Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E67
Title	:	Murine inos dimer with inhibitor 4-MAP bound
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	:	2008-08-14
Resolution	:	2.60 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:

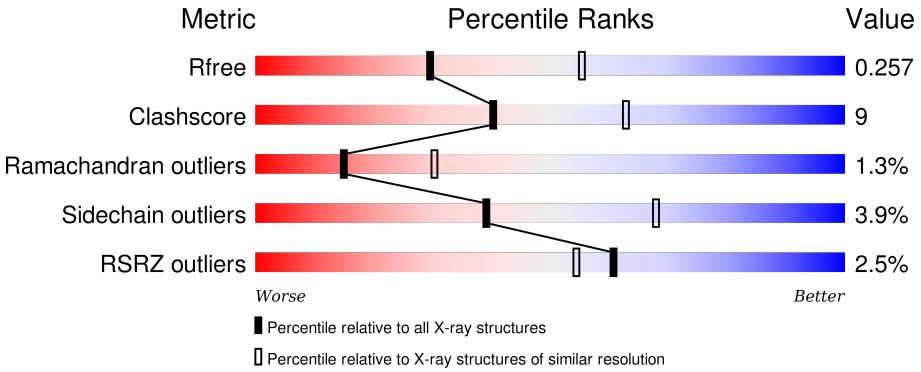
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	2% 72% 22% • 5%
1	B	433	3% 72% 22% • 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	-	-	-
3	H4B	B	902	X	-	-	-

2 Entry composition

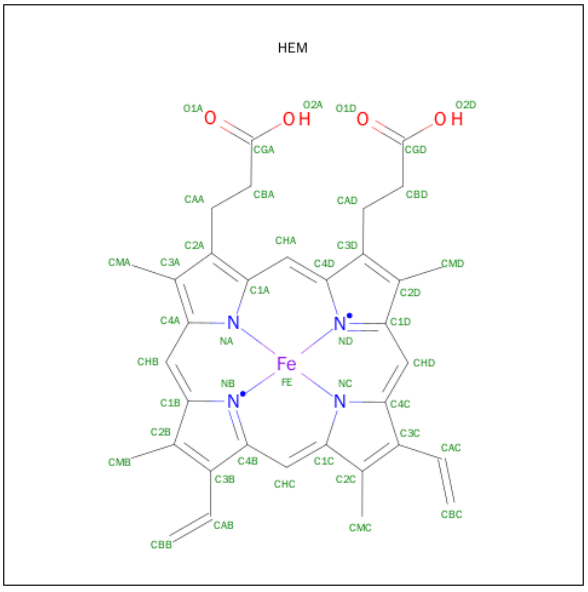
There are 5 unique types of molecules in this entry. The entry contains 6933 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

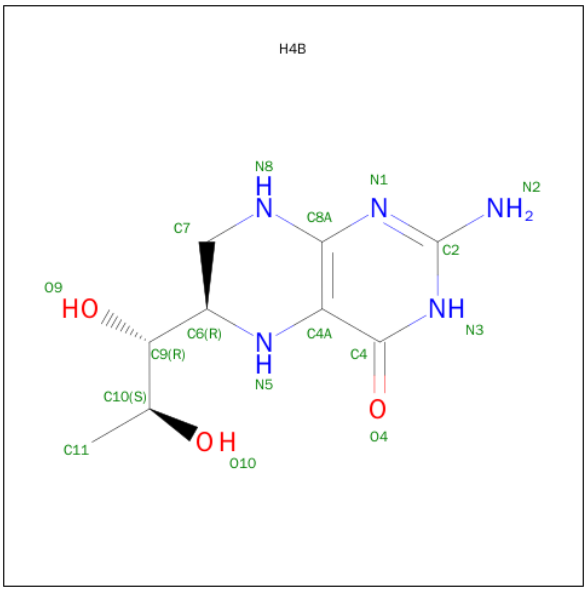
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3363	2157	580	606	20			
1	B	413	Total	C	N	O	S	0	0	0
			3359	2155	579	605	20			

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



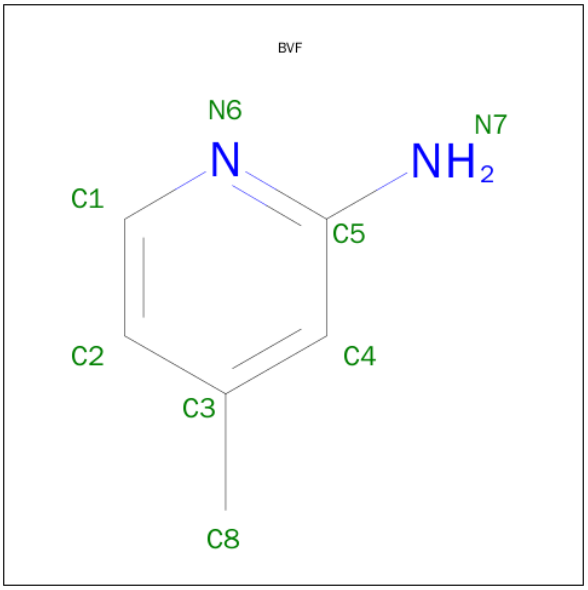
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 4 is 4-METHYLPYRIDIN-2-AMINE (three-letter code: BVF) (formula: $C_6H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 8 6 2	0	0
4	B	1	Total C N 8 6 2	0	0

- Molecule 5 is water.

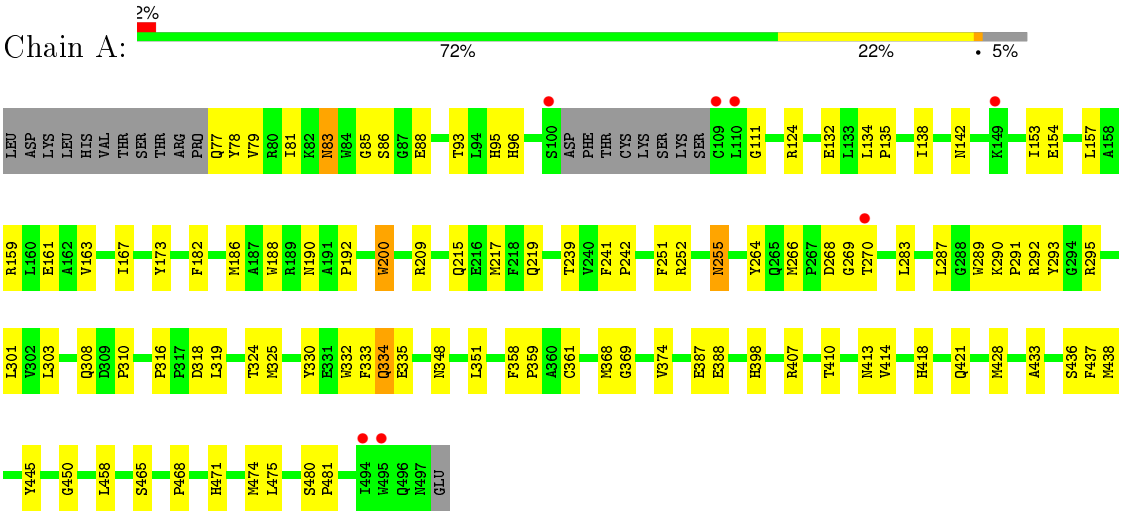
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	42	Total O 42 42	0	0
5	B	33	Total O 33 33	0	0

3 Residue-property plots (i)

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

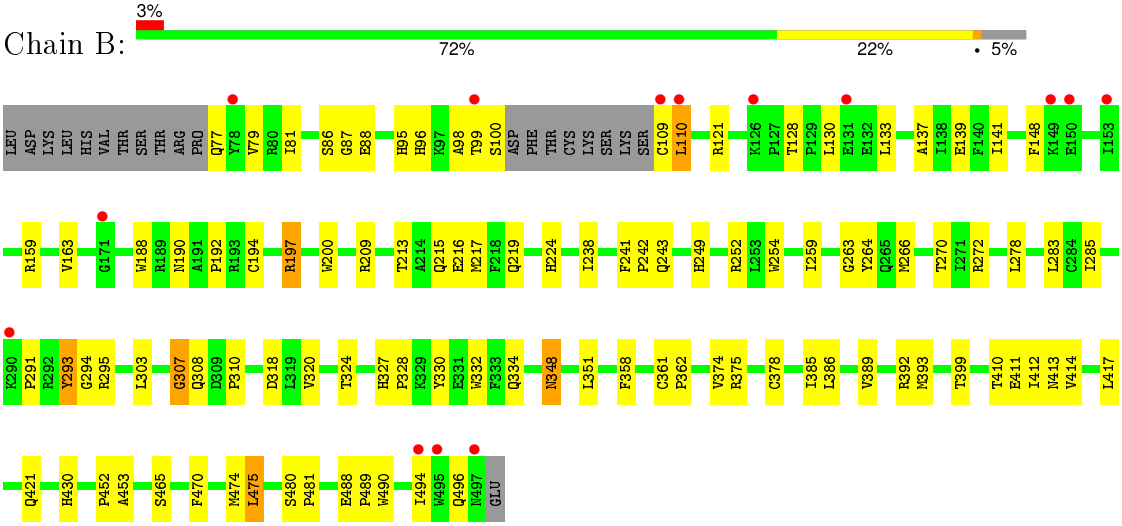
- Molecule 1: Nitric oxide synthase, inducible

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	214.09Å 214.09Å 115.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.9 (19.99-2.60) 74.5 (19.99-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.268 0.226 , 0.257	Depositor DCC
R_{free} test set	1973 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 40369 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, BVF

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	0.45	0/3461	0.63	0/4706
1	B	0.45	0/3457	0.63	0/4701
All	All	0.45	0/6918	0.63	0/9407

There are no bond length outliers.

There are no bond angle outliers.

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	3363	0	3256	52	0
1	B	3359	0	3250	62	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	17	0	14	0	0
3	B	17	0	14	1	0
4	A	8	0	8	0	0
4	B	8	0	8	0	0
5	A	42	0	0	3	0
5	B	33	0	0	0	0
All	All	6933	0	6610	117	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 9.

All (117) 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:A:410:THR:O	1:A:414:VAL:HG23	1.91	0.71
1:B:215:GLN:HE21	1:B:219:GLN:HE21	1.34	0.71
1:B:410:THR:O	1:B:414:VAL:HG23	1.93	0.68
1:A:190:ASN:O	1:A:192:PRO:HD3	1.94	0.67
1:B:194:CYS:HB3	1:B:197:ARG:HD3	1.80	0.63
1:A:209:ARG:O	1:A:242:PRO:HG3	1.99	0.62
1:A:163:VAL:O	1:A:167:ILE:HG13	2.00	0.61
1:A:301:LEU:HB3	1:A:303:LEU:HD21	1.82	0.61
1:A:83:ASN:ND2	1:A:85:GLY:H	1.99	0.60
2:B:901:HEM:HMC2	2:B:901:HEM:HBC2	1.82	0.60
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.65	0.60
1:B:266:MET:HB2	1:B:270:THR:O	2.02	0.60
1:B:385:ILE:O	1:B:389:VAL:HG23	2.01	0.59
1:A:465:SER:O	1:A:471:HIS:HE1	1.85	0.59
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.82	0.59
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.17	0.59
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.39	0.58
1:A:303:LEU:O	1:A:310:PRO:HA	2.04	0.57
1:B:190:ASN:O	1:B:192:PRO:HD3	2.05	0.57
1:A:266:MET:HB2	1:A:270:THR:O	2.05	0.56
1:A:159:ARG:O	1:A:163:VAL:HG23	2.06	0.56
1:B:77:GLN:O	1:B:96:HIS:HE1	1.89	0.55
1:B:361:CYS:SG	1:B:361:CYS:O	2.64	0.55
2:A:901:HEM:HBC2	2:A:901:HEM:HMC2	1.88	0.55
1:B:263:GLY:O	1:B:278:LEU:HD23	2.08	0.53
1:A:316:PRO:HD2	1:A:319:LEU:HD12	1.90	0.53
1:B:303:LEU:O	1:B:310:PRO:HA	2.09	0.53
1:B:393:MET:HE3	1:B:411:GLU:HG3	1.91	0.53
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.10	0.52
1:B:137:ALA:O	1:B:141:ILE:HG12	2.09	0.52
1:A:77:GLN:O	1:A:96:HIS:HE1	1.92	0.52
1:B:375:ARG:HH12	3:B:902:H4B:C4	2.23	0.52
1:A:124:ARG:HD3	5:A:930:HOH:O	2.09	0.51
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.45	0.51
1:B:98:ALA:O	1:B:100:SER:N	2.44	0.51
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.46	0.51
1:B:79:VAL:HG23	1:B:95:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH1	1:B:452:PRO:O	2.44	0.50
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.93	0.50
1:B:249:HIS:HA	1:B:307:GLY:HA3	1.94	0.49
1:A:374:VAL:CG2	1:A:413:ASN:HD21	2.25	0.49
1:A:132:GLU:O	1:A:135:PRO:HD2	2.13	0.49
1:B:480:SER:HA	1:B:481:PRO:C	2.34	0.48
1:B:215:GLN:HE21	1:B:219:GLN:NE2	2.07	0.48
1:A:445:TYR:HA	1:A:450:GLY:H	1.79	0.48
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.49	0.47
1:A:437:PHE:CE2	1:A:458:LEU:HD13	2.49	0.47
1:B:209:ARG:O	1:B:242:PRO:HG3	2.15	0.47
1:B:259:ILE:HD12	1:B:320:VAL:HG22	1.96	0.47
1:B:224:HIS:HE1	1:B:238:ILE:HA	1.79	0.46
1:A:289:TRP:HZ2	1:A:292:ARG:HH11	1.63	0.46
1:A:252:ARG:HD3	1:A:359:PRO:HB3	1.96	0.46
1:A:153:ILE:O	1:A:157:LEU:HD23	2.14	0.46
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.45	0.45
1:B:86:SER:C	1:B:88:GLU:H	2.20	0.45
1:A:217:MET:HG2	1:A:241:PHE:CE2	2.51	0.45
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.98	0.45
1:B:148:PHE:CD2	1:B:148:PHE:N	2.85	0.45
1:B:148:PHE:HD2	1:B:148:PHE:N	2.16	0.44
1:B:488:GLU:HA	1:B:489:PRO:HD2	1.81	0.44
1:B:264:TYR:HE1	1:B:294:GLY:H	1.66	0.44
1:A:351:LEU:HB3	1:A:358:PHE:HB2	1.99	0.44
1:B:266:MET:CE	1:B:272:ARG:HE	2.31	0.43
1:A:438:MET:HE1	1:A:468:PRO:O	2.19	0.43
1:B:374:VAL:CG2	1:B:413:ASN:HD21	2.31	0.43
2:A:901:HEM:HHC	2:A:901:HEM:HBB2	2.00	0.43
1:A:334:GLN:HA	5:A:946:HOH:O	2.18	0.43
1:B:159:ARG:O	1:B:163:VAL:HG23	2.19	0.43
1:B:217:MET:HG2	1:B:241:PHE:CE2	2.54	0.43
1:A:480:SER:HA	1:A:481:PRO:C	2.39	0.43
1:B:128:THR:HG22	1:B:133:LEU:HB2	2.01	0.43
1:B:389:VAL:HG21	1:B:412:ILE:HD11	2.00	0.43
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.53	0.42
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.54	0.42
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.34	0.42
1:B:430:HIS:N	1:B:430:HIS:ND1	2.65	0.42
1:A:239:THR:O	1:A:361:CYS:HA	2.18	0.42
1:A:418:HIS:HA	1:A:421:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.54	0.42
1:A:368:MET:HA	1:A:428:MET:O	2.19	0.42
1:A:242:PRO:HB2	1:A:251:PHE:CE1	2.54	0.42
1:B:238:ILE:HG13	1:B:362:PRO:O	2.19	0.42
1:A:332:TRP:O	1:A:335:GLU:HB2	2.20	0.42
1:A:79:VAL:HG23	1:A:95:HIS:CE1	2.55	0.42
1:B:254:TRP:CE3	1:B:283:LEU:HD21	2.55	0.42
1:A:78:TYR:HB3	1:A:93:THR:HG22	2.01	0.42
1:B:417:LEU:O	1:B:421:GLN:HG3	2.20	0.42
1:A:255:ASN:HD21	1:A:301:LEU:HA	1.84	0.42
1:A:330:TYR:N	1:A:330:TYR:CD2	2.87	0.42
1:A:138:ILE:O	1:A:142:ASN:ND2	2.51	0.42
1:A:289:TRP:O	1:A:291:PRO:HD3	2.18	0.42
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.88	0.42
1:A:291:PRO:HB2	1:A:293:TYR:CE2	2.55	0.41
1:A:86:SER:OG	1:A:88:GLU:HG2	2.20	0.41
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.88	0.41
1:B:197:ARG:HG3	1:B:197:ARG:HH21	1.86	0.41
1:B:197:ARG:HG3	1:B:197:ARG:NH2	2.35	0.41
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.55	0.41
1:B:385:ILE:HD11	1:B:412:ILE:HD13	2.01	0.41
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.69	0.41
1:B:81:ILE:HA	1:B:81:ILE:HD13	1.83	0.41
1:B:330:TYR:HE1	1:B:393:MET:HE3	1.85	0.41
1:A:290:LYS:HA	1:A:291:PRO:HD2	1.98	0.41
1:A:182:PHE:O	1:A:186:MET:HG2	2.21	0.41
1:A:283:LEU:O	1:A:287:LEU:HG	2.19	0.41
1:B:465:SER:HA	1:B:470:PHE:CG	2.56	0.41
1:B:351:LEU:HB3	1:B:358:PHE:HB2	2.02	0.41
1:B:453:ALA:HB3	1:B:474:MET:HB2	2.02	0.41
1:A:83:ASN:ND2	1:A:83:ASN:C	2.74	0.40
1:B:266:MET:HE1	1:B:272:ARG:HE	1.86	0.40
1:A:374:VAL:HG23	1:A:413:ASN:HD21	1.86	0.40
1:A:433:ALA:O	1:A:436:SER:HB3	2.21	0.40
1:B:348:ASN:C	1:B:348:ASN:HD22	2.24	0.40
1:A:398:HIS:HB2	5:A:908:HOH:O	2.22	0.40
1:B:109:CYS:O	1:B:110:LEU:HB2	2.20	0.40
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.86	0.40
1:B:378:CYS:SG	1:B:386:LEU:HD13	2.62	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	409/433 (94%)	374 (91%)	31 (8%)	4 (1%)	19 39
1	B	409/433 (94%)	366 (90%)	36 (9%)	7 (2%)	11 22
All	All	818/866 (94%)	740 (90%)	67 (8%)	11 (1%)	15 30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	THR
1	B	110	LEU
1	A	111	GLY
1	B	293	TYR
1	B	496	GLN
1	A	200	TRP
1	B	308	GLN
1	B	87	GLY
1	B	307	GLY
1	A	269	GLY
1	A	369	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	359/381 (94%)	342 (95%)	17 (5%)	32 59
1	B	358/381 (94%)	347 (97%)	11 (3%)	47 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	717/762 (94%)	689 (96%)	28 (4%)	39 68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	154	GLU
1	A	161	GLU
1	A	173	TYR
1	A	255	ASN
1	A	268	ASP
1	A	295	ARG
1	A	308	GLN
1	A	318	ASP
1	A	324	THR
1	A	334	GLN
1	A	348	ASN
1	A	387	GLU
1	A	388	GLU
1	A	407	ARG
1	A	474	MET
1	A	475	LEU
1	B	130	LEU
1	B	139	GLU
1	B	197	ARG
1	B	295	ARG
1	B	318	ASP
1	B	324	THR
1	B	334	GLN
1	B	348	ASN
1	B	399	THR
1	B	475	LEU
1	B	494	ILE

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	91	HIS
1	A	96	HIS
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	282	GLN
1	A	348	ASN
1	A	413	ASN
1	A	421	GLN
1	A	471	HIS
1	B	96	HIS
1	B	142	ASN
1	B	219	GLN
1	B	334	GLN
1	B	348	ASN
1	B	421	GLN
1	B	423	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

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	1	30,50,50	3.04	8 (26%)	24,82,82	2.46	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	H4B	A	902	-	13,18,18	2.30	3 (23%)	11,26,26	2.40	5 (45%)
4	BVF	A	904	-	8,8,8	0.31	0	10,10,10	0.44	0
2	HEM	B	901	1	30,50,50	3.14	9 (30%)	24,82,82	2.52	11 (45%)
3	H4B	B	902	-	13,18,18	2.30	2 (15%)	11,26,26	2.38	5 (45%)
4	BVF	B	905	-	8,8,8	0.63	0	10,10,10	0.51	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
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	BVF	A	904	-	-	0/0/0/0	0/1/1/1
2	HEM	B	901	1	-	0/10/54/54	0/0/8/8
3	H4B	B	902	-	1/1/3/5	0/8/17/17	0/2/2/2
4	BVF	B	905	-	-	0/0/0/0	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C3B-C4B	-8.08	1.44	1.51
2	A	901	HEM	C2D-C3D	-7.25	1.32	1.54
2	A	901	HEM	C3D-C4D	-7.15	1.42	1.51
2	B	901	HEM	C3D-C4D	-6.81	1.42	1.51
2	B	901	HEM	C3C-CAC	-6.81	1.38	1.51
2	A	901	HEM	C3B-C4B	-6.54	1.46	1.51
3	A	902	H4B	C6-N5	-6.49	1.33	1.45
2	B	901	HEM	C2D-C3D	-6.40	1.35	1.54
2	B	901	HEM	C3B-CAB	-6.24	1.39	1.51
2	A	901	HEM	C3B-CAB	-6.04	1.40	1.51
3	B	902	H4B	C6-N5	-5.96	1.34	1.45
2	A	901	HEM	C3C-CAC	-5.53	1.41	1.51
3	B	902	H4B	C7-N8	-5.37	1.39	1.46
3	A	902	H4B	C7-N8	-4.50	1.40	1.46
2	A	901	HEM	CAD-C3D	-4.24	1.45	1.54
2	A	901	HEM	C2C-C1C	-3.94	1.45	1.52
2	B	901	HEM	C2C-C1C	-3.53	1.45	1.52
2	B	901	HEM	C2B-C1B	-2.92	1.42	1.51
2	A	901	HEM	C2B-C1B	-2.60	1.43	1.51
3	A	902	H4B	C4A-N5	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C4C-NC	2.06	1.38	1.36
2	B	901	HEM	FE-NC	2.61	2.06	1.95

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	HEM	CBA-CAA-C2A	-4.03	105.30	112.53
3	A	902	H4B	N3-C2-N1	-2.32	121.73	125.53
3	B	902	H4B	N3-C2-N1	-2.16	122.00	125.53
2	B	901	HEM	CAA-C2A-C1A	2.00	129.18	127.01
3	A	902	H4B	C2-N1-C8A	2.19	119.47	114.54
2	B	901	HEM	CMD-C2D-C3D	2.52	125.48	114.35
2	A	901	HEM	C3B-C4B-CHC	2.52	126.72	123.16
3	B	902	H4B	C2-N1-C8A	2.58	120.33	114.54
2	B	901	HEM	C2D-C3D-C4D	2.71	106.09	101.50
2	A	901	HEM	CMD-C2D-C3D	2.76	126.57	114.35
3	B	902	H4B	C4-C4A-C8A	2.79	117.09	114.56
2	A	901	HEM	C3C-CAC-CBC	2.81	128.77	124.46
2	B	901	HEM	C4B-CHC-C1C	2.92	130.70	125.82
3	A	902	H4B	C4-C4A-C8A	2.99	117.27	114.56
3	A	902	H4B	C4-N3-C2	3.00	120.10	115.94
2	B	901	HEM	C3B-C4B-CHC	3.34	127.86	123.16
2	A	901	HEM	CAD-C3D-C4D	3.34	124.27	112.47
2	B	901	HEM	C3B-CAB-CBB	3.35	129.60	124.46
3	B	902	H4B	C4-N3-C2	3.42	120.69	115.94
2	B	901	HEM	CAD-C3D-C4D	3.65	125.36	112.47
2	B	901	HEM	CMB-C2B-C3B	3.80	126.01	116.53
2	A	901	HEM	CMB-C2B-C3B	4.23	127.09	116.53
2	A	901	HEM	CMC-C2C-C3C	4.50	127.76	116.53
2	A	901	HEM	CAD-C3D-C2D	4.52	126.21	113.22
2	A	901	HEM	C3B-CAB-CBB	4.55	131.44	124.46
2	A	901	HEM	C2D-C3D-C4D	4.58	109.27	101.50
2	B	901	HEM	CAD-C3D-C2D	4.92	127.37	113.22
3	B	902	H4B	C7-C6-N5	4.97	120.77	110.45
2	B	901	HEM	CMC-C2C-C3C	5.17	129.42	116.53
3	A	902	H4B	C7-C6-N5	5.21	121.28	110.45

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	2	0
2	B	901	HEM	1	0
3	B	902	H4B	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

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	413/433 (95%)	-0.21	7 (1%) 73 68	34, 57, 88, 107	0
1	B	413/433 (95%)	-0.18	14 (3%) 49 41	33, 57, 89, 107	0
All	All	826/866 (95%)	-0.19	21 (2%) 61 54	33, 57, 89, 107	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	CYS	10.1
1	A	110	LEU	6.4
1	B	99	THR	5.4
1	B	109	CYS	4.9
1	A	495	TRP	4.3
1	A	149	LYS	3.8
1	B	290	LYS	3.7
1	B	171	GLY	3.3
1	B	78	TYR	3.3
1	A	494	ILE	3.2
1	B	131	GLU	3.1
1	B	110	LEU	3.1
1	A	270	THR	2.7
1	B	494	ILE	2.7
1	B	495	TRP	2.3
1	B	497	ASN	2.3
1	B	149	LYS	2.3
1	B	150	GLU	2.2
1	B	126	LYS	2.1
1	B	153	ILE	2.1
1	A	100	SER	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 (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	BVF	B	905	8/8	0.96	0.13	-0.56	29,33,35,35	0
2	HEM	A	901	43/43	0.98	0.10	-0.70	28,34,38,42	0
4	BVF	A	904	8/8	0.98	0.11	-0.80	32,33,36,37	0
2	HEM	B	901	43/43	0.98	0.11	-1.19	28,33,38,45	0
3	H4B	A	902	17/17	0.96	0.10	-1.52	31,33,39,40	0
3	H4B	B	902	17/17	0.98	0.09	-2.01	26,35,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.