Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:31 PM GMT

PDB ID	:	4IMX
Title	:	Structure of bovine endothelial nitric oxide synthase heme domain in complex with 3,5-bis(2-(6-amino-4-methylpyridin-2-yl)ethyl)benzonitrile
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-01-03
Resolution	:	2.25 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 ⓘ symbol.

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

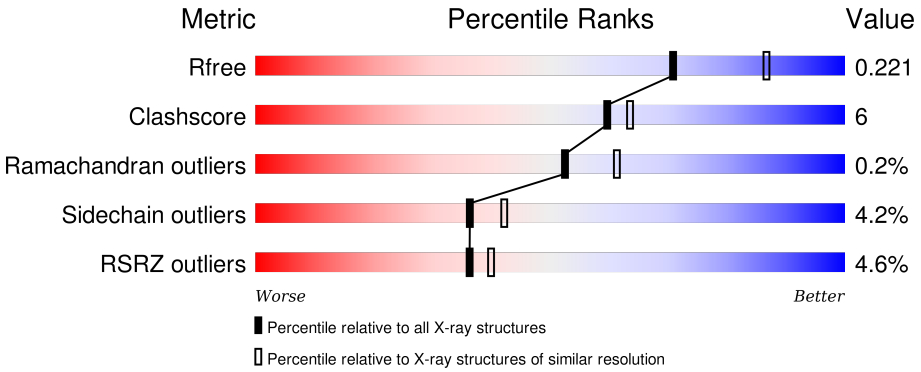
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	442	5% 82% 8% • 8%
1	B	442	3% 79% 10% • 8%

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
4	1EV	A	503	-	-	-	X
4	1EV	B	503	-	-	X	X
5	ACT	A	505	-	-	-	X
5	ACT	B	504	-	-	-	X
6	GOL	A	506	-	-	-	X
6	GOL	B	506	-	-	-	X

2 Entry composition

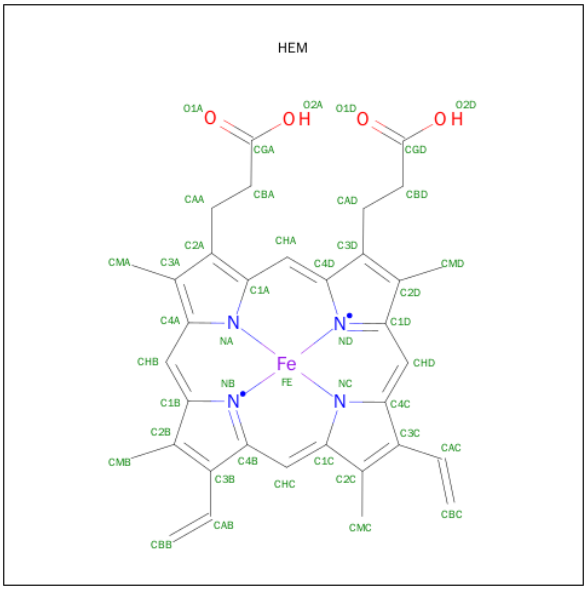
There are 9 unique types of molecules in this entry. The entry contains 6906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 subunit A.

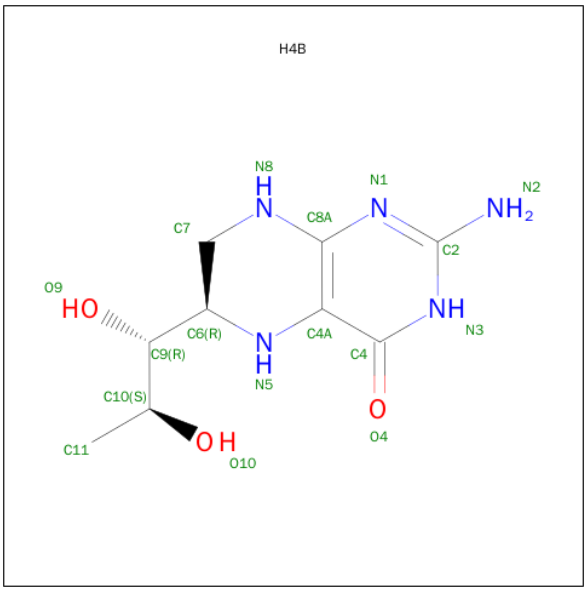
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3220	2047	568	589	16			
1	B	405	Total	C	N	O	S	0	0	0
			3226	2052	569	589	16			

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



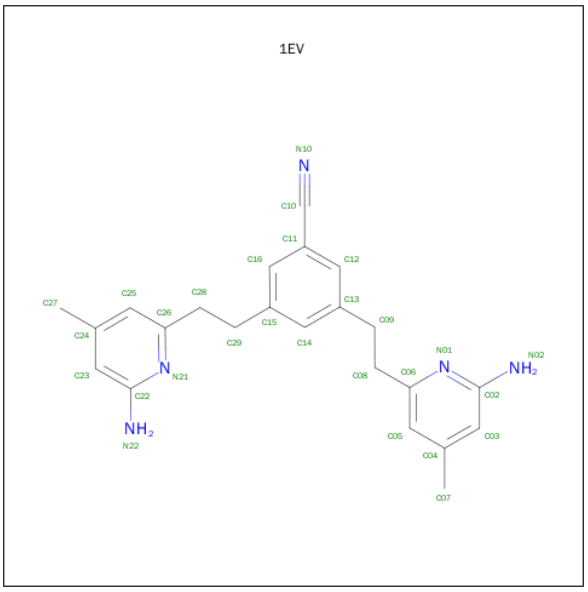
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 3,5-BIS[2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL]BENZONITRILE (three-letter code: 1EV) (formula: $C_{23}H_{25}N_5$).



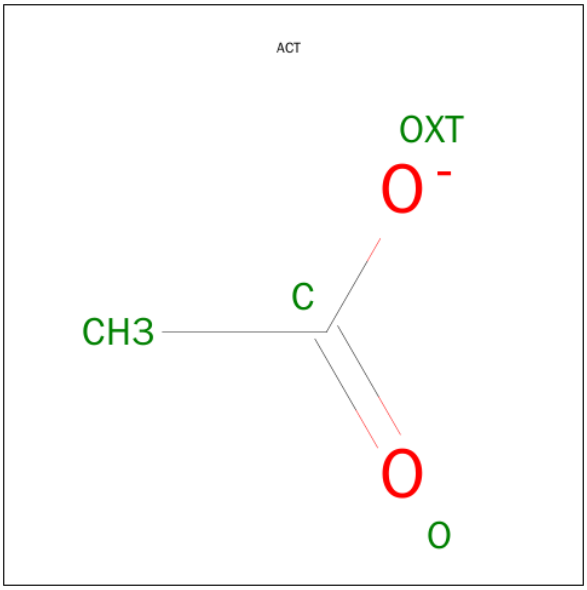
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 28 23 5	0	0

Continued on next page...

Continued from previous page...

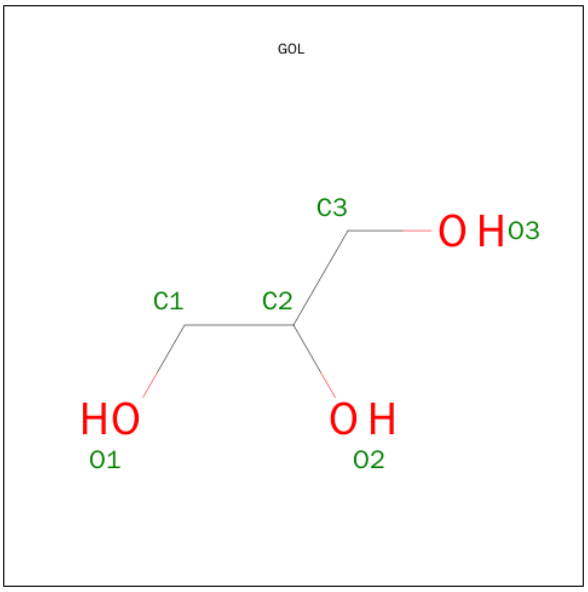
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 28 23 5	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



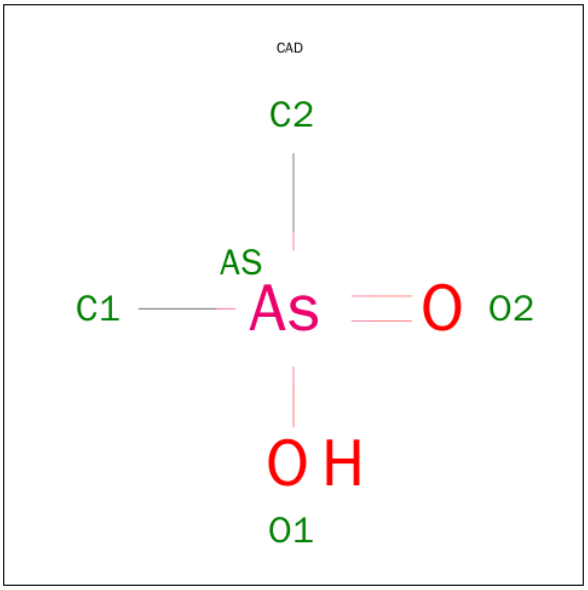
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total As C 3 1 2	0	0
7	B	1	Total As C 3 1 2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0

- Molecule 9 is water.

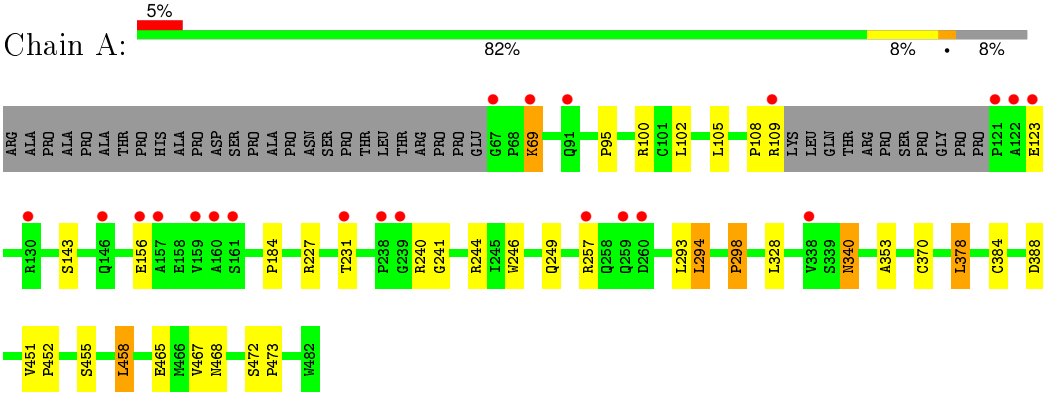
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	134	Total O 134 134	0	0
9	B	115	Total O 115 115	0	0

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.

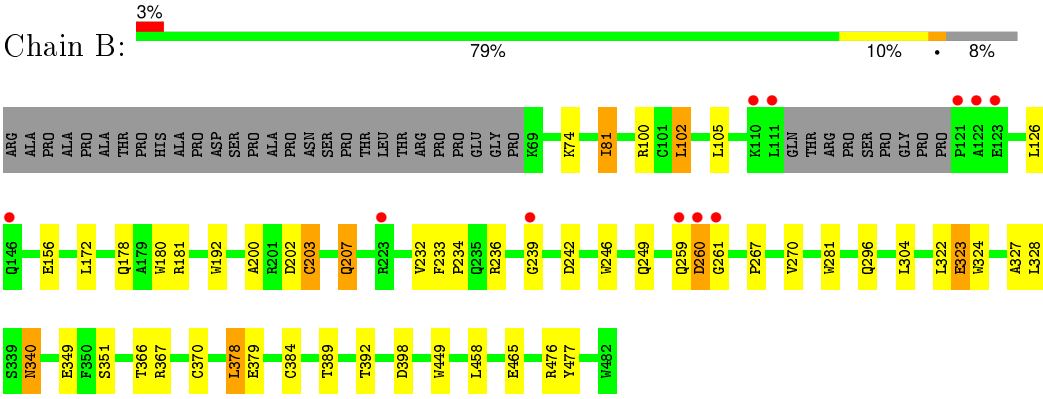
- Molecule 1: subunit A

Chain A:



- Molecule 1: subunit A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.06Å 106.60Å 156.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.26 – 2.25 39.26 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.26-2.25) 99.3 (39.26-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.222 0.179 , 0.221	Depositor DCC
R_{free} test set	2320 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 46527 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6906	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: GOL, ZN, H4B, ACT, 1EV, HEM, CAD

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	0.69	0/3310	0.70	1/4508 (0.0%)
1	B	0.71	1/3315 (0.0%)	0.70	0/4513
All	All	0.70	1/6625 (0.0%)	0.70	1/9021 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-5.26	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

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	3220	0	3128	29	0
1	B	3226	0	3142	38	0
2	A	43	0	30	2	0
2	B	43	0	30	9	0
3	A	17	0	15	1	0
3	B	17	0	15	2	0
4	A	28	0	25	3	0
4	B	28	0	25	11	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
7	A	3	0	0	1	0
7	B	3	0	0	3	0
8	A	1	0	0	0	0
9	A	134	0	0	1	0
9	B	115	0	0	2	0
All	All	6906	0	6438	75	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 6.

All (75) 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:384:CYS:SG	7:A:507:CAD:AS	2.59	1.21
1:B:384:CYS:SG	7:B:507:CAD:AS	2.59	1.20
1:B:249:GLN:HE21	4:B:503:1EV:H2	1.11	1.05
1:A:249:GLN:HE21	4:A:503:1EV:H2	1.32	0.95
1:B:249:GLN:NE2	4:B:503:1EV:H2	1.82	0.94
1:B:324:TRP:HB2	7:B:507:CAD:C1	2.12	0.80
1:B:249:GLN:HE21	4:B:503:1EV:C12	1.94	0.77
1:A:249:GLN:NE2	4:A:503:1EV:H2	2.07	0.67
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.76	0.67
2:B:501:HEM:O2D	4:B:503:1EV:H15	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.75	0.67
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.47	0.62
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.82	0.62
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.00	0.61
1:A:378:LEU:HB2	9:A:605:HOH:O	2.02	0.59
1:A:388:ASP:OD1	1:A:390:ARG:HG3	2.03	0.59
1:A:108:PRO:O	1:A:109:ARG:HG3	2.04	0.57
2:B:501:HEM:CBA	4:B:503:1EV:H5	2.35	0.56
1:B:207:GLN:HB2	9:B:612:HOH:O	2.06	0.55
1:A:340:ASN:HD22	1:A:340:ASN:H	1.54	0.54
1:B:449:TRP:HA	3:B:502:H4B:N1	2.22	0.54
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.90	0.52
1:A:388:ASP:OD1	1:A:390:ARG:CG	2.58	0.52
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.73	0.52
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.91	0.51
1:B:366:THR:O	1:B:370:CYS:HB2	2.11	0.51
1:B:74:LYS:HD2	1:B:81:ILE:HD11	1.92	0.51
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.93	0.51
1:B:246:TRP:HE1	1:B:296:GLN:NE2	2.09	0.51
1:A:240:ARG:HD2	1:A:241:GLY:O	2.11	0.51
1:A:455:SER:O	1:A:458:LEU:HB2	2.11	0.50
2:B:501:HEM:HBB2	2:B:501:HEM:HHC	1.94	0.49
3:A:502:H4B:O4	6:A:506:GOL:O2	2.29	0.49
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.42	0.49
1:A:472:SER:HA	1:A:473:PRO:C	2.33	0.49
2:B:501:HEM:HBA1	4:B:503:1EV:H5	1.95	0.48
1:B:259:GLN:C	1:B:261:GLY:H	2.17	0.47
2:B:501:HEM:O2A	4:B:503:1EV:C14	2.63	0.47
1:A:467:VAL:HG13	1:B:102:LEU:CD1	2.46	0.46
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.97	0.46
1:B:477:TYR:CE1	4:B:503:1EV:N22	2.84	0.45
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.56	0.45
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.97	0.45
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.98	0.45
1:B:259:GLN:O	1:B:261:GLY:N	2.49	0.44
2:B:501:HEM:HBA2	4:B:503:1EV:H5	1.99	0.44
1:B:340:ASN:HD22	1:B:340:ASN:H	1.63	0.44
1:B:384:CYS:CB	7:B:507:CAD:AS	3.26	0.43
1:A:69:LYS:HD2	1:A:69:LYS:HA	1.70	0.43
1:B:178:GLN:HE22	1:B:181:ARG:NH1	2.14	0.43
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:OE2	1:B:476:ARG:NH2	2.52	0.43
1:B:367:ARG:HH12	3:B:502:H4B:C4	2.32	0.43
1:B:126:LEU:HD21	1:B:156:GLU:HG2	2.01	0.43
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	2.01	0.43
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.48	0.42
1:B:324:TRP:O	1:B:327:ALA:HB3	2.18	0.42
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.59	0.42
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.47	0.42
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.79	0.42
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.35	0.42
1:B:267:PRO:O	1:B:270:VAL:HG23	2.20	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.89	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.01	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.56	0.41
1:B:323:GLU:HG3	1:B:323:GLU:H	1.47	0.41
2:B:501:HEM:C1C	4:B:503:1EV:H13	2.56	0.41
2:A:501:HEM:C1C	4:A:503:1EV:H13	2.56	0.41
1:B:172:LEU:HD11	1:B:232:VAL:HG11	2.03	0.40
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.56	0.40
1:A:108:PRO:O	1:A:109:ARG:CG	2.68	0.40
2:B:501:HEM:O2A	4:B:503:1EV:H14	2.22	0.40
1:B:200:ALA:O	1:B:203:CYS:HB2	2.22	0.40
1:A:108:PRO:O	1:A:109:ARG:CB	2.70	0.40
1:B:330:LEU:HB2	9:B:609: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	401/442 (91%)	392 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	401/442 (91%)	386 (96%)	13 (3%)	2 (0%)	34 34
All	All	802/884 (91%)	778 (97%)	22 (3%)	2 (0%)	52 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ASP
1	B	328	LEU

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	344/375 (92%)	329 (96%)	15 (4%)	35 40
1	B	345/375 (92%)	331 (96%)	14 (4%)	37 44
All	All	689/750 (92%)	660 (96%)	29 (4%)	36 42

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	123	GLU
1	A	125	LEU
1	A	127	SER
1	A	143	SER
1	A	293	LEU
1	A	294	LEU
1	A	298	PRO
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	LEU
1	B	81	ILE
1	B	100	ARG
1	B	102	LEU
1	B	202	ASP
1	B	207	GLN
1	B	260	ASP
1	B	323	GLU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	379	GLU
1	B	389	THR
1	B	398	ASP
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN
1	B	296	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	501	1	30,50,50	2.10	9 (30%)	24,82,82	2.71	13 (54%)
3	H4B	A	502	-	13,18,18	0.98	1 (7%)	11,26,26	2.86	5 (45%)
4	1EV	A	503	-	30,30,30	1.50	1 (3%)	41,41,41	2.16	13 (31%)
5	ACT	A	504	-	1,3,3	1.58	0	0,3,3	0.00	-
5	ACT	A	505	-	1,3,3	1.55	0	0,3,3	0.00	-
6	GOL	A	506	-	5,5,5	0.51	0	5,5,5	0.78	0
7	CAD	A	507	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	501	1	30,50,50	2.16	7 (23%)	24,82,82	2.67	10 (41%)
3	H4B	B	502	-	13,18,18	0.66	0	11,26,26	2.34	5 (45%)
4	1EV	B	503	-	30,30,30	1.36	1 (3%)	41,41,41	1.87	11 (26%)
5	ACT	B	504	-	1,3,3	0.50	0	0,3,3	0.00	-
5	ACT	B	505	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
6	GOL	B	506	-	5,5,5	0.38	0	5,5,5	0.52	0
7	CAD	B	507	-	0,2,4	0.00	-	0,1,6	0.00	-

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	501	1	-	0/10/54/54	0/0/8/8
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
4	1EV	A	503	-	-	0/12/12/12	0/3/3/3
5	ACT	A	504	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	A	505	-	-	0/0/0/0	0/0/0/0
6	GOL	A	506	-	-	0/4/4/4	0/0/0/0
7	CAD	A	507	-	-	0/0/0/0	0/0/0/0
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	1EV	B	503	-	-	0/12/12/12	0/3/3/3
5	ACT	B	504	-	-	0/0/0/0	0/0/0/0
5	ACT	B	505	-	-	0/0/0/0	0/0/0/0
6	GOL	B	506	-	-	0/4/4/4	0/0/0/0
7	CAD	B	507	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C4B	-6.97	1.45	1.51
4	A	503	1EV	C11-C10	-6.31	1.28	1.44
4	B	503	1EV	C11-C10	-6.20	1.29	1.44
2	A	501	HEM	C3B-C4B	-6.10	1.46	1.51
2	A	501	HEM	C3D-C4D	-5.57	1.44	1.51
2	B	501	HEM	C3D-C4D	-5.14	1.45	1.51
2	A	501	HEM	C2C-C1C	-4.10	1.44	1.52
2	B	501	HEM	C2C-C1C	-3.53	1.45	1.52
2	B	501	HEM	C2B-C1B	-2.34	1.44	1.51
2	A	501	HEM	C2B-C1B	-2.22	1.44	1.51
2	A	501	HEM	C2D-C1D	-2.14	1.44	1.51
2	A	501	HEM	C4C-NC	2.03	1.38	1.36
2	A	501	HEM	C3B-CAB	2.07	1.55	1.51
2	A	501	HEM	C1C-NC	2.10	1.38	1.36
2	B	501	HEM	CAA-C2A	2.15	1.55	1.52
3	A	502	H4B	C4-N3	2.42	1.37	1.33
2	A	501	HEM	CAA-C2A	2.44	1.56	1.52
2	B	501	HEM	FE-NC	2.44	2.05	1.95
5	B	505	ACT	CH3-C	2.78	1.52	1.48
2	B	501	HEM	C3B-CAB	2.79	1.56	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CBA-CAA-C2A	-5.28	103.06	112.53
2	A	501	HEM	CBA-CAA-C2A	-4.91	103.72	112.53
3	A	502	H4B	N3-C2-N1	-4.36	118.39	125.53
4	B	503	1EV	C09-C13-C12	-4.13	113.64	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	1EV	C08-C06-C05	-4.00	115.52	121.13
3	B	502	H4B	N3-C2-N1	-3.62	119.60	125.53
2	B	501	HEM	C3C-CAC-CBC	-3.38	119.27	124.46
4	A	503	1EV	C05-C06-N01	-3.37	119.16	122.96
2	A	501	HEM	CBD-CAD-C3D	-3.10	104.54	113.55
2	B	501	HEM	CBD-CAD-C3D	-2.91	105.08	113.55
4	A	503	1EV	C29-C15-C16	-2.80	115.88	120.56
4	A	503	1EV	C25-C26-N21	-2.79	119.81	122.96
4	B	503	1EV	C05-C06-N01	-2.77	119.83	122.96
2	A	501	HEM	C3C-CAC-CBC	-2.61	120.45	124.46
4	A	503	1EV	C09-C13-C12	-2.61	116.18	120.56
4	B	503	1EV	C25-C26-N21	-2.50	120.14	122.96
2	A	501	HEM	CAA-C2A-C1A	-2.45	124.35	127.01
4	B	503	1EV	C29-C15-C16	-2.44	116.47	120.56
4	A	503	1EV	C07-C04-C05	-2.34	117.39	120.95
2	A	501	HEM	CMA-C3A-C4A	-2.30	124.55	128.36
2	A	501	HEM	C1D-CHD-C4C	-2.08	122.35	125.82
4	A	503	1EV	C29-C15-C14	2.07	124.03	120.56
4	B	503	1EV	C08-C06-N01	2.17	118.89	115.69
4	B	503	1EV	N22-C22-N21	2.24	120.58	116.50
2	A	501	HEM	CAA-CBA-CGA	2.47	117.27	112.75
4	B	503	1EV	C11-C12-C13	2.54	123.00	120.32
2	A	501	HEM	C2D-C3D-C4D	2.57	105.86	101.50
3	A	502	H4B	N2-C2-N1	2.65	121.59	117.20
3	B	502	H4B	C2-N1-C8A	2.68	120.57	114.54
3	B	502	H4B	N2-C2-N1	2.71	121.69	117.20
2	B	501	HEM	CMD-C2D-C3D	2.78	126.65	114.35
2	A	501	HEM	CMD-C2D-C3D	2.96	127.45	114.35
2	B	501	HEM	C2D-C3D-C4D	2.97	106.53	101.50
3	A	502	H4B	C2-N1-C8A	3.02	121.32	114.54
4	B	503	1EV	C28-C26-N21	3.03	120.17	115.69
4	A	503	1EV	C22-N21-C26	3.19	120.49	118.23
4	A	503	1EV	C28-C26-N21	3.39	120.69	115.69
4	A	503	1EV	C09-C13-C14	3.39	126.24	120.56
3	B	502	H4B	C4-N3-C2	3.65	121.01	115.94
4	B	503	1EV	C22-N21-C26	3.70	120.86	118.23
2	B	501	HEM	CMC-C2C-C3C	3.87	126.20	116.53
2	B	501	HEM	CAA-CBA-CGA	4.07	120.20	112.75
3	B	502	H4B	C4-C4A-C8A	4.09	118.27	114.56
4	A	503	1EV	C02-N01-C06	4.11	121.15	118.23
4	A	503	1EV	C09-C08-C06	4.12	120.45	112.53
2	B	501	HEM	CMB-C2B-C3B	4.19	126.98	116.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAD-C3D-C2D	4.24	125.40	113.22
2	A	501	HEM	CAD-C3D-C4D	4.29	127.59	112.47
2	B	501	HEM	CAD-C3D-C4D	4.39	127.94	112.47
2	A	501	HEM	CMC-C2C-C3C	4.52	127.81	116.53
4	B	503	1EV	C09-C13-C14	4.52	128.14	120.56
3	A	502	H4B	C4-C4A-C8A	4.62	118.75	114.56
2	A	501	HEM	CAD-C3D-C2D	4.63	126.52	113.22
4	B	503	1EV	C02-N01-C06	4.75	121.60	118.23
3	A	502	H4B	C4-N3-C2	5.22	123.18	115.94
2	A	501	HEM	CMB-C2B-C3B	5.50	130.25	116.53
4	A	503	1EV	C08-C06-N01	6.47	125.25	115.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
3	A	502	H4B	1	0
4	A	503	1EV	3	0
6	A	506	GOL	1	0
7	A	507	CAD	1	0
2	B	501	HEM	9	0
3	B	502	H4B	2	0
4	B	503	1EV	11	0
7	B	507	CAD	3	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	405/442 (91%)	0.06	23 (5%)	27	30	28, 41, 67, 81	0
1	B	405/442 (91%)	0.02	14 (3%)	48	52	27, 44, 71, 95	0
All	All	810/884 (91%)	0.04	37 (4%)	36	40	27, 42, 68, 95	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	6.4
1	B	259	GLN	5.0
1	B	260	ASP	5.0
1	B	110	LYS	4.7
1	A	160	ALA	4.7
1	A	239	GLY	4.6
1	A	121	PRO	3.9
1	A	123	GLU	3.8
1	A	126	LEU	3.5
1	B	111	LEU	3.5
1	B	121	PRO	3.3
1	A	122	ALA	3.3
1	A	91	GLN	3.2
1	A	146	GLN	2.9
1	B	239	GLY	2.8
1	A	156	GLU	2.8
1	A	257	ARG	2.8
1	B	142	ARG	2.7
1	B	261	GLY	2.6
1	A	109	ARG	2.6
1	B	223	ARG	2.6
1	A	238	PRO	2.6
1	A	67	GLY	2.6
1	A	157	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	2.5
1	B	141	LYS	2.5
1	A	69	LYS	2.5
1	B	146	GLN	2.4
1	A	338	VAL	2.3
1	A	231	THR	2.3
1	B	338	VAL	2.2
1	A	260	ASP	2.2
1	A	159	VAL	2.2
1	B	122	ALA	2.2
1	A	130	ARG	2.1
1	B	123	GLU	2.1
1	A	161	SER	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
5	ACT	B	504	4/4	0.97	0.18	5.89	51,52,53,55	0
5	ACT	A	505	4/4	0.95	0.25	4.73	44,45,45,47	0
4	1EV	B	503	28/28	0.86	0.32	3.87	32,74,90,91	0
4	1EV	A	503	28/28	0.85	0.31	3.44	27,76,90,91	0
6	GOL	B	506	6/6	0.91	0.25	3.06	55,56,58,58	0
6	GOL	A	506	6/6	0.88	0.23	2.05	56,57,60,60	0
5	ACT	A	504	4/4	0.94	0.13	1.02	43,43,46,47	0
2	HEM	A	501	43/43	0.98	0.19	0.88	24,29,44,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	B	501	43/43	0.98	0.15	0.29	26,32,43,46	0
7	CAD	A	507	3/5	0.97	0.09	-0.12	84,84,84,85	0
3	H4B	A	502	17/17	0.96	0.15	-0.13	37,41,44,46	0
3	H4B	B	502	17/17	0.95	0.15	-0.24	36,39,43,47	0
7	CAD	B	507	3/5	0.99	0.13	-0.39	70,70,70,71	0
5	ACT	B	505	4/4	0.98	0.10	-1.24	43,43,46,47	0
8	ZN	A	508	1/1	0.99	0.09	-1.41	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.