



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 PM GMT

PDB ID : 3RQO  
Title : Structure of the endothelial nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((1S,2R/1R,2S)-2-(3-Clorophenyl)cyclopropylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Delker, S.L.; Poulos, T.L.  
Deposited on : 2011-04-28  
Resolution : 2.08 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

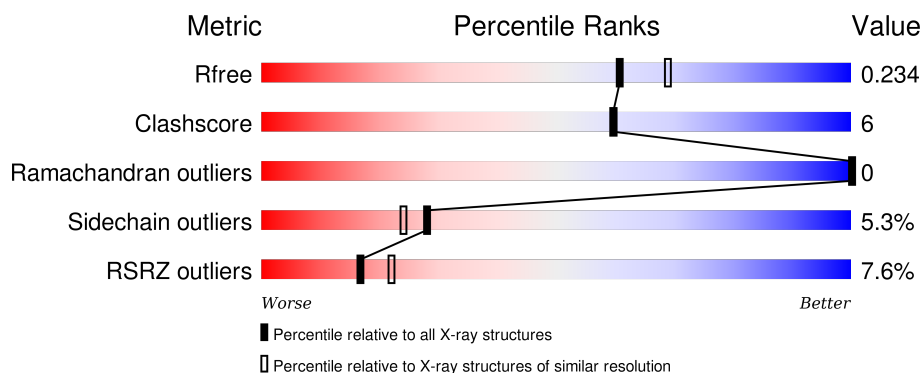
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div>
1	B	443	<div> <div>5%</div> <div>75%</div> <div>14%</div> <div>•</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
5	ACT	A	860	-	-	-	X
5	ACT	B	860	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7032 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	404	Total	C	N	O	S	0	3	0
			3228	2053	568	591	16			
1	B	402	Total	C	N	O	S	0	0	0
			3198	2034	562	586	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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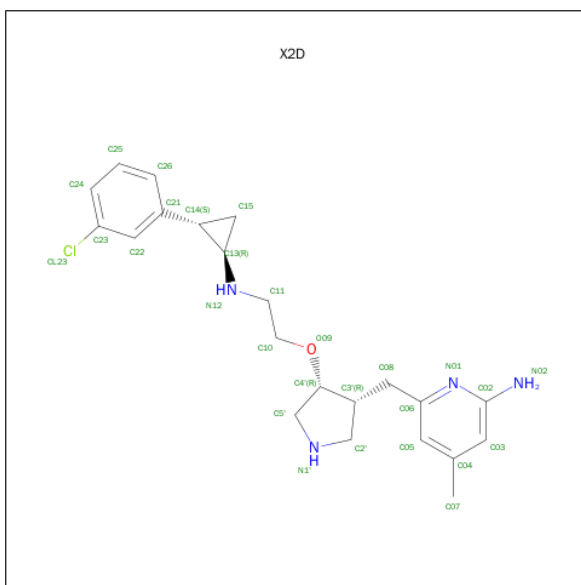
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 6-([(3R,4R)-4-(2-([(1R,2S)-2-(3-CHLOROPHENYL)CYCLOPROPYL]AMINO)ETHOXY)PYRROLIDIN-3-YL]METHYL}-4-METHYLPYRIDIN-2-AMINE (three-letter code: X2D) (formula:  $C_{22}H_{29}ClN_4O$ ).



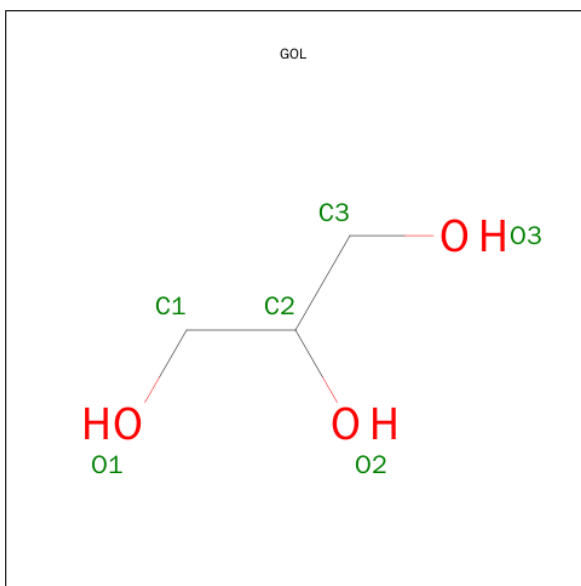
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
4	B	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		

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



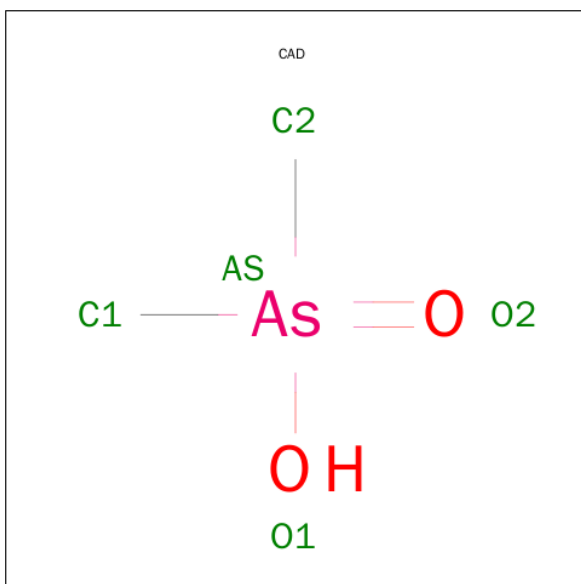
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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



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

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

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

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

- Molecule 9 is water.

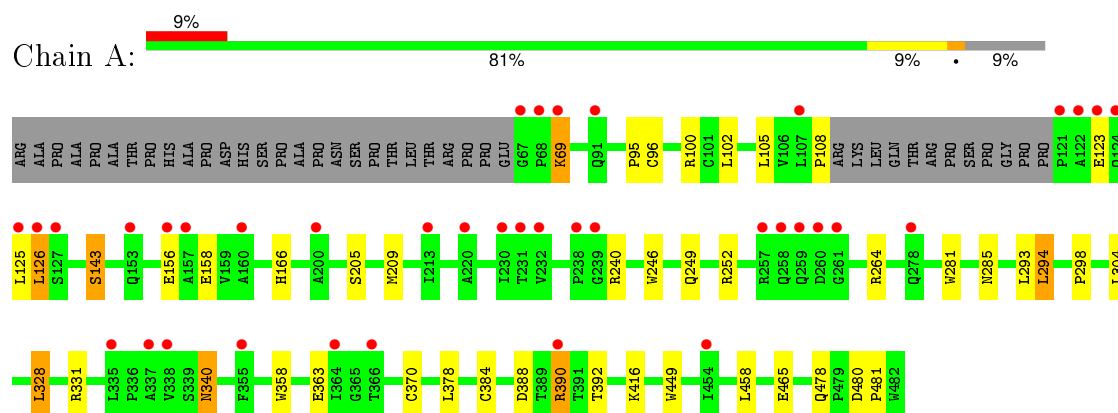
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	198	Total	O	0	0
			198	198		
9	B	205	Total	O	0	0
			205	205		



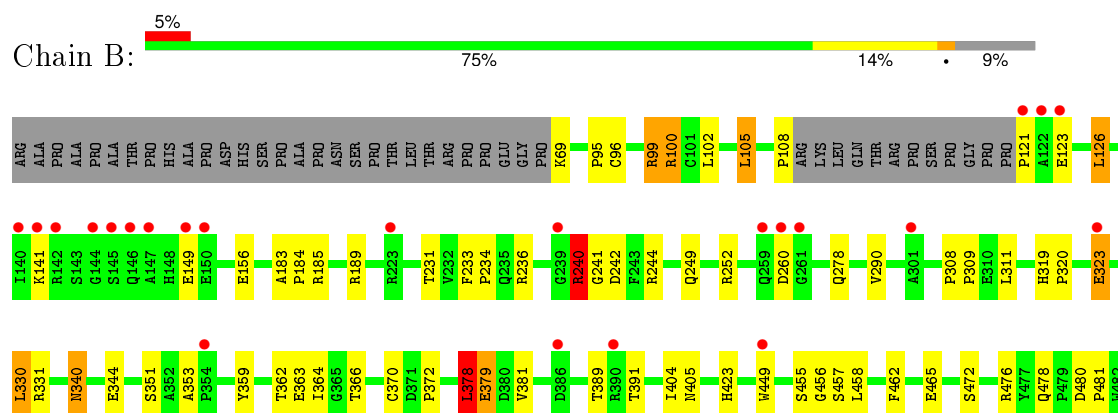
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	58.08Å 106.64Å 156.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.11 – 2.08 35.11 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.11-2.08) 99.3 (35.11-2.08)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.221 0.189 , 0.234	Depositor DCC
$R_{free}$ test set	2930 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.1	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 58735 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, X2D, 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	0.70	0/3327	0.75	1/4531 (0.0%)
1	B	0.73	0/3287	0.75	5/4477 (0.1%)
All	All	0.72	0/6614	0.75	6/9008 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	240	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	189	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	378	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	328	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	189	ARG	NE-CZ-NH2	5.70	123.15	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3140	30	0
1	B	3198	0	3104	42	0
2	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	2	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	28	0	29	2	0
4	B	28	0	29	2	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	3	0	0	3	0
7	B	3	0	0	0	0
8	A	1	0	0	0	0
9	A	198	0	0	2	0
9	B	205	0	0	7	0
All	All	7032	0	6414	74	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 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CYS:SG	7:A:950:CAD:AS	2.59	1.21
1:B:236:ARG:HD3	1:B:242:ASP:OD1	1.62	1.00
1:B:236:ARG:HD3	1:B:242:ASP:CG	2.12	0.68
1:A:340:ASN:HD22	1:A:340:ASN:H	1.41	0.67
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.76	0.66
1:B:363:GLU:OE1	4:B:800:X2D:H14	1.95	0.66
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.37	0.64
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.38	0.63
1:A:388:ASP:OD1	1:A:390:ARG:HG3	2.01	0.61
1:B:240:ARG:HD2	1:B:241:GLY:O	2.00	0.61
1:A:384:CYS:CB	7:A:950:CAD:AS	3.09	0.60
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.83	0.60
1:B:330:LEU:HB2	9:B:1008:HOH:O	2.02	0.60
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.43	0.60
1:B:240:ARG:NH2	9:B:1199:HOH:O	2.31	0.59
1:B:379:GLU:HB2	9:B:1136:HOH:O	2.03	0.58
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.85	0.57
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.35	0.55
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HB2	9:A:1010:HOH:O	2.06	0.55
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.90	0.54
1:B:362:THR:HA	1:B:405:ASN:HD21	1.74	0.53
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.90	0.53
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.90	0.53
1:B:378:LEU:HB2	9:B:1016:HOH:O	2.07	0.52
1:A:143:SER:HB2	9:A:1018:HOH:O	2.09	0.52
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.91	0.52
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.93	0.51
1:B:362:THR:HA	1:B:405:ASN:ND2	2.26	0.51
1:B:95:PRO:HG3	1:B:108:PRO:HG2	1.92	0.50
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.95	0.49
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.95	0.49
1:A:384:CYS:HB3	7:A:950:CAD:AS	2.73	0.48
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.96	0.48
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.95	0.48
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.97	0.47
1:A:340:ASN:O	1:A:478:GLN:HB2	2.15	0.46
1:B:457:SER:HA	1:B:462:PHE:CG	2.50	0.46
1:A:205:SER:O	1:A:209:MET:HG3	2.16	0.46
1:A:264:ARG:HD3	1:A:285:ASN:O	2.15	0.46
1:B:476:ARG:NH1	9:B:1071:HOH:O	2.48	0.46
1:B:231:THR:O	1:B:353:ALA:HA	2.15	0.45
1:A:363:GLU:OE1	4:A:800:X2D:H14	2.17	0.45
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.47	0.45
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.99	0.45
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.00	0.44
1:B:290:VAL:HG23	9:B:1096:HOH:O	2.18	0.44
1:B:323:GLU:CD	1:B:323:GLU:H	2.21	0.43
1:B:366:THR:O	1:B:370:CYS:HB2	2.19	0.42
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.54	0.42
1:B:308:PRO:HA	1:B:309:PRO:HD3	1.94	0.42
1:B:480:ASP:HA	1:B:481:PRO:HD3	1.91	0.42
1:A:480:ASP:HA	1:A:481:PRO:HD3	1.89	0.42
1:A:358:TRP:O	4:A:800:X2D:H25	2.20	0.42
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.54	0.42
1:B:457:SER:HA	1:B:462:PHE:CB	2.50	0.42
1:A:105:LEU:HD22	1:B:465:GLU:HB3	2.01	0.42
1:A:449:TRP:HA	3:A:600:H4B:N1	2.35	0.41
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.50	0.41
1:B:121:PRO:HG2	1:B:123:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:OE1	1:B:472:SER:OG	2.32	0.41
1:B:244:ARG:HD2	1:B:351:SER:HB2	2.02	0.41
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.50	0.41
1:B:455:SER:O	1:B:456:GLY:C	2.59	0.41
1:A:340:ASN:HD22	1:A:340:ASN:N	2.07	0.41
4:B:800:X2D:H26	9:B:1205:HOH:O	2.20	0.41
1:B:340:ASN:O	1:B:478:GLN:HG2	2.19	0.41
1:B:183:ALA:HA	1:B:184:PRO:HD3	1.85	0.41
1:A:392:THR:HB	1:B:423:HIS:HB2	2.03	0.41
1:B:340:ASN:HD22	1:B:340:ASN:H	1.67	0.41
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.86	0.41
1:A:158:GLU:OE1	1:A:166:HIS:HD2	2.04	0.41
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.56	0.41
1:B:185:ARG:HB3	1:B:449:TRP:CE3	2.56	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	403/443 (91%)	393 (98%)	10 (2%)	0	100	100
1	B	398/443 (90%)	384 (96%)	14 (4%)	0	100	100
All	All	801/886 (90%)	777 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	346/376 (92%)	331 (96%)	15 (4%)	35	33
1	B	342/376 (91%)	321 (94%)	21 (6%)	23	18
All	All	688/752 (92%)	652 (95%)	36 (5%)	28	25

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	123	GLU
1	A	125	LEU
1	A	126	LEU
1	A	143	SER
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	B	69	LYS
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	126	LEU
1	B	141	LYS
1	B	149	GLU
1	B	240	ARG
1	B	260	ASP
1	B	278	GLN
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	372	PRO
1	B	378	LEU
1	B	379	GLU

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Mol	Chain	Res	Type
1	B	389	THR
1	B	391	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 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	1.91	7 (23%)	24,82,82	2.45	12 (50%)
3	H4B	A	600	-	13,18,18	0.68	0	11,26,26	2.64	6 (54%)
4	X2D	A	800	-	26,31,31	1.10	2 (7%)	30,43,43	2.36	8 (26%)
5	ACT	A	860	-	1,3,3	1.15	0	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.45	0	5,5,5	0.14	0
7	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	1	30,50,50	2.17	7 (23%)	24,82,82	2.68	14 (58%)
3	H4B	B	600	-	13,18,18	0.82	0	11,26,26	2.17	5 (45%)
4	X2D	B	800	-	26,31,31	0.81	0	30,43,43	2.15	8 (26%)
5	ACT	B	860	-	1,3,3	0.96	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.40	0	5,5,5	0.81	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
4	X2D	A	800	-	-	0/13/30/30	0/3/4/4
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	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
4	X2D	B	800	-	-	0/13/30/30	0/3/4/4
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0
7	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-6.72	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3D-C4D	-5.13	1.45	1.51
2	A	500	HEM	C3D-C4D	-4.56	1.45	1.51
2	A	500	HEM	C3B-C4B	-4.39	1.47	1.51
2	A	500	HEM	C2C-C1C	-4.00	1.45	1.52
2	B	500	HEM	C2C-C1C	-3.46	1.46	1.52
2	A	500	HEM	C2D-C1D	-2.43	1.43	1.51
2	B	500	HEM	C2D-C1D	-2.34	1.44	1.51
2	A	500	HEM	C3B-CAB	2.14	1.55	1.51
2	B	500	HEM	C3B-CAB	2.16	1.55	1.51
4	A	800	X2D	C15-C14	2.16	1.53	1.50
2	A	500	HEM	C4C-NC	2.23	1.38	1.36
4	A	800	X2D	C23-CL23	2.31	1.79	1.74
2	B	500	HEM	FE-ND	2.56	2.11	1.97
2	B	500	HEM	FE-NC	3.13	2.08	1.95
2	A	500	HEM	C1C-NC	3.35	1.40	1.36

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	X2D	C15-C14-C21	-7.18	109.43	122.30
4	B	800	X2D	C15-C14-C21	-7.04	109.68	122.30
2	B	500	HEM	CBA-CAA-C2A	-5.14	103.32	112.53
4	A	800	X2D	C04-C05-C06	-3.80	117.90	120.28
4	B	800	X2D	C15-C13-N12	-3.77	107.89	118.20
2	B	500	HEM	CBD-CAD-C3D	-3.66	102.90	113.55
3	A	600	H4B	N3-C2-N1	-3.39	119.98	125.53
2	A	500	HEM	C3C-CAC-CBC	-3.29	119.41	124.46
2	A	500	HEM	CBA-CAA-C2A	-3.21	106.78	112.53
3	B	600	H4B	N3-C2-N1	-3.18	120.32	125.53
2	B	500	HEM	C3C-CAC-CBC	-3.16	119.61	124.46
4	A	800	X2D	C15-C13-N12	-2.86	110.37	118.20
2	B	500	HEM	CAA-C2A-C1A	-2.82	123.95	127.01
4	B	800	X2D	C04-C05-C06	-2.76	118.55	120.28
4	A	800	X2D	C06-C08-C3'	-2.62	105.48	115.57
2	B	500	HEM	C3B-C4B-NB	-2.35	107.13	111.63
4	A	800	X2D	C05-C06-N01	-2.34	120.32	122.96
2	A	500	HEM	CAA-C2A-C1A	-2.23	124.59	127.01
4	B	800	X2D	C26-C21-C14	-2.20	116.67	121.08
4	B	800	X2D	C21-C14-C13	-2.18	116.87	121.50
2	A	500	HEM	C1D-CHD-C4C	-2.12	122.28	125.82
4	B	800	X2D	C05-C06-N01	-2.11	120.58	122.96
2	A	500	HEM	C3B-C4B-NB	-2.03	107.74	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C2C-C1C-NC	-2.03	106.78	110.21
4	B	800	X2D	C11-N12-C13	2.01	116.92	113.89
3	A	600	H4B	N2-C2-N3	2.01	120.53	117.20
2	A	500	HEM	C3B-C4B-CHC	2.02	126.01	123.16
4	A	800	X2D	N02-C02-N01	2.05	120.24	116.50
2	A	500	HEM	C2D-C3D-C4D	2.33	105.46	101.50
3	B	600	H4B	N2-C2-N3	2.62	121.54	117.20
3	B	600	H4B	C4-N3-C2	2.63	119.59	115.94
2	B	500	HEM	C2C-C1C-CHC	2.67	127.74	123.68
2	B	500	HEM	CMD-C2D-C3D	2.68	126.20	114.35
2	B	500	HEM	C2D-C3D-C4D	2.72	106.11	101.50
2	A	500	HEM	CMD-C2D-C3D	2.82	126.82	114.35
3	A	600	H4B	C2-N1-C8A	2.93	121.11	114.54
3	B	600	H4B	C2-N1-C8A	2.96	121.19	114.54
2	B	500	HEM	C3B-C4B-CHC	3.17	127.62	123.16
3	A	600	H4B	C4A-C8A-N8	3.36	122.39	118.43
2	B	500	HEM	CMB-C2B-C3B	3.39	124.99	116.53
4	A	800	X2D	C11-N12-C13	3.82	119.65	113.89
3	B	600	H4B	C4-C4A-C8A	3.82	118.03	114.56
2	B	500	HEM	CMC-C2C-C3C	3.83	126.10	116.53
2	A	500	HEM	CMC-C2C-C3C	3.85	126.15	116.53
3	A	600	H4B	C4-N3-C2	3.93	121.39	115.94
2	B	500	HEM	CAD-C3D-C4D	4.22	127.34	112.47
2	A	500	HEM	CAD-C3D-C4D	4.47	128.23	112.47
2	A	500	HEM	CAD-C3D-C2D	4.55	126.28	113.22
2	B	500	HEM	CAD-C3D-C2D	4.58	126.38	113.22
3	A	600	H4B	C4-C4A-C8A	4.58	118.71	114.56
4	B	800	X2D	C02-N01-C06	4.77	121.62	118.23
2	A	500	HEM	CMB-C2B-C3B	5.28	129.72	116.53
4	A	800	X2D	C02-N01-C06	6.57	122.90	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	3	0
3	A	600	H4B	1	0
4	A	800	X2D	2	0
7	A	950	CAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	2	0
4	B	800	X2D	2	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%)	0.46	38 (9%) 11 14	26, 38, 61, 81	0
1	B	402/443 (90%)	0.30	23 (5%) 27 34	25, 39, 61, 83	0
All	All	806/886 (90%)	0.38	61 (7%) 17 22	25, 38, 61, 83	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	GLY	6.0
1	A	259	GLN	5.9
1	B	259	GLN	5.2
1	A	122	ALA	4.7
1	A	123	GLU	4.7
1	A	124	GLN	4.6
1	A	68	PRO	4.2
1	B	146	GLN	4.1
1	A	160	ALA	4.1
1	A	69	LYS	4.1
1	A	153	GLN	4.0
1	B	121	PRO	4.0
1	A	121	PRO	3.7
1	B	239	GLY	3.7
1	B	147	ALA	3.7
1	A	257	ARG	3.5
1	A	261	GLY	3.5
1	A	230	ILE	3.3
1	B	122	ALA	3.3
1	A	232	VAL	3.2
1	A	260	ASP	3.1
1	B	261	GLY	3.1
1	B	142	ARG	3.0
1	A	337	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	67	GLY	2.9
1	B	141	LYS	2.9
1	B	323	GLU	2.9
1	A	91	GLN	2.8
1	B	260	ASP	2.7
1	B	144	GLY	2.7
1	A	338	VAL	2.6
1	A	390	ARG	2.6
1	A	125	LEU	2.6
1	A	126	LEU	2.6
1	A	127	SER	2.5
1	A	156	GLU	2.5
1	B	123	GLU	2.5
1	A	213	ILE	2.5
1	A	231	THR	2.4
1	B	145	SER	2.4
1	A	200	ALA	2.3
1	B	390	ARG	2.3
1	A	107	LEU	2.3
1	B	386	ASP	2.3
1	B	449	TRP	2.3
1	A	258	GLN	2.3
1	A	335	LEU	2.3
1	A	355	PHE	2.2
1	A	220	ALA	2.2
1	B	301	ALA	2.2
1	B	223	ARG	2.1
1	A	278	GLN	2.1
1	A	364	ILE	2.1
1	B	150	GLU	2.1
1	B	149	GLU	2.1
1	A	157	ALA	2.1
1	A	366	THR	2.0
1	A	454	ILE	2.0
1	A	238	PRO	2.0
1	B	140	ILE	2.0
1	B	354	PRO	2.0

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

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

### 6.3 Carbohydrates [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
5	ACT	B	860	4/4	0.97	0.25	7.75	47,49,49,51	0
5	ACT	A	860	4/4	0.94	0.19	3.38	45,46,48,48	0
6	GOL	A	880	6/6	0.85	0.21	1.90	55,56,57,57	0
6	GOL	B	880	6/6	0.87	0.20	1.34	52,53,55,55	0
2	HEM	B	500	43/43	0.98	0.17	0.80	27,30,35,36	0
3	H4B	B	600	17/17	0.99	0.16	0.54	23,28,31,34	0
2	HEM	A	500	43/43	0.98	0.17	0.54	21,28,34,39	0
3	H4B	A	600	17/17	0.98	0.15	0.31	23,28,31,31	0
4	X2D	B	800	28/28	0.96	0.16	0.12	33,38,47,53	0
4	X2D	A	800	28/28	0.92	0.17	0.02	29,38,41,47	0
8	ZN	A	900	1/1	1.00	0.08	-0.89	32,32,32,32	0
7	CAD	A	950	3/5	0.98	0.07	-1.95	70,70,70,71	0
7	CAD	B	950	3/5	0.98	0.22	-	77,77,77,77	0

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

There are no such residues in this entry.