Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EBF
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	:	2.29 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:

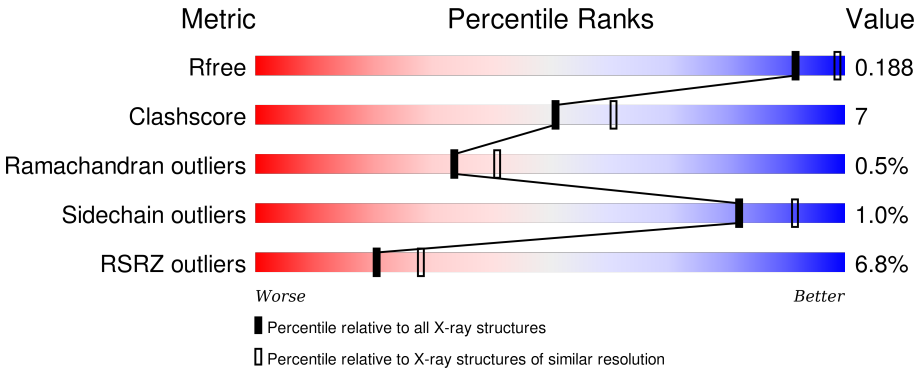
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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% 78% 19%
1	B	433	7% 84% 13%

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

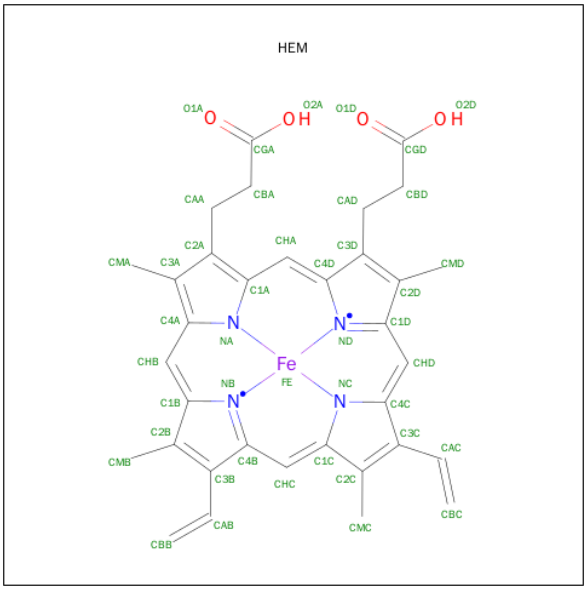
There are 6 unique types of molecules in this entry. The entry contains 7887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

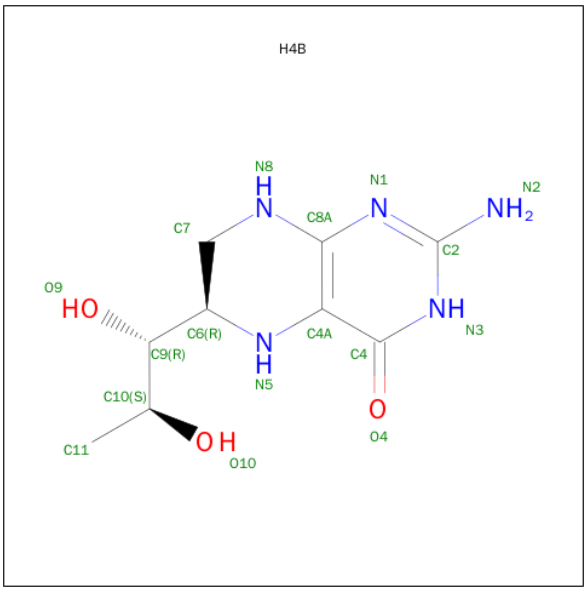
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3425	2195	590	619	21			
1	B	421	Total	C	N	O	S	0	0	0
			3421	2193	589	618	21			

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



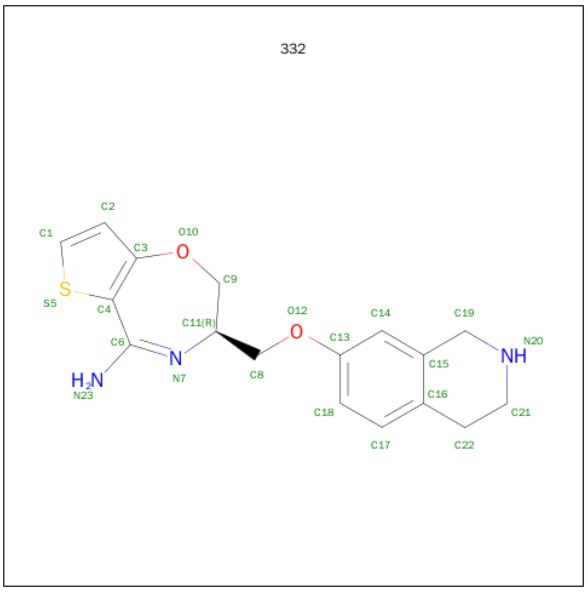
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is (3R)-3-[(1,2,3,4-TETRAHYDROISOQUINOLIN-7-YLOXY)METHYL]-2,3-DIHYDROTHIENO[2,3-F][1,4]OXAZEPIN-5-AMINE (three-letter code: 332) (formula: $C_{17}H_{19}N_3O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 23 17 3 2 1	0	0

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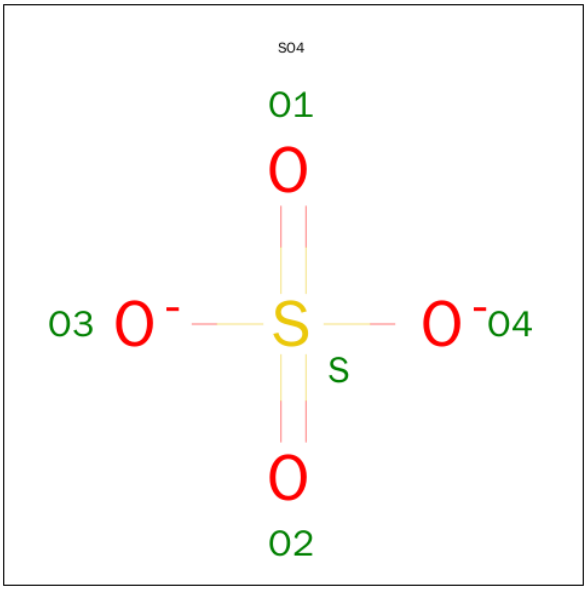
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			23	17	3	2	1		

- 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.

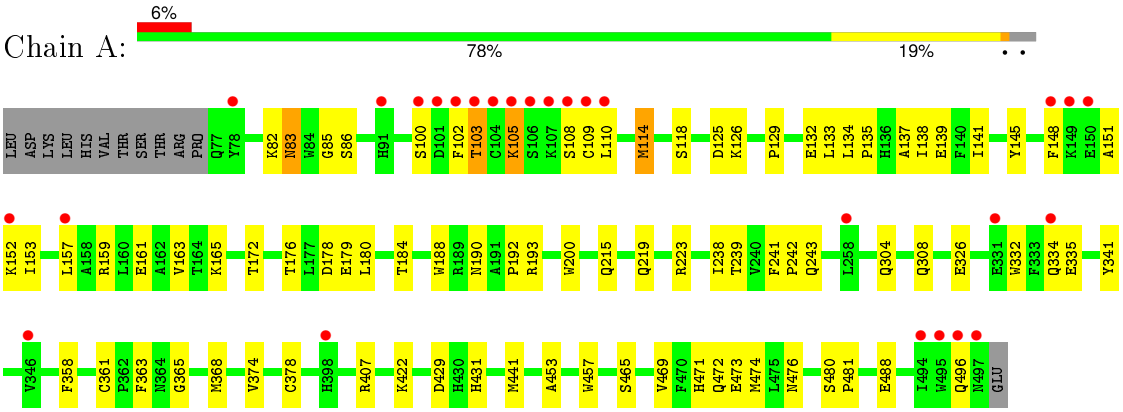
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	398	Total	O	0	0
			398	398		
6	B	457	Total	O	0	0
			457	457		

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.

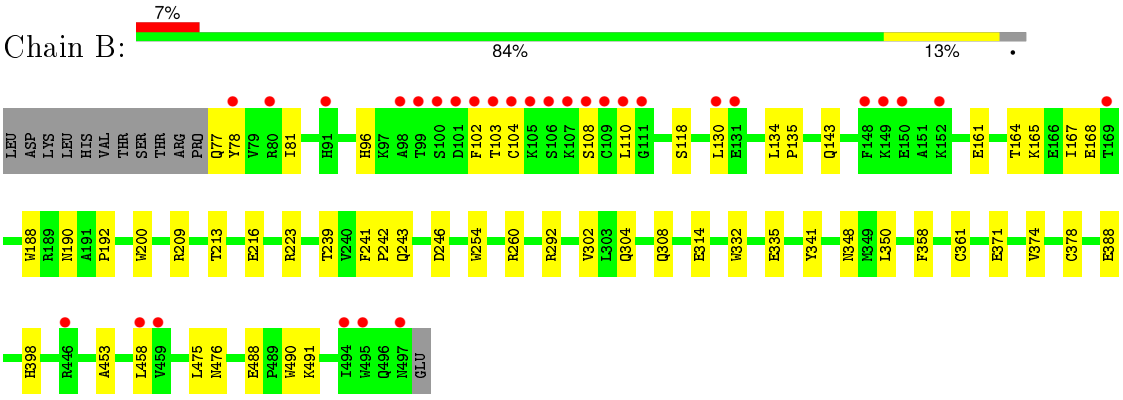
- Molecule 1: Nitric oxide synthase, inducible

Chain A:



- Molecule 1: Nitric oxide synthase, inducible

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	212.94Å 212.94Å 116.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.39 – 2.29 31.39 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.0 (31.39-2.29) 93.2 (31.39-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.203 , 0.242 0.195 , 0.188	Depositor DCC
R_{free} test set	3291 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 65348 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 332, SO4, 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	0.31	0/3525	0.58	2/4792 (0.0%)
1	B	0.32	0/3521	0.59	0/4787
All	All	0.32	0/7046	0.59	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	-5.71	98.81	113.10
1	A	368	MET	N-CA-C	-5.20	96.96	111.00

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	3425	0	3318	55	0
1	B	3421	0	3312	38	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	17	0	14	0	0
3	B	17	0	14	0	0
4	A	23	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	19	4	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	398	0	0	3	0
6	B	457	0	0	6	0
All	All	7887	0	6756	95	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 (95) 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	1.42	0.97
1:A:441:MET:HE1	1:A:472:GLN:HG2	1.52	0.90
1:A:103:THR:HG22	1:A:110:LEU:HB2	1.63	0.80
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.94	0.67
1:A:83:ASN:HD22	1:A:86:SER:H	1.42	0.67
1:B:388:GLU:HG2	6:B:4814:HOH:O	1.96	0.66
1:A:215:GLN:O	1:A:219:GLN:HG3	1.96	0.65
1:B:190:ASN:O	1:B:192:PRO:HD3	1.97	0.64
1:A:441:MET:CE	1:A:472:GLN:HG2	2.26	0.64
1:A:83:ASN:ND2	1:A:85:GLY:H	1.98	0.62
1:B:77:GLN:O	1:B:96:HIS:HE1	1.85	0.60
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.84	0.59
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.85	0.58
1:A:103:THR:CG2	1:A:110:LEU:HB2	2.32	0.58
1:B:164:THR:O	1:B:168:GLU:HG3	2.04	0.57
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.39	0.57
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.27	0.57
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.85	0.57
1:B:104:CYS:HA	1:B:110:LEU:HD12	1.88	0.56
1:A:465:SER:O	1:A:471:HIS:HE1	1.89	0.55
1:A:161:GLU:O	1:A:165:LYS:HD3	2.07	0.55
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.06	0.55
1:A:103:THR:H	1:A:118:SER:HB3	1.73	0.54
1:B:488:GLU:OE2	1:B:491:LYS:HE3	2.07	0.54
1:A:239:THR:O	1:A:361:CYS:HA	2.08	0.54
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.43	0.53
1:B:110:LEU:HD22	6:B:4647:HOH:O	2.09	0.53
1:A:153:ILE:O	1:A:157:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:HD2	1:A:108:SER:OG	2.08	0.53
1:B:332:TRP:O	1:B:335:GLU:HB2	2.08	0.53
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.44	0.52
1:A:152:LYS:HB2	1:A:152:LYS:NZ	2.24	0.52
1:A:332:TRP:O	1:A:335:GLU:HB2	2.10	0.52
1:A:407:ARG:HD2	6:A:4139:HOH:O	2.10	0.51
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.41	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.46	0.50
1:A:135:PRO:O	1:A:139:GLU:HG3	2.11	0.50
1:A:114:MET:HE1	6:A:4338:HOH:O	2.12	0.49
1:A:304:GLN:HG3	1:A:308:GLN:O	2.14	0.48
1:A:82:LYS:O	1:A:473:GLU:HG3	2.13	0.48
1:A:190:ASN:O	1:A:192:PRO:HD3	2.14	0.48
1:A:134:LEU:O	1:A:138:ILE:HG12	2.15	0.47
1:B:254:TRP:HB2	1:B:302:VAL:HB	1.96	0.47
1:A:469:VAL:HG13	1:A:474:MET:CE	2.45	0.47
1:A:308:GLN:HG2	1:A:496:GLN:HE22	1.78	0.47
1:B:304:GLN:HG3	1:B:308:GLN:O	2.15	0.47
1:A:83:ASN:ND2	1:A:86:SER:H	2.09	0.47
1:B:143:GLN:HG2	6:B:4660:HOH:O	2.15	0.47
1:A:103:THR:H	1:A:118:SER:CB	2.28	0.46
1:A:132:GLU:O	1:A:135:PRO:HD2	2.16	0.46
1:B:292:ARG:NH1	1:B:314:GLU:OE2	2.48	0.46
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.46	0.46
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.45	0.46
1:A:469:VAL:HG13	1:A:474:MET:HE3	1.98	0.46
1:A:152:LYS:HB2	1:A:152:LYS:HZ2	1.81	0.46
1:A:109:CYS:C	1:A:110:LEU:HD23	2.37	0.45
1:B:102:PHE:HZ	1:B:476:ASN:ND2	2.15	0.45
1:A:326:GLU:OE1	1:A:422:LYS:NZ	2.42	0.45
1:A:238:ILE:HG13	1:A:363:PHE:HB3	1.97	0.45
1:B:341:TYR:OH	4:B:2903:332:H17	2.17	0.45
1:B:371:GLU:OE1	4:B:2903:332:N7	2.49	0.45
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.46	0.45
1:B:239:THR:O	1:B:361:CYS:HA	2.17	0.45
1:B:374:VAL:O	1:B:378:CYS:HB2	2.18	0.44
2:B:2901:HEM:HBC2	2:B:2901:HEM:HMC1	1.99	0.44
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.18	0.44
1:B:246:ASP:HB3	6:B:4855:HOH:O	2.18	0.44
1:B:161:GLU:HG2	1:B:165:LYS:HE3	2.00	0.44
1:B:103:THR:OG1	1:B:104:CYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:O	1:A:184:THR:HG23	2.18	0.43
1:B:78:TYR:CD1	1:B:78:TYR:C	2.92	0.43
1:A:137:ALA:O	1:A:141:ILE:HG12	2.19	0.42
1:A:429:ASP:OD1	1:A:431:HIS:HB2	2.19	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.19	0.42
1:A:488:GLU:HG2	6:A:4254:HOH:O	2.19	0.42
1:A:165:LYS:HD2	1:A:165:LYS:N	2.34	0.42
1:A:341:TYR:OH	4:A:903:332:H17	2.20	0.42
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.54	0.42
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.01	0.42
1:A:133:LEU:HD21	1:A:172:THR:HA	2.02	0.41
1:A:145:TYR:HA	1:A:148:PHE:CD2	2.54	0.41
1:B:209:ARG:O	1:B:242:PRO:HG3	2.20	0.41
1:B:103:THR:HG22	1:B:118:SER:OG	2.20	0.41
1:A:453:ALA:HB3	1:A:474:MET:HB3	2.01	0.41
1:A:241:PHE:HB3	1:A:242:PRO:HD2	2.03	0.41
1:B:488:GLU:HB3	1:B:490:TRP:CE2	2.56	0.41
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.56	0.41
1:B:350:LEU:C	1:B:350:LEU:HD23	2.42	0.41
1:B:260:ARG:CZ	4:B:2903:332:H22A	2.51	0.40
1:A:159:ARG:O	1:A:163:VAL:HG23	2.21	0.40
1:B:398:HIS:HB2	6:B:4594:HOH:O	2.20	0.40
1:A:102:PHE:HZ	1:A:476:ASN:ND2	2.19	0.40
1:A:480:SER:HA	1:A:481:PRO:C	2.42	0.40
2:B:2901:HEM:HBA2	4:B:2903:332:H9A	2.02	0.40
1:B:108:SER:HB2	6:B:4582:HOH:O	2.21	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	419/433 (97%)	394 (94%)	21 (5%)	4 (1%)	19 21
1	B	419/433 (97%)	392 (94%)	27 (6%)	0	100 100
All	All	838/866 (97%)	786 (94%)	48 (6%)	4 (0%)	34 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	103	THR
1	A	151	ALA
1	A	105	LYS

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%)	362 (99%)	5 (1%)	74 86
1	B	366/381 (96%)	364 (100%)	2 (0%)	92 97
All	All	733/762 (96%)	726 (99%)	7 (1%)	82 91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	114	MET
1	A	178	ASP
1	A	223	ARG
1	A	334	GLN
1	B	223	ARG
1	B	348	ASN

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	83	ASN
1	A	96	HIS
1	A	142	ASN
1	A	202	ASN
1	A	219	GLN
1	A	249	HIS
1	A	334	GLN
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS
1	A	496	GLN
1	B	96	HIS
1	B	143	GLN
1	B	215	GLN
1	B	334	GLN
1	B	348	ASN
1	B	421	GLN

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

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	0.23	0	6,6,6	0.07	0
5	SO4	A	3004	-	4,4,4	0.23	0	6,6,6	0.11	0
2	HEM	A	901	1	30,50,50	2.63	8 (26%)	24,82,82	2.27	8 (33%)
3	H4B	A	902	-	13,18,18	1.86	1 (7%)	11,26,26	6.94	9 (81%)
4	332	A	903	-	22,26,26	2.55	12 (54%)	18,36,36	1.30	1 (5%)
2	HEM	B	2901	1	30,50,50	2.45	8 (26%)	24,82,82	2.42	9 (37%)
3	H4B	B	2902	-	13,18,18	1.88	1 (7%)	11,26,26	6.25	7 (63%)
4	332	B	2903	-	22,26,26	2.58	12 (54%)	18,36,36	1.34	1 (5%)
5	SO4	B	3003	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	B	3004	-	4,4,4	0.23	0	6,6,6	0.09	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	332	A	903	-	-	0/4/25/25	0/3/4/4
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	332	B	2903	-	-	0/4/25/25	0/3/4/4
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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C2D-C3D	-6.43	1.35	1.54
3	B	2902	H4B	C7-N8	-6.26	1.37	1.46
3	A	902	H4B	C7-N8	-6.15	1.38	1.46
2	B	2901	HEM	C2D-C3D	-6.10	1.36	1.54
2	A	901	HEM	C3C-CAC	-5.83	1.40	1.51
2	A	901	HEM	C3B-CAB	-5.71	1.40	1.51
2	B	2901	HEM	C3C-CAC	-5.44	1.41	1.51
2	B	2901	HEM	C3B-CAB	-5.21	1.41	1.51
2	A	901	HEM	C3B-C4B	-5.09	1.47	1.51
2	B	2901	HEM	C3B-C4B	-4.62	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C2C-C1C	-4.19	1.44	1.52
2	A	901	HEM	C3D-C4D	-3.95	1.46	1.51
2	B	2901	HEM	C3D-C4D	-3.84	1.46	1.51
2	B	2901	HEM	C2C-C1C	-2.75	1.47	1.52
2	B	2901	HEM	C2B-C1B	-2.52	1.43	1.51
2	A	901	HEM	C2B-C1B	-2.02	1.45	1.51
4	A	903	332	C19-N20	2.02	1.49	1.46
4	A	903	332	C22-C16	2.05	1.54	1.51
4	B	2903	332	C17-C16	2.14	1.43	1.39
4	A	903	332	C17-C16	2.25	1.43	1.39
4	B	2903	332	C19-N20	2.29	1.49	1.46
4	B	2903	332	C22-C16	2.32	1.55	1.51
4	A	903	332	O12-C13	2.54	1.43	1.37
4	A	903	332	C15-C16	2.74	1.45	1.40
4	B	2903	332	C15-C16	2.77	1.45	1.40
4	A	903	332	C18-C13	2.80	1.44	1.38
4	B	2903	332	O12-C13	2.81	1.44	1.37
2	B	2901	HEM	FE-NC	2.87	2.07	1.95
4	B	2903	332	C18-C13	2.87	1.44	1.38
4	B	2903	332	C21-C22	3.08	1.57	1.50
4	A	903	332	C21-C22	3.12	1.58	1.50
4	B	2903	332	C17-C18	3.25	1.44	1.38
4	A	903	332	C17-C18	3.43	1.44	1.38
2	A	901	HEM	FE-NC	3.48	2.09	1.95
4	B	2903	332	C9-C11	3.81	1.55	1.50
4	A	903	332	C9-C11	4.05	1.56	1.50
4	B	2903	332	C14-C13	4.26	1.46	1.38
4	A	903	332	C14-C13	4.30	1.46	1.38
4	A	903	332	C11-N7	4.47	1.51	1.47
4	B	2903	332	C8-C11	4.55	1.62	1.52
4	A	903	332	C8-C11	4.56	1.62	1.52
4	B	2903	332	C11-N7	4.58	1.51	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	H4B	C4-C4A-C8A	-16.99	99.20	114.56
3	B	2902	H4B	C4-C4A-C8A	-13.09	102.72	114.56
3	A	902	H4B	C4A-C8A-N8	-6.30	111.02	118.43
3	A	902	H4B	C4-N3-C2	-4.79	109.29	115.94
3	B	2902	H4B	C4A-C8A-N8	-4.33	113.34	118.43
3	B	2902	H4B	C2-N1-C8A	-3.78	106.03	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	H4B	N2-C2-N1	-2.68	112.77	117.20
3	A	902	H4B	C2-N1-C8A	-2.33	109.30	114.54
3	B	2902	H4B	O10-C10-C11	-2.07	103.62	109.61
2	A	901	HEM	CMD-C2D-C3D	2.27	124.38	114.35
2	A	901	HEM	CAA-C2A-C1A	2.34	129.54	127.01
2	B	2901	HEM	CMD-C2D-C3D	2.56	125.69	114.35
2	B	2901	HEM	C4B-CHC-C1C	2.65	130.25	125.82
3	A	902	H4B	N3-C2-N1	2.73	130.01	125.53
2	B	2901	HEM	C3B-C4B-CHC	2.89	127.23	123.16
2	A	901	HEM	C3B-CAB-CBB	2.90	128.90	124.46
2	B	2901	HEM	C3B-CAB-CBB	3.31	129.53	124.46
2	A	901	HEM	C2D-C3D-C4D	3.51	107.44	101.50
2	B	2901	HEM	C2D-C3D-C4D	3.51	107.45	101.50
2	A	901	HEM	CAD-C3D-C2D	3.65	123.72	113.22
4	A	903	332	O12-C8-C11	3.65	114.11	108.11
2	A	901	HEM	CMB-C2B-C3B	3.70	125.76	116.53
4	B	2903	332	O12-C8-C11	3.81	114.37	108.11
2	B	2901	HEM	CAD-C3D-C2D	3.82	124.20	113.22
2	B	2901	HEM	CMB-C2B-C3B	4.26	127.16	116.53
2	B	2901	HEM	CAD-C3D-C4D	4.38	127.91	112.47
2	A	901	HEM	CAD-C3D-C4D	4.53	128.43	112.47
2	B	2901	HEM	CMC-C2C-C3C	4.57	127.94	116.53
2	A	901	HEM	CMC-C2C-C3C	5.02	129.07	116.53
3	A	902	H4B	C7-C6-N5	6.45	123.84	110.45
3	A	902	H4B	C8A-C4A-N5	6.90	127.55	118.85
3	B	2902	H4B	C7-C6-N5	7.45	125.92	110.45
3	B	2902	H4B	C8A-C4A-N5	8.13	129.09	118.85
3	A	902	H4B	C4A-C8A-N1	8.22	135.80	118.76
3	B	2902	H4B	C4A-C8A-N1	9.68	138.82	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	332	1	0
2	B	2901	HEM	2	0
4	B	2903	332	4	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	421/433 (97%)	0.27	27 (6%)	23	31	17, 32, 56, 86	0
1	B	421/433 (97%)	0.23	30 (7%)	19	26	16, 29, 55, 84	0
All	All	842/866 (97%)	0.25	57 (6%)	20	28	16, 30, 56, 86	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	THR	13.7
1	A	103	THR	13.3
1	B	106	SER	10.0
1	A	106	SER	9.5
1	A	102	PHE	8.3
1	A	104	CYS	8.2
1	B	104	CYS	7.6
1	B	108	SER	7.2
1	B	102	PHE	7.1
1	B	101	ASP	6.9
1	B	107	LYS	6.2
1	B	100	SER	5.5
1	A	107	LYS	5.5
1	A	108	SER	4.7
1	B	99	THR	4.6
1	A	149	LYS	4.6
1	B	78	TYR	4.5
1	A	496	GLN	4.5
1	A	101	ASP	4.5
1	A	105	LYS	4.5
1	B	105	LYS	4.4
1	B	149	LYS	3.9
1	A	495	TRP	3.7
1	B	494	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	398	HIS	3.6
1	A	334	GLN	3.5
1	A	78	TYR	3.4
1	A	157	LEU	3.4
1	A	148	PHE	3.1
1	A	100	SER	3.1
1	B	497	ASN	3.1
1	B	130	LEU	3.0
1	A	150	GLU	2.9
1	B	111	GLY	2.9
1	B	150	GLU	2.9
1	A	152	LYS	2.8
1	A	91	HIS	2.7
1	B	98	ALA	2.6
1	A	110	LEU	2.6
1	B	110	LEU	2.6
1	B	91	HIS	2.5
1	B	148	PHE	2.5
1	B	446	ARG	2.5
1	A	494	ILE	2.4
1	B	495	TRP	2.4
1	A	109	CYS	2.4
1	B	459	VAL	2.3
1	A	346	VAL	2.3
1	B	169	THR	2.3
1	B	80	ARG	2.3
1	B	109	CYS	2.2
1	A	497	ASN	2.2
1	A	258	LEU	2.2
1	A	331	GLU	2.2
1	B	152	LYS	2.2
1	B	131	GLU	2.1
1	B	458	LEU	2.1

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

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
2	HEM	A	901	43/43	0.98	0.15	0.45	15,19,22,24	0
4	332	A	903	23/23	0.97	0.16	0.38	16,20,22,24	0
2	HEM	B	2901	43/43	0.98	0.15	0.13	13,16,18,19	0
4	332	B	2903	23/23	0.98	0.14	0.06	13,18,22,23	0
3	H4B	B	2902	17/17	0.97	0.13	-0.36	14,19,22,23	0
3	H4B	A	902	17/17	0.97	0.10	-1.56	13,23,26,26	0
5	SO4	B	3004	5/5	0.86	0.35	-	84,84,85,85	0
5	SO4	B	3003	5/5	0.93	0.34	-	89,89,89,90	0
5	SO4	A	3003	5/5	0.80	0.33	-	87,87,88,88	0
5	SO4	A	3004	5/5	0.79	0.33	-	82,83,84,84	0

6.5 Other polymers

There are no such residues in this entry.