



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:56 AM GMT

PDB ID : 3NLQ  
Title : Structure of neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with 6-{{(3'R,4'R)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine  
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Deposited on : 2010-06-21  
Resolution : 2.15 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

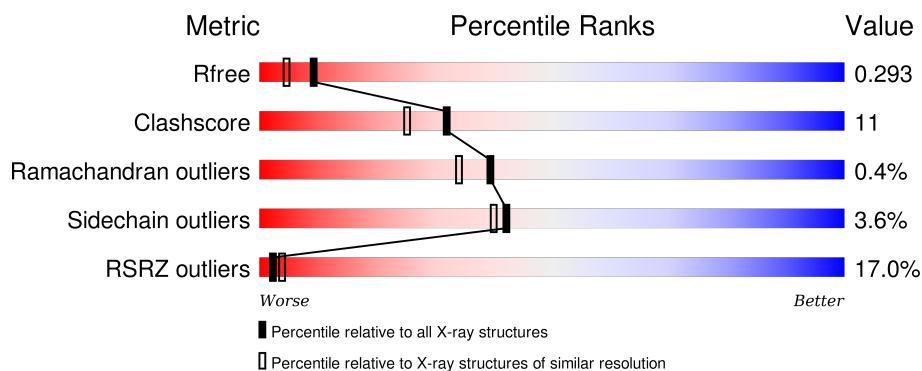
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

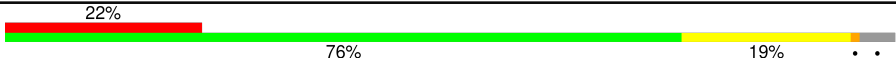

The reported resolution of this entry is 2.15 Å.

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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	
1	B	422	

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	B	860	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7063 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	1	0
			3350	2144	575	611	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:  $C_{34}H_{32}FeN_4O_4$ ).



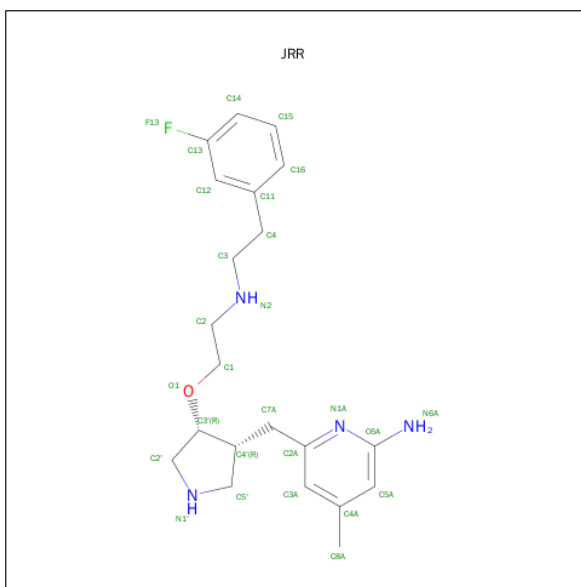
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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-[[2-(3-FLUOROPHENYL)ETHYL]AMINO]ETHOXY)PYRROLIDIN-3-YL]METHYL]-4-METHYLPYRIDIN-2-AMINE (three-letter code: JRR) (formula:  $C_{21}H_{29}FN_4O$ ).



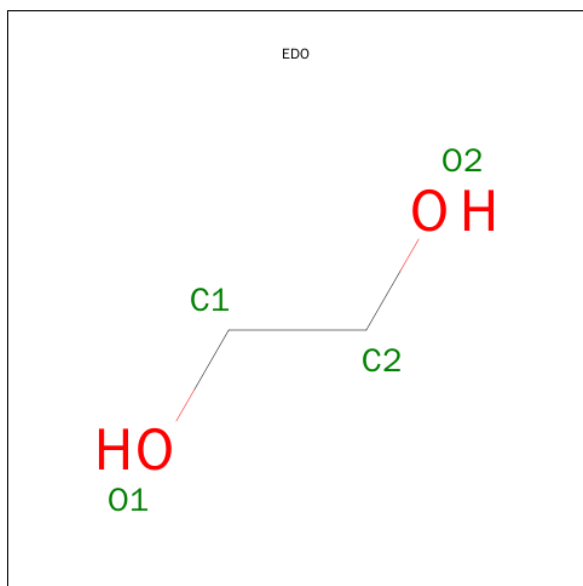
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- 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 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

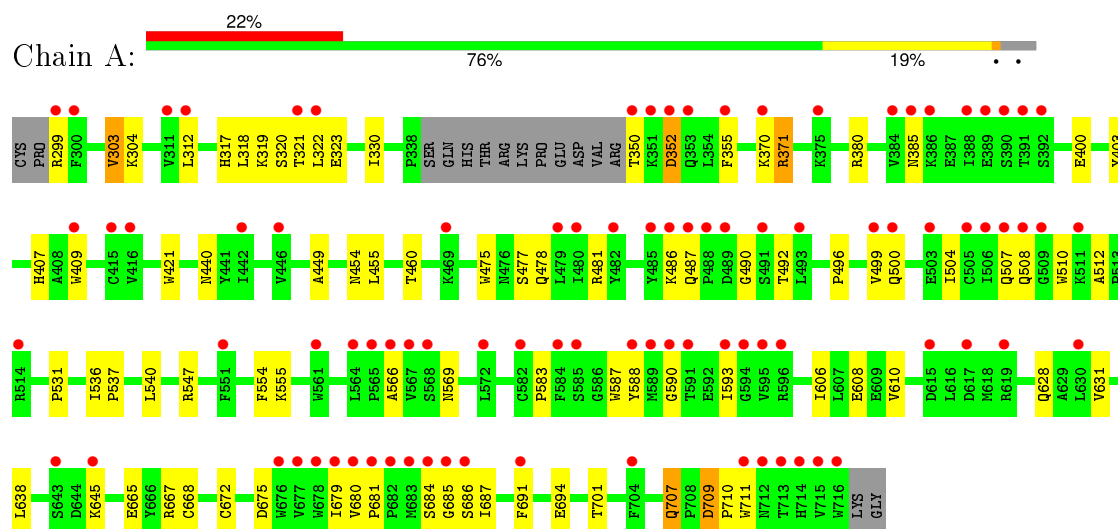
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	91	Total	O	0	0
			91	91		
8	B	123	Total	O	0	0
			123	123		

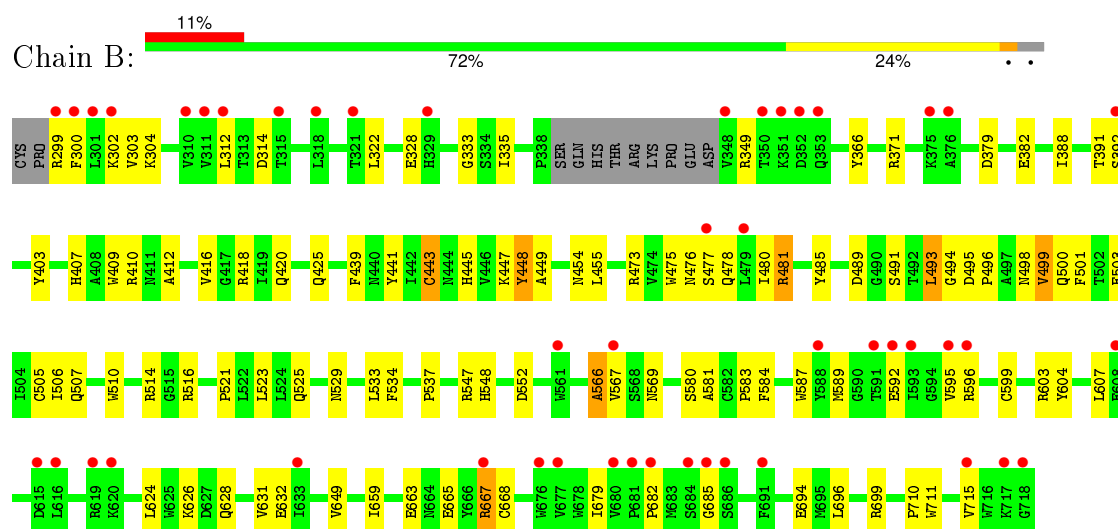
### 3 Residue-property plots

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, 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, $\alpha$ , $\beta$ , $\gamma$	51.59Å 111.23Å 163.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.82 – 2.15 37.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.82-2.15) 99.2 (37.82-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.204 , 0.259 0.249 , 0.293	Depositor DCC
$R_{free}$ test set	2594 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.0	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	1 of 51988 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: ZN, H4B, EDO, JRR, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.71	0/3405	0.75	0/4621
1	B	0.99	8/3446 (0.2%)	0.90	4/4673 (0.1%)
All	All	0.86	8/6851 (0.1%)	0.83	4/9294 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	ALA	C-O	6.59	1.35	1.23
1	B	499	VAL	CB-CG1	6.50	1.66	1.52
1	B	665	GLU	CD-OE2	6.28	1.32	1.25
1	B	441	TYR	CD1-CE1	-6.21	1.30	1.39
1	B	448	TYR	CD1-CE1	6.06	1.48	1.39
1	B	668	CYS	CB-SG	5.60	1.91	1.82
1	B	581	ALA	CA-CB	-5.42	1.41	1.52
1	B	443	CYS	CB-SG	5.07	1.90	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	B	596	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	379	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	379	ASP	CB-CG-OD1	5.48	123.23	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	59	0
1	B	3350	0	3267	80	0
2	A	43	0	30	5	0
2	B	43	0	30	10	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	4	0	6	0	0
7	A	1	0	0	0	0
8	A	91	0	0	2	0
8	B	123	0	0	3	0
All	All	7063	0	6650	143	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 (143) 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:500:GLN:HA	1:B:503:GLU:OE2	1.58	1.01
1:B:514:ARG:HG2	1:B:514:ARG:HH11	1.26	0.99
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.50	0.92
1:A:299:ARG:O	1:A:317:HIS:CE1	2.24	0.90
1:B:480:ILE:HA	8:B:1035:HOH:O	1.73	0.88
1:B:439:PHE:CE2	1:B:443:CYS:SG	2.74	0.80
1:B:514:ARG:HG2	1:B:514:ARG:NH1	1.96	0.76
1:A:299:ARG:O	1:A:317:HIS:HE1	1.67	0.76
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.51	0.76
1:B:659:ILE:O	1:B:663:GLU:HG3	1.88	0.74
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.05	0.72
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.04	0.71
1:B:663:GLU:O	1:B:667:ARG:HD2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.73	0.69
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.75	0.69
1:B:409:TRP:CH2	2:B:750:HEM:HMC1	2.28	0.68
1:B:533:LEU:O	1:B:534:PHE:CG	2.46	0.68
1:B:587:TRP:H	2:B:750:HEM:HAB	1.59	0.68
1:B:525:GLN:HG3	1:B:529:ASN:O	1.94	0.68
1:B:501:PHE:CE2	1:B:505:CYS:SG	2.87	0.68
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.60	0.66
1:A:554:PHE:HB3	8:A:1087:HOH:O	1.96	0.65
2:B:750:HEM:HBA2	4:B:800:JRR:H4	1.78	0.64
1:B:493:LEU:HD12	1:B:494:GLY:N	2.14	0.63
1:A:686:SER:OG	1:B:682:PRO:HB2	1.98	0.63
1:B:592[A]:GLU:OE1	4:B:800:JRR:H16	1.99	0.62
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.35	0.62
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.82	0.61
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.35	0.61
1:A:317:HIS:O	1:A:320:SER:HB3	2.01	0.60
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.84	0.59
2:B:750:HEM:HBA1	2:B:750:HEM:HMA2	1.85	0.59
1:A:569:ASN:O	1:A:707:GLN:HG3	2.02	0.59
1:A:492:THR:HG21	1:A:496:PRO:HB3	1.85	0.59
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.76	0.59
1:B:499:VAL:O	1:B:503:GLU:HG3	2.03	0.58
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.86	0.58
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.86	0.57
1:B:595:VAL:O	1:B:599:CYS:HB2	2.04	0.57
1:A:321:THR:HG23	1:A:322:LEU:HG	1.86	0.57
1:A:304:LYS:O	1:A:694:GLU:HG3	2.05	0.57
1:B:510:TRP:CD1	1:B:521:PRO:HG3	2.40	0.57
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.86	0.56
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.87	0.56
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.68	0.56
1:A:500:GLN:O	1:A:504:ILE:HG13	2.07	0.55
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.55
1:B:388:ILE:O	1:B:392:SER:N	2.40	0.55
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
1:B:445:HIS:C	1:B:445:HIS:CD2	2.81	0.54
1:A:478:GLN:HA	1:A:566:ALA:O	2.07	0.54
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.42	0.54
1:B:304:LYS:O	1:B:694:GLU:HG3	2.07	0.54
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLN:O	1:A:507:GLN:HG2	2.08	0.53
1:B:409:TRP:CE2	2:B:750:HEM:C2C	2.97	0.53
1:A:299:ARG:HG3	1:A:318:LEU:CD1	2.39	0.53
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.90	0.53
2:A:750:HEM:HBA2	4:A:800:JRR:H4	1.90	0.53
1:B:514:ARG:CG	1:B:514:ARG:NH1	2.70	0.52
1:A:317:HIS:O	1:A:320:SER:CB	2.58	0.52
1:B:439:PHE:CZ	1:B:443:CYS:SG	3.03	0.51
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.26	0.51
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.10	0.51
1:B:514:ARG:CG	1:B:514:ARG:HH11	2.08	0.50
1:B:476:ASN:ND2	1:B:501:PHE:CZ	2.80	0.50
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.93	0.50
1:B:567:VAL:HB	1:B:584:PHE:CE1	2.47	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.94	0.49
1:A:487:GLN:O	1:A:490:GLY:N	2.45	0.49
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.78	0.49
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.43	0.49
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.49
1:B:481:ARG:NH1	1:B:498:ASN:OD1	2.45	0.49
1:B:567:VAL:HB	1:B:584:PHE:CZ	2.48	0.49
2:A:750:HEM:O2D	4:A:800:JRR:N1A	2.46	0.49
1:B:478:GLN:HA	1:B:566:ALA:O	2.12	0.48
1:B:624:LEU:O	1:B:628:GLN:HG3	2.13	0.48
1:B:489:ASP:OD2	1:B:491:SER:OG	2.29	0.48
1:B:366:TYR:HD2	1:B:371:ARG:HB2	1.77	0.48
2:B:750:HEM:CBC	2:B:750:HEM:HMC2	2.33	0.48
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.76	0.48
1:A:665:GLU:CB	1:A:672:CYS:HB2	2.43	0.48
1:B:505:CYS:O	1:B:506:ILE:C	2.53	0.47
1:B:481:ARG:CD	1:B:498:ASN:HD21	2.23	0.46
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.50	0.46
1:B:533:LEU:C	1:B:534:PHE:CG	2.88	0.46
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.48	0.46
1:B:495:ASP:HB2	1:B:604:TYR:CE1	2.50	0.46
1:A:299:ARG:O	1:A:317:HIS:NE2	2.49	0.45
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.99	0.45
1:B:566:ALA:HA	1:B:584:PHE:O	2.16	0.45
1:A:536:ILE:O	1:A:537:PRO:C	2.54	0.45
2:A:750:HEM:O2A	4:A:800:JRR:H2'A	2.16	0.45
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:THR:O	1:A:583:PRO:HD2	2.17	0.45
1:B:302:LYS:HA	1:B:312:LEU:O	2.17	0.45
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.45
1:A:352:ASP:N	1:A:352:ASP:OD2	2.48	0.45
1:B:496:PRO:HD2	1:B:603:ARG:HA	1.98	0.45
1:B:477:SER:HA	1:B:569:ASN:HB3	1.99	0.44
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.99	0.44
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.85	0.44
1:A:606:ILE:O	1:A:610:VAL:HG23	2.18	0.44
1:B:439:PHE:HZ	1:B:537:PRO:HD3	1.82	0.44
1:A:303:VAL:HG23	1:A:312:LEU:HB2	1.99	0.43
1:B:425:GLN:HG2	1:B:448:TYR:CE2	2.53	0.43
1:A:449:ALA:O	1:A:455:LEU:HA	2.18	0.43
1:A:709:ASP:HB3	1:A:711:TRP:CE2	2.54	0.43
2:B:750:HEM:O2D	4:B:800:JRR:N1A	2.51	0.43
1:B:416:VAL:HB	8:B:1001:HOH:O	2.19	0.43
1:B:455:LEU:HD12	1:B:455:LEU:N	2.33	0.43
1:B:409:TRP:CZ2	2:B:750:HEM:HMC1	2.53	0.42
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.42
1:A:321:THR:HG23	1:A:322:LEU:N	2.34	0.42
1:B:416:VAL:HG23	1:B:679:ILE:HG23	2.00	0.42
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.92	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.18	0.42
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.55	0.42
1:A:440:ASN:ND2	8:A:1057:HOH:O	2.43	0.42
1:A:510:TRP:CE3	1:A:512:ALA:HB2	2.54	0.42
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.42
1:B:391:THR:O	1:B:392:SER:HB2	2.19	0.42
1:B:409:TRP:CH2	2:B:750:HEM:CMC	3.00	0.41
1:B:388:ILE:O	1:B:392:SER:HA	2.21	0.41
1:B:449:ALA:O	1:B:455:LEU:HA	2.20	0.41
1:A:590:GLY:HA3	1:A:638:LEU:HD21	2.01	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.96	0.41
1:A:685:GLY:O	1:A:691:PHE:HB2	2.20	0.41
1:B:505:CYS:O	1:B:507:GLN:N	2.54	0.41
1:B:418:ARG:C	1:B:420:GLN:N	2.74	0.41
1:B:567:VAL:O	1:B:583:PRO:HA	2.21	0.41
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.56	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.02	0.41
1:B:510:TRP:CG	1:B:521:PRO:HG3	2.56	0.41
1:B:412:ALA:O	1:B:418:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:CD1	1:B:455:LEU:N	2.83	0.40
1:A:492:THR:HG21	1:A:496:PRO:CB	2.50	0.40
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.40
1:B:447:LYS:HG2	8:B:1095:HOH:O	2.22	0.40
1:B:314:ASP:OD1	1:B:314:ASP:C	2.60	0.40
1:A:321:THR:HG23	1:A:322:LEU:H	1.85	0.40
1:B:710:PRO:HD2	1:B:711:TRP:CE3	2.57	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	403/422 (96%)	381 (94%)	21 (5%)	1 (0%)	52	51
1	B	408/422 (97%)	379 (93%)	27 (7%)	2 (0%)	34	26
All	All	811/844 (96%)	760 (94%)	48 (6%)	3 (0%)	39	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	GLY
1	B	685	GLY
1	A	709	ASP

### 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	363/377 (96%)	349 (96%)	14 (4%)	39	36
1	B	367/377 (97%)	355 (97%)	12 (3%)	45	44
All	All	730/754 (97%)	704 (96%)	26 (4%)	42	40

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	VAL
1	A	319	LYS
1	A	350	THR
1	A	352	ASP
1	A	371	ARG
1	A	454	ASN
1	A	477	SER
1	A	508	GLN
1	A	547	ARG
1	A	555	LYS
1	A	608	GLU
1	A	645	LYS
1	A	701	THR
1	A	707	GLN
1	B	300	PHE
1	B	303	VAL
1	B	349	ARG
1	B	382	GLU
1	B	454	ASN
1	B	481	ARG
1	B	493	LEU
1	B	516	ARG
1	B	547	ARG
1	B	552	ASP
1	B	667	ARG
1	B	715	VAL

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	317	HIS
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	364	GLN
1	A	440	ASN
1	A	454	ASN
1	A	508	GLN
1	A	605	ASN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	454	ASN
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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	30,50,50	2.46	9 (30%)	24,82,82	3.03	11 (45%)
3	H4B	A	760	-	13,18,18	1.17	2 (15%)	11,26,26	2.88	7 (63%)
4	JRR	A	800	-	26,29,29	1.04	1 (3%)	27,38,38	1.82	8 (29%)
5	ACT	A	860	-	1,3,3	0.79	0	0,3,3	0.00	-
6	EDO	A	890	-	3,3,3	0.64	0	2,2,2	0.50	0
2	HEM	B	750	1	30,50,50	2.11	6 (20%)	24,82,82	2.88	14 (58%)
3	H4B	B	760	-	13,18,18	1.30	2 (15%)	11,26,26	2.68	6 (54%)
4	JRR	B	800	-	26,29,29	0.87	0	27,38,38	2.29	10 (37%)
5	ACT	B	860	-	1,3,3	1.39	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	-	0/10/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JRR	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
6	EDO	A	890	-	-	0/1/1/1	0/0/0/0
2	HEM	B	750	1	-	0/10/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	JRR	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C4D	-7.16	1.42	1.51
2	A	750	HEM	C3B-C4B	-6.37	1.46	1.51
2	B	750	HEM	C3D-C4D	-6.00	1.43	1.51
2	B	750	HEM	C3B-C4B	-5.65	1.46	1.51
2	A	750	HEM	C2C-C1C	-3.51	1.45	1.52
2	B	750	HEM	C2C-C1C	-3.43	1.46	1.52
2	B	750	HEM	C2D-C1D	-2.48	1.43	1.51
2	B	750	HEM	CMA-C3A	2.06	1.55	1.51
2	A	750	HEM	CMA-C3A	2.15	1.56	1.51
3	B	760	H4B	O4-C4	2.29	1.30	1.24
2	A	750	HEM	CHC-C1C	2.29	1.41	1.36
3	A	760	H4B	C7-N8	2.32	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CAA-C2A	2.55	1.56	1.52
4	A	800	JRR	C2A-N1A	2.62	1.39	1.34
3	A	760	H4B	C2-N2	2.66	1.39	1.34
2	A	750	HEM	C3B-CAB	2.68	1.56	1.51
3	B	760	H4B	C7-N8	2.77	1.49	1.46
2	B	750	HEM	FE-NC	3.35	2.09	1.95
2	A	750	HEM	C1C-NC	3.47	1.40	1.36
2	A	750	HEM	FE-NC	4.10	2.12	1.95

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-6.65	100.60	112.53
2	A	750	HEM	C3C-CAC-CBC	-6.31	114.77	124.46
2	B	750	HEM	CBA-CAA-C2A	-4.58	104.32	112.53
3	A	760	H4B	N3-C2-N1	-4.49	118.17	125.53
4	B	800	JRR	C4A-C3A-C2A	-4.30	117.59	120.28
2	B	750	HEM	C3C-CAC-CBC	-4.07	118.22	124.46
4	A	800	JRR	C3-C4-C11	-3.88	104.78	112.83
2	B	750	HEM	C3B-CAB-CBB	-3.83	118.57	124.46
2	B	750	HEM	CAA-C2A-C1A	-3.70	122.99	127.01
2	B	750	HEM	CAA-CBA-CGA	-3.55	106.25	112.75
4	B	800	JRR	C14-C13-C12	-3.37	119.00	123.35
2	A	750	HEM	CBD-CAD-C3D	-3.22	104.19	113.55
3	B	760	H4B	N3-C2-N1	-3.05	120.53	125.53
4	A	800	JRR	C3A-C2A-N1A	-2.74	119.87	122.96
4	B	800	JRR	C3-C4-C11	-2.74	107.16	112.83
2	B	750	HEM	CBD-CAD-C3D	-2.50	106.28	113.55
2	A	750	HEM	CAA-C2A-C1A	-2.49	124.30	127.01
4	A	800	JRR	F13-C13-C12	-2.34	115.10	118.22
4	A	800	JRR	C4-C11-C12	-2.23	116.83	120.56
4	A	800	JRR	C16-C15-C14	-2.20	117.09	120.24
4	B	800	JRR	C3A-C2A-N1A	-2.13	120.56	122.96
4	B	800	JRR	C8A-C4A-C3A	-2.12	117.73	120.95
2	B	750	HEM	CMA-C3A-C4A	-2.10	124.89	128.36
4	B	800	JRR	C1-O1-C3'	2.03	118.75	113.95
4	B	800	JRR	F13-C13-C14	2.07	121.98	118.52
3	A	760	H4B	N2-C2-N3	2.13	120.73	117.20
2	B	750	HEM	C2C-C1C-CHC	2.34	127.24	123.68
3	A	760	H4B	N2-C2-N1	2.35	121.10	117.20
3	B	760	H4B	N2-C2-N3	2.37	121.12	117.20
4	B	800	JRR	C5A-C4A-C3A	2.37	121.11	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	C2D-C3D-C4D	2.38	105.53	101.50
2	A	750	HEM	CMD-C2D-C3D	2.55	125.61	114.35
3	B	760	H4B	C2-N1-C8A	2.62	120.44	114.54
2	A	750	HEM	C3B-C4B-CHC	2.64	126.88	123.16
2	A	750	HEM	C2C-C1C-CHC	2.81	127.96	123.68
4	A	800	JRR	F13-C13-C14	2.83	123.25	118.52
3	A	760	H4B	C4-C4A-C8A	2.84	117.13	114.56
2	B	750	HEM	CMD-C2D-C3D	3.01	127.66	114.35
2	A	750	HEM	CMB-C2B-C3B	3.23	124.59	116.53
3	B	760	H4B	C4A-C8A-N8	3.29	122.31	118.43
3	A	760	H4B	C4A-C8A-N8	3.60	122.67	118.43
4	A	800	JRR	N6A-C6A-N1A	3.65	123.16	116.50
3	B	760	H4B	C4-N3-C2	3.76	121.16	115.94
2	A	750	HEM	CAD-C3D-C4D	3.77	125.78	112.47
3	A	760	H4B	C2-N1-C8A	3.81	123.11	114.54
4	A	800	JRR	C6A-N1A-C2A	3.92	121.02	118.23
2	B	750	HEM	CMC-C2C-C3C	4.13	126.85	116.53
2	B	750	HEM	CMB-C2B-C3B	4.16	126.92	116.53
2	B	750	HEM	CAD-C3D-C4D	4.28	127.56	112.47
4	B	800	JRR	C11-C12-C13	4.53	122.60	118.84
2	A	750	HEM	CMC-C2C-C3C	4.59	127.99	116.53
2	B	750	HEM	CAD-C3D-C2D	4.75	126.89	113.22
3	A	760	H4B	C4-N3-C2	4.96	122.83	115.94
3	B	760	H4B	C4-C4A-C8A	5.47	119.52	114.56
2	A	750	HEM	CAD-C3D-C2D	5.95	130.33	113.22
4	B	800	JRR	C6A-N1A-C2A	7.13	123.29	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
4	A	800	JRR	3	0
2	B	750	HEM	10	0
4	B	800	JRR	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	407/422 (96%)	1.16	91 (22%) 1 2	34, 64, 121, 153	0
1	B	411/422 (97%)	0.68	48 (11%) 6 10	28, 53, 89, 112	0
All	All	818/844 (96%)	0.92	139 (16%) 2 4	28, 58, 110, 153	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.1
1	A	488	PRO	7.4
1	A	716	TRP	6.2
1	A	355	PHE	5.7
1	A	713	THR	5.5
1	A	712	ASN	5.1
1	B	715	VAL	5.1
1	A	506	ILE	5.0
1	A	300	PHE	4.9
1	A	352	ASP	4.8
1	A	567	VAL	4.8
1	A	351	LYS	4.7
1	B	619	ARG	4.6
1	A	486	LYS	4.5
1	A	715	VAL	4.5
1	B	592[A]	GLU	4.3
1	A	619	ARG	4.3
1	B	616	LEU	4.2
1	A	677	VAL	4.0
1	A	485	TYR	4.0
1	A	509	GLY	4.0
1	A	507	GLN	3.9
1	A	678	TRP	3.9
1	B	302	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	591	THR	3.9
1	B	350	THR	3.9
1	B	677	VAL	3.9
1	B	348	VAL	3.8
1	A	388	ILE	3.8
1	A	391	THR	3.8
1	A	593	ILE	3.8
1	A	682	PRO	3.8
1	B	718	GLY	3.8
1	B	301	LEU	3.8
1	B	310	VAL	3.8
1	A	389	GLU	3.7
1	A	479	LEU	3.7
1	A	588	TYR	3.6
1	A	685	GLY	3.6
1	B	591	THR	3.6
1	A	566	ALA	3.6
1	B	567	VAL	3.6
1	A	551	PHE	3.6
1	A	350	THR	3.5
1	A	679	ILE	3.5
1	A	415	CYS	3.4
1	A	565	PRO	3.4
1	A	686	SER	3.4
1	A	711	TRP	3.3
1	B	615	ASP	3.3
1	A	469	LYS	3.3
1	A	584	PHE	3.3
1	B	680	VAL	3.3
1	B	311	VAL	3.3
1	A	311	VAL	3.2
1	B	299	ARG	3.2
1	A	714	HIS	3.2
1	A	322	LEU	3.2
1	A	386	LYS	3.2
1	A	480	ILE	3.1
1	A	683	MET	3.1
1	B	691	PHE	3.1
1	A	681	PRO	3.1
1	B	561	TRP	3.1
1	B	684	SER	3.1
1	B	620	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	615	ASP	3.0
1	B	353	GLN	3.0
1	A	503	GLU	3.0
1	A	299	ARG	3.0
1	A	416	VAL	3.0
1	A	390	SER	3.0
1	B	667	ARG	2.9
1	A	375	LYS	2.9
1	B	681	PRO	2.9
1	A	385	ASN	2.9
1	B	588	TYR	2.9
1	B	352	ASP	2.9
1	A	594	GLY	2.8
1	A	680	VAL	2.8
1	B	329	HIS	2.8
1	A	630	LEU	2.8
1	A	487	GLN	2.7
1	A	312	LEU	2.7
1	A	704	PHE	2.7
1	A	561	TRP	2.7
1	A	489	ASP	2.6
1	B	312	LEU	2.6
1	A	491	SER	2.6
1	A	505	CYS	2.6
1	A	384	VAL	2.6
1	A	321	THR	2.6
1	B	318	LEU	2.6
1	A	511	LYS	2.6
1	B	351	LYS	2.5
1	B	477	SER	2.5
1	B	676	TRP	2.5
1	A	482	TYR	2.5
1	A	595	VAL	2.5
1	B	593	ILE	2.5
1	A	684	SER	2.5
1	B	682	PRO	2.4
1	A	676	TRP	2.4
1	A	691	PHE	2.4
1	A	409	TRP	2.4
1	B	717	LYS	2.4
1	A	643	SER	2.4
1	A	353	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	596	ARG	2.4
1	A	446	VAL	2.3
1	A	493	LEU	2.3
1	B	479	LEU	2.3
1	A	370	LYS	2.3
1	B	375	LYS	2.3
1	B	595	VAL	2.3
1	A	564	LEU	2.3
1	B	685	GLY	2.3
1	B	608	GLU	2.2
1	A	568	SER	2.2
1	A	585	SER	2.2
1	A	645	LYS	2.2
1	B	633	ILE	2.2
1	A	617	ASP	2.2
1	A	572	LEU	2.2
1	A	500	GLN	2.2
1	A	514	ARG	2.2
1	A	392	SER	2.2
1	A	590	GLY	2.1
1	B	376	ALA	2.1
1	B	686	SER	2.1
1	B	596	ARG	2.1
1	A	442	ILE	2.1
1	A	499	VAL	2.1
1	A	508	GLN	2.0
1	B	392	SER	2.0
1	B	321	THR	2.0
1	A	589	MET	2.0
1	B	315	THR	2.0
1	A	582	CYS	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 ⓘ

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	0.86	0.21	4.39	79,81,82,83	0
5	ACT	A	860	4/4	0.92	0.17	1.47	84,86,86,88	0
2	HEM	A	750	43/43	0.95	0.27	0.82	36,41,50,54	0
3	H4B	A	760	17/17	0.93	0.24	0.68	33,38,46,47	0
4	JRR	A	800	27/27	0.85	0.28	0.62	47,54,61,63	0
3	H4B	B	760	17/17	0.94	0.21	0.62	29,38,44,49	0
6	EDO	A	890	4/4	0.86	0.20	0.60	49,50,51,52	0
2	HEM	B	750	43/43	0.96	0.21	0.21	38,45,49,53	0
4	JRR	B	800	27/27	0.90	0.21	0.01	38,49,58,60	0
7	ZN	A	900	1/1	0.99	0.09	-0.87	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.