



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:56 AM GMT

PDB ID : 3NLD  
Title : Structure of endothelial nitric oxide synthase heme domain complexed with 6- $\{[(3'S,4'S)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl\}methyl\}$ -4-methylpyridin-2-amine  
Authors : Ji, H.; Delker, S.L.; Li, H.; Martasek, P.; Roman, L.; Poulos, T.L.; Silverman, R.B.  
Deposited on : 2010-06-21  
Resolution : 2.29 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 (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

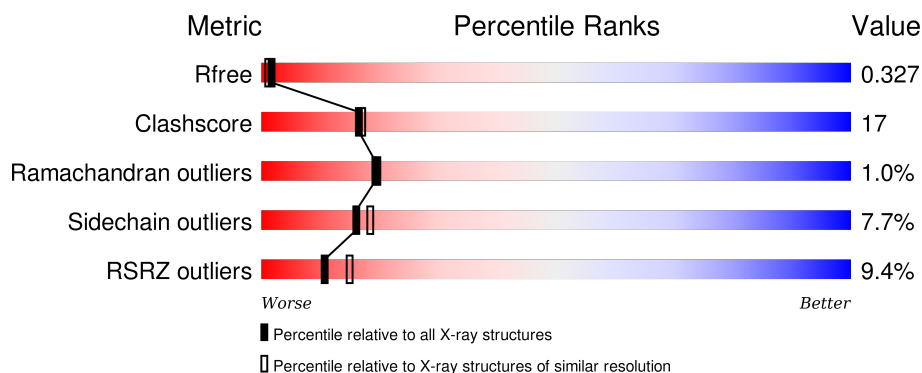
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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>10%</div> <div>65%</div> <div>23%</div> <div>•</div> <div>9%</div> </div>
1	B	444	<div> <div>7%</div> <div>58%</div> <div>28%</div> <div>5%</div> <div>9%</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
4	ACT	A	850	-	-	X	X
4	ACT	B	850	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6750 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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3202	2036	563	587	16			
1	B	403	Total	C	N	O	S	0	0	0
			3209	2040	566	587	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:  $C_{34}H_{32}FeN_4O_4$ ).



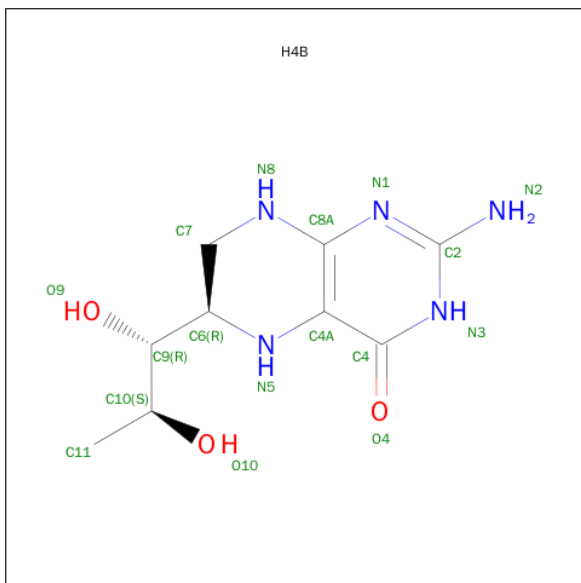
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

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



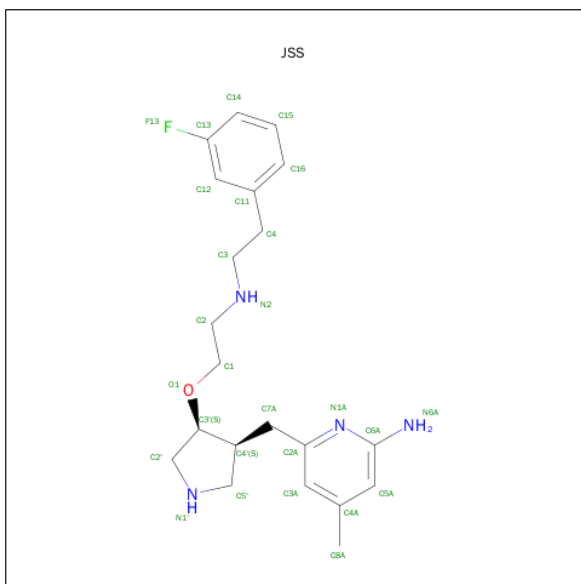
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



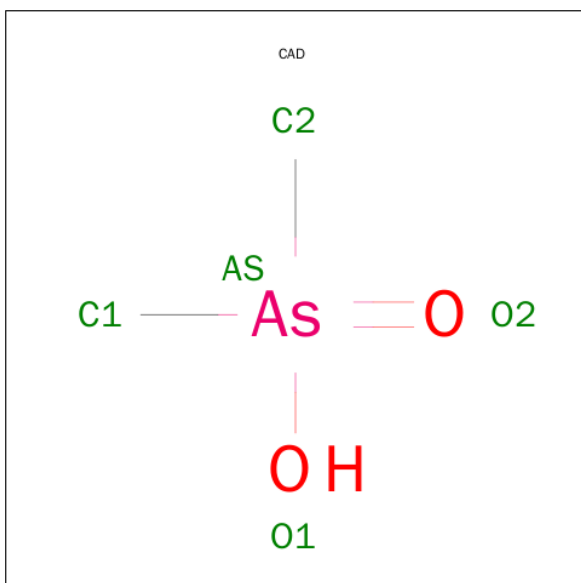
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 6-[[[(3S,4S)-4-(2-{[2-(3-FLUOROPHENYL)ETHYL]AMINO}ETHOXY)PYRROLIDIN-3-YL]METHYL]-4-METHYLPYRIDIN-2-AMINE (three-letter code: JSS) (formula: C<sub>21</sub>H<sub>29</sub>FN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
6	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- Molecule 7 is CACODYLIC ACID (three-letter code: CAD) (formula: C<sub>2</sub>H<sub>7</sub>AsO<sub>2</sub>).



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

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

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

- Molecule 9 is water.

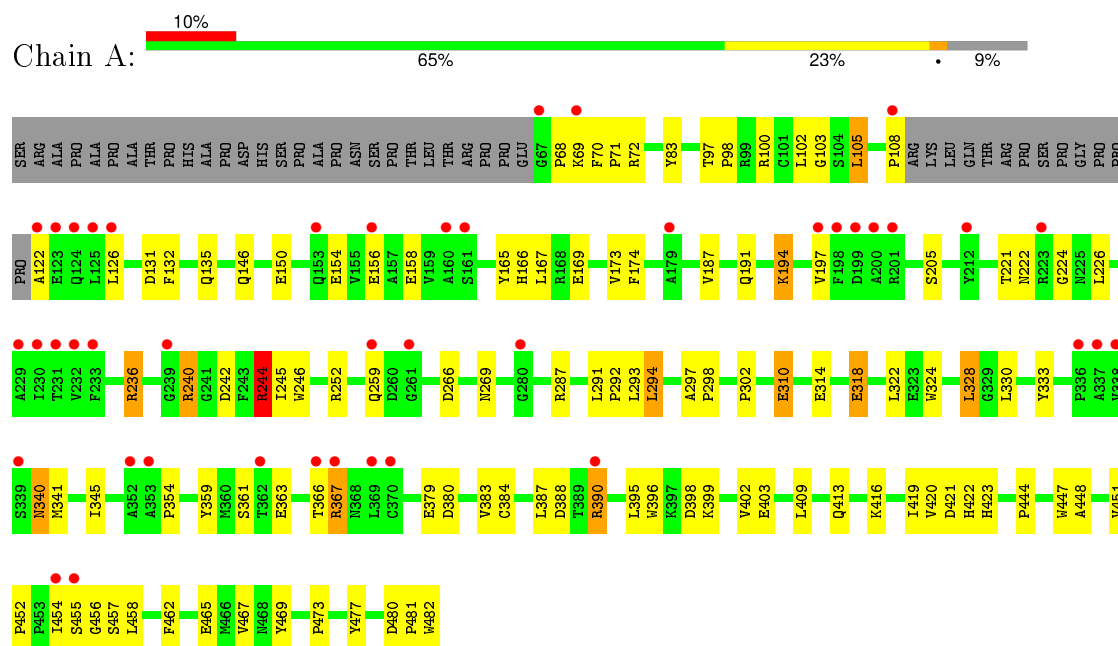
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	70	Total 70	O 70	0	0
9	B	68	Total 68	O 68	0	0



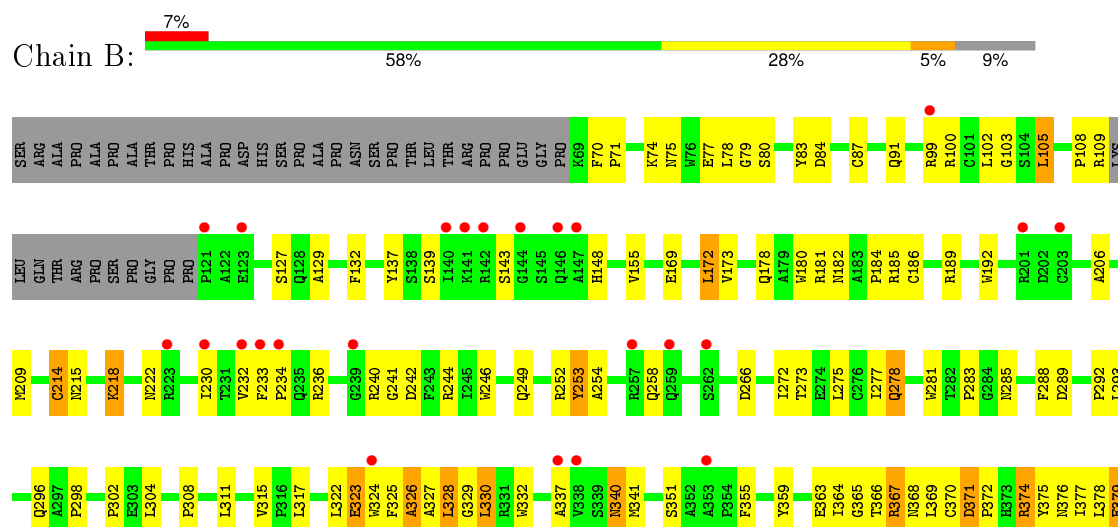
### 3 Residue-property plots [i](#)

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

- Molecule 1: Nitric oxide synthase, endothelial



- Molecule 1: Nitric oxide synthase, endothelial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.40Å 106.89Å 157.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.92 – 2.29 36.92 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (36.92-2.29) 98.8 (36.92-2.29)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.222 , 0.292 0.270 , 0.327	Depositor DCC
$R_{free}$ test set	2201 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.927	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44143 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.375 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, H4B, JSS, 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	0.89	3/3291 (0.1%)	0.87	4/4483 (0.1%)
1	B	1.08	9/3298 (0.3%)	0.98	7/4491 (0.2%)
All	All	0.99	12/6589 (0.2%)	0.93	11/8974 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	TYR	CE2-CZ	11.37	1.53	1.38
1	B	253	TYR	CG-CD2	8.30	1.50	1.39
1	B	383	VAL	CB-CG1	7.09	1.67	1.52
1	B	385	MET	CG-SD	6.66	1.98	1.81
1	B	283	PRO	C-O	6.21	1.35	1.23
1	B	326	ALA	N-CA	5.90	1.58	1.46
1	B	329	GLY	N-CA	5.48	1.54	1.46
1	B	83	TYR	CE2-CZ	5.24	1.45	1.38
1	A	477	TYR	CD2-CE2	-5.14	1.31	1.39
1	B	214	CYS	CB-SG	-5.12	1.73	1.81
1	A	318	GLU	CG-CD	5.06	1.59	1.51
1	A	448	ALA	CA-CB	5.01	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	367	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	B	367	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	374	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	395	LEU	CA-CB-CG	-5.70	102.18	115.30
1	A	244	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	285	ASN	CB-CA-C	-5.49	99.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	185	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	84	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	380	ASP	CB-CG-OD1	5.09	122.88	118.30

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	3202	0	3107	88	0
1	B	3209	0	3117	127	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	4	0	3	4	0
4	B	4	0	3	6	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
6	A	27	0	29	2	0
6	B	27	0	29	1	0
7	A	3	0	0	1	0
7	B	3	0	0	1	0
8	A	1	0	0	0	0
9	A	70	0	0	11	0
9	B	68	0	0	5	0
All	All	6750	0	6394	216	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 17.

All (216) 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:B:384:CYS:SG	7:B:950:CAD:AS	2.48	1.32
1:A:384:CYS:SG	7:A:950:CAD:AS	2.66	1.13
1:B:368:ASN:HD21	4:B:850:ACT:H2	1.10	1.11
1:A:236:ARG:HD3	1:A:242:ASP:OD1	1.68	0.93
1:B:368:ASN:ND2	4:B:850:ACT:H2	1.82	0.92
1:B:325:PHE:O	1:B:328:LEU:HB2	1.72	0.90
1:B:366:THR:O	1:B:370:CYS:HB2	1.71	0.90
1:B:481:PRO:HD2	1:B:482:TRP:CE3	2.08	0.88
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.58	0.85
1:B:74:LYS:HE3	9:B:1057:HOH:O	1.75	0.85
1:B:444:PRO:HB3	1:B:469:TYR:CZ	2.11	0.84
1:B:381:VAL:O	1:B:384:CYS:HB2	1.79	0.82
2:A:500:HEM:HBC2	2:A:500:HEM:HMC1	1.64	0.80
1:A:122:ALA:N	9:A:1060:HOH:O	2.15	0.79
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.65	0.79
1:B:359:TYR:HE1	4:B:850:ACT:H1	1.47	0.79
1:A:108:PRO:HG3	9:A:1007:HOH:O	1.82	0.78
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.65	0.78
1:A:359:TYR:OH	4:A:850:ACT:CH3	2.34	0.76
9:A:1062:HOH:O	1:B:397:LYS:HB2	1.85	0.76
1:A:359:TYR:OH	4:A:850:ACT:H3	1.86	0.75
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.68	0.74
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.23	0.74
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.19	0.72
1:B:326:ALA:C	1:B:328:LEU:H	1.91	0.72
1:A:158:GLU:HG2	1:A:165:TYR:CB	2.21	0.71
1:B:444:PRO:HB3	1:B:469:TYR:CE1	2.25	0.70
1:B:368:ASN:HD21	4:B:850:ACT:CH3	1.98	0.70
1:A:158:GLU:HG2	1:A:165:TYR:HB2	1.72	0.70
1:A:108:PRO:HD3	9:A:1007:HOH:O	1.93	0.69
1:B:281:TRP:CD1	1:B:292:PRO:HG3	2.27	0.69
1:B:369:LEU:HB3	1:B:377:ILE:CD1	2.23	0.68
1:A:457:SER:HA	1:A:462:PHE:CG	2.28	0.68
1:A:158:GLU:HG2	1:A:165:TYR:HA	1.76	0.68
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.24	0.68
1:A:345:ILE:HG12	1:A:473:PRO:HB3	1.76	0.68
1:B:404:ILE:O	1:B:408:VAL:HG23	1.94	0.67
1:B:452:PRO:HG2	1:B:459:THR:HG21	1.76	0.67
1:B:481:PRO:HD2	1:B:482:TRP:CZ3	2.29	0.67
1:A:105:LEU:N	1:A:105:LEU:CD2	2.57	0.67
1:A:423:HIS:CE1	9:A:1058:HOH:O	2.48	0.66
1:B:186:CYS:HB3	1:B:189:ARG:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ILE:HG13	1:B:272:ILE:O	1.96	0.66
1:B:182:ASN:O	1:B:184:PRO:HD3	1.96	0.65
1:A:403:GLU:OE1	1:A:403:GLU:HA	1.96	0.65
1:A:105:LEU:N	1:A:105:LEU:HD23	2.12	0.65
1:B:172:LEU:HD11	1:B:232:VAL:HG21	1.79	0.65
1:B:377:ILE:O	1:B:381:VAL:HG23	1.97	0.65
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.44	0.64
1:B:218:LYS:HD3	1:B:311:LEU:HD21	1.80	0.64
1:B:230:ILE:HG13	1:B:355:PHE:HB3	1.80	0.63
1:B:340:ASN:HD22	1:B:340:ASN:C	1.98	0.63
1:B:326:ALA:C	1:B:328:LEU:N	2.52	0.63
2:B:500:HEM:O1A	3:B:600:H4B:N3	2.31	0.62
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.29	0.62
1:A:340:ASN:HD22	1:A:340:ASN:H	1.47	0.61
1:B:266:ASP:OD2	1:B:374:ARG:NH2	2.24	0.61
1:A:422:HIS:HE1	1:B:398:ASP:OD2	1.84	0.61
1:B:369:LEU:O	1:B:377:ILE:HG12	2.01	0.61
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.83	0.60
1:B:341:MET:HE2	1:B:475:PHE:HB3	1.82	0.60
1:A:398:ASP:O	1:A:402:VAL:HG23	2.01	0.59
1:B:359:TYR:CE1	4:B:850:ACT:H1	2.34	0.59
1:A:423:HIS:CD2	9:A:1062:HOH:O	2.56	0.59
1:A:379:GLU:O	1:A:383:VAL:HG23	2.03	0.59
1:A:395:LEU:O	1:A:399:LYS:HG3	2.02	0.59
1:A:367:ARG:HH22	5:A:880:GOL:H2	1.68	0.59
1:A:310:GLU:H	1:A:310:GLU:CD	2.06	0.58
1:B:129:ALA:O	1:B:132:PHE:N	2.37	0.58
1:A:366:THR:HG21	1:A:454:ILE:HG23	1.86	0.57
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.04	0.57
4:A:850:ACT:O	6:A:800:JSS:N1'	2.37	0.57
1:B:315:VAL:HG11	1:B:412:PHE:CD1	2.40	0.57
1:A:146:GLN:O	1:A:150:GLU:HG3	2.04	0.57
1:B:240:ARG:HD2	1:B:298:PRO:HB3	1.86	0.57
1:A:419:ILE:HG13	1:A:420:VAL:N	2.20	0.57
1:B:323:GLU:HG3	1:B:324:TRP:H	1.70	0.57
1:B:324:TRP:O	1:B:325:PHE:C	2.43	0.56
1:B:244:ARG:NH2	9:B:1029:HOH:O	2.37	0.56
1:A:131:ASP:OD2	1:A:135:GLN:NE2	2.32	0.56
1:A:158:GLU:OE1	1:A:166:HIS:HD2	1.88	0.56
1:A:105:LEU:HD23	1:A:105:LEU:H	1.69	0.56
1:A:158:GLU:HG2	1:A:165:TYR:CA	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HD3	9:A:1057:HOH:O	2.05	0.55
1:B:392:THR:O	1:B:395:LEU:HD23	2.06	0.55
1:B:323:GLU:HG3	1:B:324:TRP:N	2.22	0.55
1:B:332:TRP:CD1	1:B:364:ILE:HG12	2.42	0.54
1:B:444:PRO:HB3	1:B:469:TYR:CE2	2.41	0.54
1:B:172:LEU:O	1:B:172:LEU:HG	2.06	0.54
1:B:365:GLY:HA2	1:B:404:ILE:CG2	2.37	0.54
1:B:325:PHE:C	1:B:325:PHE:CD1	2.81	0.54
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.89	0.54
2:A:500:HEM:CBC	2:A:500:HEM:HMC1	2.37	0.53
1:A:359:TYR:OH	4:A:850:ACT:H2	2.06	0.53
1:B:75:ASN:N	1:B:80:SER:O	2.35	0.53
1:A:158:GLU:CG	1:A:165:TYR:HA	2.39	0.53
1:B:365:GLY:HA2	1:B:404:ILE:HG22	1.90	0.53
1:B:218:LYS:HG2	1:B:311:LEU:HD22	1.90	0.53
1:B:395:LEU:HD23	1:B:395:LEU:N	2.22	0.53
1:B:365:GLY:CA	1:B:404:ILE:HG22	2.38	0.53
1:B:388:ASP:CG	1:B:390:ARG:NH1	2.63	0.53
1:B:340:ASN:ND2	1:B:340:ASN:C	2.62	0.53
1:A:97:THR:HB	1:A:98:PRO:CD	2.40	0.52
1:A:236:ARG:CG	1:A:236:ARG:HH11	2.23	0.52
1:B:186:CYS:HB3	1:B:189:ARG:CG	2.39	0.52
1:A:465:GLU:HB3	1:B:105:LEU:CD2	2.39	0.52
1:A:388:ASP:OD1	1:A:390:ARG:HG3	2.09	0.52
1:B:317:LEU:HD12	1:B:330:LEU:HB3	1.92	0.51
1:B:317:LEU:O	1:B:326:ALA:HA	2.10	0.51
1:A:108:PRO:CD	9:A:1007:HOH:O	2.52	0.51
1:B:169:GLU:O	1:B:173:VAL:HG23	2.11	0.51
1:A:108:PRO:CG	9:A:1007:HOH:O	2.48	0.51
1:B:372:PRO:HA	1:B:376:ASN:ND2	2.26	0.51
1:A:252:ARG:HB2	1:A:291:LEU:HD12	1.93	0.50
1:B:371:ASP:O	1:B:376:ASN:HB2	2.12	0.50
1:A:457:SER:HB3	1:B:453:PRO:HB2	1.94	0.50
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.41	0.50
1:A:399:LYS:O	1:A:403:GLU:HG2	2.11	0.50
1:B:326:ALA:O	1:B:328:LEU:N	2.45	0.50
1:B:324:TRP:CE3	1:B:325:PHE:HA	2.47	0.50
1:B:246:TRP:CD1	1:B:481:PRO:HG2	2.47	0.50
1:B:367:ARG:HD3	9:B:1002:HOH:O	2.12	0.50
1:B:240:ARG:NH1	1:B:241:GLY:O	2.42	0.49
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:HB3	1:B:377:ILE:HD11	1.95	0.49
1:A:422:HIS:H	1:A:422:HIS:CD2	2.30	0.49
1:B:189:ARG:O	1:B:192:TRP:HD1	1.95	0.49
1:B:457:SER:HA	1:B:462:PHE:CG	2.48	0.49
1:B:369:LEU:HB3	1:B:377:ILE:HD13	1.93	0.48
1:B:340:ASN:HD22	1:B:341:MET:N	2.12	0.48
1:B:366:THR:O	1:B:370:CYS:CB	2.54	0.48
1:B:324:TRP:CH2	1:B:384:CYS:HB3	2.49	0.48
1:B:364:ILE:O	1:B:369:LEU:HD12	2.14	0.47
1:A:236:ARG:NH1	1:A:236:ARG:HG3	2.28	0.47
1:A:266:ASP:HB3	1:A:269:ASN:HD22	1.79	0.47
1:A:173:VAL:HG22	1:A:197:VAL:HB	1.95	0.47
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.60	0.47
1:B:74:LYS:HE2	1:B:79:GLY:HA2	1.96	0.47
1:A:409:LEU:HD11	1:A:421:ASP:HB3	1.96	0.47
1:B:214:CYS:O	1:B:218:LYS:HG2	2.14	0.47
1:A:387:LEU:HD13	1:A:396:TRP:HA	1.95	0.47
1:B:337:ALA:HA	1:B:355:PHE:O	2.15	0.47
1:B:367:ARG:NH2	1:B:371:ASP:OD2	2.48	0.47
1:B:296:GLN:HB2	1:B:302:PRO:HB3	1.96	0.47
1:A:191:GLN:HE22	1:A:194:LYS:NZ	2.13	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.97	0.46
1:B:275:LEU:HD11	1:B:482:TRP:CE2	2.49	0.46
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.80	0.46
1:B:137:TYR:CD1	1:B:148:HIS:CD2	3.03	0.46
1:B:341:MET:CE	1:B:475:PHE:HB3	2.45	0.46
1:B:253:TYR:CD1	1:B:288:PHE:O	2.68	0.46
1:A:363:GLU:OE1	6:A:800:JSS:N1A	2.49	0.46
1:A:444:PRO:HA	1:A:467:VAL:O	2.16	0.46
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.50	0.46
1:B:324:TRP:O	1:B:327:ALA:N	2.43	0.45
1:B:206:ALA:O	1:B:209:MET:HB2	2.16	0.45
1:B:363:GLU:OE1	6:B:800:JSS:N1'	2.49	0.45
1:A:345:ILE:HG23	1:A:473:PRO:HG3	1.99	0.45
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.99	0.45
1:A:314:GLU:HA	1:A:333:TYR:HA	1.98	0.45
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.98	0.45
1:A:224:GLY:O	1:A:226:LEU:HD13	2.16	0.45
1:B:218:LYS:CD	1:B:311:LEU:HD21	2.47	0.44
1:B:308:PRO:HD2	1:B:311:LEU:HD12	2.00	0.44
1:A:221:THR:O	1:A:222:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASN:CG	4:B:850:ACT:H2	2.36	0.44
1:A:480:ASP:HB3	1:A:482:TRP:CH2	2.52	0.44
1:A:122:ALA:N	9:A:1039:HOH:O	2.49	0.44
1:B:137:TYR:CE1	1:B:148:HIS:HA	2.52	0.44
1:A:480:ASP:HB3	1:A:482:TRP:CZ3	2.52	0.44
1:B:273:THR:O	1:B:277:ILE:HG13	2.17	0.44
1:A:68:PRO:HG2	1:A:83:TYR:CD2	2.52	0.44
1:B:254:ALA:N	1:B:289:ASP:O	2.44	0.44
1:B:87:CYS:HB3	1:B:469:TYR:CD1	2.52	0.44
1:B:218:LYS:HG2	1:B:311:LEU:CD2	2.48	0.43
1:B:278:GLN:HE21	1:B:278:GLN:HB3	1.67	0.43
1:A:205:SER:HB3	9:A:1030:HOH:O	2.17	0.43
1:B:215:ASN:HA	1:B:218:LYS:HG3	1.99	0.43
1:A:457:SER:HB3	1:B:453:PRO:CB	2.48	0.43
1:B:367:ARG:HH21	1:B:371:ASP:CG	2.21	0.43
1:A:390:ARG:HH11	1:A:390:ARG:HG2	1.84	0.43
1:B:400:ALA:O	1:B:401:ALA:C	2.57	0.43
1:A:340:ASN:ND2	1:A:340:ASN:H	2.16	0.43
1:B:87:CYS:HB3	1:B:469:TYR:CE1	2.54	0.43
1:B:178:GLN:HE22	1:B:181:ARG:NH1	2.14	0.42
1:B:215:ASN:HD22	1:B:218:LYS:HE3	1.84	0.42
1:B:249:GLN:HA	1:B:337:ALA:O	2.19	0.42
1:B:258:GLN:HB3	9:B:1065:HOH:O	2.19	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.44	0.42
1:B:368:ASN:O	1:B:375:TYR:HB2	2.20	0.42
1:A:132:PHE:O	1:A:135:GLN:HB2	2.19	0.42
1:B:379:GLU:O	1:B:383:VAL:HG23	2.20	0.42
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.40	0.42
1:A:480:ASP:HA	1:A:481:PRO:HD3	1.84	0.42
1:B:70:PHE:HA	1:B:71:PRO:HD3	1.75	0.42
1:B:180:TRP:CZ3	2:B:500:HEM:HMC3	2.54	0.42
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.83	0.41
1:A:447:TRP:HZ2	1:A:462:PHE:O	2.03	0.41
1:A:245:ILE:HD11	1:A:354:PRO:HD3	2.02	0.41
1:B:472:SER:HA	1:B:473:PRO:C	2.41	0.41
1:A:97:THR:HB	1:A:98:PRO:HD2	2.01	0.41
1:A:291:LEU:HA	1:A:292:PRO:HD2	1.85	0.41
1:A:246:TRP:CH2	1:A:302:PRO:HG3	2.55	0.41
1:B:129:ALA:HB1	1:B:155:VAL:HG11	2.02	0.41
1:A:422:HIS:CD2	1:A:422:HIS:N	2.88	0.41
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:O	1:A:187:VAL:HG22	2.21	0.41
1:A:419:ILE:HG13	1:A:420:VAL:H	1.84	0.41
1:B:236:ARG:HA	9:B:1001:HOH:O	2.21	0.41
1:B:388:ASP:O	1:B:396:TRP:CD1	2.73	0.41
1:A:70:PHE:O	1:A:71:PRO:C	2.59	0.40
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.83	0.40
1:B:178:GLN:NE2	1:B:181:ARG:HD3	2.36	0.40
1:A:361:SER:OG	1:A:421:ASP:HA	2.20	0.40
1:B:77:GLU:HG2	1:B:78:LEU:HG	2.03	0.40
1:A:297:ALA:O	1:A:298:PRO:C	2.58	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	399/444 (90%)	363 (91%)	31 (8%)	5 (1%)	15	14
1	B	399/444 (90%)	352 (88%)	44 (11%)	3 (1%)	24	26
All	All	798/888 (90%)	715 (90%)	75 (9%)	8 (1%)	19	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	SER
1	A	240	ARG
1	B	103	GLY
1	B	108	PRO
1	A	103	GLY
1	A	244	ARG
1	B	371	ASP
1	A	456	GLY

### 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	342/377 (91%)	317 (93%)	25 (7%)	17	20
1	B	343/377 (91%)	315 (92%)	28 (8%)	14	16
All	All	685/754 (91%)	632 (92%)	53 (8%)	16	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	154	GLU
1	A	156	GLU
1	A	169	GLU
1	A	174	PHE
1	A	194	LYS
1	A	236	ARG
1	A	244	ARG
1	A	259	GLN
1	A	293	LEU
1	A	294	LEU
1	A	310	GLU
1	A	318	GLU
1	A	328	LEU
1	A	340	ASN
1	A	341	MET
1	A	390	ARG
1	A	413	GLN
1	A	416	LYS
1	A	458	LEU
1	A	469	TYR
1	B	91	GLN
1	B	99	ARG

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Mol	Chain	Res	Type
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	127	SER
1	B	139	SER
1	B	143	SER
1	B	172	LEU
1	B	218	LYS
1	B	222	ASN
1	B	278	GLN
1	B	293	LEU
1	B	323	GLU
1	B	328	LEU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	379	GLU
1	B	387	LEU
1	B	391	THR
1	B	397	LYS
1	B	398	ASP
1	B	406	LEU
1	B	467	VAL
1	B	469	TYR
1	B	473	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	166	HIS
1	A	191	GLN
1	A	196	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	422	HIS
1	A	468	ASN
1	B	91	GLN
1	B	146	GLN
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	191	GLN
1	B	215	ASN
1	B	222	ASN
1	B	278	GLN
1	B	285	ASN
1	B	340	ASN
1	B	368	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 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	$\# Z  > 2$
2	HEM	A	500	1	30,50,50	2.60	9 (30%)	24,82,82	2.64	12 (50%)
3	H4B	A	600	-	13,18,18	1.12	1 (7%)	11,26,26	2.42	6 (54%)
6	JSS	A	800	-	26,29,29	0.78	1 (3%)	27,38,38	1.53	3 (11%)
4	ACT	A	850	-	1,3,3	0.83	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	880	-	5,5,5	0.56	0	5,5,5	0.48	0
7	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	1	30,50,50	2.43	10 (33%)	24,82,82	2.62	12 (50%)
3	H4B	B	600	-	13,18,18	1.69	4 (30%)	11,26,26	3.11	9 (81%)
6	JSS	B	800	-	26,29,29	0.92	1 (3%)	27,38,38	1.83	5 (18%)
4	ACT	B	850	-	1,3,3	0.07	0	0,3,3	0.00	-
5	GOL	B	880	-	5,5,5	0.56	0	5,5,5	0.49	0
7	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	-	0/10/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
6	JSS	A	800	-	-	0/13/23/23	0/3/3/3
4	ACT	A	850	-	-	0/0/0/0	0/0/0/0
5	GOL	A	880	-	-	0/4/4/4	0/0/0/0
7	CAD	A	950	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
6	JSS	B	800	-	-	0/13/23/23	0/3/3/3
4	ACT	B	850	-	-	0/0/0/0	0/0/0/0
5	GOL	B	880	-	-	0/4/4/4	0/0/0/0
7	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-8.58	1.44	1.51
2	A	500	HEM	C3B-C4B	-8.12	1.44	1.51
2	B	500	HEM	C3D-C4D	-5.39	1.44	1.51
2	A	500	HEM	C3D-C4D	-5.18	1.44	1.51
3	B	600	H4B	C4A-C8A	-4.05	1.33	1.41
2	B	500	HEM	C2C-C1C	-3.31	1.46	1.52
2	B	500	HEM	C2B-C1B	-2.87	1.42	1.51
2	A	500	HEM	C2C-C1C	-2.68	1.47	1.52
2	A	500	HEM	C2B-C1B	-2.65	1.43	1.51
2	B	500	HEM	C2D-C1D	-2.06	1.45	1.51
3	B	600	H4B	C4-N3	2.04	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CMA-C3A	2.05	1.55	1.51
2	B	500	HEM	C3C-CAC	2.06	1.55	1.51
6	A	800	JSS	C5A-C4A	2.09	1.42	1.38
6	B	800	JSS	C14-C13	2.18	1.41	1.37
3	B	600	H4B	C8A-N1	2.30	1.38	1.34
3	B	600	H4B	C2-N2	2.30	1.38	1.34
2	A	500	HEM	CAA-C2A	2.35	1.56	1.52
2	B	500	HEM	FE-ND	2.37	2.10	1.97
2	A	500	HEM	FE-NB	2.81	2.12	1.97
3	A	600	H4B	C4-N3	2.96	1.38	1.33
2	B	500	HEM	C4C-NC	3.29	1.40	1.36
2	B	500	HEM	C1C-NC	3.34	1.40	1.36
2	A	500	HEM	FE-ND	3.40	2.15	1.97
2	A	500	HEM	C1C-NC	3.96	1.40	1.36
2	A	500	HEM	C4C-NC	5.46	1.42	1.36

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	H4B	N3-C2-N1	-5.73	116.15	125.53
2	B	500	HEM	CBA-CAA-C2A	-5.30	103.04	112.53
2	A	500	HEM	C3B-CAB-CBB	-4.91	116.92	124.46
2	B	500	HEM	CAA-C2A-C1A	-3.91	122.76	127.01
3	A	600	H4B	N3-C2-N1	-3.80	119.31	125.53
3	B	600	H4B	O10-C10-C11	-3.64	99.07	109.61
6	B	800	JSS	C3A-C2A-N1A	-3.27	119.27	122.96
2	B	500	HEM	CMA-C3A-C4A	-3.25	122.99	128.36
6	B	800	JSS	C3-C4-C11	-2.98	106.64	112.83
2	A	500	HEM	CBA-CAA-C2A	-2.97	107.20	112.53
2	A	500	HEM	CMA-C3A-C4A	-2.92	123.53	128.36
3	B	600	H4B	C4A-C8A-N8	-2.74	115.21	118.43
6	A	800	JSS	C3A-C2A-N1A	-2.50	120.14	122.96
2	A	500	HEM	C3C-CAC-CBC	-2.45	120.69	124.46
6	B	800	JSS	C8A-C4A-C3A	-2.39	117.32	120.95
6	A	800	JSS	C14-C13-C12	-2.38	120.28	123.35
6	B	800	JSS	C5'-C4'-C3'	-2.24	100.45	103.35
2	B	500	HEM	C3B-CAB-CBB	-2.21	121.07	124.46
2	A	500	HEM	C4B-CHC-C1C	-2.20	122.14	125.82
3	B	600	H4B	C7-C6-N5	-2.13	106.02	110.45
2	B	500	HEM	C4B-CHC-C1C	-2.06	122.38	125.82
2	A	500	HEM	CMD-C2D-C3D	2.19	124.02	114.35
3	A	600	H4B	C4-C4A-C8A	2.22	116.58	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	H4B	C8A-C4A-N5	2.38	121.85	118.85
3	B	600	H4B	N2-C2-N1	2.49	121.32	117.20
2	B	500	HEM	C3B-C4B-CHC	2.50	126.69	123.16
2	B	500	HEM	CMA-C3A-C2A	2.65	130.78	125.24
2	B	500	HEM	CMD-C2D-C3D	2.70	126.31	114.35
2	A	500	HEM	CAA-CBA-CGA	2.82	117.91	112.75
3	B	600	H4B	C8A-C4A-N5	2.86	122.45	118.85
2	B	500	HEM	CMC-C2C-C3C	2.97	123.93	116.53
3	B	600	H4B	C4-N3-C2	3.07	120.20	115.94
3	A	600	H4B	C2-N1-C8A	3.11	121.53	114.54
2	A	500	HEM	C3B-C4B-CHC	3.19	127.66	123.16
3	B	600	H4B	N2-C2-N3	3.20	122.51	117.20
3	B	600	H4B	C2-N1-C8A	3.39	122.17	114.54
2	A	500	HEM	CMC-C2C-C3C	3.55	125.38	116.53
3	A	600	H4B	N2-C2-N3	3.55	123.08	117.20
3	A	600	H4B	C4-N3-C2	3.69	121.06	115.94
2	B	500	HEM	CMB-C2B-C3B	4.45	127.64	116.53
2	A	500	HEM	CMB-C2B-C3B	4.50	127.77	116.53
2	B	500	HEM	CAD-C3D-C4D	4.54	128.50	112.47
2	A	500	HEM	CAD-C3D-C4D	4.72	129.12	112.47
2	B	500	HEM	CAD-C3D-C2D	4.79	126.98	113.22
2	A	500	HEM	CAD-C3D-C2D	4.81	127.06	113.22
6	A	800	JSS	C6A-N1A-C2A	4.96	121.76	118.23
6	B	800	JSS	C6A-N1A-C2A	6.05	122.53	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	3	0
6	A	800	JSS	2	0
4	A	850	ACT	4	0
5	A	880	GOL	1	0
7	A	950	CAD	1	0
2	B	500	HEM	3	0
3	B	600	H4B	1	0
6	B	800	JSS	1	0
4	B	850	ACT	6	0
7	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	403/444 (90%)	0.49	43 (10%) 8 11	37, 58, 84, 99	0
1	B	403/444 (90%)	0.54	33 (8%) 14 19	43, 61, 83, 107	0
All	All	806/888 (90%)	0.52	76 (9%) 11 15	37, 60, 84, 107	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	GLY	5.0
1	A	67	GLY	4.3
1	A	200	ALA	4.1
1	B	140	ILE	4.0
1	A	337	ALA	4.0
1	B	259	GLN	4.0
1	A	199	ASP	3.6
1	B	233	PHE	3.6
1	B	223	ARG	3.5
1	A	353	ALA	3.4
1	B	121	PRO	3.4
1	B	257	ARG	3.4
1	A	370	CYS	3.3
1	B	142	ARG	3.3
1	B	337	ALA	3.2
1	B	146	GLN	3.2
1	A	160	ALA	3.1
1	A	124	GLN	3.1
1	A	259	GLN	3.1
1	A	156	GLU	3.0
1	B	451	VAL	3.0
1	B	452	PRO	3.0
1	A	232	VAL	3.0
1	B	456	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	LYS	2.9
1	B	123	GLU	2.9
1	B	141	LYS	2.8
1	B	454	ILE	2.8
1	A	390	ARG	2.8
1	A	153	GLN	2.7
1	A	198	PHE	2.7
1	B	201	ARG	2.7
1	A	230	ILE	2.7
1	A	338	VAL	2.7
1	A	280	GLY	2.6
1	A	336	PRO	2.6
1	A	454	ILE	2.6
1	A	201	ARG	2.6
1	A	362	THR	2.6
1	B	455	SER	2.6
1	A	231	THR	2.5
1	A	339	SER	2.5
1	A	367	ARG	2.5
1	B	232	VAL	2.5
1	A	366	THR	2.5
1	A	123	GLU	2.4
1	A	455	SER	2.4
1	B	262	SER	2.4
1	A	126	LEU	2.4
1	A	108	PRO	2.4
1	A	239	GLY	2.3
1	A	223	ARG	2.3
1	B	458	LEU	2.3
1	A	161	SER	2.3
1	A	212	TYR	2.3
1	A	369	LEU	2.2
1	A	261	GLY	2.2
1	B	324	TRP	2.2
1	B	234	PRO	2.2
1	B	353	ALA	2.2
1	B	230	ILE	2.2
1	B	450	ILE	2.2
1	B	239	GLY	2.2
1	A	233	PHE	2.2
1	B	390	ARG	2.2
1	B	203	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	338	VAL	2.1
1	A	122	ALA	2.1
1	A	229	ALA	2.1
1	B	147	ALA	2.1
1	A	125	LEU	2.1
1	B	99	ARG	2.0
1	B	453	PRO	2.0
1	A	197	VAL	2.0
1	A	179	ALA	2.0
1	A	352	ALA	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<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
4	ACT	A	850	4/4	0.87	0.35	3.03	66,67,70,71	0
6	JSS	A	800	27/27	0.89	0.28	1.50	40,57,92,94	0
4	ACT	B	850	4/4	0.95	0.23	1.10	63,64,67,67	0
6	JSS	B	800	27/27	0.90	0.21	0.73	35,48,82,86	0
5	GOL	B	880	6/6	0.93	0.18	0.69	55,55,57,58	0
3	H4B	A	600	17/17	0.96	0.21	0.47	43,49,54,54	0
2	HEM	A	500	43/43	0.97	0.20	0.33	41,48,60,68	0
3	H4B	B	600	17/17	0.94	0.17	0.16	39,43,50,54	0
2	HEM	B	500	43/43	0.97	0.17	0.12	41,48,60,61	0
8	ZN	A	900	1/1	0.99	0.13	-0.19	60,60,60,60	0
7	CAD	A	950	3/5	0.99	0.12	-1.20	87,87,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CAD	B	950	3/5	0.98	0.10	-1.84	85,85,85,87	0
5	GOL	A	880	6/6	0.90	0.40	-	75,76,78,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.