



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:53 PM GMT

PDB ID : 1D0C
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH 3-BROMO-7-NITROINDAZOLE (H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,
T.L.
Deposited on : 1999-09-09
Resolution : 1.65 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

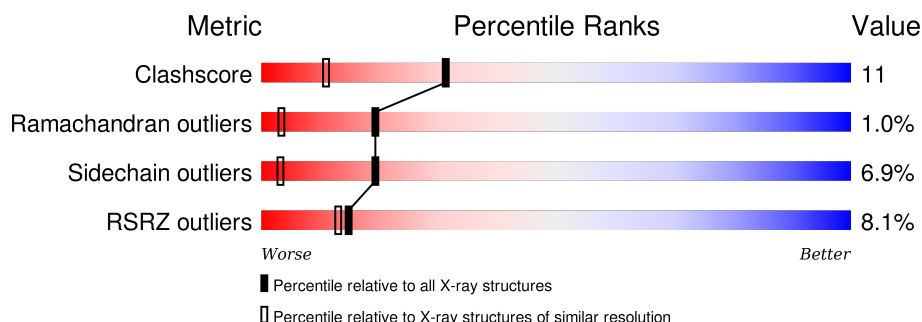
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 $\leq 5\%$. 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	444	<div> <div>8%</div> <div>75%</div> <div>14%</div> <div>5%</div> <div>6%</div> </div>
1	B	444	<div> <div>7%</div> <div>73%</div> <div>15%</div> <div>• • 7%</div> </div>

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
2	ACT	A	860	-	-	-	X
2	ACT	B	851	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CAD	A	950	-	-	-	X
6	CAD	B	951	-	-	-	X
7	GOL	B	881	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7428 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.

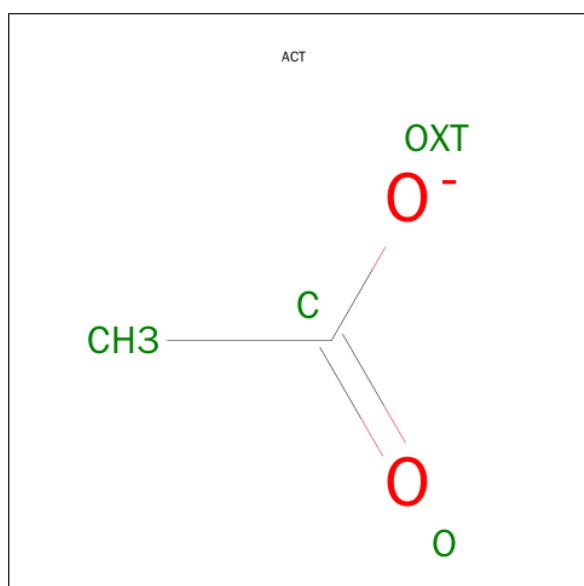
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	1	0
			3303	2099	584	604	16			
1	B	414	Total	C	N	O	S	0	1	0
			3292	2092	582	602	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	CONFLICT	UNP P29473
B	100	ARG	CYS	CONFLICT	UNP P29473

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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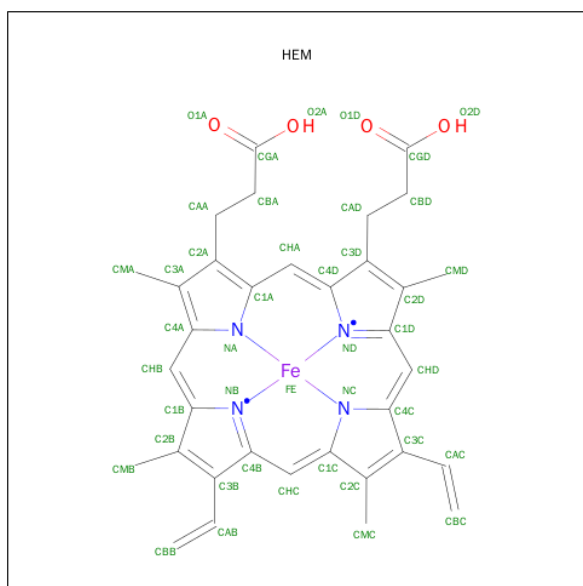
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

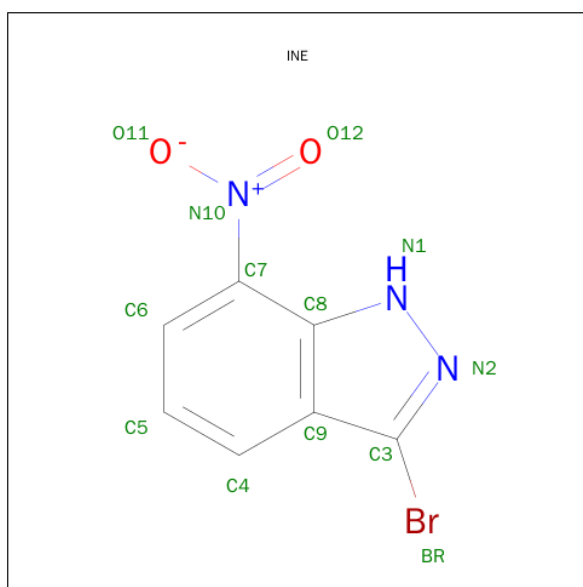
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



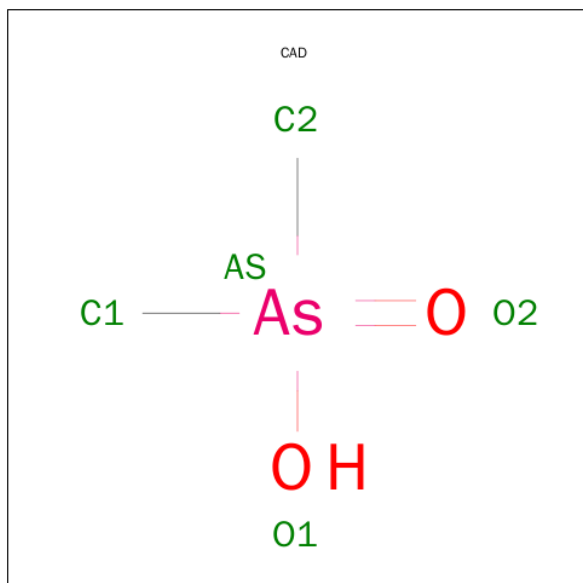
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

- Molecule 5 is 3-BROMO-7-NITROINDAZOLE (three-letter code: INE) (formula: $C_7H_4BrN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

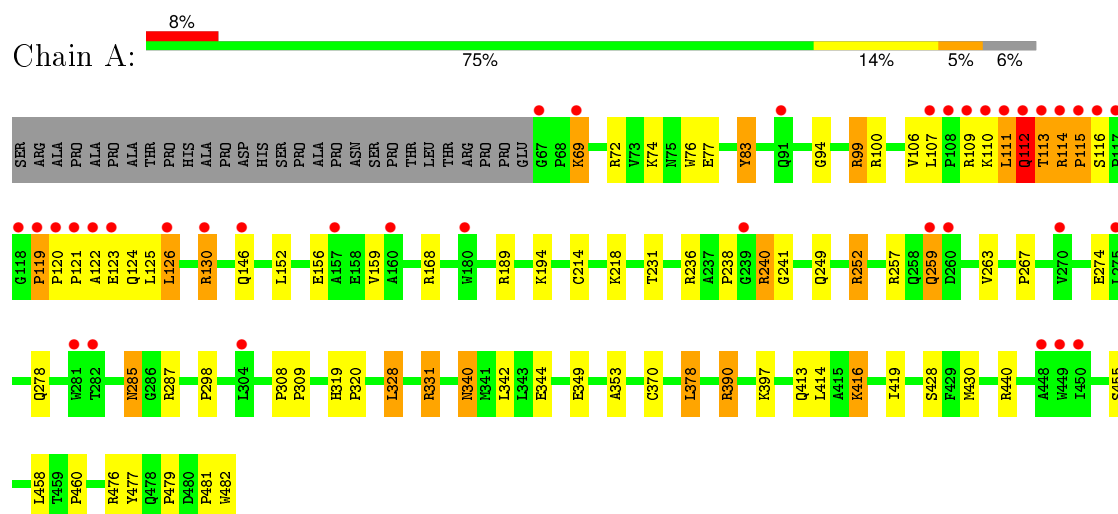
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	348	Total	O	0	0
			348	348		
8	B	307	Total	O	0	0
			307	307		

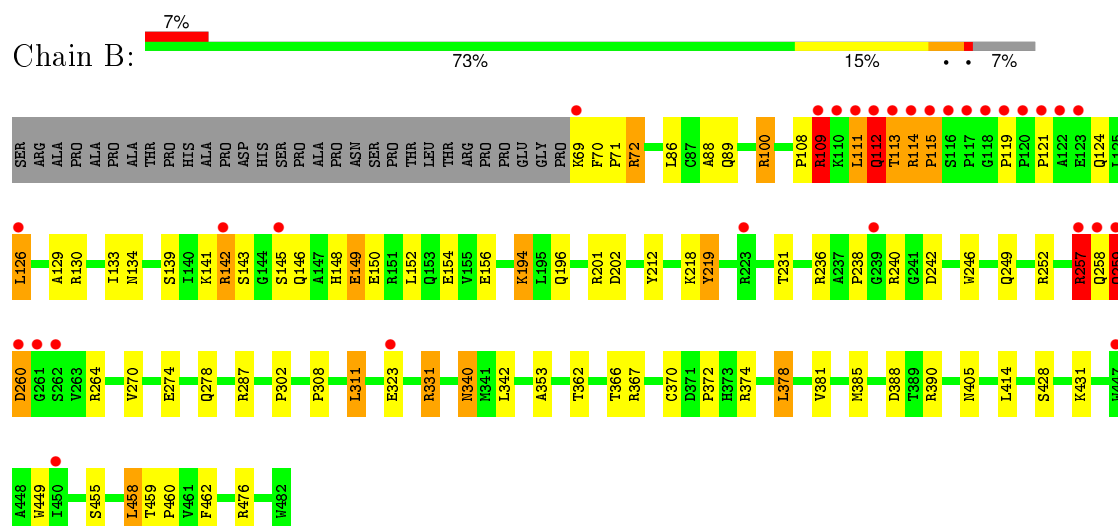
3 Residue-property plots

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

• Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN



• Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.44Å 105.98Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.65 48.04 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-1.65) 92.2 (48.04-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.65Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.213 , 0.259 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 67.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 113260 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7428	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 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, ACT, HEM, INE, 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	0.57	2/3403 (0.1%)	1.07	11/4639 (0.2%)
1	B	0.46	2/3391 (0.1%)	1.05	9/4622 (0.2%)
All	All	0.52	4/6794 (0.1%)	1.06	20/9261 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428[A]	SER	CB-OG	-15.10	1.22	1.42
1	A	428[B]	SER	CB-OG	-15.10	1.22	1.42
1	B	428[A]	SER	CB-OG	-7.79	1.32	1.42
1	B	428[B]	SER	CB-OG	-7.79	1.32	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	B	240	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	252	ARG	NH1-CZ-NH2	7.02	127.12	119.40
1	B	331	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	331	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	440	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	440	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	100	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	83	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	252	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	219	TYR	CB-CG-CD1	5.89	124.53	121.00
1	A	168	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	130	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	374	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	367	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	328	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	201	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	462	PHE	CB-CG-CD2	5.02	124.31	120.80
1	B	212	TYR	CB-CG-CD1	-5.01	117.99	121.00

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	3303	0	3216	71	0
1	B	3292	0	3206	74	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	48	0	8	3	0
5	A	26	0	8	0	0
5	B	26	0	8	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	348	0	0	12	0
8	B	307	0	0	7	0
All	All	7428	0	6504	143	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 11.

All (143) 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:111:LEU:HD23	1:A:476:ARG:HG2	1.35	1.08
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.22	1.04
1:B:115:PRO:HA	1:B:236:ARG:HH12	1.26	0.99
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.46	0.95
1:A:109:ARG:O	1:A:110:LYS:HD2	1.71	0.90
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.45	0.81
1:B:121:PRO:HD2	1:B:124:GLN:OE1	1.81	0.81
1:A:111:LEU:CD2	1:A:476:ARG:HG2	2.12	0.80
1:B:152:LEU:O	1:B:156:GLU:HG3	1.83	0.78
1:B:258:GLN:OE1	1:B:264:ARG:HB2	1.83	0.78
1:A:119:PRO:HG3	1:A:238:PRO:HG3	1.66	0.77
1:A:152:LEU:O	1:A:156:GLU:HG3	1.85	0.77
1:A:106:VAL:HG12	1:A:107:LEU:HD23	1.69	0.73
1:B:126:LEU:O	1:B:130:ARG:HG3	1.93	0.69
1:B:86:LEU:O	1:B:89:GLN:HG2	1.94	0.68
1:A:274:GLU:O	1:A:278:GLN:HG3	1.93	0.68
1:B:119:PRO:HG3	1:B:238:PRO:HG3	1.76	0.67
1:B:257:ARG:HH11	1:B:270:VAL:HG11	1.62	0.64
1:B:150:GLU:O	1:B:154:GLU:HG3	1.98	0.63
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.81	0.62
1:B:113:THR:HG21	1:B:342:LEU:HD22	1.82	0.62
1:B:126:LEU:HD22	1:B:130:ARG:HG3	1.81	0.62
1:B:115:PRO:HA	1:B:236:ARG:NH1	2.07	0.61
1:B:257:ARG:HD3	1:B:270:VAL:HG11	1.84	0.60
1:A:397:LYS:HE3	8:A:1245:HOH:O	2.01	0.59
1:A:413:GLN:O	1:A:416:LYS:HE3	2.01	0.59
1:A:74:LYS:HE2	1:A:76:TRP:CE3	2.37	0.59
1:A:94:GLY:HA3	8:A:1281:HOH:O	2.03	0.59
1:A:113:THR:O	1:A:115:PRO:HD3	2.03	0.59
1:B:126:LEU:HD21	1:B:156:GLU:HG2	1.85	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.43	0.58
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.86	0.57
1:A:126:LEU:O	1:A:130:ARG:HG3	2.04	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.51	0.57
1:A:120:PRO:HB2	1:A:125:LEU:HB2	1.87	0.57
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.85	0.57
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.40	0.56
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.87	0.56
1:A:378:LEU:HB2	8:A:1013:HOH:O	2.06	0.56
1:B:114:ARG:NH1	1:B:114:ARG:HA	2.06	0.56
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.88	0.56
1:B:119:PRO:HG3	1:B:238:PRO:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:107:LEU:CD2	2.35	0.55
1:B:381:VAL:O	1:B:385:MET:HG3	2.07	0.54
1:B:236:ARG:HD2	1:B:242:ASP:OD2	2.07	0.54
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.38	0.54
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.90	0.54
1:A:285:ASN:HB2	8:A:1190:HOH:O	2.07	0.53
1:A:69:LYS:HG2	1:A:69:LYS:O	2.06	0.53
1:A:99:ARG:HH21	1:B:88:ALA:HA	1.73	0.53
1:A:130:ARG:HD3	8:A:1148:HOH:O	2.08	0.53
1:A:99:ARG:CB	1:A:99:ARG:HH11	2.20	0.53
1:B:111:LEU:O	1:B:112:GLN:O	2.27	0.53
1:B:449:TRP:CZ3	4:B:500[B]:HEM:O1A	2.63	0.52
1:B:449:TRP:CE3	4:B:500[B]:HEM:O1A	2.63	0.52
1:A:390:ARG:N	1:A:390:ARG:HD3	2.24	0.51
1:B:274:GLU:HA	1:B:274:GLU:OE1	2.10	0.51
1:B:114:ARG:O	1:B:115:PRO:O	2.29	0.51
1:B:246:TRP:CZ2	1:B:302:PRO:HG3	2.46	0.51
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.44	0.51
1:A:72:ARG:HD2	1:A:83:TYR:CE2	2.46	0.51
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.41	0.50
1:A:390:ARG:H	1:A:390:ARG:HD3	1.76	0.50
1:A:112:GLN:NE2	1:A:477:TYR:HB2	2.25	0.50
1:B:149:GLU:OE1	1:B:149:GLU:O	2.30	0.50
1:B:414:LEU:HD23	8:B:1012:HOH:O	2.10	0.50
1:A:109:ARG:C	1:A:110:LYS:HD2	2.32	0.49
1:B:287:ARG:HD3	8:B:1060:HOH:O	2.12	0.49
1:A:236:ARG:NH1	1:A:349:GLU:OE2	2.44	0.49
1:B:126:LEU:HD22	1:B:130:ARG:CG	2.42	0.49
1:A:119:PRO:HG3	1:A:238:PRO:CG	2.39	0.48
1:A:74:LYS:HE2	1:A:76:TRP:CD2	2.48	0.48
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.94	0.48
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.54	0.48
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.78	0.48
1:A:214:CYS:O	1:A:218:LYS:HG3	2.14	0.47
1:B:308:PRO:O	1:B:311:LEU:HB2	2.13	0.47
1:B:142:ARG:O	1:B:145:SER:OG	2.30	0.47
1:A:285:ASN:N	1:A:285:ASN:HD22	2.10	0.47
1:B:202:ASP:HB3	8:B:1075:HOH:O	2.15	0.47
1:B:146:GLN:NE2	1:B:150:GLU:OE2	2.48	0.47
1:B:388:ASP:OD1	1:B:390:ARG:HG3	2.15	0.47
1:B:308:PRO:HG2	1:B:311:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HD22	1:B:378:LEU:HD21	1.96	0.46
1:B:129:ALA:O	1:B:133:ILE:HG12	2.15	0.46
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.97	0.46
1:B:108:PRO:CG	1:B:111:LEU:HB2	2.45	0.46
1:B:459:THR:HB	1:B:460:PRO:HD2	1.96	0.46
1:B:258:GLN:O	1:B:260:ASP:N	2.49	0.46
1:A:331:ARG:HD2	8:A:1242:HOH:O	2.15	0.46
1:B:257:ARG:NH1	1:B:270:VAL:HG11	2.30	0.46
1:A:430:MET:HG3	1:A:460:PRO:HB2	1.97	0.46
1:B:340:ASN:HD22	1:B:340:ASN:H	1.64	0.46
1:B:231:THR:O	1:B:353:ALA:HA	2.15	0.46
1:A:259:GLN:O	1:A:259:GLN:NE2	2.50	0.45
1:B:109:ARG:NH2	8:B:1068:HOH:O	2.48	0.45
1:A:122:ALA:O	1:A:126:LEU:HB2	2.16	0.45
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.99	0.45
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.98	0.45
1:A:107:LEU:HD22	1:A:477:TYR:CE2	2.51	0.45
1:B:112:GLN:CG	1:B:113:THR:H	2.29	0.45
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.16	0.45
1:A:240:ARG:NH2	8:A:1228:HOH:O	2.49	0.45
1:B:431:LYS:NZ	8:B:1108:HOH:O	2.49	0.45
1:B:126:LEU:HD11	1:B:156:GLU:CG	2.46	0.45
1:A:240:ARG:HD3	1:A:241:GLY:O	2.17	0.45
1:A:72:ARG:NH1	8:A:1215:HOH:O	2.49	0.45
1:B:72:ARG:NH1	8:B:1125:HOH:O	2.50	0.45
1:A:231:THR:O	1:A:353:ALA:HA	2.17	0.45
1:A:344:GLU:HG3	8:A:1075:HOH:O	2.17	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.52	0.45
5:B:765:INE:N1	5:B:765:INE:O12	2.50	0.45
1:A:111:LEU:HD21	8:A:994:HOH:O	2.17	0.44
1:A:477:TYR:HD2	8:A:1211:HOH:O	2.00	0.44
1:B:264:ARG:NH1	1:B:287:ARG:HG3	2.32	0.44
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.64	0.44
1:A:112:GLN:NE2	8:A:1211:HOH:O	2.50	0.44
1:B:257:ARG:HD3	1:B:270:VAL:CG1	2.46	0.44
1:A:340:ASN:HD22	1:A:340:ASN:N	2.17	0.43
1:B:70:PHE:HA	1:B:71:PRO:HD3	1.71	0.43
1:A:106:VAL:C	1:A:107:LEU:HD23	2.39	0.43
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.57	0.43
1:A:126:LEU:CD2	1:A:159:VAL:HG21	2.49	0.43
1:B:449:TRP:CZ3	4:B:500[A]:HEM:O1A	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HB2	1:A:124:GLN:HB2	2.00	0.42
1:A:113:THR:O	1:A:479:PRO:HD3	2.19	0.42
1:B:196:GLN:HG2	1:B:219:TYR:CE1	2.55	0.42
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.48	0.42
1:A:263:VAL:HG11	1:A:267:PRO:HA	2.01	0.42
1:B:108:PRO:HB3	1:B:111:LEU:HD22	2.00	0.41
1:B:194:LYS:HD3	8:B:1190:HOH:O	2.20	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.41
1:A:114:ARG:HH21	1:A:479:PRO:HB3	1.85	0.41
1:B:246:TRP:CH2	1:B:302:PRO:HG3	2.56	0.41
1:B:218:LYS:HE3	1:B:218:LYS:HB3	1.79	0.41
1:A:194:LYS:O	1:A:194:LYS:HG2	2.20	0.41
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.91	0.41
1:B:455:SER:O	1:B:458:LEU:HB2	2.21	0.41
1:B:264:ARG:NH1	1:B:264:ARG:HG3	2.36	0.41
1:B:86:LEU:HD12	1:B:89:GLN:HG3	2.03	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.21	0.41
1:A:77:GLU:HG3	1:B:372:PRO:HG2	2.03	0.40
1:B:362:THR:HA	1:B:405:ASN:HD21	1.86	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	415/444 (94%)	402 (97%)	10 (2%)	3 (1%)	26	7
1	B	413/444 (93%)	396 (96%)	12 (3%)	5 (1%)	16	2
All	All	828/888 (93%)	798 (96%)	22 (3%)	8 (1%)	19	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	115	PRO
1	B	259	GLN
1	A	119	PRO
1	B	257	ARG
1	B	109	ARG
1	A	112	GLN
1	A	115	PRO

5.3.2 Protein sidechains ⓘ

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	355/377 (94%)	332 (94%)	23 (6%)	21	4
1	B	354/377 (94%)	328 (93%)	26 (7%)	17	3
All	All	709/754 (94%)	660 (93%)	49 (7%)	19	3

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	111	LEU
1	A	112	GLN
1	A	113	THR
1	A	114	ARG
1	A	116	SER
1	A	123	GLU
1	A	126	LEU
1	A	146	GLN
1	A	240	ARG
1	A	257	ARG
1	A	259	GLN
1	A	285	ASN
1	A	287	ARG

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	414	LEU
1	A	416	LYS
1	A	419	ILE
1	B	69	LYS
1	B	72	ARG
1	B	100	ARG
1	B	109	ARG
1	B	111	LEU
1	B	112	GLN
1	B	113	THR
1	B	114	ARG
1	B	126	LEU
1	B	139	SER
1	B	141	LYS
1	B	142	ARG
1	B	143	SER
1	B	149	GLU
1	B	194	LYS
1	B	257	ARG
1	B	259	GLN
1	B	260	ASP
1	B	278	GLN
1	B	311	LEU
1	B	323	GLU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	458	LEU
1	B	476	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	153	GLN
1	A	191	GLN
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	146	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	340	ASN
1	B	405	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
4	HEM	A	500	1	30,50,50	2.97	10 (33%)	24,82,82	2.48	11 (45%)
5	INE	A	760	-	10,14,14	3.65	4 (40%)	6,20,20	2.41	2 (33%)
5	INE	A	766	-	10,14,14	3.85	3 (30%)	6,20,20	2.08	1 (16%)
2	ACT	A	850	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
2	ACT	A	860	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-
7	GOL	A	880	-	5,5,5	0.23	0	5,5,5	0.27	0
6	CAD	A	950	1	0,2,4	0.00	-	0,1,6	0.00	-
4	HEM	B	500[A]	-	30,50,50	3.65	12 (40%)	24,82,82	3.02	13 (54%)
4	HEM	B	500[B]	-	30,50,50	3.66	12 (40%)	24,82,82	2.69	11 (45%)
5	INE	B	761	-	10,14,14	3.19	3 (30%)	6,20,20	1.86	1 (16%)
5	INE	B	765	-	10,14,14	3.81	3 (30%)	6,20,20	2.47	1 (16%)
2	ACT	B	851	-	1,3,3	2.50	1 (100%)	0,3,3	0.00	-
2	ACT	B	861	-	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
7	GOL	B	881	-	5,5,5	0.67	0	5,5,5	0.86	0
6	CAD	B	951	1	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
4	HEM	A	500	1	-	0/10/54/54	0/0/8/8
5	INE	A	760	-	-	0/3/4/4	0/2/2/2
5	INE	A	766	-	-	0/3/4/4	0/2/2/2
2	ACT	A	850	-	-	0/0/0/0	0/0/0/0
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
7	GOL	A	880	-	-	0/4/4/4	0/0/0/0
6	CAD	A	950	1	-	0/0/0/0	0/0/0/0
4	HEM	B	500[A]	-	-	0/10/54/54	0/0/8/8
4	HEM	B	500[B]	-	-	0/10/54/54	0/0/8/8
5	INE	B	761	-	-	0/3/4/4	0/2/2/2
5	INE	B	765	-	-	0/3/4/4	0/2/2/2
2	ACT	B	851	-	-	0/0/0/0	0/0/0/0
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0
7	GOL	B	881	-	-	0/4/4/4	0/0/0/0
6	CAD	B	951	1	-	0/0/0/0	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	INE	BR-C3	-8.91	1.76	1.90
4	B	500[B]	HEM	C3B-C4B	-8.89	1.43	1.51
4	B	500[A]	HEM	C3B-C4B	-8.89	1.43	1.51
4	A	500	HEM	C3B-C4B	-8.55	1.44	1.51
5	A	766	INE	BR-C3	-8.53	1.77	1.90
5	B	765	INE	BR-C3	-8.22	1.77	1.90
5	B	761	INE	BR-C3	-7.19	1.79	1.90
4	B	500[B]	HEM	C2D-C3D	-6.26	1.35	1.54
4	B	500[A]	HEM	C2D-C3D	-6.26	1.35	1.54
4	A	500	HEM	C3C-CAC	-6.08	1.39	1.51
4	A	500	HEM	C3D-C4D	-6.07	1.43	1.51
4	A	500	HEM	C2D-C3D	-6.05	1.36	1.54
4	B	500[B]	HEM	C3B-CAB	-6.04	1.40	1.51
4	B	500[A]	HEM	C3B-CAB	-6.04	1.40	1.51
4	B	500[B]	HEM	C3D-C4D	-5.69	1.44	1.51
4	B	500[A]	HEM	C3D-C4D	-5.69	1.44	1.51
4	A	500	HEM	C3B-CAB	-5.62	1.40	1.51
4	B	500[B]	HEM	C3C-CAC	-5.60	1.40	1.51
4	B	500[A]	HEM	C3C-CAC	-5.60	1.40	1.51
4	B	500[B]	HEM	C2C-C1C	-4.04	1.44	1.52
4	B	500[A]	HEM	C2C-C1C	-4.04	1.44	1.52
4	A	500	HEM	C2C-C1C	-3.91	1.45	1.52
5	B	761	INE	C8-N1	-2.52	1.31	1.37
5	B	765	INE	C8-N1	-2.51	1.31	1.37
4	B	500[B]	HEM	C2B-C1B	-2.50	1.43	1.51
4	B	500[A]	HEM	C2B-C1B	-2.50	1.43	1.51
5	A	766	INE	C8-N1	-2.39	1.31	1.37
5	A	760	INE	C8-N1	-2.38	1.31	1.37
4	A	500	HEM	C2B-C1B	-2.34	1.44	1.51
4	A	500	HEM	C2D-C1D	-2.34	1.44	1.51
4	B	500[B]	HEM	C2D-C1D	-2.20	1.44	1.51
4	B	500[A]	HEM	C2D-C1D	-2.20	1.44	1.51
4	A	500	HEM	C4C-NC	2.02	1.38	1.36
4	B	500[B]	HEM	C4C-NC	2.11	1.38	1.36
4	B	500[A]	HEM	C4C-NC	2.11	1.38	1.36
5	A	760	INE	C5-C4	2.17	1.41	1.36
4	A	500	HEM	C1C-NC	2.19	1.38	1.36
2	A	850	ACT	CH3-C	2.37	1.52	1.48
2	B	851	ACT	CH3-C	2.50	1.52	1.48
2	A	860	ACT	CH3-C	2.51	1.52	1.48
2	B	861	ACT	CH3-C	2.79	1.52	1.48
4	B	500[B]	HEM	CMA-C3A	2.83	1.57	1.51
4	B	500[A]	HEM	CMA-C3A	2.83	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500[B]	HEM	CAD-C3D	4.47	1.63	1.54
4	B	500[A]	HEM	CAD-C3D	4.47	1.63	1.54
5	B	761	INE	C3-N2	6.28	1.42	1.34
5	A	760	INE	C3-N2	6.52	1.43	1.34
5	A	766	INE	C3-N2	8.02	1.45	1.34
5	B	765	INE	C3-N2	8.17	1.45	1.34
4	B	500[A]	HEM	CAA-C2A	10.07	1.69	1.52
4	B	500[B]	HEM	CAA-C2A	10.17	1.69	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500[A]	HEM	CBA-CAA-C2A	-6.99	99.99	112.53
4	B	500[B]	HEM	CBA-CAA-C2A	-4.00	105.37	112.53
4	B	500[A]	HEM	CAA-C2A-C1A	-2.85	123.91	127.01
4	A	500	HEM	C1D-CHD-C4C	-2.67	121.36	125.82
4	A	500	HEM	CMA-C3A-C4A	-2.53	124.17	128.36
4	B	500[B]	HEM	C1D-CHD-C4C	-2.46	121.71	125.82
4	B	500[A]	HEM	C1D-CHD-C4C	-2.46	121.71	125.82
5	A	760	INE	C5-C4-C9	-2.25	117.70	120.88
4	B	500[B]	HEM	CBD-CAD-C3D	-2.23	107.05	113.55
4	B	500[A]	HEM	CBD-CAD-C3D	-2.23	107.05	113.55
4	B	500[B]	HEM	CMD-C2D-C3D	2.14	123.80	114.35
4	B	500[A]	HEM	CMD-C2D-C3D	2.14	123.80	114.35
4	B	500[A]	HEM	CAA-CBA-CGA	2.32	117.00	112.75
4	A	500	HEM	CMD-C2D-C3D	2.48	125.31	114.35
4	A	500	HEM	CMA-C3A-C2A	2.49	130.44	125.24
4	B	500[B]	HEM	C2D-C3D-C4D	2.55	105.82	101.50
4	B	500[A]	HEM	C2D-C3D-C4D	2.55	105.82	101.50
4	A	500	HEM	C2D-C3D-C4D	2.92	106.45	101.50
4	B	500[B]	HEM	CMB-C2B-C3B	3.02	124.07	116.53
4	B	500[A]	HEM	CMB-C2B-C3B	3.02	124.07	116.53
4	A	500	HEM	CMB-C2B-C3B	3.35	124.91	116.53
4	B	500[B]	HEM	CAD-C3D-C2D	3.82	124.20	113.22
4	B	500[A]	HEM	CAD-C3D-C2D	3.82	124.20	113.22
4	A	500	HEM	CAD-C3D-C2D	3.82	124.21	113.22
4	A	500	HEM	C3B-CAB-CBB	3.98	130.56	124.46
5	B	761	INE	C6-C7-N10	4.17	121.98	116.59
4	A	500	HEM	CMC-C2C-C3C	4.27	127.18	116.53
4	B	500[B]	HEM	C3C-CAC-CBC	4.27	131.01	124.46
4	B	500[A]	HEM	C3C-CAC-CBC	4.27	131.01	124.46
5	A	766	INE	C6-C7-N10	4.30	122.16	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	HEM	C3C-CAC-CBC	4.74	131.73	124.46
4	A	500	HEM	CAD-C3D-C4D	4.78	129.33	112.47
4	B	500[B]	HEM	CAD-C3D-C4D	4.96	129.96	112.47
4	B	500[A]	HEM	CAD-C3D-C4D	4.96	129.96	112.47
5	A	760	INE	C6-C7-N10	4.98	123.04	116.59
4	B	500[B]	HEM	CMC-C2C-C3C	5.25	129.64	116.53
4	B	500[A]	HEM	CMC-C2C-C3C	5.25	129.64	116.53
5	B	765	INE	C6-C7-N10	5.40	123.59	116.59
4	B	500[B]	HEM	C3B-CAB-CBB	5.54	132.96	124.46
4	B	500[A]	HEM	C3B-CAB-CBB	5.54	132.96	124.46

There are no chirality outliers.

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
4	B	500[A]	HEM	1	0
4	B	500[B]	HEM	2	0
5	B	765	INE	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/444 (93%)	0.47	37 (8%) 12 10	17, 27, 63, 123	0
1	B	414/444 (93%)	0.39	30 (7%) 18 16	19, 29, 65, 137	0
All	All	830/888 (93%)	0.43	67 (8%) 15 13	17, 28, 65, 137	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	15.9
1	A	113	THR	15.1
1	B	113	THR	14.6
1	A	119	PRO	13.7
1	B	111	LEU	13.5
1	B	115	PRO	12.5
1	B	114	ARG	12.2
1	A	110	LYS	11.4
1	B	110	LYS	10.4
1	A	117	PRO	10.0
1	A	111	LEU	10.0
1	A	120	PRO	8.6
1	B	118	GLY	8.5
1	B	119	PRO	8.4
1	B	261	GLY	8.1
1	B	259	GLN	7.9
1	A	115	PRO	7.4
1	B	116	SER	7.1
1	B	120	PRO	6.8
1	A	121	PRO	6.4
1	A	116	SER	5.4
1	B	112	GLN	5.4
1	A	259	GLN	5.1
1	A	160	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	118	GLY	4.7
1	A	123	GLU	4.7
1	A	112	GLN	4.4
1	A	109	ARG	4.2
1	A	239	GLY	4.1
1	A	114	ARG	3.9
1	B	260	ASP	3.7
1	A	122	ALA	3.5
1	A	260	ASP	3.2
1	A	449	TRP	3.0
1	A	69	LYS	3.0
1	B	223	ARG	3.0
1	B	109	ARG	2.9
1	A	450	ILE	2.8
1	B	69	LYS	2.8
1	A	146	GLN	2.7
1	A	107	LEU	2.6
1	A	91	GLN	2.6
1	A	281	TRP	2.6
1	A	67	GLY	2.6
1	B	323	GLU	2.5
1	A	448	ALA	2.5
1	B	257	ARG	2.5
1	A	108	PRO	2.5
1	A	130	ARG	2.4
1	B	121	PRO	2.4
1	B	258	GLN	2.4
1	A	282	THR	2.4
1	B	262	SER	2.3
1	A	157	ALA	2.2
1	B	123	GLU	2.2
1	B	450	ILE	2.2
1	B	142	ARG	2.2
1	B	447	TRP	2.2
1	B	122	ALA	2.2
1	A	180	TRP	2.1
1	A	270	VAL	2.1
1	B	126	LEU	2.1
1	B	145	SER	2.1
1	B	239	GLY	2.1
1	A	126	LEU	2.0
1	A	275	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	CAD	A	950	3/5	0.94	0.46	22.37	24,24,47,53	0
7	GOL	B	881	6/6	0.76	0.27	9.01	44,54,59,62	0
6	CAD	B	951	3/5	0.97	0.41	8.66	19,19,38,50	0
2	ACT	A	860	4/4	0.93	0.18	3.41	28,34,36,39	0
2	ACT	B	851	4/4	0.97	0.10	2.44	25,32,34,35	0
7	GOL	A	880	6/6	0.81	0.16	1.73	34,45,53,61	0
4	HEM	B	500[A]	43/43	0.98	0.11	0.72	16,21,38,49	5
4	HEM	B	500[B]	43/43	0.98	0.11	0.72	16,22,32,41	5
4	HEM	A	500	43/43	0.98	0.14	0.65	15,19,42,53	0
2	ACT	B	861	4/4	0.93	0.08	0.19	24,26,31,32	0
5	INE	B	765	13/13	0.91	0.13	0.06	36,44,56,57	0
5	INE	A	760	13/13	0.99	0.11	0.02	17,21,25,32	0
5	INE	A	766	13/13	0.91	0.11	-0.01	36,42,59,59	0
5	INE	B	761	13/13	0.99	0.07	-0.35	19,24,29,36	0
2	ACT	A	850	4/4	0.98	0.07	-0.56	22,27,31,34	0
3	ZN	A	900	1/1	1.00	0.02	-3.88	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.