



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DQR  
Title : Structure of neuronal NOS D597N/M336V mutant heme domain in complex with a inhibitor (+-)-N1-{cis-4'-[(6"-aminopyridin-2"-yl)methyl]pyrrolidin-3'-yl}ethane-1,2-diamine  
Authors : Igarashi, J.; Li, H.; Poulos, T.L.  
Deposited on : 2008-07-09  
Resolution : 2.40 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

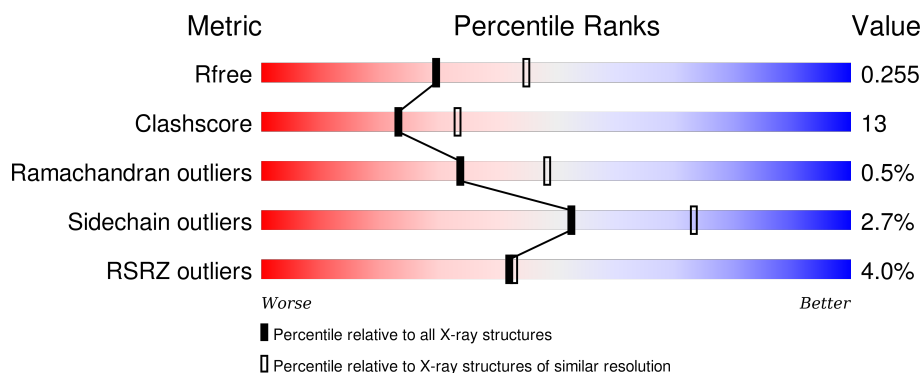
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	422	<div> <div>5%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
1	B	422	<div> <div>3%</div> <div>77%</div> <div>19%</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
2	ACT	A	860	-	-	-	X
2	ACT	B	860	-	-	-	X
6	JI2	A	800	-	-	-	X
6	JI2	B	800	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7087 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, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3312	2121	567	604	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2140	575	609	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	ENGINEERED	UNP P29476
A	597	ASN	ASP	ENGINEERED	UNP P29476
B	336	VAL	MET	ENGINEERED	UNP P29476
B	597	ASN	ASP	ENGINEERED	UNP P29476

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

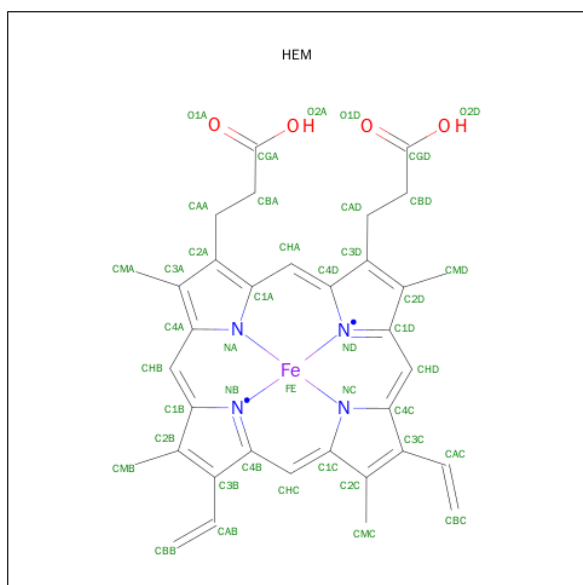


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



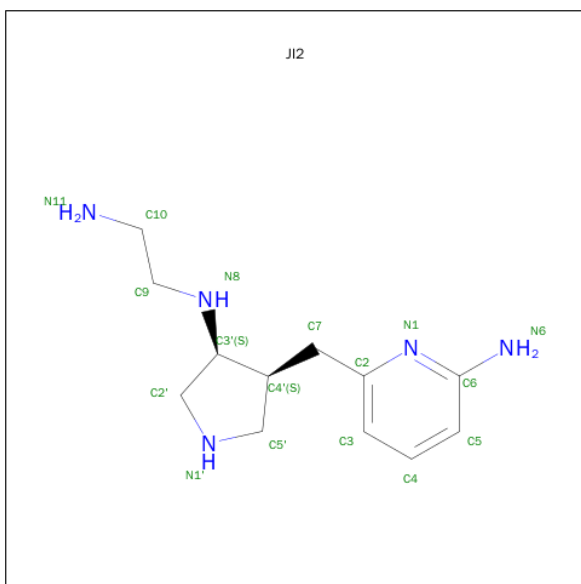
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 6 is N-[(3S,4S)-4-[(6-AMINOPYRIDIN-2-YL)METHYL]PYRROLIDIN-3-YL]ETHANE-1,2-DIAMINE (three-letter code: JI2) (formula: C<sub>12</sub>H<sub>21</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			17	12	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			17	12	5		

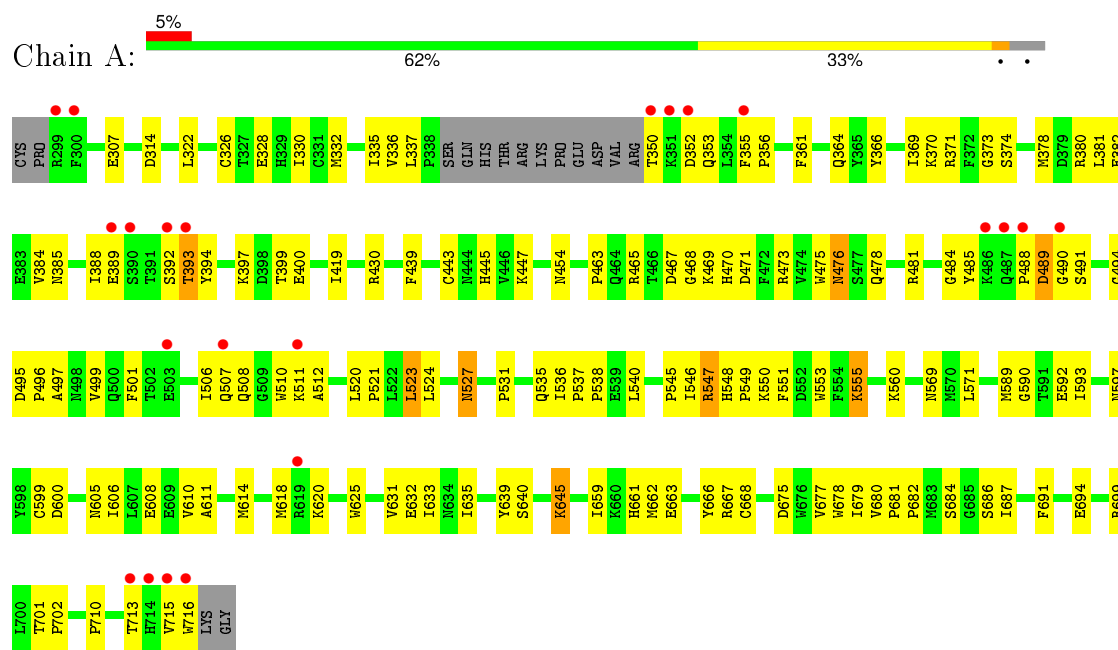
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	110	Total	O	0	0
			110	110		
7	B	158	Total	O	0	0
			158	158		

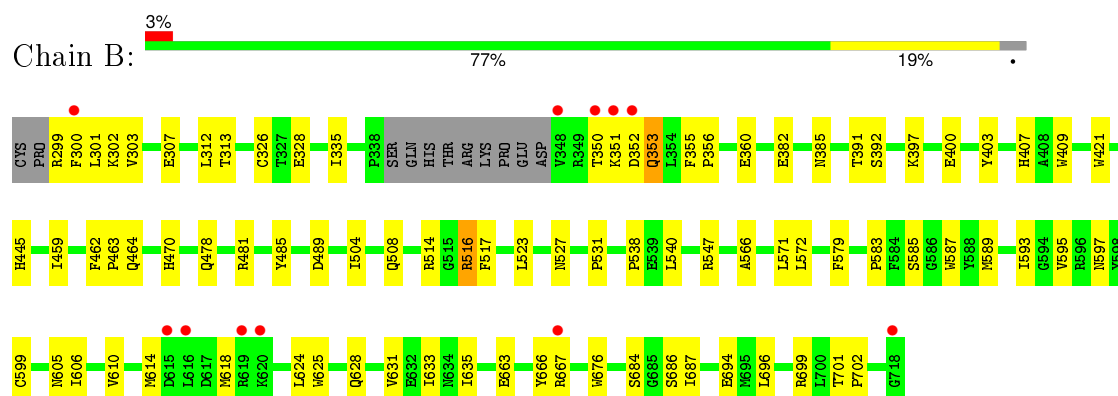
### 3 Residue-property plots [i](#)

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, brain



- Molecule 1: Nitric oxide synthase, brain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.87Å 110.70Å 164.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.94 – 2.40 38.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.94-2.40) 99.3 (38.94-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.261 0.202 , 0.255	Depositor DCC
$R_{free}$ test set	1882 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37621 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, JI2, H4B, ACT

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	0.46	0/3405	0.69	2/4621 (0.0%)
1	B	0.50	0/3437	0.69	2/4661 (0.0%)
All	All	0.48	0/6842	0.69	4/9282 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	CYS	CA-CB-SG	8.11	128.59	114.00
1	A	589	MET	N-CA-C	-6.13	94.44	111.00
1	B	589	MET	N-CA-C	-5.78	95.39	111.00
1	A	326	CYS	CA-CB-SG	5.56	124.01	114.00

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	3312	0	3223	123	0
1	B	3344	0	3261	61	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	6	0
4	B	43	0	30	2	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	17	0	21	4	0
6	B	17	0	21	1	0
7	A	110	0	0	5	0
7	B	158	0	0	3	0
All	All	7087	0	6622	180	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 13.

All (180) 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:523:LEU:HD22	1:A:531:PRO:HB2	1.34	1.10
1:A:350:THR:HB	1:A:353:GLN:HG3	1.51	0.89
1:A:380:ARG:NH1	1:A:397:LYS:HG2	1.87	0.89
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.08	0.83
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.44	0.82
1:A:307:GLU:HG3	7:B:210:HOH:O	1.81	0.81
1:A:374:SER:O	1:A:378:MET:HG2	1.82	0.78
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.70	0.74
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.71	0.73
1:B:350:THR:HG22	1:B:352:ASP:H	1.54	0.72
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.03	0.72
4:B:750:HEM:HBA2	6:B:800:JI2:H72	1.72	0.70
1:A:361:PHE:O	1:A:364:GLN:HG2	1.92	0.68
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.75	0.68
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.77	0.66
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.31	0.66
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.78	0.65
1:B:307:GLU:HG3	7:B:49:HOH:O	1.96	0.65
1:A:322:LEU:HB3	1:A:699:ARG:NH2	2.13	0.64
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.13	0.64
1:A:350:THR:HB	1:A:353:GLN:CG	2.25	0.63
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.13	0.63
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.13	0.63
1:A:373:GLY:HA2	1:A:378:MET:CE	2.30	0.62
1:A:328:GLU:H	1:A:328:GLU:CD	2.02	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:HA	1:B:312:LEU:O	2.00	0.62
1:A:659:ILE:O	1:A:663:GLU:HG3	2.00	0.61
1:B:356:PRO:O	1:B:360:GLU:HG3	2.01	0.61
1:A:399:THR:HG23	7:A:221:HOH:O	2.01	0.60
1:A:350:THR:HG22	1:A:352:ASP:H	1.65	0.60
1:B:391:THR:O	1:B:392:SER:HB2	2.02	0.60
1:A:675:ASP:O	1:A:679:ILE:HG12	2.03	0.59
1:A:715:VAL:HG23	1:A:715:VAL:O	2.02	0.58
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.86	0.58
1:A:384:VAL:O	1:A:388:ILE:HG13	2.03	0.58
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.68	0.57
4:A:750:HEM:HBA2	6:A:800:JI2:H72	1.86	0.57
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.86	0.57
1:A:608:GLU:O	1:A:611:ALA:HB3	2.05	0.56
1:A:694:GLU:HG2	1:B:335:ILE:HA	1.87	0.56
1:B:353:GLN:O	1:B:356:PRO:HG2	2.04	0.56
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.69	0.56
1:B:610:VAL:O	1:B:614:MET:HG3	2.04	0.56
1:A:382:GLU:OE1	1:A:385:ASN:HB3	2.04	0.56
1:A:373:GLY:HA2	1:A:378:MET:HE3	1.88	0.56
1:B:587:TRP:H	4:B:750:HEM:HAB	1.71	0.55
1:A:682:PRO:HB2	1:B:686:SER:OG	2.07	0.55
1:B:523:LEU:CD1	1:B:531:PRO:HB2	2.36	0.55
1:B:631:VAL:O	1:B:635:ILE:HG13	2.06	0.55
1:A:667:ARG:HG3	1:A:667:ARG:HH11	1.72	0.55
1:B:516:ARG:HG2	1:B:517:PHE:CE1	2.41	0.55
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.72	0.55
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.72	0.54
1:A:571:LEU:C	1:A:571:LEU:HD23	2.27	0.54
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.88	0.54
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.72	0.53
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.90	0.53
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.82	0.53
1:A:484:GLY:O	1:A:499:VAL:HA	2.09	0.53
1:B:593:ILE:HA	1:B:597:ASN:HB2	1.92	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.25	0.52
1:A:677:VAL:HG22	1:B:676:TRP:CE3	2.45	0.52
1:A:392:SER:O	1:A:393:THR:HB	2.10	0.51
1:A:489:ASP:O	1:A:489:ASP:OD2	2.27	0.51
1:A:489:ASP:C	1:A:491:SER:H	2.12	0.51
1:B:701:THR:HA	1:B:702:PRO:C	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.26	0.51
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.93	0.51
1:A:631:VAL:HG11	1:B:628:GLN:CG	2.38	0.50
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.11	0.50
1:A:314:ASP:HB2	1:A:666:TYR:HE2	1.77	0.50
1:A:701:THR:HA	1:A:702:PRO:C	2.32	0.50
1:A:419:ILE:HA	1:A:661:HIS:ND1	2.27	0.50
1:B:382:GLU:HA	1:B:382:GLU:OE1	2.11	0.50
4:A:750:HEM:HBB2	4:A:750:HEM:HHC	1.94	0.50
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.12	0.49
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.00	0.49
1:A:592:GLU:OE1	6:A:800:JI2:N1	2.46	0.49
1:A:606:ILE:O	1:A:610:VAL:HG23	2.11	0.49
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.42	0.49
1:A:488:PRO:C	1:A:490:GLY:H	2.15	0.49
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.78	0.49
1:A:494:GLY:O	1:A:496:PRO:HD3	2.12	0.49
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.48	0.49
1:B:699:ARG:HA	7:B:50:HOH:O	2.11	0.49
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.06	0.49
1:B:299:ARG:CB	1:B:299:ARG:NH1	2.75	0.48
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.43	0.48
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.96	0.48
1:A:549:PRO:O	1:A:550:LYS:HD3	2.14	0.48
1:A:447:LYS:HE2	7:A:185:HOH:O	2.14	0.48
1:A:445:HIS:C	1:A:445:HIS:CD2	2.86	0.48
1:A:373:GLY:HA2	1:A:378:MET:HE1	1.96	0.48
1:B:350:THR:HG22	1:B:351:LYS:N	2.29	0.48
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.49	0.48
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.49	0.47
1:A:475:TRP:CE3	1:A:523:LEU:HD13	2.49	0.47
1:A:476:ASN:OD1	1:A:476:ASN:N	2.47	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.15	0.47
1:B:303:VAL:CG2	1:B:312:LEU:HB2	2.44	0.47
1:A:667:ARG:HG3	1:A:667:ARG:NH1	2.29	0.47
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.50	0.47
1:A:370:LYS:O	1:A:371:ARG:HG3	2.15	0.47
1:A:551:PHE:CD1	1:A:553:TRP:CZ2	3.03	0.47
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.46	0.46
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.50	0.46
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.28	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:O	1:B:508:GLN:HG2	2.15	0.46
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.97	0.46
1:A:537:PRO:HD2	1:A:540:LEU:HD12	1.97	0.46
1:A:614:MET:CE	1:A:632:GLU:HG3	2.46	0.46
1:A:507:GLN:O	1:A:507:GLN:HG2	2.15	0.45
1:A:645:LYS:HB2	1:A:645:LYS:HE3	1.86	0.45
1:A:508:GLN:HA	1:A:508:GLN:NE2	2.31	0.45
1:A:635:ILE:HG13	1:B:624:LEU:HD12	1.97	0.45
1:A:380:ARG:HH11	1:A:397:LYS:HG2	1.76	0.45
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.94	0.45
1:A:508:GLN:OE1	1:A:716:TRP:CZ3	2.70	0.45
1:A:384:VAL:HG13	1:A:394:TYR:CD1	2.52	0.45
1:A:535:GLN:O	1:A:536:ILE:C	2.54	0.45
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.78	0.45
1:A:610:VAL:HG21	1:A:633:ILE:CD1	2.47	0.45
1:A:599:CYS:O	1:A:600:ASP:C	2.53	0.45
1:A:618:MET:HA	1:A:625:TRP:CD1	2.51	0.45
1:A:713:THR:HG22	1:A:713:THR:O	2.17	0.45
1:A:353:GLN:O	1:A:356:PRO:HG2	2.18	0.44
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.83	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.44
1:B:300:PHE:CD1	1:B:300:PHE:N	2.85	0.44
1:A:380:ARG:NH2	1:A:384:VAL:HG22	2.33	0.43
1:A:495:ASP:OD1	1:A:497:ALA:HB3	2.18	0.43
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.43
1:A:467:ASP:C	1:A:469:LYS:H	2.21	0.43
1:B:566:ALA:HB2	1:B:585:SER:HB3	2.01	0.43
1:A:560:LYS:HE3	7:A:125:HOH:O	2.18	0.43
1:A:380:ARG:HH12	1:A:397:LYS:HG2	1.73	0.43
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.83	0.43
1:A:488:PRO:C	1:A:490:GLY:N	2.72	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.54	0.43
1:B:301:LEU:O	1:B:313:THR:HA	2.19	0.42
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.00	0.42
1:A:467:ASP:O	1:A:469:LYS:N	2.52	0.42
1:A:336:VAL:HG12	1:A:337:LEU:HG	2.01	0.42
1:A:465:ARG:HG3	1:A:471:ASP:OD1	2.20	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.42
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.02	0.42
1:B:571:LEU:C	1:B:571:LEU:HD23	2.40	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.55	0.42
1:B:572:LEU:HB3	1:B:579:PHE:HB2	2.01	0.42
1:B:459:ILE:HG13	1:B:583:PRO:O	2.20	0.42
1:A:511:LYS:HE2	1:A:511:LYS:HB3	1.89	0.42
4:A:750:HEM:CBA	6:A:800:JI2:H72	2.50	0.42
1:A:551:PHE:CE1	1:A:614:MET:HE3	2.54	0.42
1:B:523:LEU:HD12	1:B:531:PRO:HB2	2.02	0.42
1:A:593:ILE:HA	1:A:597:ASN:ND2	2.34	0.42
1:B:397:LYS:HB2	1:B:400:GLU:HG3	2.01	0.41
1:A:590:GLY:HA3	7:A:235:HOH:O	2.20	0.41
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.50	0.41
1:B:489:ASP:OD2	1:B:489:ASP:C	2.58	0.41
1:B:470:HIS:O	1:B:527:ASN:HA	2.20	0.41
1:A:332:MET:CE	1:B:301:LEU:HD22	2.51	0.41
1:A:465:ARG:HG3	7:A:33:HOH:O	2.20	0.41
1:A:496:PRO:HA	1:A:499:VAL:CG2	2.47	0.41
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.35	0.41
4:A:750:HEM:O2D	6:A:800:JI2:H102	2.21	0.41
1:A:506:ILE:C	1:A:508:GLN:N	2.74	0.41
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.51	0.41
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.56	0.41
1:A:546:ILE:HA	1:A:640:SER:OG	2.21	0.41
1:A:678:TRP:HA	5:A:760:H4B:N1	2.36	0.41
1:B:299:ARG:HB2	1:B:299:ARG:CZ	2.51	0.40
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.03	0.40
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.35	0.40
4:A:750:HEM:CMC	4:A:750:HEM:HBC2	2.46	0.40
1:A:430:ARG:O	1:A:463:PRO:HG3	2.21	0.40
1:A:314:ASP:HB2	1:A:666:TYR:CE2	2.56	0.40
1:B:684:SER:HB3	1:B:687:ILE:HD11	2.04	0.40
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.36	0.40
1:B:618:MET:HG2	1:B:625:TRP:CD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	403/422 (96%)	368 (91%)	31 (8%)	4 (1%)	19	28
1	B	407/422 (96%)	389 (96%)	18 (4%)	0	100	100
All	All	810/844 (96%)	757 (94%)	49 (6%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	THR
1	A	468	GLY
1	A	605	ASN
1	A	489	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	350 (96%)	13 (4%)	42	63
1	B	366/377 (97%)	359 (98%)	7 (2%)	65	83
All	All	729/754 (97%)	709 (97%)	20 (3%)	52	73

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

Mol	Chain	Res	Type
1	A	381	LEU
1	A	389	GLU
1	A	454	ASN
1	A	476	ASN
1	A	523	LEU
1	A	527	ASN
1	A	538	PRO
1	A	547	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	662	MET
1	B	328	GLU
1	B	353	GLN
1	B	516	ARG
1	B	538	PRO
1	B	540	LEU
1	B	547	ARG
1	B	605	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	507	GLN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	642	GLN
1	B	697	ASN

### 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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
4	HEM	A	750	1	30,50,50	2.90	10 (33%)	24,82,82	2.58	8 (33%)
5	H4B	A	760	-	13,18,18	2.23	3 (23%)	11,26,26	4.06	6 (54%)
6	JI2	A	800	-	15,18,18	2.06	5 (33%)	16,23,23	2.33	3 (18%)
2	ACT	A	860	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
4	HEM	B	750	1	30,50,50	2.61	9 (30%)	24,82,82	2.69	9 (37%)
5	H4B	B	760	-	13,18,18	2.43	3 (23%)	11,26,26	4.02	6 (54%)
6	JI2	B	800	-	15,18,18	2.04	5 (33%)	16,23,23	2.44	3 (18%)
2	ACT	B	860	-	1,3,3	2.72	1 (100%)	0,3,3	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
4	HEM	A	750	1	-	0/10/54/54	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	JI2	A	800	-	-	0/8/18/18	0/2/2/2
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/10/54/54	0/0/8/8
5	H4B	B	760	-	-	0/8/17/17	0/2/2/2
6	JI2	B	800	-	-	0/8/18/18	0/2/2/2
2	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	HEM	C3D-C4D	-7.46	1.42	1.51
4	B	750	HEM	C3D-C4D	-7.28	1.42	1.51
4	A	750	HEM	C3C-CAC	-6.31	1.39	1.51
4	A	750	HEM	C2D-C3D	-5.97	1.36	1.54
4	A	750	HEM	C3B-C4B	-5.83	1.46	1.51
4	B	750	HEM	C2D-C3D	-5.56	1.37	1.54
4	B	750	HEM	C3B-CAB	-5.42	1.41	1.51
4	A	750	HEM	C3B-CAB	-4.60	1.42	1.51
4	B	750	HEM	C2C-C1C	-4.57	1.43	1.52
4	B	750	HEM	C3C-CAC	-4.57	1.42	1.51
4	A	750	HEM	C2C-C1C	-3.80	1.45	1.52
4	B	750	HEM	C3B-C4B	-3.25	1.49	1.51
4	A	750	HEM	C2D-C1D	-2.86	1.42	1.51
4	B	750	HEM	C2D-C1D	-2.50	1.43	1.51
4	A	750	HEM	C2B-C1B	-2.04	1.45	1.51
4	B	750	HEM	CMD-C2D	2.15	1.58	1.53
6	B	800	JI2	C2-N1	2.55	1.39	1.34
2	B	860	ACT	CH3-C	2.72	1.52	1.48
4	A	750	HEM	C1C-NC	2.78	1.39	1.36
4	B	750	HEM	C1C-NC	2.80	1.39	1.36
6	B	800	JI2	C3-C2	2.90	1.45	1.38
6	A	800	JI2	C3-C2	2.90	1.45	1.38
6	B	800	JI2	C4-C3	2.91	1.44	1.38
6	A	800	JI2	C4-C3	2.97	1.45	1.38
6	A	800	JI2	C4-C5	3.03	1.45	1.38
4	A	750	HEM	CHC-C1C	3.06	1.43	1.36
6	B	800	JI2	C4-C5	3.23	1.45	1.38
6	A	800	JI2	C2-N1	3.28	1.40	1.34
2	A	860	ACT	CH3-C	3.53	1.53	1.48
6	A	800	JI2	C7-C4'	3.63	1.59	1.53
5	A	760	H4B	C4A-N5	3.74	1.46	1.38
5	B	760	H4B	C4A-N5	3.93	1.47	1.38
5	A	760	H4B	C6-N5	4.11	1.54	1.45
6	B	800	JI2	C7-C4'	4.27	1.60	1.53
5	B	760	H4B	C6-N5	4.38	1.54	1.45
5	A	760	H4B	C4-N3	4.93	1.42	1.33
5	B	760	H4B	C4-N3	5.79	1.43	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-5.48	102.70	112.53
5	A	760	H4B	N3-C2-N1	-4.54	118.09	125.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	760	H4B	N3-C2-N1	-4.38	118.35	125.53
4	A	750	HEM	CBA-CAA-C2A	-4.02	105.32	112.53
4	B	750	HEM	CAA-C2A-C1A	-3.19	123.54	127.01
6	A	800	JI2	C5'-C4'-C3'	-2.12	100.86	103.80
6	B	800	JI2	C5-C6-N1	-2.10	119.14	121.80
4	B	750	HEM	C3B-C4B-CHC	2.76	127.05	123.16
4	B	750	HEM	CAD-C3D-C4D	2.78	122.28	112.47
5	B	760	H4B	N2-C2-N1	2.83	121.89	117.20
4	A	750	HEM	CAD-C3D-C4D	2.83	122.47	112.47
4	A	750	HEM	CMD-C2D-C3D	3.02	127.70	114.35
5	A	760	H4B	N2-C2-N1	3.06	122.27	117.20
6	B	800	JI2	C9-N8-C3'	3.21	118.72	113.89
4	B	750	HEM	C2D-C3D-C4D	3.31	107.11	101.50
6	A	800	JI2	C9-N8-C3'	3.38	118.99	113.89
4	A	750	HEM	C3B-C4B-CHC	3.47	128.05	123.16
5	B	760	H4B	C2-N1-C8A	3.52	122.46	114.54
5	A	760	H4B	C4A-C8A-N8	3.75	122.84	118.43
4	B	750	HEM	CMD-C2D-C3D	3.76	130.97	114.35
5	A	760	H4B	C2-N1-C8A	3.84	123.18	114.54
5	B	760	H4B	C4A-C8A-N8	3.90	123.02	118.43
4	A	750	HEM	C2D-C3D-C4D	3.91	108.13	101.50
4	A	750	HEM	CMB-C2B-C3B	4.56	127.92	116.53
4	B	750	HEM	CMC-C2C-C3C	4.63	128.08	116.53
4	B	750	HEM	CMB-C2B-C3B	5.13	129.33	116.53
4	A	750	HEM	CMC-C2C-C3C	5.58	130.46	116.53
4	A	750	HEM	CAD-C3D-C2D	5.61	129.35	113.22
4	B	750	HEM	CAD-C3D-C2D	6.04	130.59	113.22
5	B	760	H4B	C4-N3-C2	6.20	124.55	115.94
5	A	760	H4B	C4-N3-C2	6.46	124.91	115.94
6	A	800	JI2	C6-N1-C2	7.40	123.49	118.23
6	B	800	JI2	C6-N1-C2	8.08	123.97	118.23
5	A	760	H4B	C4-C4A-C8A	8.77	122.50	114.56
5	B	760	H4B	C4-C4A-C8A	8.93	122.65	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	760	H4B	1	0
6	A	800	JI2	4	0
4	B	750	HEM	2	0
6	B	800	JI2	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	407/422 (96%)	0.28	22 (5%) 29 30	25, 45, 74, 88	0
1	B	411/422 (97%)	-0.19	11 (2%) 58 57	21, 37, 62, 83	0
All	All	818/844 (96%)	0.04	33 (4%) 42 43	21, 41, 70, 88	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	5.6
1	B	348	VAL	4.8
1	B	300	PHE	4.7
1	A	488	PRO	4.7
1	A	715	VAL	4.6
1	A	716	TRP	3.7
1	B	619	ARG	3.7
1	A	351	LYS	3.6
1	A	490	GLY	3.5
1	B	350	THR	3.4
1	A	392	SER	3.1
1	A	714	HIS	3.0
1	A	299	ARG	3.0
1	A	713	THR	3.0
1	B	615	ASP	3.0
1	B	352	ASP	2.8
1	A	486	LYS	2.8
1	A	619	ARG	2.8
1	B	718	GLY	2.6
1	A	487	GLN	2.6
1	B	620	LYS	2.6
1	A	355	PHE	2.6
1	A	389	GLU	2.5
1	A	300	PHE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	350	THR	2.4
1	B	351	LYS	2.3
1	A	393	THR	2.3
1	A	507	GLN	2.2
1	A	390	SER	2.2
1	B	616	LEU	2.2
1	A	511	LYS	2.2
1	B	667	ARG	2.1
1	A	503	GLU	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
2	ACT	A	860	4/4	0.97	0.20	9.44	59,59,61,62	0
2	ACT	B	860	4/4	0.93	0.25	4.75	43,44,46,47	0
6	JI2	A	800	17/17	0.94	0.32	3.00	39,44,57,59	0
6	JI2	B	800	17/17	0.94	0.27	2.65	39,44,56,56	0
4	HEM	B	750	43/43	0.97	0.16	0.62	22,29,38,42	0
5	H4B	B	760	17/17	0.96	0.18	0.41	28,31,35,35	0
4	HEM	A	750	43/43	0.97	0.19	0.35	22,30,40,45	0
5	H4B	A	760	17/17	0.96	0.17	0.20	33,35,37,37	0
3	ZN	B	900	1/1	1.00	0.09	-1.21	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.