



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 10:17 AM EDT

PDB ID : 3NLR  
Title : Structure of neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with 6-{{(3'R,4'S)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine  
Authors : Li, H.; Delker, S.L.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 2.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

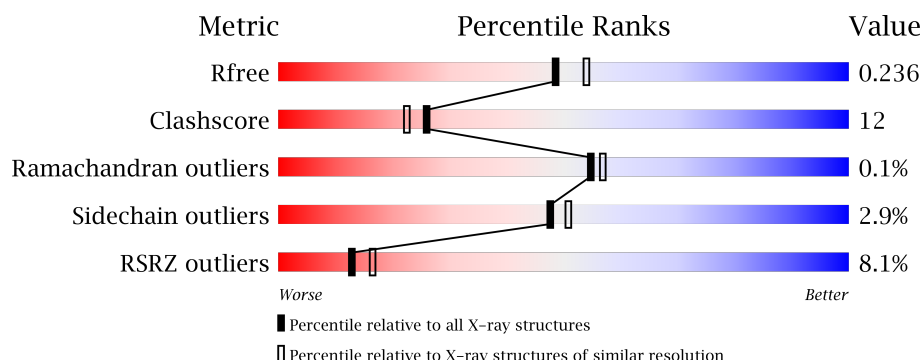
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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>11%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	422	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>21%</div> <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
4	JRS	B	800	-	-	-	X
5	ACT	A	860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7039 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.

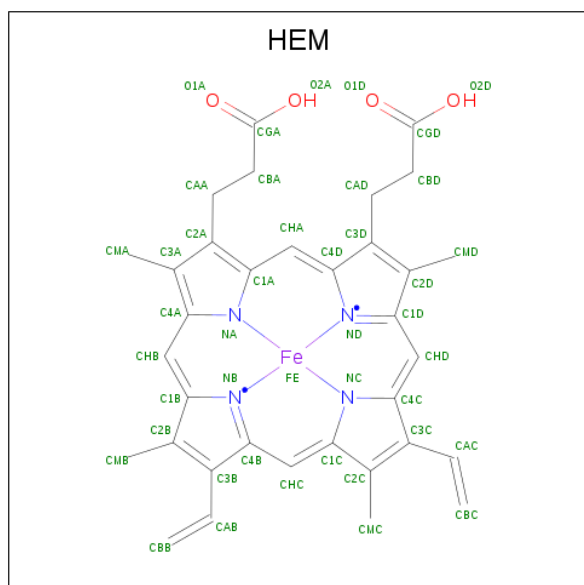
- Molecule 1 is a protein called Nitric oxide synthase, brain.

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:

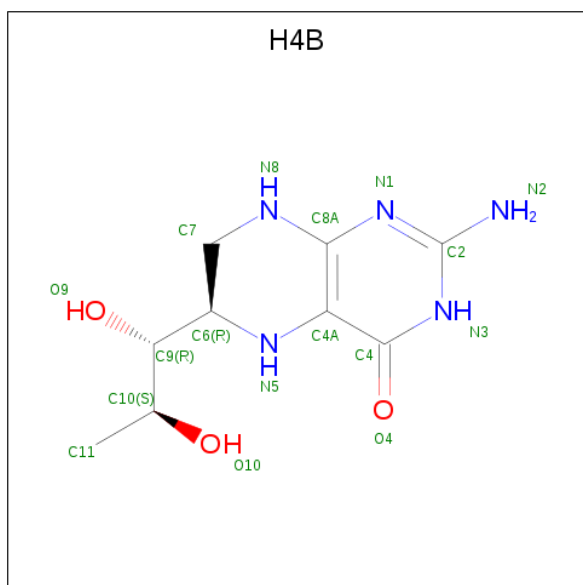
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
A	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476
B	336	VAL	MET	ENGINEERED MUTATION	UNP P29476
B	597	ASN	ASP	ENGINEERED MUTATION	UNP P29476

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



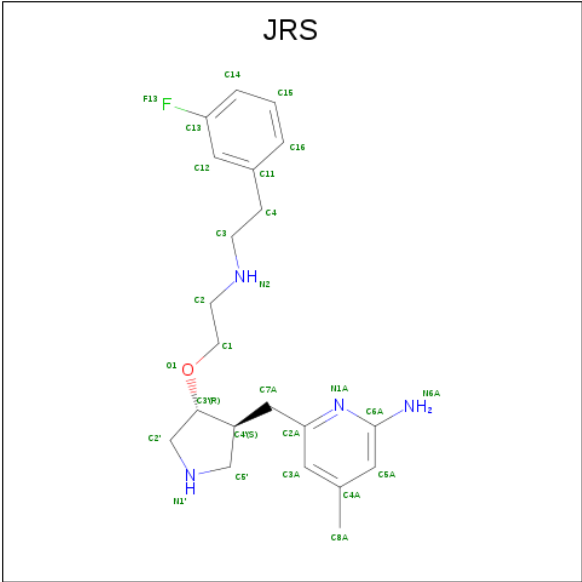
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



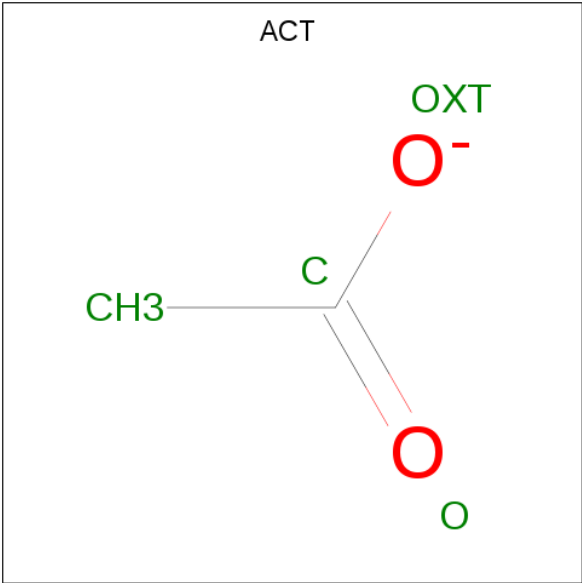
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			17	9	5	3		
3	B	1	Total	C	N	O		
			17	9	5	3		

- Molecule 4 is 6-{[(3S,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: JRS) (formula:  $C_{21}H_{29}FN_4O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- Molecule 5 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
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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

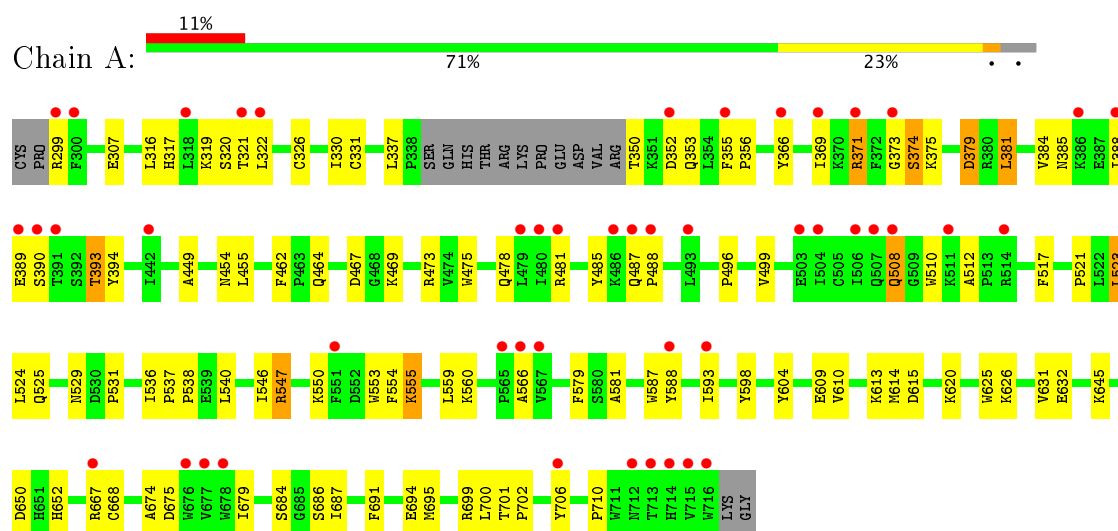
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total 87	O 87	0	0
7	B	113	Total 113	O 113	0	0

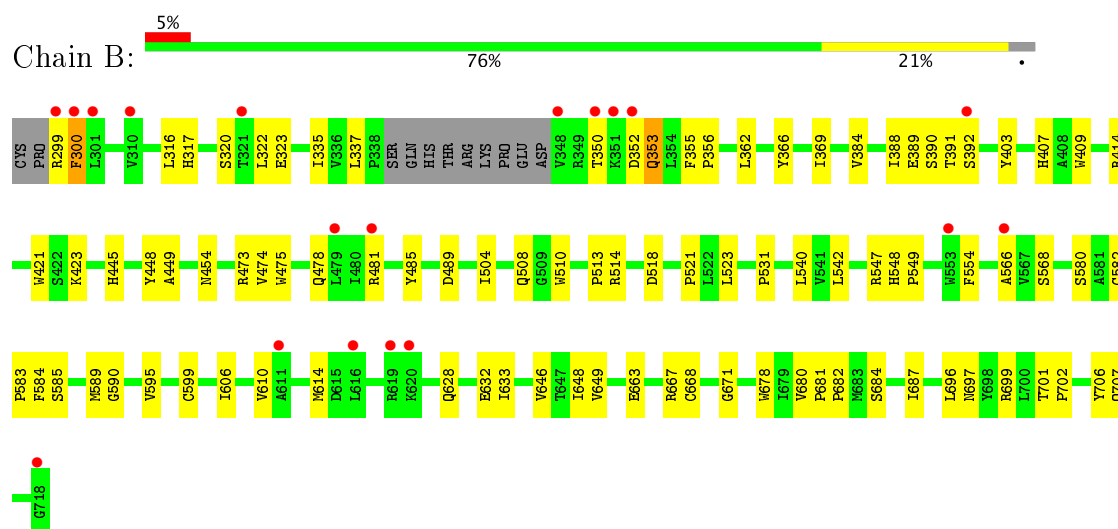
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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, $\alpha$ , $\beta$ , $\gamma$	51.45Å 110.58Å 164.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.56 – 2.10 40.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.56-2.10) 93.7 (40.55-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.10Å)	Xtriage
Refinement program	CNS, REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.186 , 0.235 0.187 , 0.236	Depositor DCC
$R_{free}$ test set	2574 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: HEM, ZN, JRS, 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	0.83	1/3405 (0.0%)	0.87	5/4621 (0.1%)
1	B	0.90	0/3437	0.86	2/4661 (0.0%)
All	All	0.87	1/6842 (0.0%)	0.86	7/9282 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	CYS	CB-SG	-5.61	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASP	CB-CG-OD1	-10.13	109.19	118.30
1	A	547	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	B	489	ASP	CB-CG-OD2	8.75	126.18	118.30
1	A	547	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	A	381	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	668	CYS	CA-CB-SG	-5.21	104.62	114.00
1	A	379	ASP	CB-CG-OD2	5.00	122.81	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	3312	0	3223	82	0
1	B	3344	0	3261	68	0
2	A	43	0	30	10	0
2	B	43	0	30	9	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	29	3	0
4	B	27	0	29	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	87	0	0	8	0
7	B	113	0	0	5	0
All	All	7039	0	6638	159	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 12.

All (159) 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	1.45	0.99
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.49	0.93
1:B:299:ARG:HD2	7:B:74:HOH:O	1.79	0.82
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.62	0.81
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.62	0.81
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.99	0.79
1:A:554:PHE:HB3	7:A:8:HOH:O	1.85	0.74
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.70	0.74
1:A:307:GLU:HG3	7:B:41:HOH:O	1.87	0.73
1:A:322:LEU:HD12	7:A:119:HOH:O	1.89	0.73
1:A:467:ASP:OD2	1:A:469:LYS:HB2	1.91	0.69
2:A:750:HEM:O2D	4:A:800:JRS:H3A	1.96	0.66
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.23	0.66
1:B:391:THR:O	1:B:392:SER:HB2	1.97	0.64
1:B:299:ARG:CZ	1:B:299:ARG:HB3	2.28	0.64
2:B:750:HEM:O2D	4:B:800:JRS:H3A	1.98	0.64
1:B:668:CYS:HB3	7:B:43:HOH:O	1.96	0.64
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.13	0.63
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.81	0.63
1:A:375:LYS:NZ	1:A:379:ASP:OD1	2.32	0.63
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.29	0.62
1:B:355:PHE:N	1:B:356:PRO:HD2	2.15	0.62
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.29	0.62
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.24	0.62
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.82	0.61
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.83	0.61
1:B:388:ILE:O	1:B:392:SER:N	2.32	0.61
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.16	0.60
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.84	0.60
1:A:508:GLN:HA	1:A:508:GLN:OE1	2.00	0.59
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.68	0.59
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.85	0.59
1:A:337:LEU:HD21	4:A:800:JRS:H15	1.85	0.58
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.38	0.58
1:A:598:TYR:HA	7:A:82:HOH:O	2.04	0.57
1:A:699:ARG:HB3	7:A:119:HOH:O	2.05	0.57
1:B:389:GLU:HG3	1:B:390:SER:N	2.20	0.56
1:A:449:ALA:O	1:A:455:LEU:HA	2.06	0.55
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.89	0.55
1:A:384:VAL:O	1:A:388:ILE:HG13	2.06	0.55
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.88	0.55
1:B:353:GLN:O	1:B:356:PRO:HG2	2.06	0.55
1:B:350:THR:HG22	1:B:352:ASP:H	1.72	0.54
1:B:337:LEU:HD21	4:B:800:JRS:H15	1.88	0.54
1:A:496:PRO:O	1:A:499:VAL:HG23	2.08	0.54
1:B:317:HIS:O	1:B:320:SER:HB3	2.07	0.54
1:A:525:GLN:HG3	1:A:529:ASN:O	2.07	0.54
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.41	0.54
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.43	0.54
1:A:546:ILE:HG13	1:A:598:TYR:OH	2.08	0.54
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.22	0.54
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.43	0.53
1:B:701:THR:HA	1:B:702:PRO:C	2.28	0.53
1:A:604:TYR:HB2	7:A:82:HOH:O	2.06	0.53
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.90	0.53
1:A:350:THR:HG22	1:A:352:ASP:H	1.73	0.53
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.92	0.52
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.40	0.51
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.76	0.51
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.75	0.51
1:A:610:VAL:O	1:A:614:MET:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:VAL:O	1:B:614:MET:HG3	2.11	0.51
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.24	0.51
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.45	0.51
1:A:536:ILE:O	1:A:537:PRO:C	2.48	0.51
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.77	0.49
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.94	0.49
1:B:542:LEU:HD21	1:B:646:VAL:HG22	1.94	0.49
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.95	0.48
1:A:604:TYR:CB	7:A:82:HOH:O	2.60	0.48
1:B:504:ILE:O	1:B:508:GLN:HG2	2.14	0.48
2:A:750:HEM:O1A	7:A:141:HOH:O	2.20	0.48
1:A:675:ASP:O	1:A:679:ILE:HG12	2.14	0.48
1:A:553:TRP:CZ3	1:A:613:LYS:HB3	2.49	0.47
2:A:750:HEM:HBB2	2:A:750:HEM:CHC	2.36	0.47
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.47
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.44	0.47
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.48	0.47
2:A:750:HEM:CBB	2:A:750:HEM:HHC	2.41	0.47
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.30	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.49	0.46
1:A:467:ASP:CG	1:A:469:LYS:H	2.19	0.46
1:A:355:PHE:N	1:A:356:PRO:CD	2.78	0.46
1:A:478:GLN:HA	1:A:566:ALA:O	2.17	0.46
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.31	0.46
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.98	0.45
1:A:321:THR:HG23	1:A:322:LEU:H	1.82	0.45
1:B:523:LEU:CD1	1:B:531:PRO:HB2	2.47	0.45
1:B:391:THR:O	1:B:392:SER:CB	2.63	0.45
1:A:373:GLY:O	1:A:374:SER:O	2.34	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.52	0.45
1:A:625:TRP:CH2	1:A:626:LYS:HE3	2.52	0.45
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.99	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.17	0.44
1:B:300:PHE:N	1:B:300:PHE:CD1	2.84	0.44
1:B:554:PHE:HB3	7:B:190:HOH:O	2.17	0.44
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.47	0.44
1:A:393:THR:OG1	1:A:394:TYR:N	2.51	0.44
1:A:517:PHE:CB	1:A:560:LYS:HE3	2.48	0.44
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.53	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.46	0.43
2:B:750:HEM:HMC1	2:B:750:HEM:HBC2	1.98	0.43
1:A:321:THR:HG23	1:A:322:LEU:N	2.32	0.43
1:B:322:LEU:HB3	1:B:699:ARG:CZ	2.49	0.43
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.01	0.43
1:A:546:ILE:HB	1:A:559:LEU:HB2	2.01	0.43
1:B:448:TYR:C	1:B:448:TYR:CD2	2.92	0.43
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.88	0.43
1:B:566:ALA:HB2	1:B:585:SER:HB3	2.00	0.43
1:B:316:LEU:HB3	1:B:671:GLY:HA3	2.01	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.43
1:A:701:THR:HA	1:A:702:PRO:C	2.39	0.43
2:B:750:HEM:HMC1	2:B:750:HEM:CBC	2.48	0.43
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.51	0.42
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.55	0.42
1:A:667:ARG:HG3	1:A:667:ARG:NH1	2.34	0.42
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.55	0.42
1:A:353:GLN:O	1:A:356:PRO:HD2	2.19	0.42
1:A:553:TRP:CZ3	1:A:613:LYS:CB	3.02	0.42
1:B:449:ALA:HB1	7:B:17:HOH:O	2.20	0.42
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.35	0.42
1:B:353:GLN:HG2	1:B:353:GLN:H	1.51	0.42
1:B:606:ILE:O	1:B:610:VAL:HG23	2.20	0.42
1:A:299:ARG:O	1:A:317:HIS:CE1	2.73	0.42
1:A:462:PHE:HB2	1:A:581:ALA:HB3	2.01	0.42
1:B:582:CYS:O	1:B:583:PRO:C	2.57	0.42
2:B:750:HEM:CBC	2:B:750:HEM:CMC	2.94	0.42
1:B:474:VAL:HG11	1:B:568:SER:HB2	2.02	0.41
1:A:706:TYR:OH	2:A:750:HEM:CGD	2.68	0.41
1:B:706:TYR:CZ	4:B:800:JRS:H16	2.55	0.41
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.02	0.41
1:A:686:SER:OG	1:B:682:PRO:HB2	2.21	0.41
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.79	0.41
2:B:750:HEM:CBB	2:B:750:HEM:HHC	2.50	0.41
1:A:320:SER:HA	1:A:700:LEU:HD23	2.03	0.41
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.56	0.41
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.56	0.41
1:A:537:PRO:HA	1:A:538:PRO:HD2	1.98	0.41
1:B:589:MET:HA	1:B:649:VAL:O	2.20	0.41
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.03	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.96	0.41
2:A:750:HEM:HBA2	4:A:800:JRS:H7AA	2.03	0.41
1:B:445:HIS:CD2	1:B:445:HIS:C	2.95	0.41
1:B:473:ARG:HD3	1:B:580:SER:HB2	2.02	0.41
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	0.41
1:A:555:LYS:N	7:A:8:HOH:O	2.54	0.40
1:B:323:GLU:O	1:B:699:ARG:HD3	2.21	0.40
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.42	0.40
1:B:566:ALA:HA	1:B:584:PHE:O	2.21	0.40
1:A:650:ASP:OD2	1:A:652:HIS:HB2	2.21	0.40
1:B:355:PHE:N	1:B:356:PRO:CD	2.84	0.40
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.10	0.40
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.40
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.03	0.40
1:B:590:GLY:HA2	1:B:648:ILE:HD11	2.02	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%)	382 (95%)	20 (5%)	1 (0%)	51	52
1	B	407/422 (96%)	391 (96%)	16 (4%)	0	100	100
All	All	810/844 (96%)	773 (95%)	36 (4%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER

### 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%)	349 (96%)	14 (4%)	37	37
1	B	366/377 (97%)	359 (98%)	7 (2%)	62	68
All	All	729/754 (97%)	708 (97%)	21 (3%)	48	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ARG
1	A	381	LEU
1	A	389	GLU
1	A	390	SER
1	A	393	THR
1	A	454	ASN
1	A	508	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	609	GLU
1	A	615	ASP
1	A	620	LYS
1	A	645	LYS
1	B	300	PHE
1	B	353	GLN
1	B	423	LYS
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	707	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	425	GLN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	436	HIS
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	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 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
2	HEM	A	750	1	28,50,50	2.16	10 (35%)	17,82,82	3.00	7 (41%)
3	H4B	A	760	-	14,18,18	0.87	0	12,26,26	2.63	5 (41%)
4	JRS	A	800	-	26,29,29	0.71	0	31,38,38	1.57	7 (22%)
5	ACT	A	860	-	1,3,3	0.92	0	0,3,3	0.00	-
2	HEM	B	750	1	28,50,50	2.41	10 (35%)	17,82,82	2.30	4 (23%)
3	H4B	B	760	-	14,18,18	0.84	1 (7%)	12,26,26	2.15	4 (33%)
4	JRS	B	800	-	26,29,29	0.74	0	31,38,38	1.64	5 (16%)
5	ACT	B	860	-	1,3,3	1.12	0	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
2	HEM	A	750	1	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JRS	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	JRS	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-5.55	1.33	1.40
2	B	750	HEM	C3C-C2C	-5.25	1.33	1.40
2	A	750	HEM	C3B-C2B	-4.54	1.34	1.40
2	A	750	HEM	C3C-C2C	-3.32	1.36	1.40
2	B	750	HEM	CMB-C2B	2.10	1.56	1.51
2	B	750	HEM	CMC-C2C	2.22	1.56	1.51
3	B	760	H4B	C4-N3	2.25	1.37	1.33
2	A	750	HEM	CMB-C2B	2.27	1.56	1.51
2	A	750	HEM	CMD-C2D	2.30	1.56	1.51
2	A	750	HEM	C1D-ND	2.37	1.41	1.36
2	B	750	HEM	C3B-CAB	2.44	1.52	1.47
2	B	750	HEM	CMD-C2D	2.65	1.57	1.51
2	B	750	HEM	C3C-CAC	2.76	1.53	1.47
2	A	750	HEM	C3C-CAC	2.83	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMC-C2C	3.19	1.58	1.51
2	B	750	HEM	C1B-NB	3.53	1.40	1.36
2	A	750	HEM	C3B-CAB	3.79	1.55	1.47
2	A	750	HEM	C4D-ND	4.04	1.41	1.36
2	B	750	HEM	C3D-C2D	4.20	1.50	1.37
2	A	750	HEM	C3D-C2D	4.28	1.50	1.37
2	B	750	HEM	C4D-ND	4.81	1.42	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-8.32	96.57	112.48
2	B	750	HEM	CBD-CAD-C3D	-6.20	100.64	112.47
2	A	750	HEM	CBD-CAD-C3D	-5.47	102.03	112.47
3	A	760	H4B	N3-C2-N1	-4.17	118.70	125.45
2	B	750	HEM	C1D-C2D-C3D	-3.93	104.26	107.00
2	A	750	HEM	C1D-C2D-C3D	-3.62	104.48	107.00
4	B	800	JRS	C3A-C2A-N1A	-3.11	119.53	122.91
4	A	800	JRS	C4-C11-C12	-2.87	115.85	120.56
2	B	750	HEM	CMA-C3A-C4A	-2.77	124.21	128.46
4	B	800	JRS	C4-C11-C12	-2.44	116.55	120.56
4	A	800	JRS	O1-C1-C2	-2.38	101.42	109.44
3	B	760	H4B	N3-C2-N1	-2.32	121.68	125.45
4	B	800	JRS	O1-C1-C2	-2.29	101.72	109.44
2	A	750	HEM	CAD-CBD-CGD	-2.25	108.81	112.66
4	B	800	JRS	O1-C3'-C2'	-2.25	105.41	111.42
4	A	800	JRS	C3A-C2A-N1A	-2.14	120.59	122.91
2	A	750	HEM	CAA-CBA-CGA	2.14	116.31	112.66
4	A	800	JRS	F13-C13-C14	2.22	122.42	118.53
4	A	800	JRS	C1-C2-N2	2.27	117.07	111.45
3	B	760	H4B	C2-N1-C8A	2.43	119.98	114.51
3	B	760	H4B	C4-N3-C2	2.44	119.57	116.06
2	A	750	HEM	CMC-C2C-C3C	2.44	129.43	124.89
4	A	800	JRS	C3-N2-C2	2.75	123.31	113.33
4	A	800	JRS	C6A-N1A-C2A	2.90	120.22	118.17
3	A	760	H4B	N2-C2-N3	3.11	122.21	117.24
2	B	750	HEM	C4C-C3C-C2C	3.19	109.12	106.90
3	A	760	H4B	C2-N1-C8A	3.21	121.75	114.51
3	A	760	H4B	C4-C4A-C8A	3.36	117.61	114.56
2	A	750	HEM	C4C-C3C-C2C	3.58	109.40	106.90
3	A	760	H4B	C4-N3-C2	4.97	123.20	116.06
3	B	760	H4B	C4-C4A-C8A	4.97	119.06	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	JRS	C6A-N1A-C2A	5.91	122.35	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	10	0
4	A	800	JRS	3	0
2	B	750	HEM	9	0
4	B	800	JRS	3	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%)	0.59	47 (11%) <b>5</b> <b>7</b>	34, 64, 116, 149	1 (0%)
1	B	411/422 (97%)	0.21	19 (4%) <b>33</b> <b>39</b>	35, 54, 87, 113	1 (0%)
All	All	818/844 (96%)	0.40	66 (8%) <b>13</b> <b>16</b>	34, 59, 110, 149	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.8
1	A	716	TRP	6.6
1	A	715	VAL	6.4
1	B	348	VAL	4.8
1	B	352	ASP	4.8
1	B	718	GLY	4.2
1	B	616	LEU	4.0
1	A	355	PHE	4.0
1	A	352	ASP	3.9
1	A	507	GLN	3.9
1	A	300	PHE	3.8
1	B	350	THR	3.6
1	B	619	ARG	3.5
1	A	713	THR	3.4
1	A	712	ASN	3.4
1	B	301	LEU	3.4
1	B	481	ARG	3.3
1	A	388	ILE	3.3
1	A	506	ILE	3.3
1	B	299	ARG	3.2
1	A	503	GLU	3.1
1	A	366	TYR	3.1
1	A	486	LYS	3.1
1	A	488	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	514	ARG	3.0
1	A	322	LEU	3.0
1	A	714	HIS	3.0
1	A	318	LEU	3.0
1	A	321	THR	3.0
1	B	351	LYS	3.0
1	B	392	SER	2.9
1	A	373	GLY	2.9
1	A	511	LYS	2.9
1	A	588	TYR	2.8
1	A	667	ARG	2.7
1	A	369	ILE	2.7
1	A	371	ARG	2.7
1	A	299	ARG	2.6
1	A	493	LEU	2.6
1	A	386	LYS	2.5
1	A	677	VAL	2.5
1	A	481	ARG	2.5
1	A	567	VAL	2.5
1	A	508	GLN	2.5
1	A	389	GLU	2.4
1	A	566	ALA	2.4
1	A	442	ILE	2.4
1	A	391	THR	2.4
1	A	480	ILE	2.4
1	B	566	ALA	2.3
1	B	321	THR	2.3
1	A	487	GLN	2.3
1	A	706	TYR	2.3
1	A	565	PRO	2.3
1	A	479	LEU	2.3
1	A	504	ILE	2.2
1	B	620	LYS	2.2
1	B	479	LEU	2.2
1	A	390	SER	2.1
1	A	593	ILE	2.1
1	B	310	VAL	2.1
1	B	611	ALA	2.1
1	A	676	TRP	2.1
1	A	551	PHE	2.0
1	A	678	TRP	2.0
1	B	553	TRP	2.0

## 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
5	ACT	A	860	4/4	0.94	0.29	5.66	82,84,84,84	0
4	JRS	B	800	27/27	0.92	0.23	2.05	44,56,85,92	0
5	ACT	B	860	4/4	0.94	0.17	1.68	63,66,66,67	0
4	JRS	A	800	27/27	0.90	0.25	1.30	34,60,87,92	0
2	HEM	B	750	43/43	0.98	0.17	1.08	35,42,60,65	0
2	HEM	A	750	43/43	0.98	0.20	0.51	37,44,64,68	0
6	ZN	A	900	1/1	0.98	0.12	0.26	51,51,51,51	0
3	H4B	A	760	17/17	0.96	0.14	-0.05	39,45,52,52	0
3	H4B	B	760	17/17	0.95	0.15	-0.10	39,45,52,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.