A	902	H4B	O10-C10-C11	-5.85	92.68	109.61
3	A	902	H4B	N2-C2-N1	-5.06	108.82	117.20
3	B	2902	H4B	O10-C10-C11	-2.46	102.49	109.61
2	B	2901	HEM	CAA-C2A-C3A	-2.39	122.17	129.00
4	B	2903	329	C7-S1-C6	-2.33	88.71	91.50
3	B	2902	H4B	C2-N1-C8A	-2.24	109.51	114.54
3	B	2902	H4B	N2-C2-N3	-2.03	113.83	117.20
2	A	901	HEM	C3B-C4B-CHC	2.25	126.33	123.16
2	A	901	HEM	CMD-C2D-C3D	2.29	124.46	114.35
2	B	2901	HEM	CMD-C2D-C3D	2.48	125.33	114.35
2	B	2901	HEM	C3B-C4B-CHC	2.62	126.86	123.16
2	A	901	HEM	CAA-C2A-C1A	2.66	129.89	127.01
2	B	2901	HEM	CAA-C2A-C1A	2.91	130.16	127.01
2	A	901	HEM	C2D-C3D-C4D	2.96	106.52	101.50
3	B	2902	H4B	C4A-C8A-N8	3.04	122.01	118.43
2	B	2901	HEM	C2D-C3D-C4D	3.10	106.75	101.50
2	B	2901	HEM	CAD-C3D-C2D	3.31	122.72	113.22
2	A	901	HEM	CMB-C2B-C3B	3.53	125.35	116.53
2	A	901	HEM	CAD-C3D-C2D	3.60	123.56	113.22
3	B	2902	H4B	N3-C2-N1	3.69	131.59	125.53
3	B	2902	H4B	C7-C6-N5	3.81	118.35	110.45
2	B	2901	HEM	CMB-C2B-C3B	4.20	127.03	116.53
3	A	902	H4B	N2-C2-N3	4.26	124.25	117.20
2	A	901	HEM	CMC-C2C-C3C	4.65	128.14	116.53
2	A	901	HEM	C3B-CAB-CBB	4.65	131.59	124.46
2	A	901	HEM	CAD-C3D-C4D	4.77	129.30	112.47
2	B	2901	HEM	CAD-C3D-C4D	4.92	129.82	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2901	HEM	CMC-C2C-C3C	5.29	129.72	116.53
3	A	902	H4B	C7-C6-N5	6.31	123.55	110.45
3	B	2902	H4B	C4A-C8A-N1	8.18	135.72	118.76
3	A	902	H4B	C4A-C8A-N1	8.62	136.62	118.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6
3	B	2902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	1	0
4	A	903	329	1	0
2	B	2901	HEM	1	0
3	B	2902	H4B	1	0
4	B	2903	329	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	421/433 (97%)	0.04	27 (6%)	23	23	23, 44, 74, 98	0
1	B	421/433 (97%)	-0.05	23 (5%)	29	29	24, 41, 72, 100	0
All	All	842/866 (97%)	-0.00	50 (5%)	26	26	23, 43, 73, 100	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	THR	5.4
1	A	106	SER	5.4
1	A	104	CYS	4.7
1	B	108	SER	4.6
1	A	103	THR	4.5
1	B	99	THR	4.3
1	B	107	LYS	4.3
1	A	495	TRP	4.1
1	B	106	SER	3.7
1	B	125	ASP	3.7
1	A	102	PHE	3.5
1	B	149	LYS	3.4
1	B	267	PRO	3.4
1	A	270	THR	3.1
1	A	497	ASN	3.1
1	A	149	LYS	2.9
1	A	150	GLU	2.9
1	A	107	LYS	2.9
1	A	496	GLN	2.8
1	A	101	ASP	2.8
1	B	102	PHE	2.8
1	A	398	HIS	2.7
1	A	91	HIS	2.7
1	A	78	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	494	ILE	2.6
1	B	270	THR	2.5
1	B	497	ASN	2.5
1	B	104	CYS	2.5
1	A	108	SER	2.5
1	B	495	TRP	2.4
1	A	99	THR	2.4
1	B	391	ARG	2.4
1	A	96	HIS	2.4
1	A	152	LYS	2.3
1	A	334	GLN	2.3
1	A	77	GLN	2.3
1	A	267	PRO	2.2
1	A	268	ASP	2.2
1	B	249	HIS	2.2
1	A	148	PHE	2.2
1	B	78	TYR	2.2
1	A	494	ILE	2.1
1	B	446	ARG	2.1
1	B	152	LYS	2.1
1	B	101	ASP	2.1
1	A	266	MET	2.0
1	A	271	ILE	2.0
1	B	268	ASP	2.0
1	B	150	GLU	2.0
1	B	294	GLY	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, 95th 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(Å²)	Q<0.9
4	329	B	2903	12/12	0.98	0.22	1.83	25,27,30,31	0
4	329	A	903	12/12	0.98	0.20	0.63	26,27,30,30	0
2	HEM	B	2901	43/43	0.97	0.17	0.42	18,23,27,29	0
2	HEM	A	901	43/43	0.98	0.18	0.39	19,23,26,31	0
3	H4B	A	902	17/17	0.98	0.18	0.27	17,25,30,33	0
3	H4B	B	2902	17/17	0.99	0.19	-0.03	16,24,26,28	0
5	SO4	A	3004	5/5	0.91	0.23	-	95,95,96,96	0
5	SO4	B	3003	5/5	0.88	0.19	-	112,113,113,114	0
5	SO4	A	3003	5/5	0.89	0.26	-	115,116,116,116	0
5	SO4	B	3004	5/5	0.90	0.23	-	103,103,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.