



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:48 am GMT

PDB ID : 3N5R  
Title : Structure of endothelial nitric oxide synthase heme domain complexed with 4-(3-(2-(6-amino-4-methylpyridin-2-yl)ethyl)phenethyl)-6-methylpyridin-2-amine  
Authors : Delker, S.L.; Li, H.; Poulos, T.L.  
Deposited on : 2010-05-25  
Resolution : 2.57 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

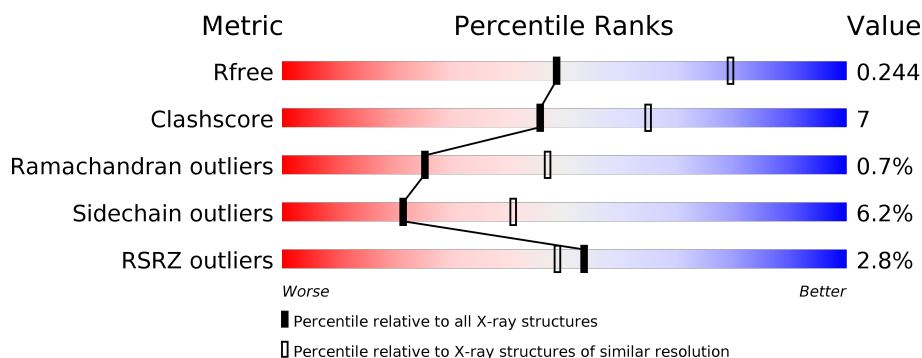
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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))
$R_{free}$	100719	2899 (2.60-2.56)
Clashscore	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

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  $\geq 3$ , 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>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>9%</div> </div> </div>
1	B	444	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>9%</div> </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
3	ACT	A	860	-	-	-	X
3	ACT	B	860	-	-	-	X
4	GOL	A	880	-	-	-	X
4	GOL	B	880	-	-	-	X
7	XFH	A	800	-	-	-	X
7	XFH	B	800	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6763 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.

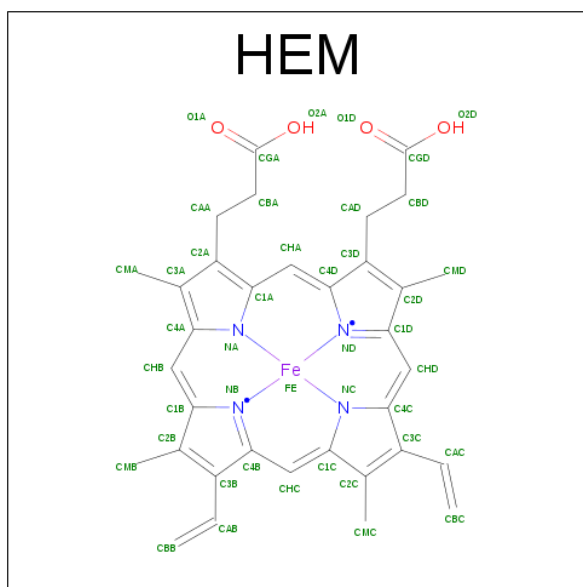
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3227	2052	569	590	16			
1	B	405	Total	C	N	O	S	0	0	0
			3223	2050	568	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- 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		

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



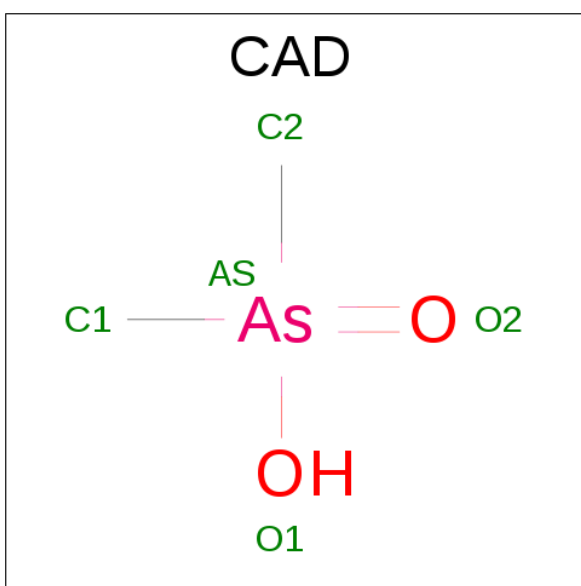
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



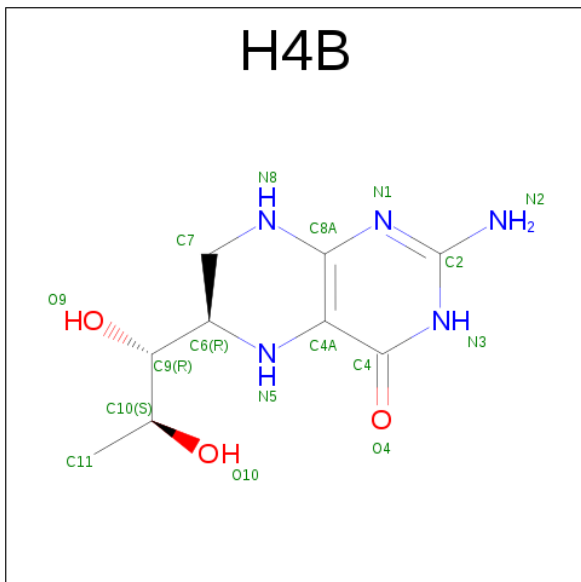
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CACODYLIC ACID (three-letter code: CAD) (formula:  $C_2H_7AsO_2$ ).



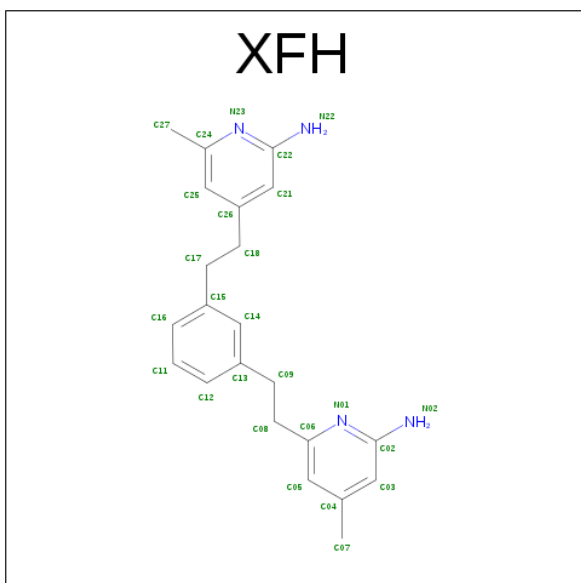
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	As	C	0	0
			3	1	2		
5	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$ ).



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

- Molecule 7 is 6-(2-{3-[2-(2-AMINO-6-METHYLPYRIDIN-4-YL)ETHYL]PHENYL}ETHYL)-4-METHYLPYRIDIN-2-AMINE (three-letter code: XFH) (formula: C<sub>22</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			26	22	4		
7	B	1	Total	C	N	0	0
			26	22	4		

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

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

- Molecule 9 is water.

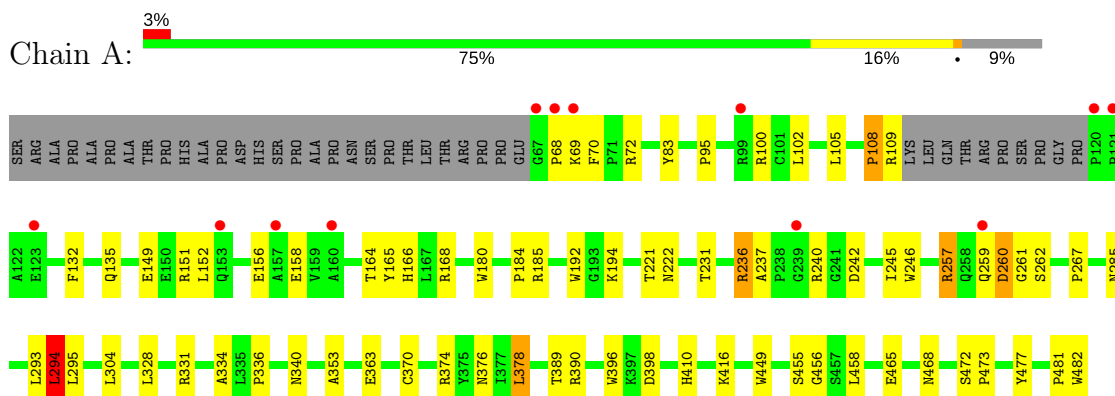
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	56	Total	O	0	0
			56	56		
9	B	54	Total	O	0	0
			54	54		



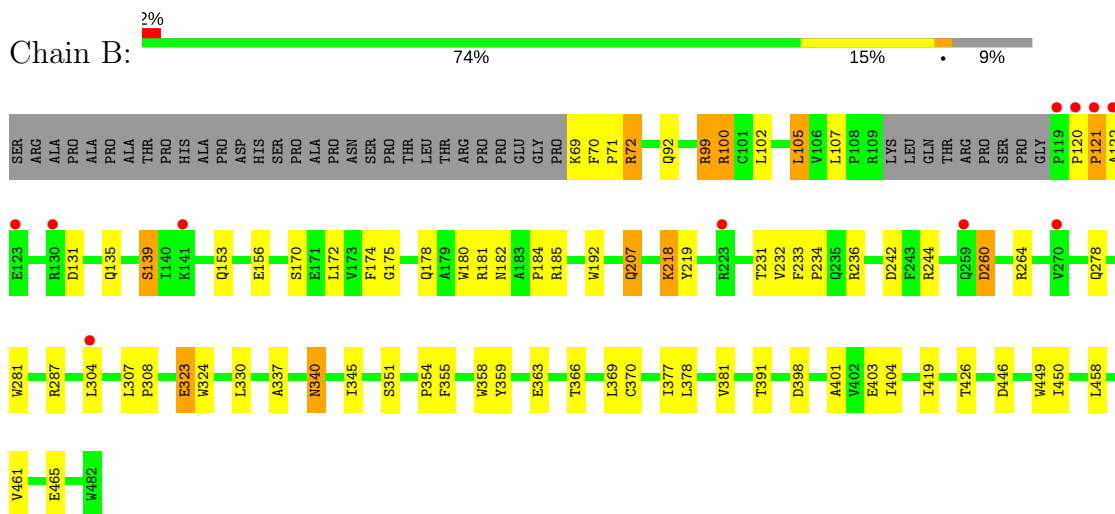
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



#### • Molecule 1: Nitric oxide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.93Å 106.71Å 156.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.12 – 2.57 44.12 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.12-2.57) 98.9 (44.12-2.57)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.182 , 0.244 0.185 , 0.244	Depositor DCC
$R_{free}$ test set	1548 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, H4B, XFH, ACT, 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	0/3318	0.72	1/4520 (0.0%)
1	B	0.72	0/3314	0.73	0/4515
All	All	0.70	0/6632	0.73	1/9035 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3227	0	3134	48	0
1	B	3223	0	3131	44	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	0	0
5	B	3	0	0	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	26	0	26	4	0
7	B	26	0	26	5	0
8	A	1	0	0	0	0
9	A	56	0	0	4	0
9	B	54	0	0	4	0
All	All	6763	0	6432	95	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 7.

All (95) 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:236:ARG:HG3	1:A:236:ARG:HH11	1.03	1.13
1:A:236:ARG:HG3	1:A:236:ARG:NH1	1.78	0.90
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.62	0.81
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.50	0.75
1:A:236:ARG:CG	1:A:236:ARG:HH11	1.89	0.73
1:B:287:ARG:HD3	9:B:1091:HOH:O	1.92	0.69
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.94	0.68
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.58	0.66
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.79	0.65
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.54	0.65
1:B:378:LEU:HB2	9:B:1062:HOH:O	1.99	0.62
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.13	0.61
1:A:285:ASN:HB3	9:A:1006:HOH:O	2.00	0.61
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.85	0.58
1:B:182:ASN:O	1:B:184:PRO:HD3	2.05	0.57
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.45	0.57
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.87	0.56
1:B:403:GLU:OE1	1:B:403:GLU:HA	2.05	0.56
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.89	0.55
1:B:324:TRP:HB2	5:B:950:CAD:C1	2.37	0.54
1:A:378:LEU:HB2	9:A:1004:HOH:O	2.08	0.54
1:B:99:ARG:HB2	1:B:99:ARG:NH1	2.23	0.53
1:A:481:PRO:HD2	1:A:482:TRP:CE3	2.45	0.52
2:A:500:HEM:HBA1	7:A:800:XFH:H09A	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:THR:O	1:B:370:CYS:HB2	2.10	0.51
1:B:369:LEU:O	1:B:377:ILE:HG12	2.11	0.51
1:A:68:PRO:HB2	1:A:70:PHE:HD1	1.76	0.51
1:B:231:THR:O	1:B:354:PRO:HD2	2.11	0.50
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.11	0.50
1:B:72:ARG:NH1	9:B:1077:HOH:O	2.45	0.50
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.47	0.50
1:B:446:ASP:O	1:B:450:ILE:HG12	2.11	0.50
1:A:455:SER:O	1:A:458:LEU:HB2	2.11	0.49
1:B:340:ASN:HD22	1:B:340:ASN:H	1.59	0.49
2:B:500:HEM:C1C	7:B:800:XFH:H07B	2.47	0.49
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.49
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.25	0.48
1:A:257:ARG:CG	1:A:257:ARG:HH11	2.22	0.48
1:A:158:GLU:OE1	1:A:166:HIS:HD2	1.95	0.48
1:B:218:LYS:HD3	1:B:219:TYR:N	2.29	0.48
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.94	0.48
1:B:175:GLY:HA3	1:B:345:ILE:HD13	1.95	0.48
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.49	0.48
1:A:363:GLU:OE1	7:A:800:XFH:N01	2.47	0.48
1:B:244:ARG:HD2	1:B:351:SER:HB2	1.96	0.48
1:B:120:PRO:O	1:B:121:PRO:C	2.52	0.47
1:A:158:GLU:OE1	1:A:166:HIS:CD2	2.68	0.47
1:A:334:ALA:O	1:A:336:PRO:HD3	2.14	0.47
1:B:207:GLN:HB2	9:B:1076:HOH:O	2.13	0.47
1:B:358:TRP:O	7:B:800:XFH:N02	2.47	0.47
1:A:72:ARG:HB2	1:A:83:TYR:CE2	2.50	0.46
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.98	0.46
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.31	0.46
1:B:359:TYR:HA	7:B:800:XFH:N02	2.31	0.46
1:A:376:ASN:ND2	9:A:1004:HOH:O	2.49	0.46
1:A:245:ILE:HG23	1:A:295:LEU:HD23	1.98	0.45
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.31	0.45
1:B:426:THR:HB	1:B:461:VAL:HG13	1.98	0.45
1:B:449:TRP:HA	6:B:600:H4B:N1	2.32	0.44
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.00	0.44
1:B:131:ASP:O	1:B:135:GLN:HG3	2.17	0.44
1:A:246:TRP:HB2	1:A:294:LEU:HB3	2.00	0.44
1:A:152:LEU:O	1:A:156:GLU:HG2	2.18	0.44
1:A:237:ALA:HB3	1:A:240:ARG:HB3	2.00	0.44
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG23	1:A:165:TYR:N	2.33	0.43
1:B:323:GLU:HG3	1:B:323:GLU:H	1.52	0.43
1:B:363:GLU:OE2	7:B:800:XFH:N02	2.45	0.43
1:A:267:PRO:HD2	1:A:374:ARG:HA	1.99	0.43
1:B:70:PHE:HA	1:B:71:PRO:HD2	1.83	0.43
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.53	0.43
1:A:260:ASP:O	1:A:262:SER:N	2.47	0.43
1:A:410:HIS:ND1	9:A:1001:HOH:O	2.26	0.42
1:A:389:THR:HA	1:A:396:TRP:CD1	2.54	0.42
1:B:185:ARG:HB2	2:B:500:HEM:HAD2	2.01	0.42
1:A:95:PRO:HG3	1:A:108:PRO:HG2	2.00	0.42
1:B:307:LEU:HA	1:B:308:PRO:HD3	1.94	0.42
2:A:500:HEM:CBA	7:A:800:XFH:H09A	2.49	0.42
1:A:132:PHE:O	1:A:135:GLN:HB2	2.19	0.42
1:A:184:PRO:HB3	1:A:468:ASN:HD21	1.84	0.42
1:A:477:TYR:CD1	7:A:800:XFH:C25	3.03	0.42
2:B:500:HEM:HBA2	7:B:800:XFH:H09A	2.02	0.42
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.68	0.42
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.02	0.42
1:B:337:ALA:HA	1:B:355:PHE:O	2.20	0.41
2:B:500:HEM:CBB	2:B:500:HEM:HHC	2.40	0.41
1:A:231:THR:O	1:A:353:ALA:HA	2.20	0.41
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.60	0.41
1:A:294:LEU:HD13	1:A:304:LEU:HD13	2.02	0.41
1:A:185:ARG:HB2	2:A:500:HEM:HAD2	2.01	0.41
1:A:260:ASP:C	1:A:262:SER:H	2.23	0.41
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.85	0.41
1:A:221:THR:O	1:A:222:ASN:C	2.58	0.41
1:B:139:SER:CB	1:B:174:PHE:CE1	3.04	0.41
1:A:449:TRP:HA	6:A:600:H4B:N1	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	402/444 (90%)	380 (94%)	19 (5%)	3 (1%)	25	47
1	B	401/444 (90%)	379 (94%)	19 (5%)	3 (1%)	25	47
All	All	803/888 (90%)	759 (94%)	38 (5%)	6 (1%)	25	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	GLY
1	A	456	GLY
1	B	122	ALA
1	A	108	PRO
1	B	121	PRO
1	B	260	ASP

### 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	345/377 (92%)	326 (94%)	19 (6%)	25	47
1	B	345/377 (92%)	321 (93%)	24 (7%)	18	34
All	All	690/754 (92%)	647 (94%)	43 (6%)	21	41

All (43) 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	109	ARG
1	A	149	GLU
1	A	194	LYS
1	A	236	ARG

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Mol	Chain	Res	Type
1	A	257	ARG
1	A	259	GLN
1	A	260	ASP
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	398	ASP
1	A	416	LYS
1	B	69	LYS
1	B	72	ARG
1	B	92	GLN
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	107	LEU
1	B	139	SER
1	B	153	GLN
1	B	156	GLU
1	B	170	SER
1	B	207	GLN
1	B	218	LYS
1	B	260	ASP
1	B	264	ARG
1	B	278	GLN
1	B	323	GLU
1	B	330	LEU
1	B	340	ASN
1	B	391	THR
1	B	398	ASP
1	B	419	ILE
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	166	HIS

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Mol	Chain	Res	Type
1	A	178	GLN
1	A	191	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	340	ASN
1	B	376	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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	500	1	28,50,50	2.16	7 (25%)	17,82,82	1.30	2 (11%)
6	H4B	A	600	-	14,18,18	0.80	0	12,26,26	2.31	5 (41%)
7	XFH	A	800	-	28,28,28	0.86	0	38,38,38	1.63	6 (15%)
3	ACT	A	850	-	1,3,3	1.55	0	0,3,3	0.00	-
3	ACT	A	860	-	1,3,3	1.79	0	0,3,3	0.00	-
4	GOL	A	880	-	5,5,5	0.44	0	5,5,5	0.34	0
5	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	1	28,50,50	2.28	7 (25%)	17,82,82	2.26	3 (17%)
6	H4B	B	600	-	14,18,18	0.99	1 (7%)	12,26,26	2.19	5 (41%)
7	XFH	B	800	-	28,28,28	0.62	0	38,38,38	1.58	5 (13%)
3	ACT	B	860	-	1,3,3	1.36	0	0,3,3	0.00	-
4	GOL	B	880	-	5,5,5	0.57	0	5,5,5	1.16	0
5	CAD	B	950	-	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	500	1	-	0/6/54/54	0/0/8/8
6	H4B	A	600	-	-	0/8/17/17	0/2/2/2
7	XFH	A	800	-	-	0/10/10/10	0/3/3/3
3	ACT	A	850	-	-	0/0/0/0	0/0/0/0
3	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	GOL	A	880	-	-	0/4/4/4	0/0/0/0
5	CAD	A	950	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/6/54/54	0/0/8/8
6	H4B	B	600	-	-	0/8/17/17	0/2/2/2
7	XFH	B	800	-	-	0/10/10/10	0/3/3/3
3	ACT	B	860	-	-	0/0/0/0	0/0/0/0
4	GOL	B	880	-	-	0/4/4/4	0/0/0/0
5	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C2B	-5.24	1.33	1.40
2	A	500	HEM	C3B-C2B	-5.10	1.33	1.40
2	B	500	HEM	C3C-C2C	-4.80	1.34	1.40
2	A	500	HEM	C3C-C2C	-4.55	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	H4B	C4-C4A	-2.33	1.38	1.41
2	B	500	HEM	C1D-ND	2.17	1.40	1.36
2	A	500	HEM	CMA-C3A	2.19	1.56	1.51
2	A	500	HEM	C4D-ND	2.37	1.39	1.36
2	B	500	HEM	C4D-ND	3.17	1.40	1.36
2	B	500	HEM	C3B-CAB	3.60	1.55	1.47
2	A	500	HEM	C3C-CAC	3.62	1.54	1.47
2	B	500	HEM	C3C-CAC	3.79	1.55	1.47
2	A	500	HEM	C3B-CAB	3.94	1.55	1.47
2	A	500	HEM	C3D-C2D	4.32	1.50	1.37
2	B	500	HEM	C3D-C2D	5.04	1.52	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CBA-CAA-C2A	-7.50	98.14	112.48
7	A	800	XFH	C05-C06-N01	-3.92	118.66	122.91
6	B	600	H4B	N3-C2-N1	-3.41	119.91	125.45
6	A	600	H4B	N3-C2-N1	-3.32	120.07	125.45
2	B	500	HEM	C1D-C2D-C3D	-3.21	104.76	107.00
7	B	800	XFH	C05-C06-N01	-3.09	119.56	122.91
2	B	500	HEM	CAD-CBD-CGD	-2.85	107.80	112.66
2	A	500	HEM	CBA-CAA-C2A	-2.61	107.50	112.48
7	A	800	XFH	C17-C15-C16	-2.48	115.06	121.24
6	A	600	H4B	C6-C7-N8	-2.39	107.22	111.01
6	B	600	H4B	N2-C2-N1	2.20	120.76	117.24
7	A	800	XFH	C09-C13-C14	2.45	124.58	120.56
2	A	500	HEM	C4C-C3C-C2C	2.54	108.67	106.90
7	A	800	XFH	C17-C15-C14	2.66	124.92	120.56
7	B	800	XFH	C26-C21-C22	2.76	120.02	117.97
6	B	600	H4B	C2-N1-C8A	2.76	120.73	114.51
7	B	800	XFH	C27-C24-N23	2.94	121.59	116.55
7	B	800	XFH	N22-C22-N23	3.02	121.72	116.64
6	A	600	H4B	C2-N1-C8A	3.02	121.32	114.51
6	A	600	H4B	C4-N3-C2	3.24	120.72	116.06
6	B	600	H4B	C4-N3-C2	3.32	120.84	116.06
6	B	600	H4B	C4-C4A-C8A	3.77	117.97	114.56
7	A	800	XFH	C08-C06-N01	3.78	121.25	115.78
6	A	600	H4B	C4-C4A-C8A	3.98	118.17	114.56
7	A	800	XFH	C02-N01-C06	4.24	121.17	118.17
7	B	800	XFH	C02-N01-C06	5.33	121.94	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	3	0
6	A	600	H4B	1	0
7	A	800	XFH	4	0
2	B	500	HEM	5	0
6	B	600	H4B	1	0
7	B	800	XFH	5	0
5	B	950	CAD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	406/444 (91%)	0.02	12 (2%) 51 46	27, 41, 68, 92	0
1	B	405/444 (91%)	-0.12	11 (2%) 55 50	27, 43, 69, 95	0
All	All	811/888 (91%)	-0.05	23 (2%) 53 49	27, 42, 69, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	4.7
1	A	121	PRO	4.4
1	B	119	PRO	4.3
1	A	67	GLY	4.2
1	B	120	PRO	4.1
1	A	160	ALA	4.0
1	A	259	GLN	3.6
1	B	304	LEU	3.4
1	B	121	PRO	3.2
1	B	259	GLN	3.2
1	A	69	LYS	2.8
1	B	130	ARG	2.8
1	B	123	GLU	2.7
1	A	68	PRO	2.6
1	A	123	GLU	2.6
1	B	223	ARG	2.5
1	B	122	ALA	2.4
1	B	141	LYS	2.3
1	A	99	ARG	2.2
1	A	157	ALA	2.2
1	A	239	GLY	2.2
1	B	270	VAL	2.1
1	A	153	GLN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ACT	B	860	4/4	0.88	0.26	6.22	58,59,60,61	0
7	XFH	B	800	26/26	0.82	0.33	5.98	65,88,101,102	0
7	XFH	A	800	26/26	0.84	0.33	3.80	44,72,84,86	0
4	GOL	B	880	6/6	0.95	0.24	3.35	48,49,50,53	0
3	ACT	A	860	4/4	0.91	0.20	2.70	47,50,50,51	0
4	GOL	A	880	6/6	0.94	0.24	2.44	56,59,61,64	0
2	HEM	A	500	43/43	0.98	0.20	1.23	27,35,45,46	0
2	HEM	B	500	43/43	0.98	0.14	0.52	30,32,42,50	0
3	ACT	A	850	4/4	0.95	0.14	0.22	43,44,45,46	0
6	H4B	A	600	17/17	0.97	0.15	-0.08	29,34,37,40	0
8	ZN	A	900	1/1	1.00	0.12	-0.22	34,34,34,34	0
5	CAD	A	950	3/5	1.00	0.11	-0.37	53,53,53,56	0
6	H4B	B	600	17/17	0.97	0.17	-0.46	29,32,36,38	0
5	CAD	B	950	3/5	0.99	0.10	-	51,51,53,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.