



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DQT  
Title : Structure of endothelial NOS heme domain in complex with a inhibitor (+-)-N1-{trans-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(3'-chlorobenzyl)ethane-1,2-diamine  
Authors : Igarashi, J.; Li, H.; Poulos, T.L.  
Deposited on : 2008-07-09  
Resolution : 2.54 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

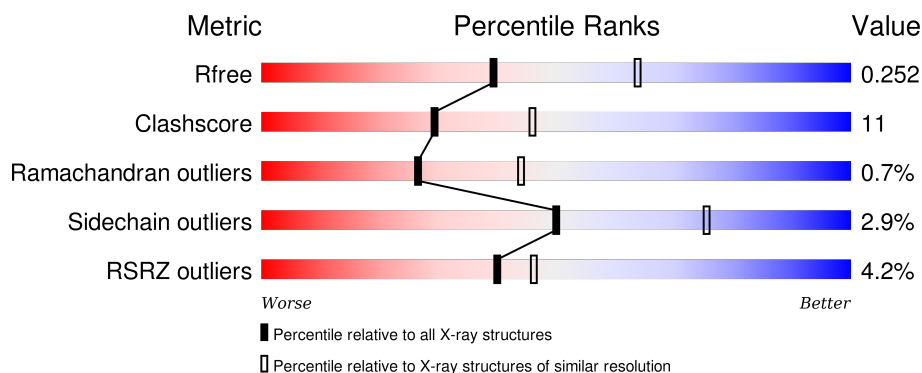
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	416	<div> <div>5%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	B	416	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	860	-	-	-	X
6	H4B	B	760	-	-	-	X
7	JI7	A	800	-	-	-	X
7	JI7	B	800	-	-	-	X
8	GOL	A	880	-	-	-	X
8	GOL	B	880	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6822 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.

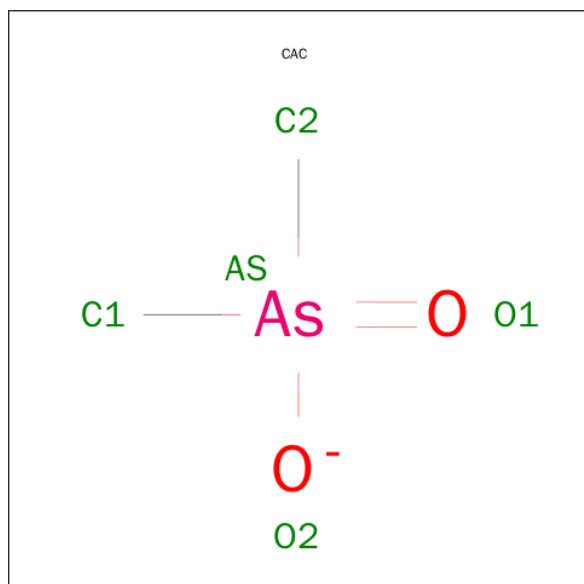
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3216	2046	565	589	16			
1	B	405	Total	C	N	O	S	0	0	0
			3223	2050	568	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	VARIANT	UNP P29473
B	100	ARG	CYS	VARIANT	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



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

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

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



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

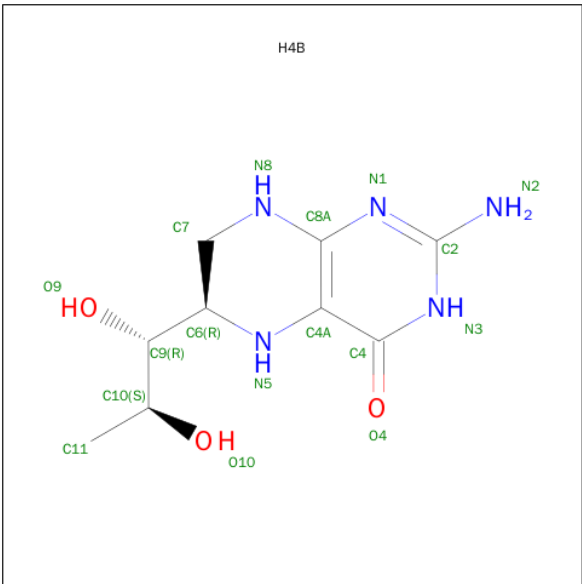
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

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



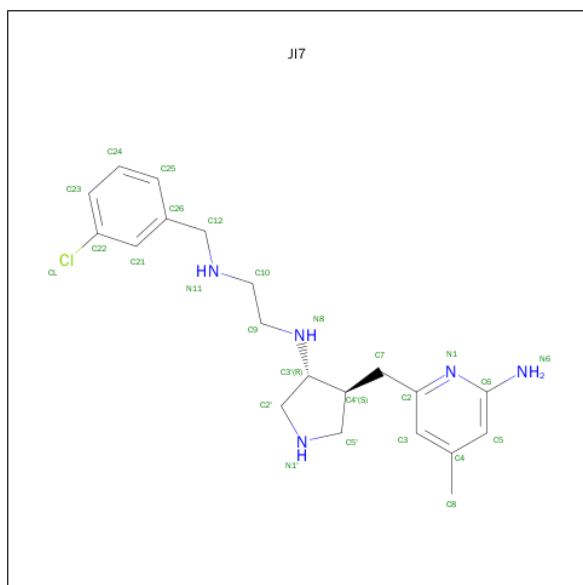
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

- Molecule 7 is N-{(3R,4S)-4-[(6-AMINO-4-METHYLPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL}-N'-(3-CHLOROBENZYL)ETHANE-1,2-DIAMINE (three-letter code: JI7) (formula: C<sub>20</sub>H<sub>28</sub>ClN<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Cl	N	0	0
			26	20	1	5		
7	B	1	Total	C	Cl	N	0	0
			26	20	1	5		

- Molecule 8 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
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

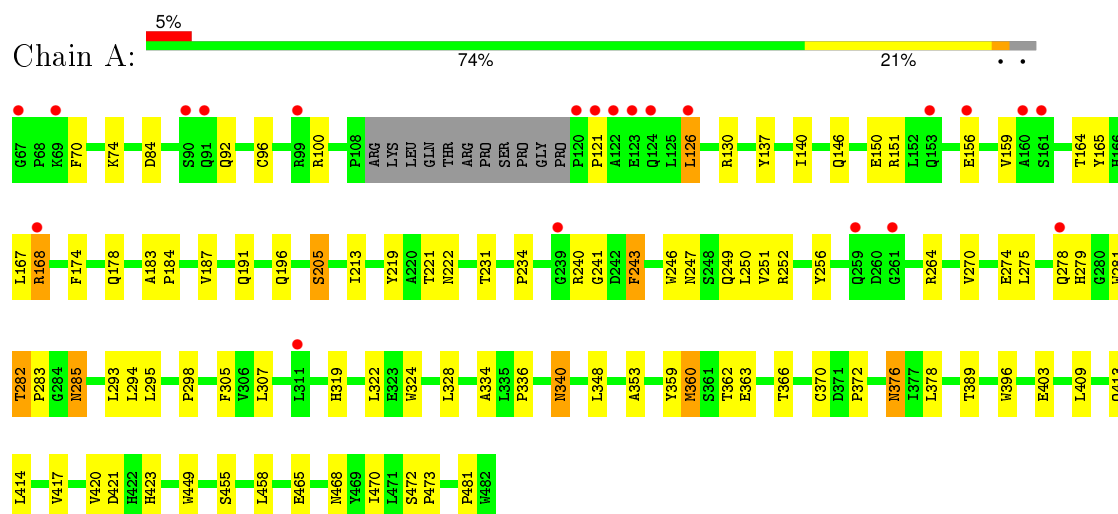
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	102	Total	O	0	0
			102	102		
9	B	82	Total	O	0	0
			82	82		



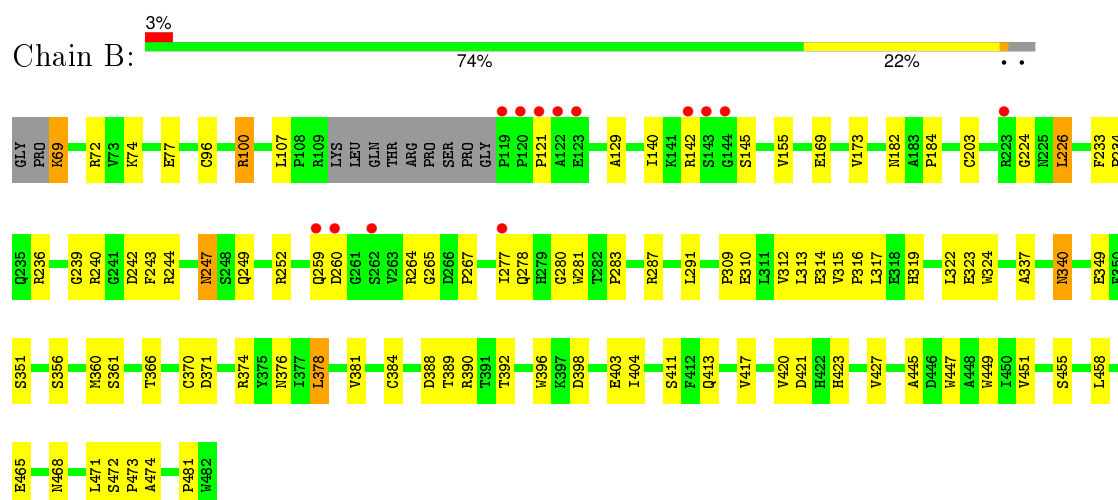
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	58.25Å 106.49Å 156.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 2.54 42.78 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.78-2.54) 99.7 (42.78-2.54)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.197 , 0.258 0.193 , 0.252	Depositor DCC
$R_{free}$ test set	1616 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 32770 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6822	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 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, JI7, ACT, CAC, 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	0.50	0/3307	0.71	2/4506 (0.0%)
1	B	0.48	0/3314	0.71	1/4515 (0.0%)
All	All	0.49	0/6621	0.71	3/9021 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	MET	N-CA-C	-5.57	95.95	111.00
1	B	280	GLY	N-CA-C	5.16	126.01	113.10
1	A	243	PHE	N-CA-C	-5.14	97.12	111.00

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	3216	0	3121	75	0
1	B	3223	0	3131	66	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	43	0	30	4	0
5	B	43	0	30	5	0
6	A	17	0	15	1	0
6	B	17	0	15	2	0
7	A	26	0	28	3	0
7	B	26	0	28	4	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	102	0	0	4	0
9	B	82	0	0	2	0
All	All	6822	0	6420	148	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 11.

All (148) 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:249:GLN:HB2	1:B:252:ARG:HD3	1.39	1.00
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.51	0.92
1:B:69:LYS:HE3	1:B:69:LYS:N	1.86	0.90
1:B:107:LEU:HD21	7:B:800:JI7:H24	1.69	0.75
1:A:205:SER:HB3	9:A:930:HOH:O	1.92	0.69
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.28	0.68
5:B:700:HEM:HMC2	5:B:700:HEM:HBC2	1.75	0.68
1:B:323:GLU:CD	1:B:323:GLU:H	1.97	0.68
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.26	0.66
1:A:126:LEU:HD12	1:A:130:ARG:NH2	2.11	0.65
1:B:310:GLU:H	1:B:310:GLU:CD	1.96	0.65
1:A:126:LEU:O	1:A:130:ARG:HG3	1.97	0.64
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.28	0.63
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.81	0.63
1:B:312:VAL:O	1:B:312:VAL:HG12	1.98	0.62
1:B:310:GLU:OE2	1:B:310:GLU:N	2.31	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.40	0.61
1:B:278:GLN:HG2	1:B:278:GLN:O	2.02	0.60
1:A:151:ARG:NH2	1:A:168:ARG:HD3	2.17	0.59
1:A:372:PRO:HA	1:A:376:ASN:ND2	2.17	0.59
1:B:277:ILE:HD11	1:B:283:PRO:HB3	1.85	0.59
1:B:236:ARG:HG3	1:B:349:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.69	0.58
1:A:151:ARG:CZ	1:A:168:ARG:HD3	2.33	0.58
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.26	0.57
1:A:409:LEU:O	1:A:413:GLN:HG3	2.04	0.57
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.85	0.57
5:B:700:HEM:HHC	5:B:700:HEM:HBB2	1.86	0.57
1:A:378:LEU:HB2	9:A:901:HOH:O	2.04	0.56
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.20	0.56
1:B:361:SER:OG	1:B:421:ASP:HA	2.06	0.56
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.88	0.55
5:B:700:HEM:HBA1	7:B:800:JI7:H72	1.89	0.55
5:A:700:HEM:HBA2	7:A:800:JI7:H72	1.87	0.55
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.22	0.55
1:A:472:SER:HA	1:A:473:PRO:O	2.06	0.55
1:B:324:TRP:CZ3	1:B:384:CYS:HB3	2.43	0.54
1:A:340:ASN:H	1:A:340:ASN:HD22	1.54	0.54
1:B:366:THR:O	1:B:370:CYS:HB2	2.08	0.53
1:B:265:GLY:O	1:B:267:PRO:HD3	2.08	0.53
1:B:337:ALA:CB	1:B:356:SER:HB3	2.38	0.52
1:A:472:SER:HA	1:A:473:PRO:C	2.29	0.52
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.90	0.52
9:A:952:HOH:O	1:B:392:THR:HG22	2.09	0.52
1:B:242:ASP:HB3	1:B:351:SER:OG	2.10	0.51
1:A:295:LEU:HD12	1:A:305:PHE:CD1	2.45	0.51
1:B:247:ASN:N	1:B:247:ASN:OD1	2.44	0.51
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.45	0.50
5:B:700:HEM:CGA	6:B:760:H4B:HN3	2.24	0.50
1:A:414:LEU:HD23	1:A:414:LEU:C	2.32	0.50
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.94	0.50
1:B:313:LEU:HD12	1:B:314:GLU:H	1.78	0.49
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.42	0.49
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.28	0.49
1:B:281:TRP:O	1:B:283:PRO:HD3	2.13	0.49
1:A:389:THR:HA	1:A:396:TRP:CD1	2.48	0.49
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.48	0.48
1:A:340:ASN:HD22	1:A:340:ASN:N	2.11	0.48
1:A:246:TRP:HB2	1:A:294:LEU:HB2	1.95	0.48
1:A:146:GLN:O	1:A:150:GLU:HG3	2.14	0.48
1:A:274:GLU:O	1:A:278:GLN:HG3	2.12	0.48
1:B:423:HIS:O	1:B:427:VAL:HG23	2.14	0.48
1:A:360:MET:HA	1:A:420:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:700:HEM:C1C	7:B:800:JI7:H83	2.49	0.47
1:B:472:SER:HA	1:B:473:PRO:C	2.35	0.47
1:A:168:ARG:HD2	1:A:168:ARG:N	2.29	0.47
1:A:241:GLY:O	1:A:298:PRO:HB3	2.15	0.47
1:B:234:PRO:HB2	1:B:243:PHE:CE1	2.50	0.47
1:A:247:ASN:OD1	1:A:247:ASN:N	2.48	0.47
1:A:174:PHE:CZ	1:A:178:GLN:HG3	2.49	0.47
1:A:275:LEU:O	1:A:279:HIS:HD2	1.97	0.47
1:B:340:ASN:HD22	1:B:340:ASN:H	1.63	0.47
1:B:389:THR:HA	1:B:396:TRP:CD1	2.50	0.47
1:B:313:LEU:HD12	1:B:314:GLU:N	2.30	0.46
7:B:800:JI7:H121	7:B:800:JI7:H91	1.82	0.46
1:A:70:PHE:HB3	1:A:84:ASP:O	2.16	0.46
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.66	0.46
1:A:168:ARG:CZ	9:A:957:HOH:O	2.64	0.46
5:A:700:HEM:O2D	7:A:800:JI7:H92	2.15	0.46
1:A:256:TYR:CE1	1:A:285:ASN:HA	2.51	0.46
1:A:74:LYS:O	1:A:465:GLU:HG3	2.15	0.46
1:A:231:THR:O	1:A:353:ALA:HA	2.16	0.46
1:B:224:GLY:O	1:B:417:VAL:HA	2.16	0.45
1:A:187:VAL:O	1:A:187:VAL:HG22	2.15	0.45
1:A:240:ARG:HG2	1:A:241:GLY:N	2.30	0.45
1:B:72:ARG:NH2	9:B:957:HOH:O	2.42	0.45
1:A:366:THR:O	1:A:370:CYS:HB2	2.17	0.45
1:B:319:HIS:NE2	1:B:403:GLU:OE2	2.44	0.45
1:B:340:ASN:N	1:B:340:ASN:HD22	2.14	0.45
1:A:319:HIS:NE2	1:A:403:GLU:OE1	2.49	0.45
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.97	0.44
1:A:92:GLN:HG2	1:A:470:ILE:HD12	2.00	0.44
1:B:129:ALA:HB1	1:B:155:VAL:HG11	1.98	0.44
1:A:449:TRP:HA	6:A:760:H4B:N1	2.33	0.44
1:A:340:ASN:H	1:A:340:ASN:ND2	2.15	0.44
1:A:363:GLU:OE2	7:A:800:JI7:N1	2.50	0.44
1:B:226:LEU:N	1:B:226:LEU:CD1	2.81	0.43
1:B:360:MET:HA	1:B:420:VAL:O	2.17	0.43
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.00	0.43
1:B:74:LYS:O	1:B:465:GLU:HG3	2.18	0.43
1:B:100:ARG:HG2	1:B:100:ARG:HH11	1.82	0.43
1:A:389:THR:HG22	1:A:396:TRP:CD2	2.54	0.43
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.48	0.43
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ALA:O	1:B:468:ASN:HB2	2.19	0.43
5:A:700:HEM:HMC1	5:A:700:HEM:HBC2	2.01	0.43
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.49	0.43
1:A:270:VAL:O	1:A:274:GLU:HG3	2.19	0.43
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.53	0.43
1:A:360:MET:CE	1:A:362:THR:OG1	2.67	0.43
1:B:169:GLU:O	1:B:173:VAL:HG23	2.18	0.42
1:B:264:ARG:NH1	1:B:287:ARG:HG3	2.35	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.42
1:A:282:THR:HG22	1:A:282:THR:O	2.18	0.42
1:A:191:GLN:HE21	1:A:191:GLN:HB3	1.67	0.42
5:A:700:HEM:HBB2	5:A:700:HEM:HHC	2.01	0.42
1:A:213:ILE:HG23	1:A:250:LEU:HD13	2.02	0.42
1:B:100:ARG:HG2	1:B:100:ARG:NH1	2.35	0.42
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.00	0.42
1:A:293:LEU:HD11	1:A:307:LEU:HD21	2.01	0.42
1:B:471:LEU:O	1:B:474:ALA:HB2	2.20	0.42
1:A:159:VAL:HA	1:A:164:THR:O	2.20	0.42
1:B:226:LEU:HD13	1:B:226:LEU:H	1.85	0.42
1:B:376:ASN:HA	9:B:928:HOH:O	2.20	0.42
1:B:323:GLU:N	1:B:323:GLU:CD	2.70	0.42
1:B:340:ASN:ND2	1:B:340:ASN:H	2.16	0.42
1:A:458:LEU:HD22	1:B:378:LEU:HD21	2.02	0.42
1:B:182:ASN:O	1:B:184:PRO:HD3	2.20	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.94	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.55	0.41
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.20	0.41
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.55	0.41
1:B:317:LEU:HA	1:B:411:SER:OG	2.20	0.41
1:A:96:CYS:HB3	1:B:96:CYS:HB3	2.03	0.41
1:A:251:VAL:O	1:A:252:ARG:HG2	2.20	0.41
1:A:281:TRP:O	1:A:283:PRO:HD3	2.21	0.41
1:B:324:TRP:CZ3	1:B:384:CYS:CB	3.03	0.40
1:B:315:VAL:HA	1:B:316:PRO:HD3	1.86	0.40
1:A:196:GLN:HG2	1:A:219:TYR:CZ	2.56	0.40
1:B:252:ARG:HB2	1:B:291:LEU:HD12	2.03	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.96	0.40
1:A:221:THR:O	1:A:222:ASN:C	2.59	0.40
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.34	0.40
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.03	0.40
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG23	1:A:165:TYR:N	2.37	0.40
1:B:449:TRP:HA	6:B:760:H4B:N1	2.36	0.40
1:A:137:TYR:HA	1:A:140:ILE:HG12	2.03	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	401/416 (96%)	375 (94%)	25 (6%)	1 (0%)	52	73
1	B	401/416 (96%)	367 (92%)	29 (7%)	5 (1%)	16	27
All	All	802/832 (96%)	742 (92%)	54 (7%)	6 (1%)	26	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	SER
1	B	240	ARG
1	A	121	PRO
1	B	239	GLY
1	B	309	PRO
1	B	121	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	344/354 (97%)	335 (97%)	9 (3%)	54	79
1	B	345/354 (98%)	334 (97%)	11 (3%)	46	72
All	All	689/708 (97%)	669 (97%)	20 (3%)	50	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	126	LEU
1	A	168	ARG
1	A	205	SER
1	A	282	THR
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	376	ASN
1	B	69	LYS
1	B	100	ARG
1	B	203	CYS
1	B	226	LEU
1	B	247	ASN
1	B	259	GLN
1	B	260	ASP
1	B	340	ASN
1	B	378	LEU
1	B	398	ASP
1	B	413	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	153	GLN
1	A	191	GLN
1	A	207	GLN
1	A	259	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN

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Mol	Chain	Res	Type
1	B	124	GLN
1	B	146	GLN
1	B	222	ASN
1	B	279	HIS
1	B	340	ASN
1	B	405	ASN
1	B	413	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
5	HEM	A	700	1	30,50,50	2.82	10 (33%)	24,82,82	2.66	10 (41%)
6	H4B	A	760	-	13,18,18	2.06	4 (30%)	11,26,26	4.17	6 (54%)
7	JI7	A	800	-	25,28,28	1.51	4 (16%)	30,37,37	1.16	3 (10%)
2	CAC	A	850	-	0,2,4	0.00	-	0,1,6	0.00	-
3	ACT	A	860	-	1,3,3	2.55	1 (100%)	0,3,3	0.00	-
8	GOL	A	880	-	5,5,5	0.11	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	B	700	1	30,50,50	2.65	8 (26%)	24,82,82	2.49	11 (45%)
6	H4B	B	760	-	13,18,18	2.16	4 (30%)	11,26,26	4.15	6 (54%)
7	JI7	B	800	-	25,28,28	1.42	4 (16%)	30,37,37	1.34	3 (10%)
2	CAC	B	850	-	0,2,4	0.00	-	0,1,6	0.00	-
3	ACT	B	860	-	1,3,3	2.00	1 (100%)	0,3,3	0.00	-
8	GOL	B	880	-	5,5,5	0.12	0	5,5,5	0.26	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
5	HEM	A	700	1	-	0/10/54/54	0/0/8/8
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	JI7	A	800	-	-	0/12/22/22	0/3/3/3
2	CAC	A	850	-	-	0/0/0/0	0/0/0/0
3	ACT	A	860	-	-	0/0/0/0	0/0/0/0
8	GOL	A	880	-	-	0/4/4/4	0/0/0/0
5	HEM	B	700	1	-	0/10/54/54	0/0/8/8
6	H4B	B	760	-	-	0/8/17/17	0/2/2/2
7	JI7	B	800	-	-	0/12/22/22	0/3/3/3
2	CAC	B	850	-	-	0/0/0/0	0/0/0/0
3	ACT	B	860	-	-	0/0/0/0	0/0/0/0
8	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	HEM	C2D-C3D	-6.88	1.33	1.54
5	B	700	HEM	C2D-C3D	-6.14	1.36	1.54
5	A	700	HEM	C3B-CAB	-6.06	1.40	1.51
5	A	700	HEM	C3D-C4D	-6.05	1.43	1.51
5	B	700	HEM	C3C-CAC	-6.00	1.40	1.51
5	B	700	HEM	C3B-CAB	-5.97	1.40	1.51
5	B	700	HEM	C3B-C4B	-5.63	1.46	1.51
5	A	700	HEM	C3B-C4B	-5.28	1.47	1.51
5	A	700	HEM	C3C-CAC	-5.19	1.41	1.51
5	B	700	HEM	C3D-C4D	-4.87	1.45	1.51
5	A	700	HEM	C2C-C1C	-4.23	1.44	1.52
5	B	700	HEM	C2C-C1C	-4.04	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	700	HEM	C2B-C1B	-2.71	1.43	1.51
5	A	700	HEM	C2B-C1B	-2.40	1.44	1.51
5	A	700	HEM	C2D-C1D	-2.15	1.44	1.51
3	B	860	ACT	CH3-C	2.00	1.51	1.48
7	A	800	JI7	C5-C6	2.01	1.43	1.40
7	B	800	JI7	C24-C23	2.01	1.43	1.38
5	B	700	HEM	C1C-NC	2.11	1.38	1.36
6	A	760	H4B	C8A-N1	2.12	1.38	1.34
7	A	800	JI7	C3-C4	2.26	1.42	1.38
7	B	800	JI7	C23-C22	2.55	1.43	1.38
3	A	860	ACT	CH3-C	2.55	1.52	1.48
6	B	760	H4B	C8A-N1	2.64	1.39	1.34
7	B	800	JI7	C21-C22	2.74	1.43	1.38
5	A	700	HEM	C4C-NC	3.11	1.39	1.36
7	A	800	JI7	C21-C22	3.15	1.43	1.38
7	B	800	JI7	C21-C26	3.17	1.44	1.39
6	A	760	H4B	C6-N5	3.18	1.52	1.45
5	A	700	HEM	C1C-NC	3.28	1.40	1.36
6	B	760	H4B	C6-N5	3.30	1.52	1.45
6	A	760	H4B	C4A-N5	3.41	1.45	1.38
6	B	760	H4B	C4A-N5	3.59	1.46	1.38
7	A	800	JI7	C21-C26	3.64	1.45	1.39
6	A	760	H4B	C4-N3	4.82	1.42	1.33
6	B	760	H4B	C4-N3	4.90	1.42	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	HEM	CBA-CAA-C2A	-7.05	99.89	112.53
6	A	760	H4B	N3-C2-N1	-4.92	117.47	125.53
6	B	760	H4B	N3-C2-N1	-4.69	117.84	125.53
5	B	700	HEM	CBA-CAA-C2A	-4.08	105.21	112.53
5	A	700	HEM	CAA-C2A-C1A	-3.14	123.60	127.01
7	B	800	JI7	C4-C3-C2	-2.52	118.70	120.28
5	B	700	HEM	CAA-C2A-C3A	-2.30	122.44	129.00
5	A	700	HEM	CMA-C3A-C2A	2.09	129.61	125.24
5	A	700	HEM	CMD-C2D-C3D	2.10	123.62	114.35
7	A	800	JI7	N6-C6-N1	2.34	120.76	116.50
5	A	700	HEM	C2D-C3D-C4D	2.37	105.51	101.50
5	B	700	HEM	CMD-C2D-C3D	2.38	124.89	114.35
7	A	800	JI7	C10-C9-N8	2.42	114.14	110.67
5	B	700	HEM	C2D-C3D-C4D	2.47	105.68	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	HEM	C3C-CAC-CBC	2.53	128.34	124.46
5	B	700	HEM	CAA-C2A-C1A	3.05	130.32	127.01
5	B	700	HEM	CMC-C2C-C3C	3.08	124.22	116.53
7	B	800	JI7	N6-C6-N1	3.08	122.12	116.50
5	B	700	HEM	C3B-CAB-CBB	3.12	129.25	124.46
5	A	700	HEM	CAD-C3D-C2D	3.13	122.23	113.22
7	A	800	JI7	C6-N1-C2	3.15	120.47	118.23
6	A	760	H4B	C4A-C8A-N8	3.31	122.33	118.43
6	B	760	H4B	C4A-C8A-N8	3.33	122.36	118.43
6	B	760	H4B	C2-N1-C8A	3.45	122.29	114.54
6	A	760	H4B	N2-C2-N1	3.52	123.03	117.20
6	A	760	H4B	C2-N1-C8A	3.52	122.46	114.54
6	B	760	H4B	N2-C2-N1	3.58	123.12	117.20
5	B	700	HEM	C3C-CAC-CBC	4.12	130.78	124.46
5	A	700	HEM	CMC-C2C-C3C	4.29	127.24	116.53
5	B	700	HEM	CAD-C3D-C4D	4.36	127.86	112.47
5	B	700	HEM	CAD-C3D-C2D	4.60	126.44	113.22
5	B	700	HEM	CMB-C2B-C3B	4.80	128.50	116.53
7	B	800	JI7	C6-N1-C2	4.86	121.68	118.23
5	A	700	HEM	CMB-C2B-C3B	4.87	128.69	116.53
5	A	700	HEM	CAD-C3D-C4D	5.61	132.25	112.47
6	A	760	H4B	C4-N3-C2	6.52	124.98	115.94
6	B	760	H4B	C4-N3-C2	6.54	125.02	115.94
6	A	760	H4B	C4-C4A-C8A	9.22	122.91	114.56
6	B	760	H4B	C4-C4A-C8A	9.22	122.91	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	HEM	4	0
6	A	760	H4B	1	0
7	A	800	JI7	3	0
5	B	700	HEM	5	0
6	B	760	H4B	2	0
7	B	800	JI7	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	405/416 (97%)	0.08	21 (5%) 31 36	31, 47, 73, 101	0
1	B	405/416 (97%)	0.16	13 (3%) 51 57	31, 51, 77, 117	0
All	All	810/832 (97%)	0.12	34 (4%) 40 46	31, 49, 75, 117	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	PRO	13.2
1	B	120	PRO	6.0
1	B	259	GLN	3.9
1	A	259	GLN	3.7
1	A	120	PRO	3.7
1	A	160	ALA	3.6
1	A	123	GLU	3.5
1	A	121	PRO	3.4
1	B	121	PRO	3.3
1	A	161	SER	3.0
1	B	142	ARG	3.0
1	A	91	GLN	2.8
1	B	277	ILE	2.8
1	A	67	GLY	2.7
1	A	239	GLY	2.7
1	A	156	GLU	2.7
1	A	126	LEU	2.7
1	A	69	LYS	2.6
1	A	99	ARG	2.6
1	A	122	ALA	2.6
1	B	123	GLU	2.5
1	B	122	ALA	2.5
1	A	311	LEU	2.4
1	B	223	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	2.3
1	A	278	GLN	2.3
1	A	168	ARG	2.2
1	B	260	ASP	2.2
1	A	90	SER	2.2
1	B	143	SER	2.1
1	A	124	GLN	2.1
1	B	144	GLY	2.1
1	A	153	GLN	2.1
1	B	262	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	GOL	B	880	6/6	0.92	0.30	4.93	69,71,74,75	0
8	GOL	A	880	6/6	0.92	0.21	3.68	66,66,69,69	0
7	JI7	A	800	26/26	0.86	0.29	2.70	29,51,88,88	0
3	ACT	B	860	4/4	0.97	0.21	2.64	45,50,50,57	0
7	JI7	B	800	26/26	0.89	0.26	2.54	38,50,86,87	0
6	H4B	B	760	17/17	0.93	0.21	2.10	54,61,71,72	0
6	H4B	A	760	17/17	0.95	0.17	1.87	58,61,64,64	0
3	ACT	A	860	4/4	0.97	0.13	0.97	44,45,46,47	0
5	HEM	B	700	43/43	0.98	0.18	0.42	29,34,62,69	0
5	HEM	A	700	43/43	0.98	0.16	0.32	26,35,60,63	0
2	CAC	B	850	3/5	0.97	0.14	-1.07	87,87,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CAC	A	850	3/5	0.99	0.09	-1.31	61,61,63,71	0
4	ZN	B	900	1/1	0.99	0.06	-1.90	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.