Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N62
Title	:	Structure of neuronal nitric oxide synthase D597N mutant heme domain in complex with 6,6'-(2,2'-(pyridine-3,5-diyl)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors	:	Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on	:	2010-05-25
Resolution	:	1.95 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:

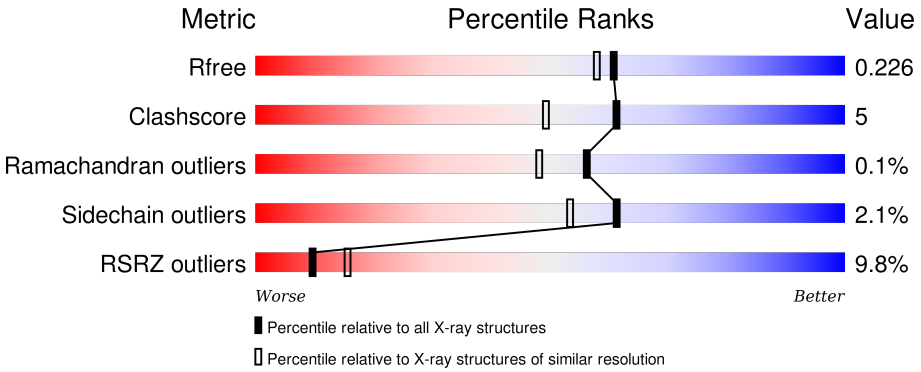
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	422	14% 87% 9%
1	B	422	5% 90% 7%

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	XFJ	B	719[A]	-	-	-	X
3	XFJ	B	805[A]	-	-	-	X
4	ACT	A	860	-	-	-	X
4	ACT	B	860	-	-	-	X
5	MTL	A	870	-	-	-	X
8	H4B	A	760[B]	-	-	X	X
8	H4B	B	760[B]	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7372 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.

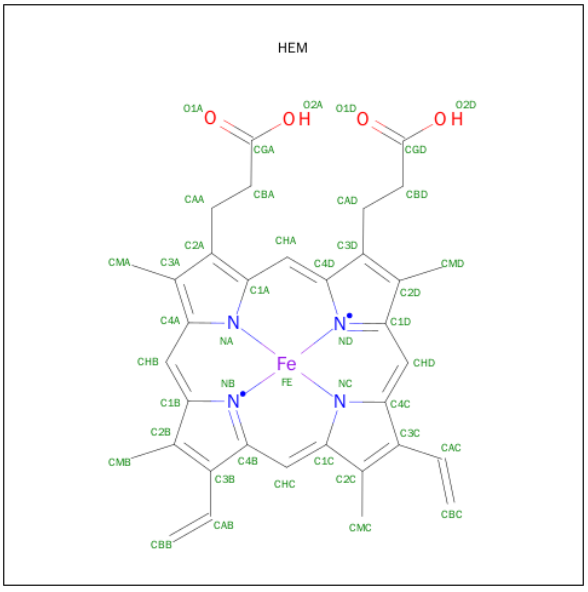
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	7	0
			3342	2142	570	608	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	575	612	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

- 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	1
			48	37	1	4	6		

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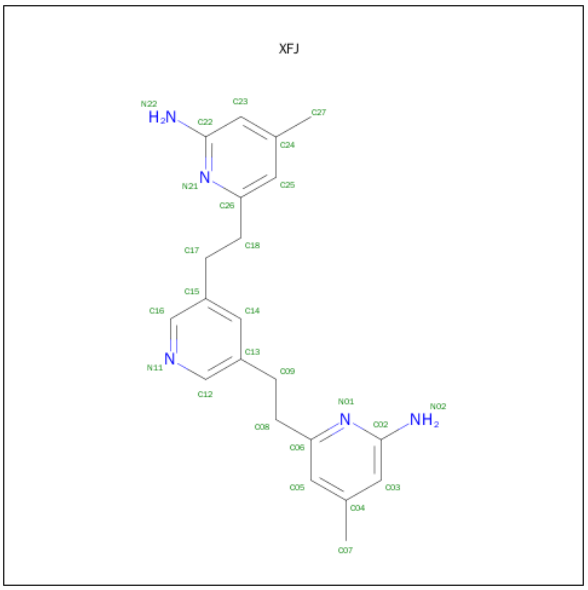
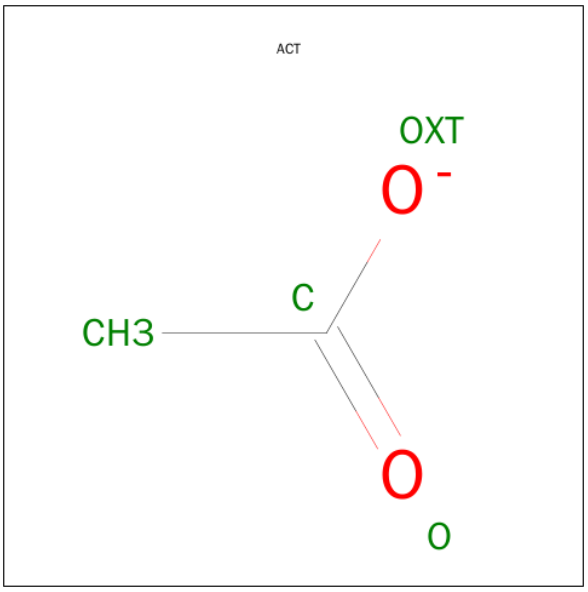
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

- Molecule 3 is 6,6'-(PYRIDINE-3,5-DIYLDIETHANE-2,1-DIYL)BIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: XFJ) (formula: $C_{21}H_{25}N_5$).



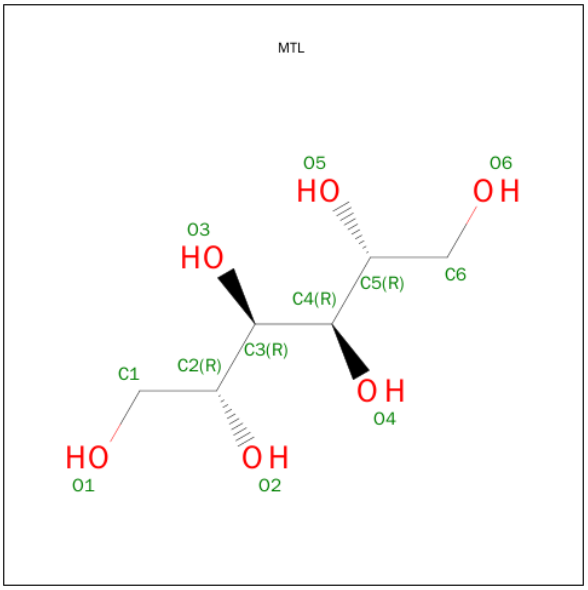
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N		0	0
			26	21	5			
3	B	1	Total	C	N		0	1
			26	21	5			
3	B	1	Total	C	N		0	0
			26	21	5			
3	B	1	Total	C	N		0	1
			26	21	5			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is D-MANNITOL (three-letter code: MTL) (formula: $C_6H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 6 6	0	0
5	B	1	Total C O 12 6 6	0	0

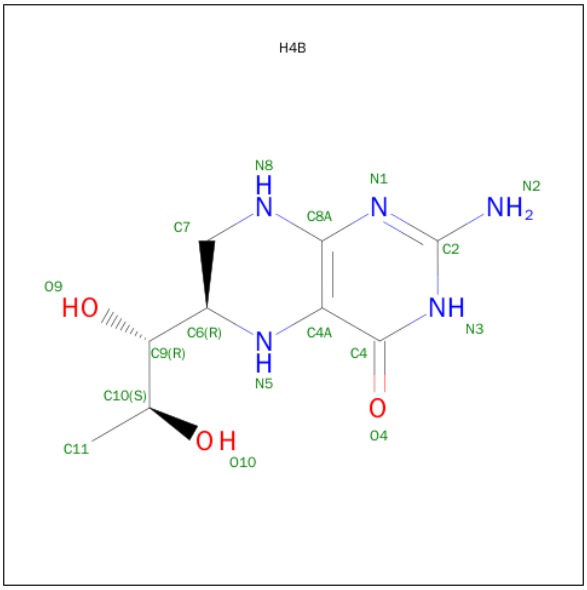
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Zn 3 3	0	0

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	169	Total O 169 169	0	2

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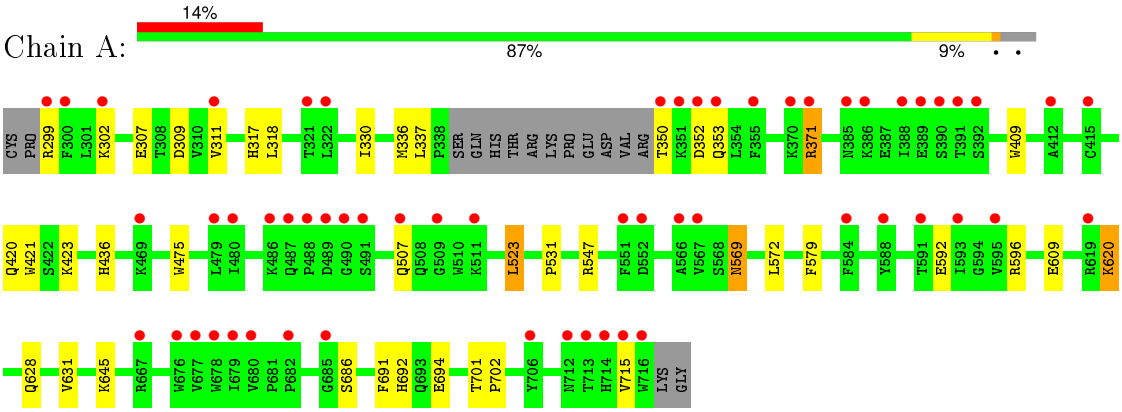
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	233	Total 233	O 233	0	2

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.

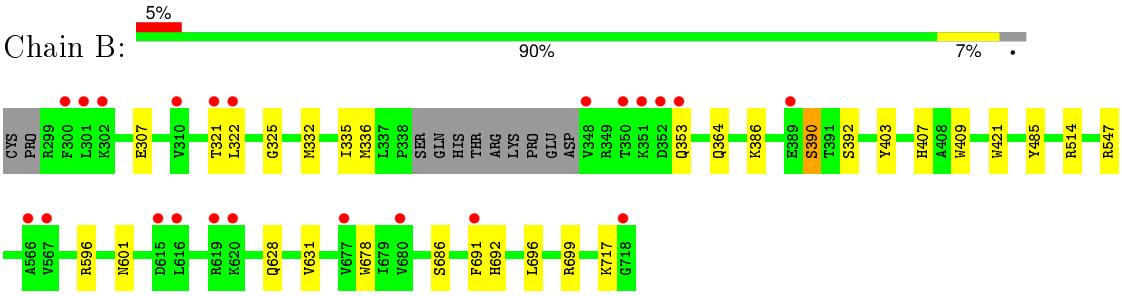
- Molecule 1: Nitric oxide synthase

Chain A:



- Molecule 1: Nitric oxide synthase

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	51.81Å 110.39Å 164.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.95 38.46 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.64-1.95) 99.6 (38.46-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.173 , 0.208 0.187 , 0.226	Depositor DCC
R_{free} test set	3436 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 69715 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7372	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: ZN, XFJ, H4B, CL, MTL, ACT, HEM

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	0.60	0/3456	0.61	0/4689
1	B	0.65	0/3459	0.65	0/4689
All	All	0.63	0/6915	0.63	0/9378

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	3342	0	3274	34	0
1	B	3357	0	3277	24	0
2	A	48	0	8	7	0
2	B	48	0	8	9	0
3	A	26	0	25	2	0
3	B	78	0	70	10	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	12	0	14	3	0
5	B	12	0	14	0	0
6	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	1	0
7	A	3	0	0	0	0
8	A	17	0	11	7	0
8	B	17	0	13	6	0
9	A	169	0	0	3	0
9	B	233	0	0	2	0
All	All	7372	0	6720	71	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 5.

All (71) 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)
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:O1A	1.61	1.30
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:N2	1.64	1.30
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:CGA	2.11	1.13
8:A:760[B]:H4B:C2	2:B:750[B]:HEM:O1A	1.97	1.12
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:C2	1.97	1.11
2:A:750[B]:HEM:O1A	8:B:760[B]:H4B:N3	1.87	1.07
2:A:750[B]:HEM:CGA	8:B:760[B]:H4B:N2	2.21	1.02
8:A:760[B]:H4B:N3	2:B:750[B]:HEM:O1A	1.92	1.01
2:B:750[A]:HEM:O2A	3:B:719[A]:XFJ:H09	1.81	0.80
1:A:701[A]:THR:HG22	1:A:702:PRO:HA	1.65	0.77
1:A:299:ARG:HD2	1:A:318:LEU:CD2	2.19	0.72
1:A:299:ARG:O	1:A:317:HIS:CE1	2.44	0.70
1:A:299:ARG:O	1:A:317:HIS:HE1	1.78	0.67
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.06	0.67
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.77	0.66
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.60	0.66
1:A:596:ARG:NH1	2:A:750[B]:HEM:O2A	2.30	0.64
1:A:302:LYS:HE3	1:A:311:VAL:HG11	1.80	0.64
1:A:436:HIS:CE1	9:A:1163:HOH:O	2.51	0.63
1:B:325:GLY:O	1:B:332:MET:HG3	2.00	0.62
8:A:760[B]:H4B:H9	1:B:336:MET:HE2	1.82	0.61
1:A:299:ARG:HD2	1:A:318:LEU:HD21	1.85	0.58
1:A:299:ARG:HD2	1:A:318:LEU:HD22	1.83	0.58
1:A:336:MET:HE2	8:B:760[B]:H4B:H9	1.87	0.57
1:B:596:ARG:NH1	2:B:750[B]:HEM:O2A	2.38	0.56
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:SER:HA	1:A:691:PHE:CG	2.43	0.53
1:B:678:TRP:CH2	3:B:719[A]:XFJ:H08	2.44	0.53
2:A:750[A]:HEM:O2A	3:B:805[A]:XFJ:H09	2.09	0.53
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.97	0.53
2:B:750[A]:HEM:O2A	3:B:719[A]:XFJ:C09	2.55	0.51
5:A:870:MTL:H12	3:B:805[A]:XFJ:H27	1.91	0.51
1:B:678:TRP:CZ3	3:B:719[A]:XFJ:H08	2.47	0.50
1:A:330[A]:ILE:HD11	1:B:696:LEU:HB3	1.93	0.50
1:B:596:ARG:HB2	6:B:910:CL:CL	2.49	0.49
1:A:609:GLU:HG3	9:A:1009:HOH:O	2.13	0.48
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.14	0.47
1:A:592:GLU:HB3	1:A:596:ARG:NH2	2.29	0.47
1:A:596:ARG:NH1	2:A:750[A]:HEM:O2A	2.48	0.47
1:B:686:SER:HA	1:B:691:PHE:CG	2.50	0.47
1:A:336:MET:CE	8:B:760[B]:H4B:H9	2.44	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:307:GLU:HG2	1:A:692:HIS:CG	2.50	0.46
1:B:364:GLN:NE2	9:B:1314:HOH:O	2.49	0.45
1:A:337:LEU:HD21	3:A:800:XFJ:H23	1.97	0.45
5:A:870:MTL:O3	3:B:805[A]:XFJ:H27B	2.17	0.44
1:A:701[A]:THR:CG2	1:A:702:PRO:HA	2.42	0.44
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.44
1:A:569:ASN:H	1:A:569:ASN:HD22	1.65	0.44
8:A:760[B]:H4B:H9	1:B:336:MET:CE	2.47	0.43
8:A:760[B]:H4B:N2	2:B:750[B]:HEM:O2A	2.45	0.43
1:B:386:LYS:O	1:B:390:SER:HB3	2.17	0.43
1:A:436:HIS:HE1	9:A:1163:HOH:O	1.91	0.43
1:A:620:LYS:HE3	1:A:620:LYS:HB2	1.81	0.43
1:B:307:GLU:HG2	1:B:692:HIS:CG	2.54	0.43
6:A:910:CL:CL	3:B:805[A]:XFJ:H12	2.56	0.42
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.84	0.42
1:B:601:ASN:HB2	9:B:1347:HOH:O	2.19	0.42
1:B:596:ARG:NH1	2:B:750[A]:HEM:O2A	2.54	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.03	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.41
1:B:321:THR:HG23	1:B:322:LEU:HG	2.02	0.41
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.56	0.41
1:A:572:LEU:HB3	1:A:579:PHE:HB2	2.03	0.41
5:A:870:MTL:O3	3:B:805[A]:XFJ:C27	2.69	0.41
1:B:353:GLN:HG2	1:B:353:GLN:H	1.78	0.41
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLN:CG	1:B:631:VAL:HG11	2.51	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	410/422 (97%)	399 (97%)	10 (2%)	1 (0%)	52 43
1	B	410/422 (97%)	402 (98%)	8 (2%)	0	100 100
All	All	820/844 (97%)	801 (98%)	18 (2%)	1 (0%)	56 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ASP

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	370/377 (98%)	359 (97%)	11 (3%)	48 36
1	B	369/377 (98%)	365 (99%)	4 (1%)	80 77
All	All	739/754 (98%)	724 (98%)	15 (2%)	61 55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	352	ASP
1	A	353	GLN
1	A	371	ARG
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	390	SER
1	B	392	SER
1	B	547	ARG
1	B	717	LYS

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	317	HIS
1	A	436	HIS
1	A	454	ASN
1	A	487	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	605	ASN
1	B	697	ASN

5.3.3 RNA

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)

Of 19 ligands modelled in this entry, 5 are 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	750[A]	-	30,50,50	2.30	12 (40%)	24,82,82	2.66	10 (41%)
2	HEM	A	750[B]	-	30,50,50	2.28	11 (36%)	24,82,82	2.93	12 (50%)
8	H4B	A	760[B]	-	13,18,18	0.83	0	11,26,26	2.56	4 (36%)
3	XFJ	A	800	-	28,28,28	0.72	0	38,38,38	1.98	11 (28%)
4	ACT	A	860	-	1,3,3	1.19	0	0,3,3	0.00	-
5	MTL	A	870	-	11,11,11	0.43	0	14,14,14	0.82	0
3	XFJ	B	719[A]	7	28,28,28	0.36	0	38,38,38	1.88	11 (28%)
2	HEM	B	750[A]	-	30,50,50	1.99	8 (26%)	24,82,82	2.57	13 (54%)
2	HEM	B	750[B]	-	30,50,50	1.96	7 (23%)	24,82,82	2.68	13 (54%)
8	H4B	B	760[B]	-	13,18,18	0.81	0	11,26,26	2.55	5 (45%)
3	XFJ	B	800	-	28,28,28	0.75	1 (3%)	38,38,38	1.96	10 (26%)
3	XFJ	B	805[A]	7	28,28,28	0.38	0	38,38,38	1.82	13 (34%)
4	ACT	B	860	-	1,3,3	1.34	0	0,3,3	0.00	-
5	MTL	B	870	-	11,11,11	0.73	0	14,14,14	0.65	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	750[A]	-	-	0/10/54/54	0/0/8/8
2	HEM	A	750[B]	-	-	0/10/54/54	0/0/8/8
8	H4B	A	760[B]	-	-	0/8/17/17	0/2/2/2
3	XFJ	A	800	-	-	0/10/10/10	0/3/3/3
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
5	MTL	A	870	-	-	0/16/16/16	0/0/0/0
3	XFJ	B	719[A]	7	-	0/10/10/10	0/3/3/3
2	HEM	B	750[A]	-	-	0/10/54/54	0/0/8/8
2	HEM	B	750[B]	-	-	0/10/54/54	0/0/8/8
8	H4B	B	760[B]	-	-	0/8/17/17	0/2/2/2
3	XFJ	B	800	-	-	0/10/10/10	0/3/3/3
3	XFJ	B	805[A]	7	-	0/10/10/10	0/3/3/3
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0
5	MTL	B	870	-	-	0/16/16/16	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750[A]	HEM	C3B-C4B	-6.96	1.45	1.51
2	A	750[B]	HEM	C3B-C4B	-6.96	1.45	1.51
2	B	750[A]	HEM	C3D-C4D	-5.55	1.44	1.51
2	B	750[B]	HEM	C3D-C4D	-5.55	1.44	1.51
2	A	750[A]	HEM	C3D-C4D	-5.49	1.44	1.51
2	A	750[B]	HEM	C3D-C4D	-5.49	1.44	1.51
2	A	750[A]	HEM	C2C-C1C	-4.41	1.44	1.52
2	A	750[B]	HEM	C2C-C1C	-4.41	1.44	1.52
2	B	750[A]	HEM	C2C-C1C	-4.33	1.44	1.52
2	B	750[B]	HEM	C2C-C1C	-4.33	1.44	1.52
2	B	750[A]	HEM	C3B-C4B	-3.65	1.48	1.51
2	B	750[B]	HEM	C3B-C4B	-3.65	1.48	1.51
2	B	750[A]	HEM	C2D-C1D	-2.45	1.43	1.51
2	B	750[B]	HEM	C2D-C1D	-2.45	1.43	1.51
2	A	750[A]	HEM	C2D-C1D	-2.33	1.44	1.51
2	A	750[B]	HEM	C2D-C1D	-2.33	1.44	1.51
2	A	750[A]	HEM	C2B-C1B	-2.15	1.44	1.51
2	A	750[B]	HEM	C2B-C1B	-2.15	1.44	1.51
2	A	750[A]	HEM	C1C-NC	2.01	1.38	1.36
2	A	750[B]	HEM	C1C-NC	2.01	1.38	1.36
3	B	800	XFJ	C06-N01	2.04	1.38	1.34
2	A	750[A]	HEM	C3B-CAB	2.06	1.55	1.51
2	A	750[B]	HEM	C3B-CAB	2.06	1.55	1.51
2	B	750[A]	HEM	C3C-CAC	2.20	1.55	1.51
2	B	750[B]	HEM	C3C-CAC	2.20	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750[A]	HEM	CMA-C3A	2.21	1.56	1.51
2	A	750[B]	HEM	CMA-C3A	2.21	1.56	1.51
2	A	750[A]	HEM	FE-ND	2.24	2.09	1.97
2	A	750[B]	HEM	FE-ND	2.24	2.09	1.97
2	A	750[A]	HEM	FE-NB	2.27	2.09	1.97
2	A	750[B]	HEM	FE-NB	2.27	2.09	1.97
2	B	750[A]	HEM	CAA-C2A	2.28	1.55	1.52
2	A	750[A]	HEM	CAA-C2A	2.30	1.56	1.52
2	B	750[A]	HEM	C3B-CAB	2.47	1.55	1.51
2	B	750[B]	HEM	C3B-CAB	2.47	1.55	1.51
2	A	750[A]	HEM	FE-NC	2.52	2.05	1.95
2	A	750[B]	HEM	FE-NC	2.52	2.05	1.95
2	B	750[A]	HEM	FE-NC	2.56	2.05	1.95
2	B	750[B]	HEM	FE-NC	2.56	2.05	1.95

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	750[B]	HEM	CAA-CBA-CGA	-5.40	102.85	112.75
2	A	750[A]	HEM	CBD-CAD-C3D	-4.68	99.92	113.55
2	A	750[B]	HEM	CBD-CAD-C3D	-4.68	99.92	113.55
2	B	750[A]	HEM	CBD-CAD-C3D	-4.23	101.23	113.55
2	B	750[B]	HEM	CBD-CAD-C3D	-4.23	101.23	113.55
2	B	750[B]	HEM	CAA-CBA-CGA	-4.04	105.34	112.75
2	A	750[A]	HEM	C3C-CAC-CBC	-3.65	118.86	124.46
2	A	750[B]	HEM	C3C-CAC-CBC	-3.65	118.86	124.46
3	B	800	XFJ	C05-C06-N01	-3.60	118.90	122.96
3	A	800	XFJ	C05-C06-N01	-3.45	119.06	122.96
2	A	750[B]	HEM	CAA-C2A-C1A	-3.16	123.58	127.01
8	B	760[B]	H4B	N3-C2-N1	-3.13	120.41	125.53
3	B	805[A]	XFJ	C17-C18-C26	-3.10	106.56	112.53
8	A	760[B]	H4B	N3-C2-N1	-3.07	120.50	125.53
2	B	750[A]	HEM	CMA-C3A-C4A	-2.95	123.48	128.36
2	B	750[B]	HEM	CMA-C3A-C4A	-2.95	123.48	128.36
3	A	800	XFJ	C15-C14-C13	-2.91	117.48	121.25
2	A	750[A]	HEM	CMA-C3A-C4A	-2.89	123.58	128.36
2	A	750[B]	HEM	CMA-C3A-C4A	-2.89	123.58	128.36
3	B	805[A]	XFJ	C05-C06-N01	-2.65	119.97	122.96
3	A	800	XFJ	C24-C25-C26	-2.58	118.66	120.28
3	B	800	XFJ	C17-C15-C16	-2.58	117.47	121.85
3	B	800	XFJ	C15-C14-C13	-2.58	117.91	121.25
3	B	800	XFJ	C09-C13-C12	-2.53	117.54	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750[B]	HEM	CAA-C2A-C1A	-2.52	124.27	127.01
3	B	800	XFJ	C25-C26-N21	-2.47	120.17	122.96
3	B	719[A]	XFJ	C24-C25-C26	-2.36	118.80	120.28
3	B	719[A]	XFJ	C05-C06-N01	-2.35	120.31	122.96
2	B	750[A]	HEM	CAA-CBA-CGA	-2.34	108.45	112.75
3	B	719[A]	XFJ	C13-C12-N11	-2.33	119.30	123.66
3	B	719[A]	XFJ	C17-C18-C26	-2.28	108.13	112.53
3	A	800	XFJ	C09-C13-C12	-2.22	118.08	121.85
2	B	750[A]	HEM	CAA-C2A-C1A	-2.13	124.70	127.01
2	B	750[A]	HEM	C3C-CAC-CBC	-2.11	121.22	124.46
2	B	750[B]	HEM	C3C-CAC-CBC	-2.11	121.22	124.46
3	B	805[A]	XFJ	C15-C14-C13	-2.05	118.60	121.25
3	B	805[A]	XFJ	C25-C26-N21	-2.04	120.66	122.96
2	B	750[A]	HEM	C2C-C1C-CHC	2.01	126.74	123.68
2	B	750[B]	HEM	C2C-C1C-CHC	2.01	126.74	123.68
3	B	719[A]	XFJ	C14-C15-C16	2.03	118.79	116.57
3	B	805[A]	XFJ	N02-C02-N01	2.22	120.55	116.50
3	B	800	XFJ	C12-N11-C16	2.25	120.89	117.50
3	B	805[A]	XFJ	N22-C22-N21	2.25	120.60	116.50
8	B	760[B]	H4B	C4A-C8A-N8	2.33	121.18	118.43
3	B	805[A]	XFJ	C18-C26-N21	2.34	119.14	115.69
8	A	760[B]	H4B	C2-N1-C8A	2.36	119.84	114.54
3	B	805[A]	XFJ	C12-N11-C16	2.44	121.18	117.50
3	A	800	XFJ	C14-C13-C12	2.46	119.26	116.57
2	B	750[A]	HEM	C2D-C3D-C4D	2.49	105.72	101.50
2	B	750[B]	HEM	C2D-C3D-C4D	2.49	105.72	101.50
3	A	800	XFJ	C12-N11-C16	2.51	121.29	117.50
2	B	750[A]	HEM	C3B-C4B-CHC	2.54	126.74	123.16
2	B	750[B]	HEM	C3B-C4B-CHC	2.54	126.74	123.16
3	B	805[A]	XFJ	C14-C13-C12	2.57	119.37	116.57
2	B	750[A]	HEM	CMD-C2D-C3D	2.66	126.13	114.35
2	B	750[B]	HEM	CMD-C2D-C3D	2.66	126.13	114.35
3	B	719[A]	XFJ	C18-C26-N21	2.70	119.68	115.69
3	B	805[A]	XFJ	C22-N21-C26	2.79	120.21	118.23
8	B	760[B]	H4B	C2-N1-C8A	2.83	120.91	114.54
3	B	805[A]	XFJ	C14-C15-C16	2.86	119.70	116.57
3	A	800	XFJ	C08-C06-N01	2.90	119.97	115.69
2	A	750[A]	HEM	C2D-C3D-C4D	2.92	106.44	101.50
2	A	750[B]	HEM	C2D-C3D-C4D	2.92	106.44	101.50
2	A	750[A]	HEM	CMD-C2D-C3D	2.97	127.47	114.35
2	A	750[B]	HEM	CMD-C2D-C3D	2.97	127.47	114.35
3	A	800	XFJ	C18-C26-N21	3.03	120.17	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	719[A]	XFJ	C12-N11-C16	3.08	122.14	117.50
3	B	805[A]	XFJ	C08-C06-N01	3.12	120.30	115.69
3	A	800	XFJ	C14-C15-C16	3.16	120.02	116.57
3	B	719[A]	XFJ	C14-C13-C12	3.19	120.06	116.57
3	B	800	XFJ	C14-C15-C16	3.32	120.20	116.57
3	B	719[A]	XFJ	C08-C06-N01	3.33	120.60	115.69
8	B	760[B]	H4B	C4-N3-C2	3.33	120.57	115.94
2	A	750[A]	HEM	C3B-C4B-CHC	3.47	128.05	123.16
2	A	750[B]	HEM	C3B-C4B-CHC	3.47	128.05	123.16
3	B	800	XFJ	C08-C06-N01	3.58	120.97	115.69
8	A	760[B]	H4B	C4-N3-C2	3.83	121.25	115.94
3	B	719[A]	XFJ	C22-N21-C26	3.89	120.99	118.23
2	B	750[A]	HEM	CAD-C3D-C2D	4.16	125.17	113.22
2	B	750[B]	HEM	CAD-C3D-C2D	4.16	125.17	113.22
2	A	750[A]	HEM	CAD-C3D-C4D	4.18	127.21	112.47
2	A	750[B]	HEM	CAD-C3D-C4D	4.18	127.21	112.47
2	A	750[A]	HEM	CMB-C2B-C3B	4.19	126.99	116.53
2	A	750[B]	HEM	CMB-C2B-C3B	4.19	126.99	116.53
3	A	800	XFJ	C02-N01-C06	4.44	121.38	118.23
2	B	750[A]	HEM	CMC-C2C-C3C	4.47	127.70	116.53
2	B	750[B]	HEM	CMC-C2C-C3C	4.47	127.70	116.53
2	A	750[A]	HEM	CAD-C3D-C2D	4.53	126.24	113.22
2	A	750[B]	HEM	CAD-C3D-C2D	4.53	126.24	113.22
3	B	800	XFJ	C22-N21-C26	4.57	121.48	118.23
3	B	719[A]	XFJ	C02-N01-C06	4.64	121.53	118.23
2	B	750[A]	HEM	CAD-C3D-C4D	4.70	129.04	112.47
2	B	750[B]	HEM	CAD-C3D-C4D	4.70	129.04	112.47
3	B	805[A]	XFJ	C02-N01-C06	4.71	121.58	118.23
3	B	800	XFJ	C02-N01-C06	4.71	121.58	118.23
2	B	750[A]	HEM	CMB-C2B-C3B	4.77	128.45	116.53
2	B	750[B]	HEM	CMB-C2B-C3B	4.77	128.45	116.53
2	A	750[A]	HEM	CMC-C2C-C3C	5.20	129.52	116.53
2	A	750[B]	HEM	CMC-C2C-C3C	5.20	129.52	116.53
3	A	800	XFJ	C22-N21-C26	5.30	122.00	118.23
8	B	760[B]	H4B	C4-C4A-C8A	5.64	119.67	114.56
8	A	760[B]	H4B	C4-C4A-C8A	5.85	119.86	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750[A]	HEM	2	0
2	A	750[B]	HEM	5	0
8	A	760[B]	H4B	7	0
3	A	800	XFJ	2	0
5	A	870	MTL	3	0
3	B	719[A]	XFJ	4	0
2	B	750[A]	HEM	3	0
2	B	750[B]	HEM	6	0
8	B	760[B]	H4B	6	0
3	B	800	XFJ	1	0
3	B	805[A]	XFJ	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	407/422 (96%)	0.73	58 (14%) 4 6	20, 38, 68, 86	0
1	B	411/422 (97%)	0.32	22 (5%) 29 41	19, 30, 52, 79	0
All	All	818/844 (96%)	0.52	80 (9%) 10 15	19, 34, 63, 86	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	7.3
1	B	348	VAL	6.7
1	B	350	THR	6.6
1	A	300	PHE	6.5
1	A	716	TRP	6.5
1	B	300	PHE	6.5
1	A	352	ASP	6.1
1	A	715	VAL	5.8
1	B	718	GLY	5.8
1	A	350	THR	5.7
1	A	351	LYS	5.0
1	A	488	PRO	5.0
1	A	486	LYS	4.7
1	A	355	PHE	4.6
1	A	321	THR	4.5
1	A	392	SER	4.3
1	B	352	ASP	4.3
1	B	619	ARG	4.2
1	A	489	ASP	3.8
1	A	713	THR	3.7
1	B	351	LYS	3.7
1	A	385	ASN	3.4
1	A	712	ASN	3.4
1	B	567	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	3.3
1	A	680	VAL	3.2
1	B	322	LEU	3.2
1	A	511	LYS	3.2
1	A	509	GLY	3.1
1	A	390	SER	3.1
1	A	678	TRP	3.0
1	A	551	PHE	2.9
1	A	388	ILE	2.9
1	A	593	ILE	2.9
1	A	386	LYS	2.9
1	A	567	VAL	2.9
1	A	469	LYS	2.8
1	A	491	SER	2.7
1	A	415	CYS	2.7
1	A	353	GLN	2.7
1	B	691	PHE	2.7
1	B	566	ALA	2.7
1	A	584	PHE	2.6
1	A	667[A]	ARG	2.6
1	A	487	GLN	2.6
1	A	490	GLY	2.6
1	A	389	GLU	2.6
1	B	680	VAL	2.6
1	A	619	ARG	2.5
1	A	677	VAL	2.5
1	B	677	VAL	2.5
1	A	371	ARG	2.4
1	A	311	VAL	2.4
1	A	591	THR	2.4
1	B	616	LEU	2.4
1	A	507	GLN	2.4
1	A	676	TRP	2.4
1	A	679	ILE	2.4
1	A	682	PRO	2.4
1	B	321	THR	2.4
1	A	370	LYS	2.3
1	B	302	LYS	2.3
1	A	714	HIS	2.3
1	B	301	LEU	2.3
1	A	302	LYS	2.3
1	B	310	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	620	LYS	2.2
1	A	552	ASP	2.2
1	A	588	TYR	2.1
1	A	706	TYR	2.1
1	B	389	GLU	2.1
1	A	391	THR	2.1
1	A	412	ALA	2.1
1	A	479	LEU	2.1
1	A	595	VAL	2.1
1	A	685	GLY	2.0
1	B	353	GLN	2.0
1	A	566	ALA	2.0
1	A	480	ILE	2.0
1	B	615	ASP	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	MTL	A	870	12/12	0.78	0.39	8.93	20,30,33,34	12
4	ACT	A	860	4/4	0.94	0.18	3.26	48,48,49,49	0
3	XFJ	B	719[A]	26/26	0.92	0.28	2.94	25,27,32,35	26
8	H4B	A	760[B]	17/17	0.89	0.25	2.73	32,33,35,35	17
3	XFJ	B	805[A]	26/26	0.93	0.29	2.25	22,27,38,41	26
8	H4B	B	760[B]	17/17	0.90	0.26	2.11	38,40,42,43	17
4	ACT	B	860	4/4	0.96	0.10	2.03	35,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	XFJ	A	800	26/26	0.90	0.23	1.31	23,34,39,41	0
5	MTL	B	870	12/12	0.89	0.14	1.28	31,39,40,42	0
2	HEM	B	750[B]	43/43	0.98	0.17	1.10	18,21,34,39	5
2	HEM	B	750[A]	43/43	0.98	0.17	1.10	18,21,33,36	5
2	HEM	A	750[A]	43/43	0.98	0.20	0.97	20,24,34,37	5
2	HEM	A	750[B]	43/43	0.98	0.20	0.97	20,24,35,39	5
3	XFJ	B	800	26/26	0.94	0.18	0.85	22,31,35,36	0
6	CL	A	910	1/1	0.98	0.15	-0.64	33,33,33,33	0
6	CL	B	910	1/1	0.98	0.13	-0.69	32,32,32,32	0
7	ZN	A	900	1/1	0.99	0.06	-1.75	28,28,28,28	0
7	ZN	A	901	1/1	0.99	0.12	-	24,24,24,24	1
7	ZN	A	719	1/1	0.99	0.11	-	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.