



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:41 PM GMT

PDB ID : 4D34  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)-N-(3- fluorophenethyl)ethan-1-amine  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : 2014-10-20  
Resolution : 2.25 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.

---

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

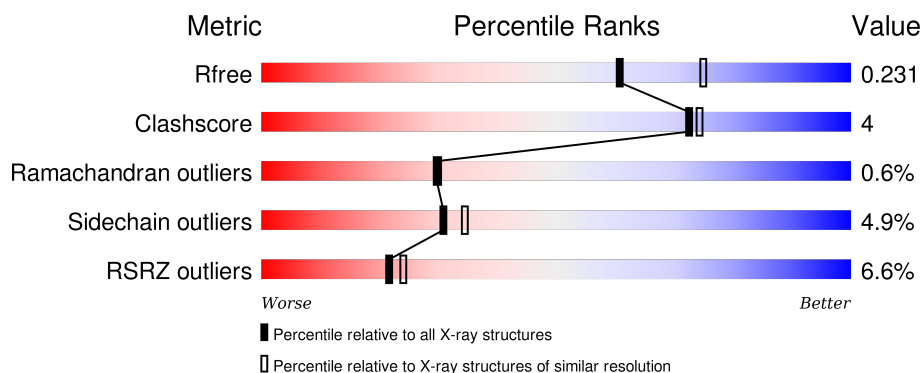
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	
1	B	443	

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
6	GOL	A	880	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6818 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.

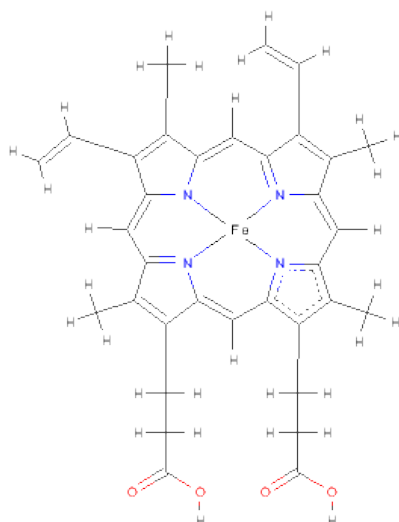
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	1	0
			3229	1	2053	568	591	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:  $C_{34}H_{32}FeN_4O_4$ ).



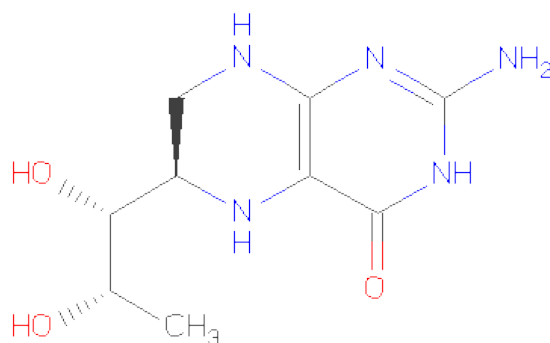
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

Continued from previous page...

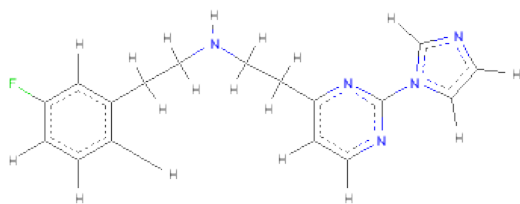
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



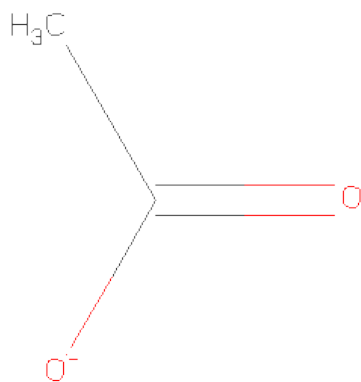
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 2-(3-FLUOROPHENYL)-N-{2-[2-(1H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL]ETHYL}ETHANAMINE (three-letter code: E2Z) (formula:  $C_{17}H_{18}FN_5$ ).



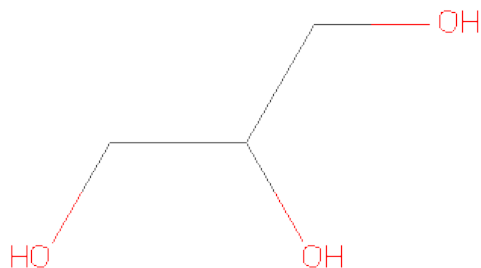
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	17	1	5		
4	B	1	Total	C	F	N	0	0
			23	17	1	5		

- 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	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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		

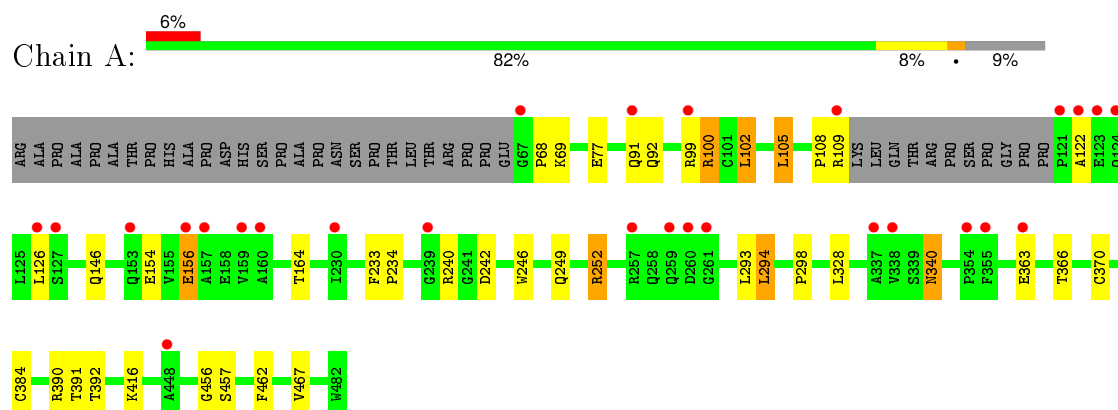
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	93	Total	O	0	0
			93	93		
8	B	80	Total	O	0	0
			80	80		

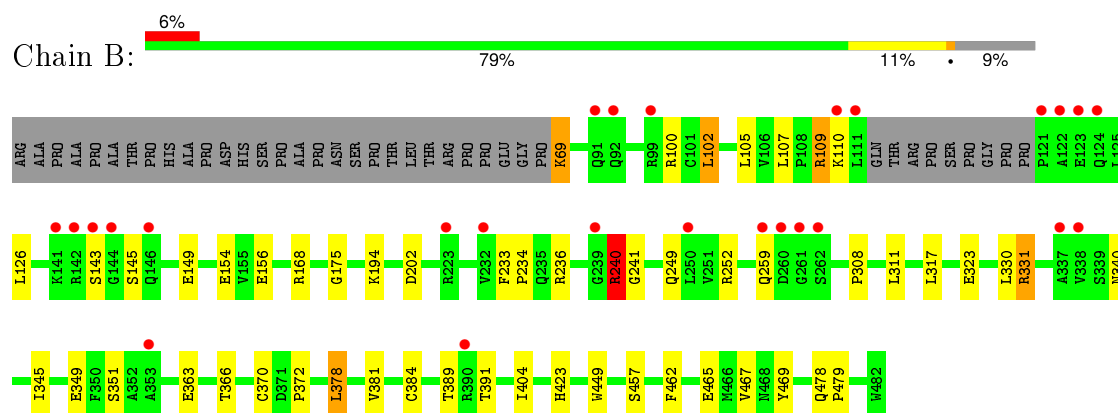
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	58.16Å 106.63Å 156.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.25 39.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.25) 98.7 (39.30-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.176 , 0.231 0.184 , 0.231	Depositor DCC
$R_{free}$ test set	2320 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46571 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, E2Z, 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	0.74	2/3312 (0.1%)	0.86	4/4509 (0.1%)
1	B	0.69	1/3308 (0.0%)	0.80	3/4502 (0.1%)
All	All	0.72	3/6620 (0.0%)	0.83	7/9011 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	GLU	CG-CD	9.61	1.66	1.51
1	A	363[A]	GLU	CG-CD	7.69	1.63	1.51
1	A	363[B]	GLU	CG-CD	7.69	1.63	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363[A]	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	363[B]	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	252	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	B	363	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	B	240	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	363	GLU	CA-CB-CG	5.78	126.11	113.40
1	A	242	ASP	CB-CG-OD1	5.14	122.93	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	3229	0	3133	22	0
1	B	3229	0	3141	28	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	23	0	18	1	0
4	B	23	0	18	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	93	0	0	2	0
8	B	80	0	0	0	0
All	All	6818	0	6422	55	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 4.

All (55) 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	2.49	1.30
1:A:384:CAS:AS	1:A:384:CAS:SG	2.59	1.21
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.68	0.74
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.71	0.73
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.75	0.68
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.77	0.67
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.80	0.64
1:A:105:LEU:N	1:A:105:LEU:HD23	2.16	0.60
1:B:107:LEU:HD21	4:B:800:E2Z:H5'	1.83	0.59
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.86	0.58
8:A:2001:HOH:O	1:B:109:ARG:HG2	2.03	0.57
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.86	0.57
2:B:500:HEM:O1D	4:B:800:E2Z:N19	2.37	0.57
1:A:384:CAS:CB	1:A:384:CAS:AS	3.14	0.56
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.36	0.55
1:B:366:THR:O	1:B:370:CYS:HB2	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.90	0.53
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.90	0.53
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.39	0.52
2:B:500:HEM:C1A	4:B:800:E2Z:H02	2.45	0.52
1:A:384:CAS:CE2	1:A:384:CAS:SG	2.98	0.51
1:A:68:PRO:O	1:B:109:ARG:NH2	2.43	0.51
1:B:175:GLY:HA3	1:B:345:ILE:HD13	1.92	0.50
2:A:500:HEM:C1A	4:A:800:E2Z:H02	2.47	0.49
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.93	0.49
1:A:467:VAL:HG13	1:B:102:LEU:CD1	2.43	0.48
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.96	0.47
1:B:384:CAS:AS	1:B:384:CAS:CB	3.23	0.47
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.75	0.47
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.45	0.47
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.55	0.47
1:B:240:ARG:HD2	1:B:241:GLY:O	2.15	0.46
1:B:69:LYS:HA	1:B:69:LYS:HE3	1.97	0.46
1:B:449:TRP:HA	3:B:600:H4B:N1	2.30	0.46
1:B:154:GLU:OE1	1:B:168:ARG:NH2	2.47	0.45
1:B:236:ARG:HG3	1:B:349:GLU:O	2.17	0.45
1:B:202:ASP:CG	1:B:202:ASP:O	2.55	0.45
1:B:126:LEU:HD11	1:B:156:GLU:HA	1.99	0.44
1:A:457:SER:HA	1:A:462:PHE:CG	2.52	0.44
1:A:105:LEU:N	1:A:105:LEU:CD2	2.80	0.44
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.99	0.44
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.59	0.44
1:A:246:TRP:HB2	1:A:294:LEU:HB3	2.00	0.43
1:B:457:SER:HA	1:B:462:PHE:CG	2.54	0.43
1:A:392:THR:HB	1:B:423:HIS:HB2	2.01	0.43
1:A:164:THR:HG21	8:A:2016:HOH:O	2.19	0.42
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.49	0.42
1:B:249:GLN:HB2	1:B:252:ARG:HG2	2.02	0.42
2:A:500:HEM:HBB2	2:A:500:HEM:CHC	2.44	0.42
1:A:340:ASN:HD22	1:A:340:ASN:H	1.66	0.42
1:B:478:GLN:HB2	1:B:479:PRO:HD2	2.01	0.42
1:A:100:ARG:CZ	1:A:102:LEU:HD22	2.51	0.41
1:B:467:VAL:HG12	1:B:469:TYR:CD1	2.55	0.41
1:B:317:LEU:HG	1:B:331:ARG:HA	2.01	0.41
1:A:366:THR:O	1:A:370:CYS:HB2	2.22	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	401/443 (90%)	380 (95%)	18 (4%)	3 (1%)	26	26
1	B	400/443 (90%)	384 (96%)	14 (4%)	2 (0%)	34	34
All	All	801/886 (90%)	764 (95%)	32 (4%)	5 (1%)	30	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	LYS
1	A	122	ALA
1	A	456	GLY
1	A	108	PRO
1	B	145	SER

### 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	344/375 (92%)	327 (95%)	17 (5%)	31	34
1	B	344/375 (92%)	327 (95%)	17 (5%)	31	34
All	All	688/750 (92%)	654 (95%)	34 (5%)	31	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	91	GLN
1	A	92	GLN
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	109	ARG
1	A	146	GLN
1	A	154	GLU
1	A	156	GLU
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	391	THR
1	A	416	LYS
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	143	SER
1	B	149	GLU
1	B	194	LYS
1	B	240	ARG
1	B	259	GLN
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	391	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	153	GLN
1	A	166	HIS
1	A	178	GLN
1	A	191	GLN
1	A	340	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	376	ASN
1	A	468	ASN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
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	1.43	1 (20%)	2,9,11	1.10	0
1	CAS	B	384	1	5,8,9	1.45	2 (40%)	2,9,11	1.53	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	2.10	2.01	1.96
1	B	384	CAS	AS-CE1	2.14	2.01	1.96
1	A	384	CAS	AS-CE1	2.81	2.03	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	-2.04	120.17	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	4	0
1	B	384	CAS	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	2.40	8 (26%)	24,82,82	2.58	12 (50%)
3	H4B	A	600	-	13,18,18	0.98	0	11,26,26	2.64	6 (54%)
4	E2Z	A	800	2	23,25,25	1.86	3 (13%)	28,32,32	2.14	6 (21%)
5	ACT	A	860	-	1,3,3	1.50	0	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.30	0	5,5,5	0.85	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	500	1,4	30,50,50	2.25	6 (20%)	24,82,82	2.50	9 (37%)
3	H4B	B	600	-	13,18,18	0.78	0	11,26,26	2.26	5 (45%)
4	E2Z	B	800	2	23,25,25	1.35	3 (13%)	28,32,32	2.40	10 (35%)
5	ACT	B	861	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.36	0	5,5,5	0.77	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	E2Z	A	800	2	-	0/8/12/12	0/3/3/3
5	ACT	A	860	-	-	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	E2Z	B	800	2	-	0/8/12/12	0/3/3/3
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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C2C-C1C	-7.16	1.39	1.52
2	B	500	HEM	C2D-C3D	-7.02	1.33	1.54
2	A	500	HEM	C2D-C3D	-6.98	1.33	1.54
2	A	500	HEM	C2C-C1C	-6.54	1.40	1.52
4	A	800	E2Z	C04-N03	-4.67	1.32	1.39
2	A	500	HEM	C3D-C4D	-4.16	1.46	1.51
4	B	800	E2Z	C04-N03	-3.85	1.33	1.39
2	A	500	HEM	C3B-CAB	-3.47	1.44	1.51
2	A	500	HEM	C3B-C4B	-3.09	1.49	1.51
2	A	500	HEM	C2B-C1B	-3.09	1.41	1.51
2	B	500	HEM	C3C-CAC	-2.73	1.46	1.51
2	B	500	HEM	C3D-C4D	-2.53	1.48	1.51
2	B	500	HEM	C2B-C1B	-2.48	1.43	1.51
2	A	500	HEM	C3C-CAC	-2.03	1.47	1.51
2	A	500	HEM	FE-NC	2.36	2.05	1.95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	861	ACT	CH3-C	2.37	1.52	1.48
4	B	800	E2Z	C12-N13	2.37	1.35	1.32
2	B	500	HEM	FE-NC	2.61	2.06	1.95
4	A	800	E2Z	C12-N13	2.82	1.36	1.32
4	B	800	E2Z	C12-N11	3.51	1.35	1.31
4	A	800	E2Z	C12-N11	6.19	1.38	1.31

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	E2Z	N11-C12-N13	-6.35	118.47	126.44
2	B	500	HEM	CBA-CAA-C2A	-6.06	101.67	112.53
4	B	800	E2Z	N11-C12-N13	-5.66	119.34	126.44
4	A	800	E2Z	C15-C16-N11	-4.30	118.99	123.90
4	B	800	E2Z	C15-C16-N11	-3.98	119.36	123.90
2	A	500	HEM	C1D-CHD-C4C	-3.28	120.33	125.82
2	A	500	HEM	C3B-C4B-NB	-3.20	105.51	111.63
4	B	800	E2Z	C15-C14-N13	-3.09	118.64	122.41
3	A	600	H4B	N3-C2-N1	-2.59	121.28	125.53
3	B	600	H4B	N3-C2-N1	-2.45	121.51	125.53
2	B	500	HEM	C3B-C4B-NB	-2.20	107.43	111.63
2	B	500	HEM	C1D-CHD-C4C	-2.05	122.40	125.82
2	B	500	HEM	C2D-C3D-C4D	2.08	105.02	101.50
2	A	500	HEM	C2C-C1C-CHC	2.13	126.92	123.68
4	B	800	E2Z	C04-N03-C02	2.16	112.55	108.53
4	A	800	E2Z	C04-N03-C02	2.17	112.57	108.53
3	B	600	H4B	C4A-C8A-N8	2.34	121.19	118.43
4	B	800	E2Z	F7'-C3'-C4'	2.37	122.48	118.52
2	A	500	HEM	CHC-C4B-NB	2.38	130.26	124.52
3	A	600	H4B	C4-N3-C2	2.47	119.36	115.94
4	B	800	E2Z	C1'-C2'-C3'	2.49	120.91	118.84
2	A	500	HEM	CMD-C2D-C3D	2.57	125.70	114.35
2	A	500	HEM	CHD-C1D-ND	2.57	130.70	124.52
2	A	500	HEM	C2D-C3D-C4D	2.70	106.08	101.50
2	B	500	HEM	CMD-C2D-C3D	2.81	126.80	114.35
4	B	800	E2Z	N11-C12-N03	2.88	119.84	115.16
3	B	600	H4B	N2-C2-N3	3.20	122.49	117.20
3	B	600	H4B	C2-N1-C8A	3.22	121.78	114.54
4	A	800	E2Z	N13-C12-N03	3.27	119.66	114.82
2	A	500	HEM	CAA-CBA-CGA	3.29	118.77	112.75
3	A	600	H4B	C2-N1-C8A	3.40	122.19	114.54
2	B	500	HEM	CMB-C2B-C3B	3.49	125.25	116.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	H4B	C4A-C8A-N8	3.75	122.85	118.43
2	A	500	HEM	CAD-C3D-C2D	3.89	124.41	113.22
3	A	600	H4B	N2-C2-N3	3.90	123.65	117.20
2	A	500	HEM	CMC-C2C-C3C	4.00	126.51	116.53
4	B	800	E2Z	N13-C12-N03	4.04	120.80	114.82
4	A	800	E2Z	N11-C12-N03	4.08	121.80	115.16
4	B	800	E2Z	C17-C14-N13	4.13	121.79	115.69
2	B	500	HEM	CAD-C3D-C4D	4.33	127.73	112.47
2	B	500	HEM	CMC-C2C-C3C	4.47	127.68	116.53
4	A	800	E2Z	C12-N13-C14	4.47	121.10	115.26
3	A	600	H4B	C4-C4A-C8A	4.53	118.66	114.56
3	B	600	H4B	C4-C4A-C8A	4.57	118.70	114.56
2	A	500	HEM	CAD-C3D-C4D	4.83	129.50	112.47
4	B	800	E2Z	C12-N13-C14	4.84	121.59	115.26
2	B	500	HEM	CAD-C3D-C2D	4.87	127.21	113.22
2	A	500	HEM	CMB-C2B-C3B	5.64	130.61	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	5	0
4	A	800	E2Z	1	0
2	B	500	HEM	5	0
3	B	600	H4B	1	0
4	B	800	E2Z	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	27 (6%) 21 23	38, 50, 79, 120	0
1	B	404/443 (91%)	0.16	26 (6%) 23 25	37, 55, 86, 115	0
All	All	808/886 (91%)	0.17	53 (6%) 22 24	37, 52, 82, 120	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	GLU	5.6
1	B	259	GLN	5.5
1	A	259	GLN	5.2
1	B	141	LYS	4.8
1	A	160	ALA	4.4
1	A	239	GLY	4.2
1	B	111	LEU	4.1
1	A	126	LEU	3.9
1	B	146	GLN	3.8
1	A	122	ALA	3.8
1	A	338	VAL	3.7
1	B	123	GLU	3.3
1	A	363[A]	GLU	3.3
1	B	338	VAL	3.3
1	A	124	GLN	3.3
1	A	109	ARG	3.2
1	B	261	GLY	3.2
1	B	110	LYS	3.2
1	A	121	PRO	3.2
1	A	156	GLU	3.2
1	B	122	ALA	3.1
1	B	260	ASP	3.1
1	B	223	ARG	3.0
1	B	142	ARG	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	127	SER	2.8
1	B	239	GLY	2.8
1	B	353	ALA	2.7
1	A	261	GLY	2.6
1	B	232	VAL	2.6
1	A	159	VAL	2.5
1	A	67	GLY	2.4
1	A	337	ALA	2.4
1	B	121	PRO	2.4
1	B	337	ALA	2.4
1	A	230	ILE	2.4
1	A	448	ALA	2.4
1	A	260	ASP	2.4
1	B	250	LEU	2.3
1	A	355	PHE	2.3
1	B	91	GLN	2.3
1	B	262	SER	2.3
1	B	143	SER	2.2
1	A	157	ALA	2.2
1	A	257	ARG	2.2
1	B	99	ARG	2.1
1	B	144	GLY	2.1
1	A	99	ARG	2.1
1	A	153	GLN	2.1
1	B	124	GLN	2.1
1	A	354	PRO	2.1
1	B	390	ARG	2.0
1	A	91	GLN	2.0
1	B	92	GLN	2.0

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

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	B	384	9/10	0.96	0.13	-	63,67,104,112	0
1	CAS	A	384	9/10	0.94	0.11	-	47,49,79,88	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(Å <sup>2</sup> )	Q<0.9
6	GOL	A	880	6/6	0.91	0.38	4.47	70,73,78,90	0
5	ACT	B	861	4/4	0.92	0.29	1.97	53,64,64,65	0
6	GOL	B	880	6/6	0.93	0.25	1.82	59,63,68,71	0
3	H4B	B	600	17/17	0.94	0.18	0.63	49,52,56,57	0
4	E2Z	B	800	23/23	0.97	0.21	0.56	37,46,70,77	0
4	E2Z	A	800	23/23	0.95	0.23	0.21	41,46,68,77	0
2	HEM	A	500	43/43	0.98	0.20	0.14	33,38,62,68	0
2	HEM	B	500	43/43	0.98	0.14	-0.27	39,45,59,80	0
3	H4B	A	600	17/17	0.97	0.16	-0.38	45,50,54,55	0
5	ACT	A	860	4/4	0.96	0.10	-0.72	53,60,60,62	0
7	ZN	A	900	1/1	1.00	0.07	-1.39	51,51,51,51	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.