Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:58 PM GMT

PDB ID : 1DM6

Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN COMPLEXED WITH N-(4-CHLOROPHENYL)-N'-HYDROXYGUANIDINE(H4B FREE)

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Deposited on : 1999-12-13

Resolution : 1.95 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683
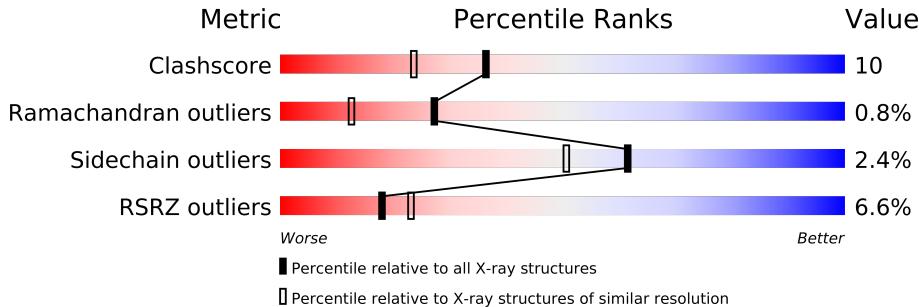
1 Overall quality at a glance ⓘ
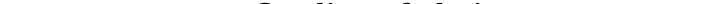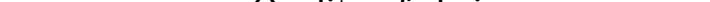
The reported resolution of this entry is 1.95 Å.

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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0.8%
Sidechain outliers		2.4%
RSRZ outliers		6.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	A	1850	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7266 atoms, of which 0 are hydrogen and 0 are deuterium.

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.
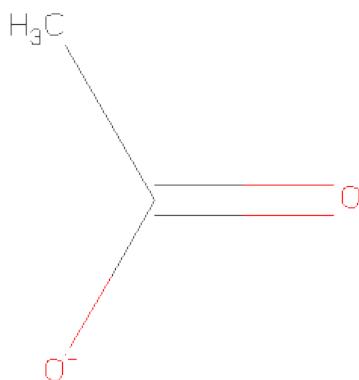
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total 3302	C 2099	N 584	O 603	S 16	0	0	0
1	B	414	Total 3291	C 2092	N 582	O 601	S 16	0	0	0

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: $C_2H_3O_2$).
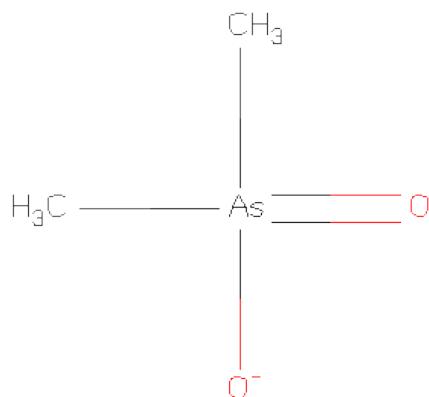
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0

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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).
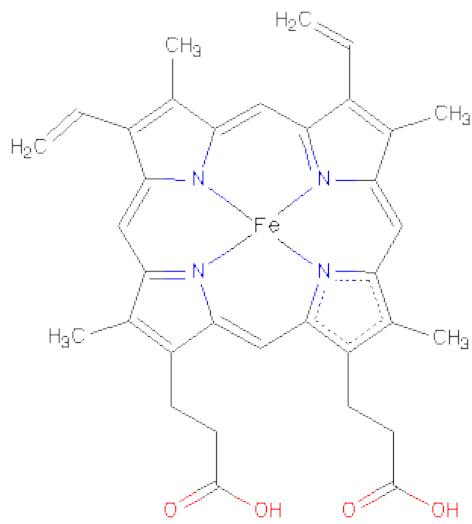
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	As 1	C 2	0	0
3	B	1	Total 3	As 1	C 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).
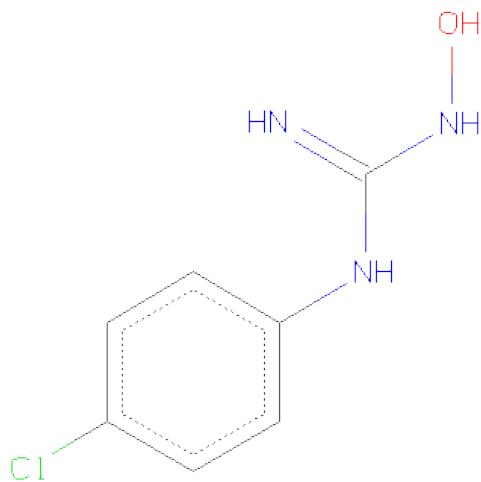
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

- Molecule 6 is N-(CHLOROPHENYL)-N'-HYDROXYGUANIDINE (three-letter code: PH3) (formula: $C_7H_8ClN_3O$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			12	7	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Cl	N	O	0	0
			12	7	1	3	1		
6	A	1	Total	C	Cl	N	O	0	0
			12	7	1	3	1		
6	B	1	Total	C	Cl	N	O	0	0
			12	7	1	3	1		

- Molecule 7 is water.
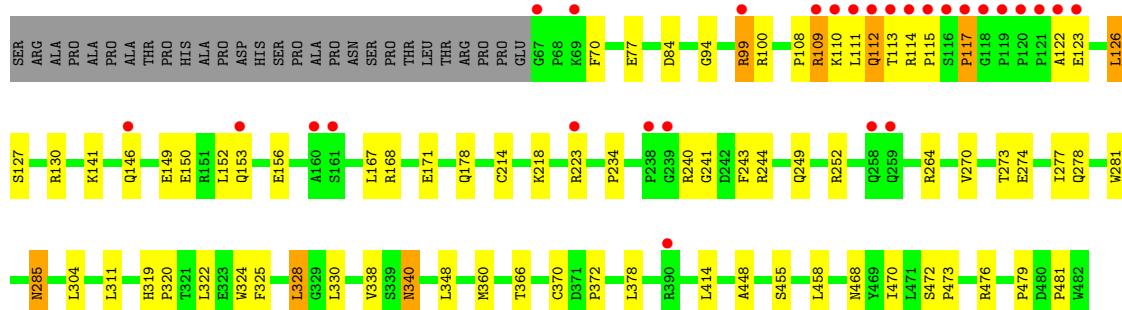
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	276	Total	O	0	0
			276	276		
7	B	240	Total	O	0	0
			240	240		

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.
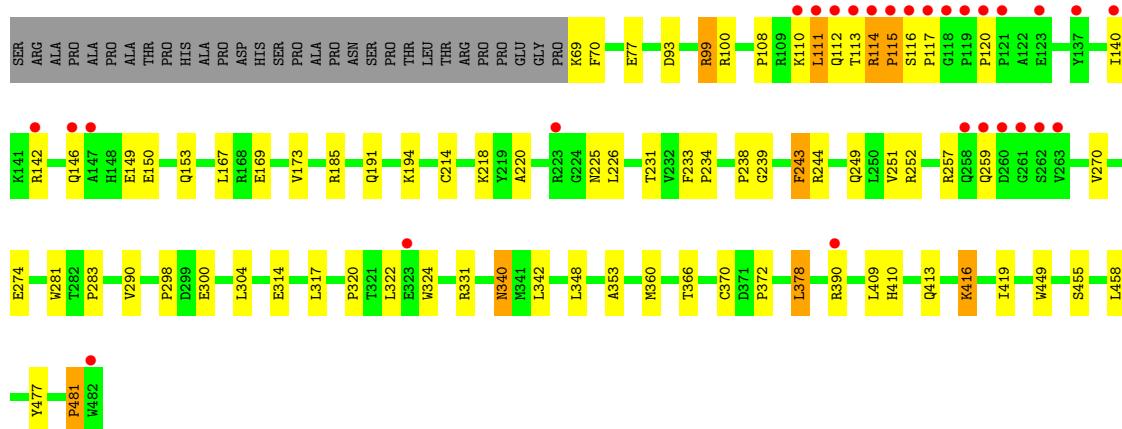
• Molecule 1: NITRIC OXIDE SYNTHASE

Chain A:

• Molecule 1: NITRIC OXIDE SYNTHASE

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.88Å　　106.43Å　　155.92Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	28.20　–　1.95 28.20　–　1.95	Depositor EDS
% Data completeness (in resolution range)	82.9 (28.20-1.95) 65.8 (28.20-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.77 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220　,　　　0.255 0.211　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.47$, $<L^2> = 0.31$	Xtriage
Outliers	4 of 55136 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7266	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: PH3, CAC, ZN, HEM, ACT

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	0.34	0/3397	0.60	1/4631 (0.0%)
1	B	0.33	0/3385	0.61	2/4614 (0.0%)
All	All	0.33	0/6782	0.60	3/9245 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	MET	N-CA-C	-6.09	94.54	111.00
1	B	360	MET	N-CA-C	-5.53	96.06	111.00
1	B	243	PHE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3302	0	3215	72	0
1	B	3291	0	3205	64	0
2	A	8	0	6	1	0
2	B	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	2	0
6	A	24	0	14	2	0
6	B	24	0	14	5	0
7	A	276	0	0	5	0
7	B	240	0	0	3	0
All	All	7266	0	6520	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:GLN:HB2	1:A:252:ARG:HD3	1.35	1.08
1:B:249:GLN:HB2	1:B:252:ARG:HD3	1.21	1.08
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.36	1.07
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.37	0.90
1:B:112:GLN:HG3	1:B:113:THR:H	1.39	0.85
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.44	0.83
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.44	0.80
1:A:146:GLN:O	1:A:150:GLU:HG3	1.81	0.80
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.66	0.76
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.68	0.73
1:A:223:ARG:HB2	1:A:223:ARG:HH11	1.54	0.72
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.17	0.70
1:A:378:LEU:HB2	7:A:3021:HOH:O	1.93	0.69
1:B:140:ILE:HB	1:B:142:ARG:NH1	2.08	0.68
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.29	0.67
1:A:126:LEU:HD21	1:A:156:GLU:HA	1.77	0.66
1:B:378:LEU:HB2	7:B:2870:HOH:O	1.95	0.66
1:B:146:GLN:O	1:B:150:GLU:HG3	1.95	0.65
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.79	0.65
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.79	0.65
1:B:116:SER:O	1:B:238:PRO:HA	1.97	0.64
1:A:111:LEU:H	1:A:111:LEU:HD12	1.62	0.64
1:A:152:LEU:O	1:A:156:GLU:HG3	1.97	0.64
1:B:477:TYR:OH	5:B:2500:HEM:O1D	2.11	0.64
1:A:115:PRO:O	1:A:117:PRO:HD3	1.99	0.62
1:A:168:ARG:HB2	1:A:171:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:GLU:O	1:A:153:GLN:HG3	1.99	0.62
1:B:366:THR:O	1:B:370:CYS:HB2	2.00	0.61
1:B:314:GLU:CD	1:B:331:ARG:HH21	2.04	0.61
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.14	0.61
1:B:416:LYS:HA	1:B:416:LYS:HE3	1.82	0.61
1:B:149:GLU:O	1:B:153:GLN:HG3	2.01	0.60
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.83	0.60
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.84	0.60
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.82	0.60
1:A:340:ASN:HD22	1:A:340:ASN:H	1.49	0.60
1:B:110:LYS:C	1:B:112:GLN:H	2.06	0.58
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.85	0.58
1:A:270:VAL:O	1:A:274:GLU:HG3	2.03	0.58
1:A:94:GLY:O	1:A:110:LYS:HE2	2.02	0.58
1:B:409:LEU:O	1:B:413:GLN:HG3	2.03	0.57
1:B:120:PRO:HD2	7:B:3074:HOH:O	2.04	0.57
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.39	0.57
6:B:2780:PH3:HN1	6:B:2780:PH3:H2	1.69	0.57
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.44	0.57
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.87	0.56
1:A:274:GLU:O	1:A:278:GLN:HG3	2.04	0.56
1:A:99:ARG:NH1	1:A:99:ARG:HB2	2.16	0.55
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.47	0.55
1:B:112:GLN:HG3	1:B:113:THR:N	2.15	0.55
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.24	0.55
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.89	0.54
1:B:340:ASN:HD22	1:B:340:ASN:H	1.53	0.54
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.89	0.54
1:A:249:GLN:HB2	1:A:252:ARG:CD	2.24	0.53
1:B:110:LYS:O	1:B:112:GLN:N	2.41	0.53
1:B:390:ARG:NH1	1:B:390:ARG:HB2	2.24	0.53
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.25	0.52
1:B:117:PRO:HA	1:B:239:GLY:H	1.75	0.52
1:B:114:ARG:NH1	1:B:114:ARG:HA	2.20	0.52
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.74	0.52
1:B:140:ILE:HD12	1:B:142:ARG:HH11	1.74	0.52
1:A:109:ARG:O	1:A:110:LYS:HD2	2.11	0.51
1:A:285:ASN:HD22	1:A:285:ASN:C	2.12	0.51
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.40	0.50
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.21	0.50
1:B:231:THR:O	1:B:353:ALA:HA	2.12	0.50
1:B:320:PRO:HG3	1:B:410:HIS:CG	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:LYS:HG2	1:B:70:PHE:CD1	2.47	0.49
1:A:325:PHE:O	1:A:328:LEU:HB2	2.12	0.49
1:B:234:PRO:HB2	1:B:243:PHE:CE1	2.47	0.49
1:A:240:ARG:HG2	1:A:241:GLY:N	2.28	0.48
1:A:99:ARG:CB	1:A:99:ARG:HH11	2.19	0.48
6:B:2780:PH3:C2	6:B:2780:PH3:HN1	2.25	0.48
1:A:223:ARG:NH1	1:A:223:ARG:HB2	2.26	0.48
1:A:123:GLU:HB2	7:A:2946:HOH:O	2.12	0.48
1:A:285:ASN:C	1:A:285:ASN:ND2	2.67	0.47
1:B:390:ARG:HH11	1:B:390:ARG:CB	2.27	0.47
1:A:127:SER:HA	1:A:130:ARG:CZ	2.45	0.47
1:A:338:VAL:HG21	6:A:1780:PH3:C4	2.44	0.47
1:A:115:PRO:C	1:A:117:PRO:HD3	2.34	0.47
1:A:113:THR:CG2	1:A:476:ARG:HD2	2.44	0.46
1:A:126:LEU:O	1:A:130:ARG:HG3	2.15	0.46
1:B:340:ASN:HD22	1:B:340:ASN:N	2.10	0.46
1:B:270:VAL:O	1:B:274:GLU:HG3	2.15	0.46
1:A:122:ALA:O	1:A:126:LEU:HB2	2.15	0.46
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.97	0.46
1:A:252:ARG:NH2	2:A:1850:ACT:OXT	2.49	0.46
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.98	0.45
1:A:114:ARG:HD2	1:A:479:PRO:HG3	1.99	0.45
1:B:281:TRP:O	1:B:283:PRO:HD3	2.16	0.45
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.31	0.45
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.52	0.45
1:A:472:SER:HA	1:A:473:PRO:C	2.37	0.45
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.83	0.45
1:A:108:PRO:O	1:A:110:LYS:N	2.50	0.44
1:B:340:ASN:H	1:B:340:ASN:ND2	2.15	0.44
1:A:109:ARG:HA	1:A:109:ARG:HD3	1.83	0.44
1:B:251:VAL:O	1:B:252:ARG:HD2	2.18	0.44
1:B:99:ARG:HH11	1:B:99:ARG:HB2	1.82	0.44
1:A:340:ASN:HD22	1:A:340:ASN:N	2.10	0.44
1:A:273:THR:O	1:A:277:ILE:HG13	2.18	0.44
1:A:70:PHE:HB3	1:A:84:ASP:O	2.18	0.43
1:B:390:ARG:NH1	1:B:390:ARG:CB	2.80	0.43
1:A:249:GLN:CB	1:A:252:ARG:HD3	2.26	0.43
1:B:298:PRO:O	1:B:300:GLU:HG2	2.18	0.43
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.34	0.43
1:B:169:GLU:O	1:B:173:VAL:HG23	2.18	0.43
1:B:191:GLN:NE2	1:B:194:LYS:HE3	2.34	0.43
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:ARG:HD2	1:A:252:ARG:HA	1.93	0.42
1:A:111:LEU:O	1:A:112:GLN:C	2.57	0.42
1:A:114:ARG:HD2	1:A:479:PRO:CG	2.49	0.42
1:B:116:SER:N	1:B:117:PRO:CD	2.83	0.42
1:A:338:VAL:HG21	6:A:1780:PH3:C3	2.50	0.42
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.01	0.42
1:A:366:THR:O	1:A:370:CYS:HB2	2.20	0.42
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.50	0.42
1:B:220:ALA:O	1:B:226:LEU:HA	2.20	0.42
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.54	0.42
5:B:2500:HEM:HBD2	6:B:2780:PH3:CL	2.57	0.41
1:A:178:GLN:HG2	7:A:2817:HOH:O	2.19	0.41
1:A:111:LEU:HG	1:A:470:ILE:HD13	2.02	0.41
1:B:317:LEU:HG	1:B:331:ARG:HA	2.02	0.41
1:B:140:ILE:HB	1:B:142:ARG:HH12	1.82	0.41
1:A:448:ALA:O	6:B:1785:PH3:NH2	2.53	0.41
1:B:290:VAL:HG23	7:B:3089:HOH:O	2.21	0.41
1:A:214:CYS:O	1:A:218:LYS:HG3	2.21	0.41
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.85	0.41
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.45	0.41
1:A:141:LYS:NZ	7:A:2931:HOH:O	2.52	0.41
1:B:110:LYS:C	1:B:112:GLN:N	2.73	0.40
1:A:168:ARG:HD2	7:A:2949:HOH:O	2.22	0.40
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.56	0.40
6:B:2780:PH3:H2	6:B:2780:PH3:NH1	2.35	0.40
1:B:214:CYS:O	1:B:218:LYS:HG3	2.20	0.40
1:B:93:ASP:O	1:B:111:LEU:HD21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	414/444 (93%)	392 (95%)	19 (5%)	3 (1%)	30	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/444 (93%)	380 (92%)	28 (7%)	4 (1%)	22	9
All	All	826/888 (93%)	772 (94%)	47 (6%)	7 (1%)	27	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	A	112	GLN
1	B	111	LEU
1	A	117	PRO
1	A	109	ARG
1	B	115	PRO
1	B	481	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	354/377 (94%)	346 (98%)	8 (2%)	63	53
1	B	353/377 (94%)	344 (98%)	9 (2%)	60	48
All	All	707/754 (94%)	690 (98%)	17 (2%)	61	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	126	LEU
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	414	LEU
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	114	ARG

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Mol	Chain	Res	Type
1	B	225	ASN
1	B	257	ARG
1	B	340	ASN
1	B	378	LEU
1	B	416	LYS
1	B	419	ILE

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	259	GLN
1	A	278	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	112	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	279	HIS
1	B	340	ASN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	#$|Z| > 2$
5	HEM	A	1500	1	49,50,50	2.02	15 (30%)	46,82,82	1.56	7 (15%)
6	PH3	A	1780	-	12,12,12	4.26	5 (41%)	15,15,15	1.99	4 (26%)
2	ACT	A	1850	-	1,3,3	2.86	1 (100%)	0,3,3	0.00	-
2	ACT	A	1860	-	1,3,3	2.32	1 (100%)	0,3,3	0.00	-
6	PH3	A	2785	-	12,12,12	2.09	3 (25%)	15,15,15	1.69	2 (13%)
3	CAC	A	950	1	2,2,4	0.48	0	0,1,6	0.00	-
6	PH3	B	1785	-	12,12,12	1.98	3 (25%)	15,15,15	1.76	2 (13%)
5	HEM	B	2500	1	49,50,50	1.97	12 (24%)	46,82,82	1.38	7 (15%)
6	PH3	B	2780	-	12,12,12	4.36	6 (50%)	15,15,15	1.96	4 (26%)
2	ACT	B	2850	-	1,3,3	2.55	1 (100%)	0,3,3	0.00	-
2	ACT	B	2860	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
3	CAC	B	950	1	2,2,4	0.46	0	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
5	HEM	A	1500	1	-	0/14/114/114	0/0/8/8
6	PH3	A	1780	-	-	0/5/6/6	0/1/1/1
2	ACT	A	1850	-	-	0/0/0/0	0/0/0/0
2	ACT	A	1860	-	-	0/0/0/0	0/0/0/0
6	PH3	A	2785	-	-	0/5/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAC	A	950	1	-	0/0/0/0	0/0/0/0
6	PH3	B	1785	-	-	0/5/6/6	0/1/1/1
5	HEM	B	2500	1	-	0/14/114/114	0/0/8/8
6	PH3	B	2780	-	-	0/5/6/6	0/1/1/1
2	ACT	B	2850	-	-	0/0/0/0	0/0/0/0
2	ACT	B	2860	-	-	0/0/0/0	0/0/0/0
3	CAC	B	950	1	-	0/0/0/0	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2780	PH3	C2-C1	11.09	1.57	1.39
6	A	1780	PH3	C2-C1	10.98	1.57	1.39
6	B	2780	PH3	C3-C2	7.57	1.53	1.38
6	A	1780	PH3	C3-C2	7.49	1.53	1.38
6	A	2785	PH3	OH-NH1	-4.98	1.30	1.39
6	B	1785	PH3	OH-NH1	-4.93	1.30	1.39
5	A	1500	HEM	C2D-C1D	4.87	1.45	1.44
5	B	2500	HEM	C3C-C2C	-4.86	1.35	1.43
5	A	1500	HEM	C3D-C2D	-4.82	1.35	1.43
5	B	2500	HEM	CHA-C4D	4.71	1.42	1.35
5	A	1500	HEM	C4A-C3A	4.28	1.45	1.40
5	B	2500	HEM	C4A-C3A	4.22	1.45	1.40
6	A	2785	PH3	C4-CL	-4.15	1.64	1.74
5	B	2500	HEM	C3B-C2B	-4.08	1.36	1.43
6	A	1780	PH3	OH-NH1	-4.01	1.32	1.39
5	A	1500	HEM	CHB-C1B	3.80	1.41	1.35
6	B	2780	PH3	C5-C4	3.76	1.45	1.38
5	B	2500	HEM	C3D-C2D	-3.73	1.37	1.43
6	B	2780	PH3	OH-NH1	-3.73	1.33	1.39
5	A	1500	HEM	C4C-NC	3.59	1.43	1.38
5	A	1500	HEM	C3B-C2B	-3.56	1.37	1.43
5	B	2500	HEM	C2B-C1B	3.50	1.45	1.44
5	A	1500	HEM	C4A-NA	3.46	1.43	1.36
5	A	1500	HEM	CHA-C4D	3.25	1.40	1.35
5	B	2500	HEM	C3D-C4D	3.24	1.45	1.44
5	A	1500	HEM	C3D-C4D	3.13	1.45	1.44
6	B	1785	PH3	C4-CL	-3.10	1.67	1.74
6	B	1785	PH3	C2-C1	3.06	1.44	1.39
6	A	1780	PH3	C5-C4	3.02	1.44	1.38
2	A	1850	ACT	CH3-C	2.86	1.52	1.48
6	A	2785	PH3	C2-C1	2.80	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2500	HEM	CHB-C1B	2.77	1.39	1.35
2	B	2860	ACT	CH3-C	2.73	1.52	1.48
5	B	2500	HEM	C1A-NA	2.60	1.41	1.36
2	B	2850	ACT	CH3-C	2.55	1.52	1.48
6	B	2780	PH3	C6-C5	2.47	1.43	1.38
5	A	1500	HEM	C3C-C2C	-2.45	1.39	1.43
5	B	2500	HEM	CMD-C2D	2.44	1.55	1.47
5	B	2500	HEM	CMB-C2B	2.38	1.54	1.47
2	A	1860	ACT	CH3-C	2.32	1.52	1.48
6	B	2780	PH3	C3-C4	2.31	1.42	1.38
5	A	1500	HEM	C1A-NA	2.27	1.41	1.36
5	B	2500	HEM	FE-NA	2.26	2.02	1.92
5	A	1500	HEM	CHC-C1C	2.25	1.40	1.36
6	A	1780	PH3	C3-C4	2.20	1.42	1.38
5	A	1500	HEM	CMC-C2C	2.04	1.53	1.47
5	A	1500	HEM	CMD-C2D	2.03	1.53	1.47
5	A	1500	HEM	FE-NA	2.03	2.01	1.92

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1500	HEM	C3B-C4B-NB	-4.99	110.43	114.00
6	B	2780	PH3	OH-NH1-CZ	4.68	126.48	117.44
6	A	1780	PH3	OH-NH1-CZ	4.66	126.44	117.44
6	B	1785	PH3	OH-NH1-CZ	4.44	126.02	117.44
6	B	1785	PH3	C1-NE-CZ	4.24	139.30	126.45
6	A	2785	PH3	C1-NE-CZ	4.11	138.91	126.45
5	B	2500	HEM	C3B-C4B-NB	-3.79	111.29	114.00
5	A	1500	HEM	C3A-C4A-NA	3.71	112.21	109.41
6	A	2785	PH3	OH-NH1-CZ	3.64	124.46	117.44
5	A	1500	HEM	C4A-NA-C1A	-3.59	102.03	106.76
5	A	1500	HEM	C4A-CHB-C1B	-3.37	123.03	127.47
6	A	1780	PH3	NE-CZ-NH1	3.21	124.61	117.28
6	A	1780	PH3	C2-C3-C4	-3.17	115.69	119.22
6	B	2780	PH3	C2-C3-C4	-3.16	115.70	119.22
6	B	2780	PH3	NE-CZ-NH1	3.13	124.43	117.28
5	B	2500	HEM	C1A-CHA-C4D	-3.10	123.39	127.47
5	B	2500	HEM	C3A-C4A-NA	3.00	111.67	109.41
5	B	2500	HEM	C4A-NA-C1A	-2.83	103.04	106.76
5	B	2500	HEM	C4C-NC-C1C	-2.76	102.66	105.53
5	A	1500	HEM	C4C-NC-C1C	-2.69	102.74	105.53
5	A	1500	HEM	C1A-CHA-C4D	-2.53	124.14	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2500	HEM	CAA-C2A-C3A	-2.48	121.93	129.00
6	B	2780	PH3	C5-C4-C3	2.06	124.26	121.26
5	A	1500	HEM	CHC-C1C-NC	-2.04	122.96	124.73
6	A	1780	PH3	C5-C4-C3	2.03	124.21	121.26
5	B	2500	HEM	C4A-CHB-C1B	-2.01	124.82	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.45	28 (6%)	17	22	23, 33, 60, 100	0
1	B	414/444 (93%)	0.53	28 (6%)	17	22	24, 36, 66, 100	0
All	All	830/888 (93%)	0.49	56 (6%)	18	22	23, 34, 65, 100	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	THR	12.4
1	A	119	PRO	11.1
1	A	113	THR	10.7
1	B	117	PRO	9.6
1	A	115	PRO	9.5
1	B	111	LEU	9.4
1	B	115	PRO	9.3
1	B	110	LYS	9.3
1	A	117	PRO	7.7
1	B	114	ARG	7.0
1	A	116	SER	6.7
1	A	118	GLY	6.4
1	B	116	SER	6.1
1	B	259	GLN	6.1
1	A	114	ARG	5.4
1	B	121	PRO	5.4
1	A	112	GLN	5.3
1	A	121	PRO	5.2
1	A	122	ALA	5.2
1	B	112	GLN	5.1
1	A	110	LYS	5.1
1	B	260	ASP	5.0
1	A	120	PRO	4.8
1	A	239	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	118	GLY	4.8
1	B	119	PRO	4.6
1	B	261	GLY	4.4
1	A	111	LEU	4.3
1	A	259	GLN	4.2
1	A	123	GLU	4.1
1	B	142	ARG	4.0
1	B	258	GLN	3.8
1	B	223	ARG	3.5
1	B	120	PRO	3.2
1	B	146	GLN	3.1
1	A	146	GLN	3.0
1	B	262	SER	2.9
1	A	99	ARG	2.9
1	B	123	GLU	2.8
1	B	482	TRP	2.8
1	B	323	GLU	2.6
1	B	140	ILE	2.6
1	A	69	LYS	2.5
1	B	147	ALA	2.5
1	B	263	VAL	2.5
1	A	109	ARG	2.4
1	B	137	TYR	2.4
1	A	160	ALA	2.3
1	A	67	GLY	2.3
1	A	390	ARG	2.2
1	A	238	PRO	2.2
1	A	153	GLN	2.1
1	A	258	GLN	2.1
1	A	161	SER	2.1
1	B	390	ARG	2.0
1	A	223	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ACT	A	1850	4/4	0.20	2.91	50,50,50,50	0
6	PH3	B	2780	12/12	0.18	1.92	37,42,45,46	0
2	ACT	B	2860	4/4	0.13	1.86	43,43,44,45	0
5	HEM	A	1500	43/43	0.14	0.60	23,25,40,43	0
6	PH3	A	1780	12/12	0.14	0.52	35,36,40,42	0
2	ACT	A	1860	4/4	0.10	0.13	40,41,41,42	0
2	ACT	B	2850	4/4	0.12	0.11	44,45,46,47	0
5	HEM	B	2500	43/43	0.12	-0.04	23,27,40,42	0
6	PH3	A	2785	12/12	0.10	-0.29	35,36,37,37	0
3	CAC	A	950	3/5	0.07	-0.86	41,41,41,45	0
6	PH3	B	1785	12/12	0.09	-0.87	32,34,37,37	0
3	CAC	B	950	3/5	0.08	-1.01	51,51,51,51	0
4	ZN	A	900	1/1	0.05	-2.33	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.