



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:40 PM GMT

PDB ID : 4D35  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with N-2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)ethyl-3-(3- fluorophenyl)propan-1-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-10-20  
Resolution : 2.18 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

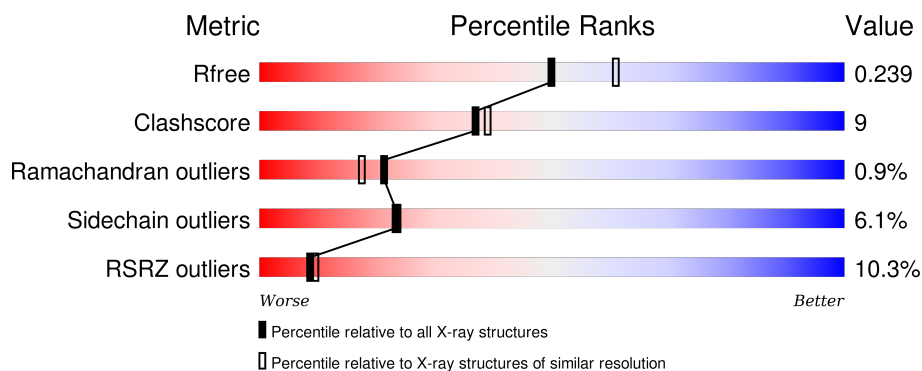
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	443	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</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
5	ACT	A	861	-	-	-	X
5	ACT	B	860	-	-	-	X
5	ACT	B	861	-	-	-	X
6	GOL	A	880	-	-	-	X
6	GOL	B	880	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6844 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.

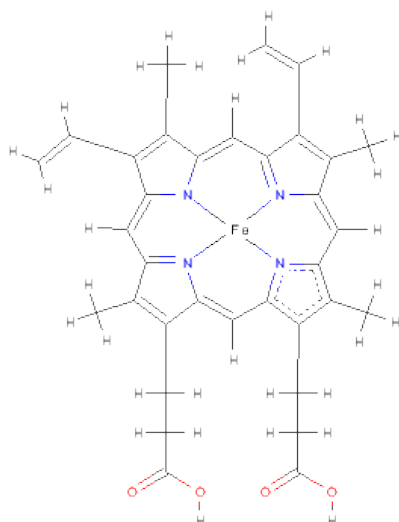
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



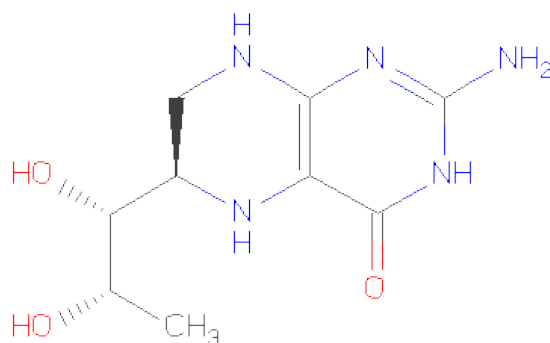
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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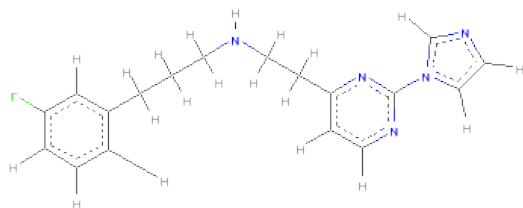
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



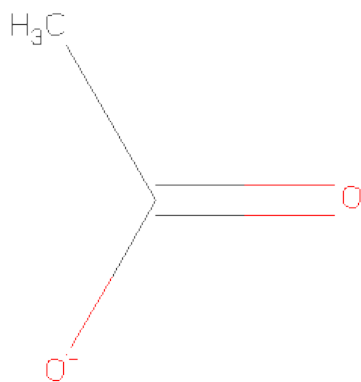
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 3-(3-FLUOROPHENYL)-N-{2-[2-(1H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL]ETHYL}PROPAN-1-AMINE (three-letter code: 4E8) (formula:  $C_{18}H_{20}FN_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			24	18	1	5		
4	B	1	Total	C	F	N	0	0
			24	18	1	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



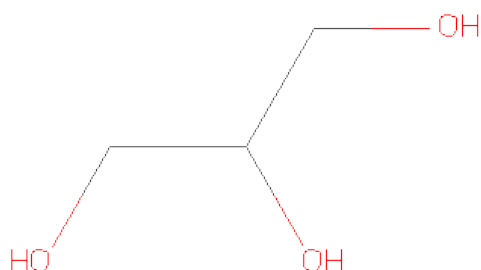
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 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
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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

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

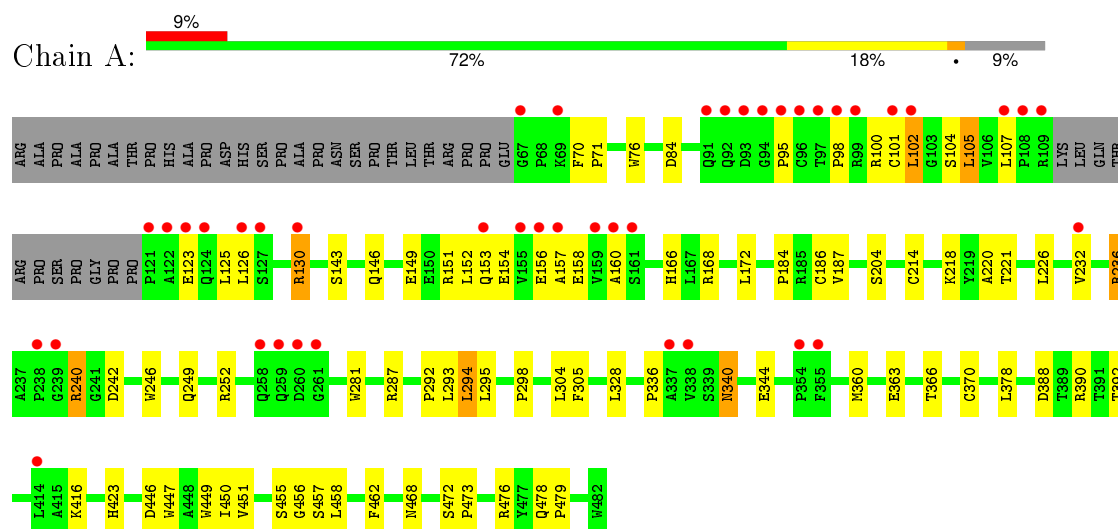
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	0
			126	126		
8	B	69	Total	O	0	0
			69	69		

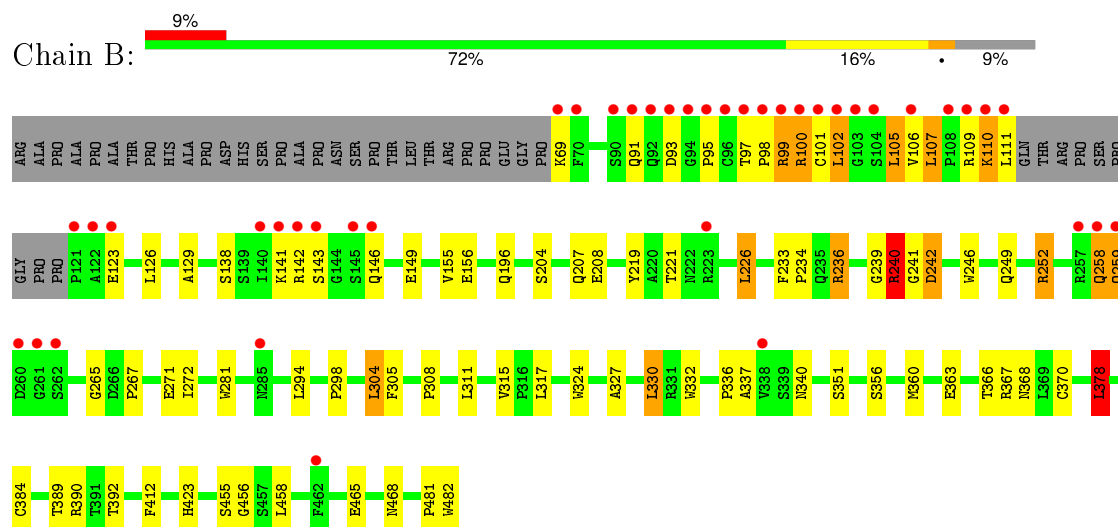
### 3 Residue-property plots [i](#)

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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.63Å 105.90Å 156.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.78 – 2.18 39.24 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.5 (87.78-2.18) 98.6 (39.24-2.18)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.186 , 0.240 0.185 , 0.239	Depositor DCC
$R_{free}$ test set	2515 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 50568 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CAS, 4E8, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.85	0/3303	0.89	1/4497 (0.0%)
1	B	0.77	1/3308 (0.0%)	0.88	8/4502 (0.2%)
All	All	0.81	1/6611 (0.0%)	0.89	9/8999 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	GLU	CG-CD	5.74	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	240	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	105	LEU	CA-CB-CG	6.64	130.58	115.30
1	B	242	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	378	LEU	CA-CB-CG	5.63	128.26	115.30
1	B	107	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	360	MET	CA-CB-CG	-5.41	104.11	113.30
1	B	304	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	240	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

## 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	3223	0	3129	59	0
1	B	3229	0	3142	61	0
2	A	43	0	30	7	0
2	B	43	0	30	4	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	24	0	20	1	0
4	B	24	0	20	6	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	4	0
7	A	1	0	0	0	0
8	A	126	0	0	9	0
8	B	69	0	0	3	0
All	All	6844	0	6429	123	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 9.

All (123) 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:CAS:AS	1:B:384:CAS:SG	2.69	1.11
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.16	1.04
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.49	0.94
1:A:236:ARG:HG3	1:A:236:ARG:NH1	1.74	0.94
1:A:236:ARG:CG	1:A:236:ARG:HH11	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.59	0.84
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.59	0.82
1:A:236:ARG:HD3	1:A:242:ASP:OD1	1.86	0.75
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.89	0.73
8:A:2007:HOH:O	1:B:100:ARG:HD2	1.88	0.73
1:B:258:GLN:HA	1:B:258:GLN:HE21	1.52	0.72
1:B:106:VAL:HG21	6:B:880:GOL:O3	1.91	0.69
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.24	0.68
1:A:152:LEU:O	1:A:156:GLU:HG2	1.93	0.67
8:A:2007:HOH:O	1:B:99:ARG:HG2	1.97	0.65
1:B:481:PRO:HD2	1:B:482:TRP:CE3	2.32	0.64
1:B:252:ARG:HE	1:B:252:ARG:HA	1.63	0.63
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.81	0.63
1:B:258:GLN:HE21	1:B:258:GLN:CA	2.10	0.63
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.31	0.60
1:A:455:SER:O	1:A:458:LEU:HB2	2.01	0.60
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.85	0.59
4:B:800:4E8:H22	6:B:880:GOL:H32	1.86	0.57
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.85	0.57
1:A:101:CYS:HB3	1:B:468:ASN:HB3	1.86	0.57
1:B:106:VAL:HG21	6:B:880:GOL:HO3	1.69	0.57
1:B:221:THR:O	1:B:226:LEU:HD12	2.04	0.56
2:B:500:HEM:C1A	4:B:800:4E8:H02	2.42	0.54
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.48	0.54
2:B:500:HEM:O1D	4:B:800:4E8:N19	2.41	0.54
1:B:146:GLN:HA	1:B:146:GLN:OE1	2.08	0.53
1:B:249:GLN:HB2	1:B:252:ARG:HG2	1.90	0.53
1:A:294:LEU:HD13	1:A:304:LEU:HD13	1.91	0.53
1:A:149:GLU:O	1:A:153:GLN:HG3	2.08	0.53
1:B:138:SER:HA	1:B:143:SER:OG	2.09	0.53
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.49	0.53
1:A:98:PRO:HG3	1:B:97:THR:HG22	1.90	0.53
1:A:157:ALA:O	1:A:160:ALA:HB3	2.09	0.53
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.24	0.52
1:A:70:PHE:HB3	1:A:84:ASP:O	2.10	0.52
1:A:340:ASN:HD22	1:A:340:ASN:H	1.57	0.51
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.92	0.51
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.41	0.51
1:B:378:LEU:HB2	8:B:2051:HOH:O	2.11	0.50
1:B:240:ARG:HD3	1:B:298:PRO:HB3	1.92	0.50
1:A:363:GLU:HG2	8:A:2125:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:NH1	1:B:390:ARG:HB2	2.27	0.50
1:A:214:CYS:O	1:A:218:LYS:HG3	2.12	0.49
1:B:204:SER:N	1:B:208:GLU:OE1	2.41	0.49
1:B:265:GLY:O	1:B:267:PRO:HD3	2.13	0.49
1:B:240:ARG:HD2	1:B:241:GLY:O	2.13	0.48
1:A:220:ALA:HB1	8:A:2048:HOH:O	2.13	0.48
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.28	0.48
8:A:2007:HOH:O	1:B:99:ARG:CG	2.57	0.48
1:B:324:TRP:O	1:B:327:ALA:HB3	2.13	0.48
1:A:449:TRP:HA	3:A:600:H4B:N1	2.29	0.47
1:B:95:PRO:HB2	1:B:102:LEU:HB3	1.96	0.47
1:A:378:LEU:HB2	8:A:2091:HOH:O	2.14	0.47
1:A:478:GLN:HB2	1:A:479:PRO:HD2	1.96	0.47
1:A:392:THR:HB	1:B:423:HIS:HB2	1.96	0.47
1:A:143:SER:HB3	8:A:2016:HOH:O	2.15	0.47
1:A:221:THR:O	1:A:226:LEU:HD12	2.14	0.47
1:B:366:THR:O	1:B:370:CYS:HB2	2.14	0.47
1:A:105:LEU:HD23	1:A:105:LEU:N	2.31	0.47
1:A:457:SER:HA	1:A:462:PHE:CG	2.50	0.46
1:A:252:ARG:HA	1:A:252:ARG:HE	1.80	0.46
1:B:455:SER:O	1:B:458:LEU:HB2	2.15	0.46
1:A:105:LEU:HD23	1:A:105:LEU:H	1.81	0.46
1:B:367:ARG:HH12	3:B:600:H4B:C4	2.28	0.46
1:A:388:ASP:OD1	1:A:390:ARG:HB2	2.15	0.46
1:A:105:LEU:N	1:A:105:LEU:CD2	2.79	0.46
1:B:258:GLN:HA	1:B:258:GLN:NE2	2.26	0.45
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.98	0.45
1:B:246:TRP:HB2	1:B:294:LEU:HB2	1.99	0.45
1:A:172:LEU:HD11	1:A:232:VAL:HG11	1.98	0.45
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.51	0.45
1:A:423:HIS:HB2	1:B:392:THR:HB	1.98	0.45
1:B:249:GLN:HA	1:B:337:ALA:O	2.17	0.45
2:B:500:HEM:O2A	4:B:800:4E8:H17	2.17	0.44
1:A:366:THR:O	1:A:370:CYS:HB2	2.18	0.44
1:A:472:SER:HA	1:A:473:PRO:C	2.38	0.44
2:A:500:HEM:C1A	4:A:800:4E8:H02	2.53	0.44
1:B:337:ALA:HB2	1:B:356:SER:HB3	2.00	0.44
1:B:129:ALA:HB1	1:B:155:VAL:HG11	2.00	0.44
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.80	0.44
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.48	0.44
1:B:110:LYS:HG3	1:B:110:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TRP:CG	1:A:292:PRO:HG3	2.52	0.44
8:A:2007:HOH:O	1:B:100:ARG:HB3	2.18	0.43
4:B:800:4E8:H21	8:B:2068:HOH:O	2.18	0.43
1:A:98:PRO:O	1:B:93:ASP:HA	2.18	0.43
1:A:446:ASP:O	1:A:450:ILE:HG12	2.19	0.43
1:B:315:VAL:HG11	1:B:412:PHE:CD1	2.54	0.43
1:A:95:PRO:HB2	1:A:102:LEU:HB3	2.00	0.43
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.54	0.42
1:A:158:GLU:OE2	1:A:166:HIS:HD2	2.01	0.42
2:B:500:HEM:C1C	4:B:800:4E8:H05	2.54	0.42
2:A:500:HEM:HBB2	2:A:500:HEM:CHC	2.49	0.42
1:B:272:ILE:HG22	8:B:2031:HOH:O	2.19	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.42
1:A:186:CYS:HB2	2:A:500:HEM:ND	2.34	0.42
1:B:97:THR:HB	1:B:98:PRO:HD2	2.02	0.42
1:B:196:GLN:HG2	1:B:219:TYR:CE2	2.55	0.42
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.55	0.42
1:B:106:VAL:CG2	6:B:880:GOL:O3	2.65	0.42
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.50	0.42
1:A:71:PRO:HB3	1:B:102:LEU:HD21	2.02	0.42
1:B:126:LEU:HD11	1:B:156:GLU:HA	2.01	0.42
1:A:187:VAL:O	1:A:187:VAL:HG22	2.19	0.41
1:A:252:ARG:HB2	8:A:2054:HOH:O	2.19	0.41
1:B:317:LEU:HD12	1:B:330:LEU:HB3	2.01	0.41
1:B:142:ARG:HD3	1:B:142:ARG:HA	1.89	0.41
1:B:258:GLN:CA	1:B:258:GLN:NE2	2.81	0.41
1:B:110:LYS:O	1:B:110:LYS:CG	2.68	0.41
1:B:332:TRP:CZ2	1:B:368:ASN:ND2	2.89	0.41
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.53	0.41
1:A:344:GLU:OE1	1:A:476:ARG:NH2	2.53	0.41
1:B:384:CAS:AS	1:B:384:CAS:CB	3.29	0.41
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.51	0.41
1:A:105:LEU:HA	1:B:465:GLU:HG2	2.02	0.41
1:B:281:TRP:CB	1:B:304:LEU:HD21	2.41	0.41
1:A:295:LEU:HD12	1:A:305:PHE:CD2	2.56	0.40
1:B:207:GLN:NE2	1:B:305:PHE:HE2	2.18	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	400/443 (90%)	380 (95%)	18 (4%)	2 (0%)	34	33
1	B	400/443 (90%)	377 (94%)	18 (4%)	5 (1%)	15	10
All	All	800/886 (90%)	757 (95%)	36 (4%)	7 (1%)	21	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLY
1	B	109	ARG
1	B	259	GLN
1	B	110	LYS
1	B	456	GLY
1	A	336	PRO
1	B	336	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/375 (92%)	324 (94%)	19 (6%)	27	28
1	B	344/375 (92%)	321 (93%)	23 (7%)	20	19
All	All	687/750 (92%)	645 (94%)	42 (6%)	23	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	102	LEU
1	A	104	SER
1	A	105	LEU
1	A	107	LEU
1	A	123	GLU
1	A	125	LEU
1	A	130	ARG
1	A	146	GLN
1	A	154	GLU
1	A	204	SER
1	A	236	ARG
1	A	287	ARG
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	360	MET
1	A	416	LYS
1	B	69	LYS
1	B	91	GLN
1	B	99	ARG
1	B	100	ARG
1	B	101	CYS
1	B	102	LEU
1	B	105	LEU
1	B	107	LEU
1	B	111	LEU
1	B	123	GLU
1	B	141	LYS
1	B	149	GLU
1	B	226	LEU
1	B	236	ARG
1	B	240	ARG
1	B	252	ARG
1	B	258	GLN
1	B	259	GLN
1	B	271	GLU
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	389	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	HIS
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	91	GLN
1	B	222	ASN
1	B	258	GLN
1	B	259	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	CAS	A	384	1	5,8,9	1.58	1 (20%)	2,9,11	1.41	0
1	CAS	B	384	1	5,8,9	1.39	1 (20%)	2,9,11	1.72	1 (50%)

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
1	CAS	A	384	1	-	0/0/7/9	0/0/0/0
1	CAS	B	384	1	-	0/0/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE1	2.17	2.01	1.96
1	A	384	CAS	AS-CE1	3.40	2.05	1.96

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	CAS	O-C-CA	-2.41	119.21	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	384	CAS	2	0

## 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	1,4	30,50,50	2.34	8 (26%)	24,82,82	2.95	17 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	H4B	A	600	-	13,18,18	0.87	0	11,26,26	2.63	6 (54%)
4	4E8	A	800	2	24,26,26	1.68	3 (12%)	30,33,33	2.29	10 (33%)
5	ACT	A	860	-	1,3,3	1.44	0	0,3,3	0.00	-
5	ACT	A	861	-	1,3,3	2.80	1 (100%)	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.27	0	5,5,5	1.40	2 (40%)
2	HEM	B	500	1,4	30,50,50	1.98	6 (20%)	24,82,82	2.63	9 (37%)
3	H4B	B	600	-	13,18,18	0.90	1 (7%)	11,26,26	2.46	6 (54%)
4	4E8	B	800	2	24,26,26	1.48	4 (16%)	30,33,33	2.26	9 (30%)
5	ACT	B	860	-	1,3,3	1.30	0	0,3,3	0.00	-
5	ACT	B	861	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.33	0	5,5,5	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,4	-	0/10/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	4E8	A	800	2	-	0/9/13/13	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
5	ACT	A	861	-	-	0/0/0/0	0/0/0/0
6	GOL	A	880	-	-	0/4/4/4	0/0/0/0
2	HEM	B	500	1,4	-	0/10/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	4E8	B	800	2	-	0/9/13/13	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
5	ACT	B	861	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C2D-C3D	-6.66	1.34	1.54
2	A	500	HEM	C2D-C3D	-6.24	1.35	1.54
2	A	500	HEM	C3D-C4D	-5.97	1.43	1.51
2	A	500	HEM	C2C-C1C	-5.50	1.42	1.52
2	B	500	HEM	C2C-C1C	-4.98	1.43	1.52
4	B	800	4E8	C04-N03	-4.08	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	4E8	C04-N03	-3.83	1.33	1.39
2	A	500	HEM	C3B-C4B	-3.65	1.48	1.51
2	B	500	HEM	C3D-C4D	-2.60	1.48	1.51
2	A	500	HEM	FE-ND	-2.45	1.84	1.97
2	A	500	HEM	C2B-C1B	-2.32	1.44	1.51
4	B	800	4E8	C2'-C3'	2.10	1.41	1.37
2	B	500	HEM	FE-NB	2.25	2.09	1.97
2	B	500	HEM	CHC-C1C	2.42	1.42	1.36
2	A	500	HEM	C4C-NC	2.49	1.39	1.36
5	B	861	ACT	CH3-C	2.71	1.52	1.48
3	B	600	H4B	C4-N3	2.73	1.38	1.33
5	A	861	ACT	CH3-C	2.80	1.52	1.48
2	A	500	HEM	FE-NC	3.00	2.07	1.95
4	B	800	4E8	C12-N11	3.20	1.34	1.31
4	A	800	4E8	C12-N13	3.31	1.37	1.32
4	B	800	4E8	C12-N13	3.52	1.37	1.32
2	B	500	HEM	FE-NC	3.55	2.09	1.95
4	A	800	4E8	C12-N11	5.51	1.37	1.31

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CBA-CAA-C2A	-7.41	99.24	112.53
4	A	800	4E8	N11-C12-N13	-5.80	119.16	126.44
4	B	800	4E8	N11-C12-N13	-5.40	119.66	126.44
2	A	500	HEM	C1D-CHD-C4C	-5.36	116.86	125.82
2	A	500	HEM	CAA-C2A-C1A	-4.45	122.17	127.01
2	A	500	HEM	CBA-CAA-C2A	-4.14	105.10	112.53
4	A	800	4E8	C04-N03-C12	-3.52	121.75	125.61
3	A	600	H4B	N3-C2-N1	-3.25	120.20	125.53
4	A	800	4E8	C4'-C3'-C2'	-3.19	119.23	123.35
4	A	800	4E8	C15-C16-N11	-2.93	120.56	123.90
3	B	600	H4B	N3-C2-N1	-2.85	120.85	125.53
2	A	500	HEM	C3C-CAC-CBC	-2.74	120.25	124.46
2	A	500	HEM	C3B-CAB-CBB	-2.74	120.26	124.46
2	A	500	HEM	CMA-C3A-C4A	-2.68	123.93	128.36
4	B	800	4E8	C15-C14-N13	-2.53	119.31	122.41
4	B	800	4E8	C15-C16-N11	-2.39	121.17	123.90
2	A	500	HEM	C4B-CHC-C1C	-2.25	122.05	125.82
6	A	880	GOL	O1-C1-C2	-2.25	99.27	110.18
4	B	800	4E8	C17-C14-C15	-2.10	117.47	121.74
4	B	800	4E8	C4'-C3'-C2'	-2.08	120.66	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C3B-C4B-NB	-2.08	107.66	111.63
6	A	880	GOL	O3-C3-C2	-2.06	100.19	110.18
2	A	500	HEM	C3B-C4B-NB	-2.05	107.72	111.63
2	A	500	HEM	C3B-C4B-CHC	-2.00	120.34	123.16
2	B	500	HEM	CHC-C4B-NB	2.01	129.37	124.52
4	A	800	4E8	N11-C12-N03	2.05	118.50	115.16
2	B	500	HEM	C2C-C1C-CHC	2.06	126.81	123.68
4	A	800	4E8	F7'-C3'-C2'	2.22	121.18	118.22
2	A	500	HEM	C2D-C3D-C4D	2.30	105.40	101.50
2	A	500	HEM	CMD-C2D-C3D	2.32	124.61	114.35
3	A	600	H4B	C2-N1-C8A	2.40	119.93	114.54
3	A	600	H4B	C4A-C8A-N8	2.57	121.45	118.43
3	B	600	H4B	N2-C2-N3	2.62	121.53	117.20
4	B	800	4E8	C04-N03-C02	2.63	113.43	108.53
2	A	500	HEM	CMA-C3A-C2A	2.66	130.80	125.24
2	B	500	HEM	CMD-C2D-C3D	2.74	126.47	114.35
4	A	800	4E8	C04-N03-C02	2.82	113.79	108.53
3	B	600	H4B	C2-N1-C8A	2.84	120.91	114.54
2	A	500	HEM	CMB-C2B-C3B	2.92	123.82	116.53
3	A	600	H4B	N2-C2-N3	3.01	122.18	117.20
2	A	500	HEM	CHC-C4B-NB	3.08	131.94	124.52
3	B	600	H4B	C4A-C8A-N8	3.16	122.15	118.43
2	B	500	HEM	CMB-C2B-C3B	3.18	124.48	116.53
3	B	600	H4B	C4-N3-C2	3.30	120.51	115.94
2	B	500	HEM	CMC-C2C-C3C	3.53	125.35	116.53
4	A	800	4E8	C17-C14-N13	3.76	121.25	115.69
4	A	800	4E8	C12-N13-C14	4.03	120.52	115.26
2	B	500	HEM	CAD-C3D-C4D	4.28	127.56	112.47
2	A	500	HEM	CMC-C2C-C3C	4.38	127.45	116.53
3	A	600	H4B	C4-N3-C2	4.47	122.14	115.94
2	A	500	HEM	CAD-C3D-C2D	4.50	126.16	113.22
2	A	500	HEM	CAD-C3D-C4D	4.53	128.44	112.47
3	B	600	H4B	C4-C4A-C8A	4.60	118.73	114.56
4	B	800	4E8	C12-N13-C14	4.64	121.32	115.26
3	A	600	H4B	C4-C4A-C8A	4.71	118.82	114.56
4	A	800	4E8	N13-C12-N03	5.08	122.33	114.82
4	B	800	4E8	C17-C14-N13	5.09	123.21	115.69
4	B	800	4E8	N13-C12-N03	5.09	122.35	114.82
2	B	500	HEM	CAD-C3D-C2D	5.26	128.34	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	7	0
3	A	600	H4B	1	0
4	A	800	4E8	1	0
2	B	500	HEM	4	0
3	B	600	H4B	1	0
4	B	800	4E8	6	0
6	B	880	GOL	4	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	404/443 (91%)	0.44	42 (10%) <b>8</b> <b>9</b>	31, 44, 87, 131	0
1	B	404/443 (91%)	0.49	41 (10%) <b>9</b> <b>10</b>	30, 49, 91, 128	0
All	All	808/886 (91%)	0.47	83 (10%) <b>9</b> <b>9</b>	30, 46, 90, 131	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ARG	8.8
1	B	110	LYS	7.6
1	A	98	PRO	7.1
1	B	259	GLN	6.6
1	A	108	PRO	6.6
1	A	67	GLY	6.4
1	A	121	PRO	6.1
1	B	98	PRO	6.0
1	B	99	ARG	5.9
1	B	146	GLN	5.7
1	B	111	LEU	5.6
1	A	93	ASP	5.4
1	A	99	ARG	5.3
1	B	96	CYS	5.2
1	B	109	ARG	5.0
1	A	101	CYS	4.9
1	B	122	ALA	4.9
1	A	123	GLU	4.8
1	A	97	THR	4.8
1	A	122	ALA	4.8
1	A	160	ALA	4.7
1	A	95	PRO	4.7
1	B	93	ASP	4.7
1	A	126	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	121	PRO	4.3
1	A	91	GLN	4.2
1	B	92	GLN	4.2
1	B	91	GLN	4.2
1	A	69	LYS	3.9
1	B	94	GLY	3.9
1	B	141	LYS	3.7
1	B	143	SER	3.7
1	B	108	PRO	3.7
1	A	259	GLN	3.7
1	B	97	THR	3.5
1	B	101	CYS	3.5
1	B	261	GLY	3.5
1	A	107	LEU	3.3
1	B	106	VAL	3.3
1	B	142	ARG	3.2
1	A	94	GLY	3.2
1	A	338	VAL	3.1
1	B	123	GLU	3.1
1	B	223	ARG	3.0
1	A	124	GLN	3.0
1	A	239	GLY	2.8
1	B	260	ASP	2.7
1	B	69	LYS	2.7
1	B	145	SER	2.6
1	A	414	LEU	2.6
1	A	92	GLN	2.6
1	B	100	ARG	2.6
1	A	157	ALA	2.5
1	A	159	VAL	2.5
1	A	102	LEU	2.5
1	A	161	SER	2.5
1	B	338	VAL	2.5
1	A	337	ALA	2.5
1	B	258	GLN	2.5
1	A	354	PRO	2.4
1	A	127	SER	2.4
1	A	130	ARG	2.4
1	B	104	SER	2.4
1	B	140	ILE	2.4
1	B	103	GLY	2.3
1	A	258	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	2.3
1	A	153	GLN	2.3
1	A	156	GLU	2.3
1	B	90	SER	2.2
1	B	285	ASN	2.2
1	A	96	CYS	2.2
1	B	262	SER	2.2
1	A	355	PHE	2.2
1	B	257	ARG	2.2
1	B	102	LEU	2.1
1	B	462	PHE	2.1
1	A	155	VAL	2.1
1	A	232	VAL	2.1
1	B	95	PRO	2.1
1	A	260	ASP	2.1
1	A	261	GLY	2.1
1	B	70	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAS	A	384	9/10	0.95	0.08	-	41,42,60,86	0
1	CAS	B	384	9/10	0.94	0.13	-	56,59,77,104	0

## 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( $\text{\AA}^2$ )	Q<0.9
5	ACT	B	860	4/4	0.97	0.20	5.71	60,60,62,69	0
5	ACT	A	861	4/4	0.77	0.30	5.04	46,47,60,60	0
5	ACT	B	861	4/4	0.76	0.34	4.89	60,68,70,74	0
6	GOL	A	880	6/6	0.89	0.28	3.65	60,76,78,78	0
4	4E8	B	800	24/24	0.97	0.24	1.37	27,42,117,119	0
4	4E8	A	800	24/24	0.96	0.26	1.27	37,44,122,126	0
6	GOL	B	880	6/6	0.88	0.22	1.08	60,70,75,76	0
2	HEM	A	500	43/43	0.99	0.19	0.70	25,32,50,55	0
2	HEM	B	500	43/43	0.98	0.15	0.26	33,39,47,68	0
3	H4B	B	600	17/17	0.95	0.15	-0.34	44,50,54,54	0
3	H4B	A	600	17/17	0.97	0.14	-0.46	38,45,52,52	0
5	ACT	A	860	4/4	0.98	0.09	-0.55	53,53,55,56	0
7	ZN	A	900	1/1	0.97	0.05	-4.78	84,84,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.