



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1K2T  
Title : Structure of rat brain nNOS heme domain complexed with S-ethyl-N-phenyl-isothiourea  
Authors : Li, H.; Martasek, P.; Masters, B.S.S.; Poulos, T.L.; Raman, C.S.  
Deposited on : 2001-09-28  
Resolution : 2.20 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

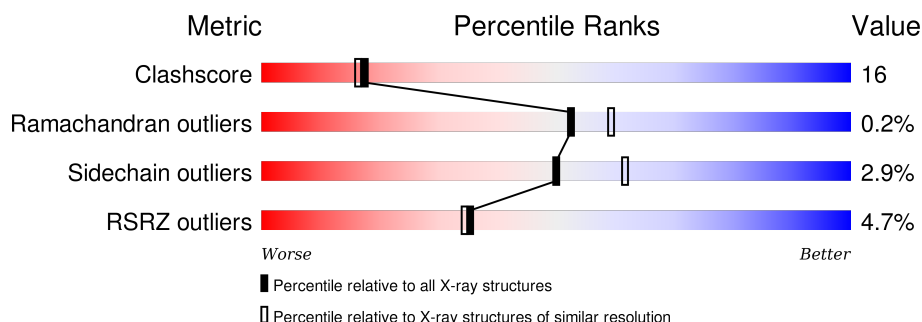
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	419	<div> <div>6%</div> <div>62%</div> <div>34%</div> <div>..</div> </div>
1	B	419	<div> <div>3%</div> <div>68%</div> <div>28%</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	1860	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7129 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

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

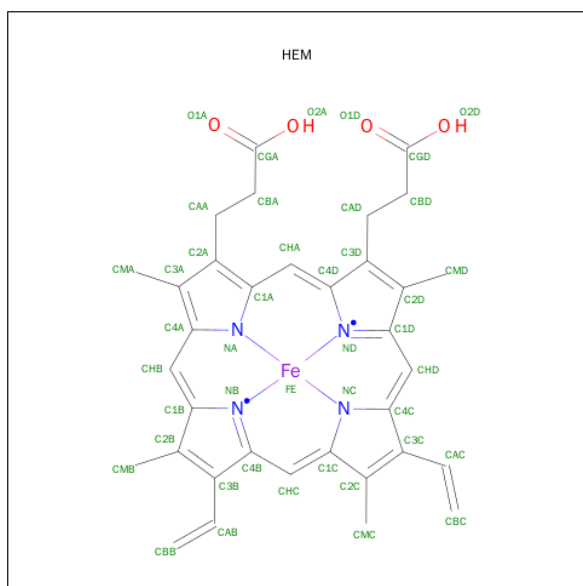


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

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

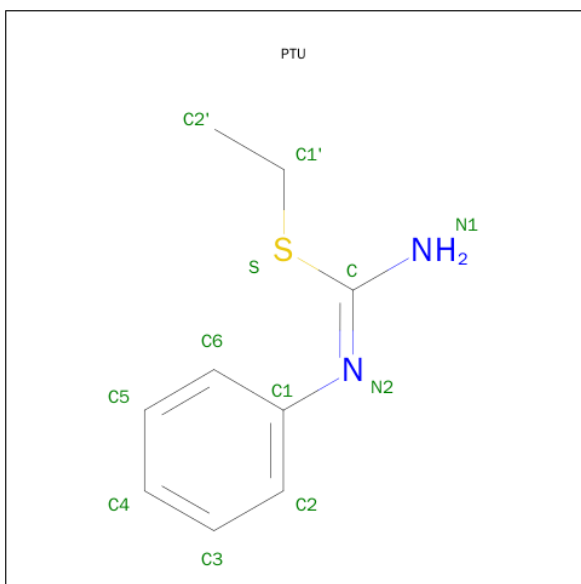
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 2-ETHYL-1-PHENYL-ISOTHIIOUREA (three-letter code: PTU) (formula:  $C_9H_{12}N_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			12	9	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	S	0	0
			12	9	2	1		

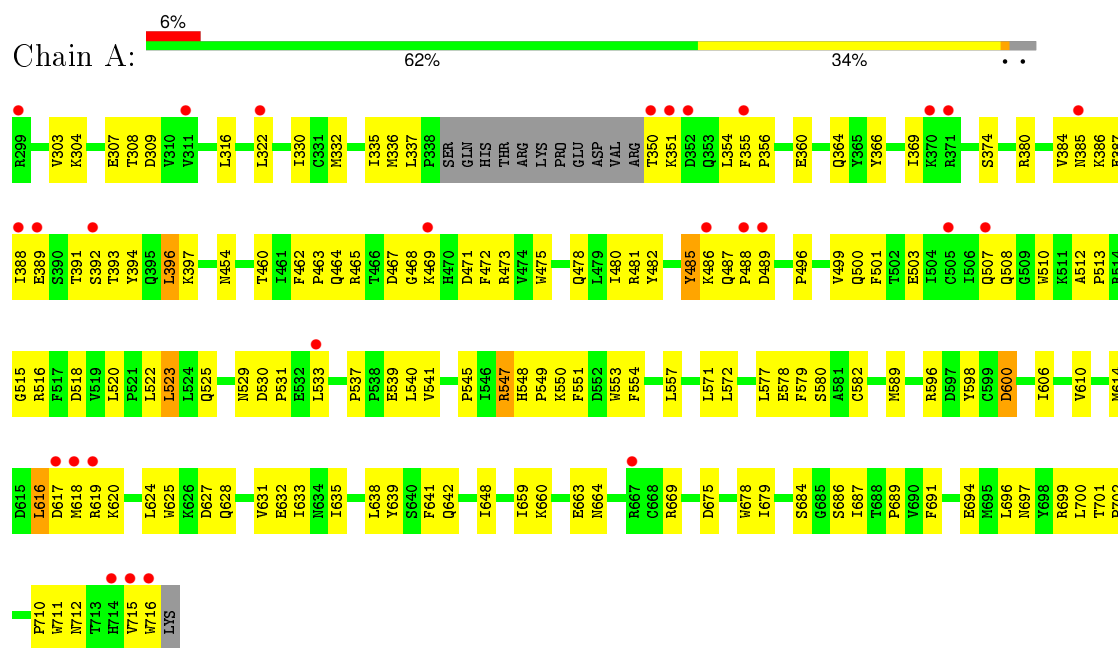
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	130	Total	O	0	0
			130	130		
7	B	192	Total	O	0	0
			192	192		

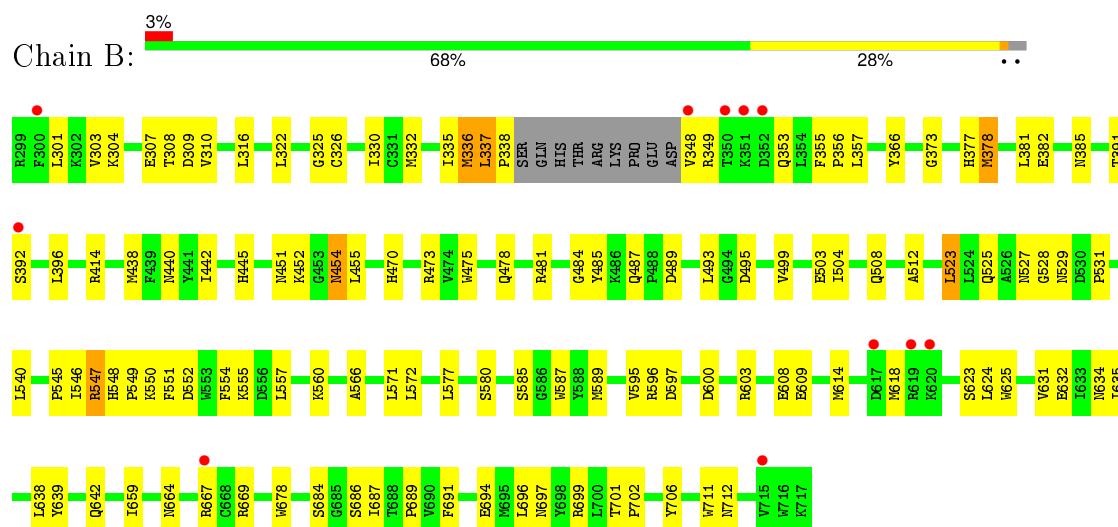
### 3 Residue-property plots

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



#### • Molecule 1: nitric-oxide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.00Å 111.24Å 165.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.20 29.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.70-2.20) 82.1 (29.70-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.265 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.4	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	1 of 45814 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: PTU, HEM, ZN, 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	0.34	0/3406	0.60	1/4621 (0.0%)
1	B	0.35	0/3434	0.60	2/4656 (0.0%)
All	All	0.34	0/6840	0.60	3/9277 (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	B	326	CYS	CA-CB-SG	6.33	125.39	114.00
1	B	589	MET	N-CA-C	-5.70	95.62	111.00
1	A	589	MET	N-CA-C	-5.41	96.39	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	3313	0	3221	122	0
1	B	3341	0	3256	102	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	2	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	130	0	0	6	0
7	B	192	0	0	12	0
All	All	7129	0	6597	214	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 16.

All (214) 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	1.40	1.02
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.49	0.94
1:A:537:PRO:HB2	1:A:540:LEU:HD13	1.49	0.94
1:B:373:GLY:H	1:B:377:HIS:HD2	1.14	0.91
1:A:635:ILE:HD11	1:B:624:LEU:HB2	1.58	0.85
1:B:322:LEU:HB3	1:B:699:ARG:HH21	1.41	0.85
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.16	0.81
1:B:631:VAL:O	1:B:635:ILE:HG12	1.81	0.80
1:B:382:GLU:HG3	7:B:2952:HOH:O	1.85	0.77
1:A:596:ARG:O	1:A:600:ASP:HB2	1.86	0.75
1:B:548:HIS:HD2	1:B:550:LYS:H	1.35	0.74
1:A:385:ASN:O	1:A:389:GLU:HG3	1.87	0.74
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.03	0.73
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.23	0.73
1:A:635:ILE:CD1	1:B:624:LEU:HB2	2.19	0.72
1:B:348:VAL:HG12	1:B:349:ARG:H	1.54	0.71
1:B:499:VAL:O	1:B:503:GLU:HG3	1.93	0.69
1:B:489:ASP:HB2	7:B:3010:HOH:O	1.93	0.68
1:A:554:PHE:O	1:A:557:LEU:HD13	1.94	0.67
1:A:316:LEU:HD11	1:A:669:ARG:HD3	1.77	0.66
1:A:322:LEU:HB2	1:A:699:ARG:HD3	1.78	0.66
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.77	0.65
1:B:348:VAL:HG12	1:B:349:ARG:N	2.13	0.64
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.61	0.64
1:B:373:GLY:H	1:B:377:HIS:CD2	2.06	0.64
1:A:553:TRP:CZ3	1:A:557:LEU:HD11	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ASP:O	1:A:631:VAL:HG23	1.98	0.64
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.79	0.63
1:B:548:HIS:CD2	1:B:550:LYS:H	2.16	0.62
1:B:545:PRO:HG2	1:B:547:ARG:NH1	2.15	0.62
1:A:571:LEU:HD12	1:A:572:LEU:N	2.15	0.61
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.00	0.61
1:A:350:THR:O	1:A:354:LEU:N	2.33	0.61
1:B:504:ILE:O	1:B:508:GLN:HG2	2.00	0.61
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.65	0.60
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.36	0.60
1:A:307:GLU:HG3	7:B:2982:HOH:O	2.00	0.60
1:B:608:GLU:HG3	7:B:3028:HOH:O	2.01	0.59
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.84	0.59
1:A:316:LEU:HD22	1:A:700:LEU:HD11	1.84	0.59
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.84	0.59
1:A:304:LYS:O	1:A:694:GLU:HG3	2.01	0.59
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.38	0.59
1:A:638:LEU:O	1:A:642:GLN:HG3	2.02	0.59
1:B:525:GLN:HG3	1:B:529:ASN:O	2.03	0.59
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.18	0.58
1:B:332:MET:HB3	1:B:335:ILE:HG13	1.84	0.58
1:B:336:MET:HE2	1:B:678:TRP:HZ2	1.68	0.58
1:A:660:LYS:HE2	7:A:1911:HOH:O	2.03	0.57
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.86	0.57
1:B:701:THR:HA	1:B:702:PRO:C	2.25	0.57
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.69	0.56
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.87	0.56
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.88	0.56
1:A:508:GLN:HE22	1:A:716:TRP:HZ3	1.52	0.56
1:A:516:ARG:HG3	1:A:516:ARG:HH11	1.70	0.56
1:B:669:ARG:HD3	7:B:2996:HOH:O	2.06	0.56
1:A:571:LEU:HD11	1:A:578:GLU:HB3	1.88	0.56
1:A:388:ILE:O	1:A:392:SER:HA	2.05	0.56
1:A:316:LEU:HD11	1:A:669:ARG:CD	2.35	0.55
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.87	0.55
1:A:525:GLN:HG3	1:A:529:ASN:O	2.06	0.55
1:A:360:GLU:O	1:A:364:GLN:HG3	2.07	0.55
1:B:664:ASN:O	1:B:667:ARG:HG2	2.07	0.55
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.87	0.55
1:A:507:GLN:O	1:A:507:GLN:HG2	2.06	0.55
1:B:332:MET:HE3	1:B:338:PRO:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.37	0.55
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.37	0.54
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.88	0.54
1:B:391:THR:O	1:B:392:SER:HB2	2.08	0.54
1:B:322:LEU:HB2	1:B:699:ARG:HE	1.71	0.54
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.89	0.54
4:B:750:HEM:HBC2	4:B:750:HEM:HMC1	1.90	0.54
1:A:549:PRO:HG3	1:A:639:TYR:CD1	2.43	0.53
1:B:493:LEU:HD22	7:B:2942:HOH:O	2.07	0.53
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.38	0.53
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.91	0.53
4:B:750:HEM:CMC	4:B:750:HEM:HBC2	2.38	0.53
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.91	0.53
1:A:554:PHE:HA	1:A:557:LEU:HD13	1.91	0.52
1:A:354:LEU:CD2	1:A:393:THR:HA	2.39	0.52
1:A:701:THR:HA	1:A:702:PRO:C	2.30	0.52
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.92	0.52
1:A:510:TRP:HB2	1:A:533:LEU:HD13	1.92	0.52
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.40	0.52
1:B:440:ASN:ND2	7:B:3007:HOH:O	2.43	0.51
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.93	0.51
1:A:522:LEU:O	1:A:533:LEU:HA	2.11	0.51
1:B:548:HIS:CD2	1:B:551:PHE:H	2.29	0.51
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.93	0.50
1:A:624:LEU:HB2	1:B:635:ILE:CD1	2.41	0.50
1:B:470:HIS:HB3	1:B:527:ASN:HD22	1.75	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.47	0.50
1:A:355:PHE:N	1:A:356:PRO:HD2	2.27	0.50
1:B:487:GLN:NE2	7:B:3040:HOH:O	2.45	0.50
1:B:308:THR:OG1	1:B:310:VAL:HG23	2.12	0.50
1:A:624:LEU:HB2	1:B:635:ILE:HD13	1.94	0.49
1:B:308:THR:O	1:B:309:ASP:HB2	2.12	0.49
1:B:485:TYR:CE2	1:B:512:ALA:HB1	2.46	0.49
1:A:548:HIS:CD2	1:A:549:PRO:HD2	2.47	0.49
1:A:354:LEU:HD23	1:A:388:ILE:HG23	1.95	0.49
1:B:332:MET:HB3	1:B:335:ILE:CG1	2.42	0.49
1:A:380:ARG:NH1	1:A:397:LYS:HE3	2.27	0.49
1:B:485:TYR:HE2	1:B:512:ALA:HB1	1.78	0.48
1:B:445:HIS:CD2	1:B:445:HIS:C	2.87	0.48
1:A:686:SER:HA	1:A:691:PHE:CG	2.48	0.48
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:O	1:A:503:GLU:HB2	2.14	0.48
1:B:638:LEU:O	1:B:642:GLN:HG3	2.14	0.48
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.44	0.48
1:A:675:ASP:O	1:A:679:ILE:HG12	2.14	0.48
1:A:486:LYS:HG3	7:A:1889:HOH:O	2.14	0.48
1:B:597:ASP:OD1	1:B:603:ARG:NH1	2.46	0.48
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.30	0.47
1:A:641:PHE:CG	1:A:648:ILE:HD12	2.48	0.47
1:B:548:HIS:CD2	1:B:549:PRO:HD2	2.49	0.47
1:A:659:ILE:O	1:A:663:GLU:HG3	2.15	0.47
1:B:596:ARG:O	1:B:600:ASP:HB2	2.14	0.47
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.97	0.47
1:A:316:LEU:CD2	1:A:700:LEU:HD11	2.43	0.47
1:B:332:MET:CE	1:B:338:PRO:HB3	2.43	0.47
1:B:566:ALA:CB	1:B:585:SER:HB3	2.45	0.47
1:A:617:ASP:OD1	1:A:619:ARG:NE	2.37	0.47
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.79	0.46
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.30	0.46
1:B:322:LEU:HB3	1:B:699:ARG:NH2	2.22	0.46
1:A:557:LEU:N	1:A:557:LEU:HD12	2.30	0.46
1:B:470:HIS:HA	1:B:528:GLY:HA3	1.96	0.46
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.96	0.46
1:A:632:GLU:O	1:A:635:ILE:HB	2.15	0.46
1:A:616:LEU:O	1:A:616:LEU:HD12	2.15	0.46
1:A:473:ARG:HD3	1:A:580:SER:HB2	1.98	0.46
1:A:316:LEU:HD23	1:A:316:LEU:O	2.16	0.45
7:A:1896:HOH:O	1:B:337:LEU:HD12	2.15	0.45
1:B:455:LEU:HD12	1:B:587:TRP:HB3	1.99	0.45
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.98	0.45
1:B:451:ASN:O	1:B:452:LYS:HB2	2.16	0.45
1:B:711:TRP:HD1	1:B:712:ASN:ND2	2.15	0.45
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.16	0.45
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.80	0.45
1:A:354:LEU:HD21	1:A:393:THR:HA	1.98	0.45
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.51	0.45
1:B:348:VAL:CG1	1:B:349:ARG:H	2.27	0.45
1:A:715:VAL:O	1:A:715:VAL:HG23	2.17	0.45
1:B:618:MET:HG2	1:B:625:TRP:CD2	2.52	0.45
1:B:686:SER:HA	1:B:691:PHE:CG	2.53	0.44
1:B:355:PHE:N	1:B:356:PRO:HD2	2.31	0.44
1:A:350:THR:HG22	1:A:351:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:HG	1:B:577:LEU:HD12	1.99	0.44
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.99	0.44
1:A:468:GLY:HA2	1:A:471:ASP:OD1	2.18	0.44
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.48	0.44
1:B:304:LYS:O	1:B:694:GLU:HG3	2.17	0.44
1:A:380:ARG:CZ	1:A:397:LYS:HE3	2.48	0.44
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.53	0.44
1:B:549:PRO:HG3	1:B:639:TYR:CD2	2.53	0.43
1:B:659:ILE:HG13	1:B:689:PRO:HB2	2.00	0.43
1:B:307:GLU:HG3	7:B:2955:HOH:O	2.17	0.43
1:A:515:GLY:N	1:A:518:ASP:OD2	2.43	0.43
1:B:451:ASN:HB3	1:B:454:ASN:O	2.18	0.43
1:B:571:LEU:HD12	1:B:572:LEU:N	2.33	0.43
1:B:557:LEU:HD23	1:B:609:GLU:OE2	2.18	0.43
1:A:635:ILE:CD1	1:B:623:SER:O	2.66	0.43
1:A:396:LEU:HD13	1:A:577:LEU:HD12	2.01	0.43
1:A:553:TRP:CE3	1:A:557:LEU:HD11	2.52	0.43
1:A:618:MET:HA	1:A:625:TRP:CD1	2.54	0.43
1:B:325:GLY:O	1:B:332:MET:HE2	2.18	0.43
1:A:659:ILE:HG13	1:A:689:PRO:HB2	2.01	0.43
1:A:539:GLU:HG2	1:A:540:LEU:HD12	2.00	0.43
1:A:384:VAL:O	1:A:388:ILE:HG13	2.18	0.43
1:A:548:HIS:HD2	1:A:550:LYS:H	1.66	0.43
1:A:322:LEU:HD12	1:A:699:ARG:HD3	2.01	0.43
1:A:478:GLN:HB2	1:A:481:ARG:HG3	2.00	0.43
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.29	0.42
1:A:465:ARG:NE	1:A:471:ASP:OD2	2.50	0.42
1:A:598:TYR:O	1:A:606:ILE:HG12	2.20	0.42
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.54	0.42
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.52	0.42
1:B:552:ASP:OD1	1:B:555:LYS:NZ	2.51	0.42
1:B:554:PHE:HB3	7:B:2977:HOH:O	2.19	0.42
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.50	0.42
1:B:438:MET:O	1:B:442:ILE:HG13	2.19	0.42
1:B:684:SER:O	1:B:687:ILE:HG12	2.20	0.42
1:A:620:LYS:NZ	7:A:1971:HOH:O	2.52	0.42
1:B:487:GLN:C	1:B:489:ASP:N	2.73	0.42
1:A:391:THR:O	1:A:393:THR:HG22	2.19	0.42
1:B:378:MET:HE1	1:B:381:LEU:HD12	2.02	0.41
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.02	0.41
1:A:391:THR:O	1:A:392:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:TYR:HA	1:A:518:ASP:O	2.21	0.41
1:B:322:LEU:CB	1:B:699:ARG:HE	2.33	0.41
1:A:557:LEU:CD1	1:A:557:LEU:N	2.83	0.41
1:A:465:ARG:CZ	7:A:1925:HOH:O	2.68	0.41
1:B:366:TYR:CD2	1:B:377:HIS:HB2	2.56	0.41
1:A:322:LEU:CB	1:A:699:ARG:HD3	2.48	0.41
1:B:508:GLN:NE2	7:B:3014:HOH:O	2.50	0.41
1:B:473:ARG:CD	1:B:580:SER:HB2	2.50	0.41
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.53	0.41
1:B:614:MET:CE	1:B:632:GLU:HG3	2.51	0.41
1:A:460:THR:O	1:A:582:CYS:HA	2.21	0.41
1:B:632:GLU:O	1:B:635:ILE:HB	2.21	0.41
1:A:664:ASN:ND2	7:A:1911:HOH:O	2.48	0.41
1:B:706:TYR:HA	7:B:2939:HOH:O	2.20	0.41
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.96	0.41
1:A:308:THR:O	1:A:309:ASP:HB2	2.21	0.40
1:B:484:GLY:HA3	1:B:495:ASP:O	2.21	0.40
1:A:332:MET:HE1	1:B:301:LEU:HD22	2.03	0.40
1:B:353:GLN:O	1:B:357:LEU:HG	2.21	0.40
1:A:480:ILE:HD13	1:A:541:VAL:HG13	2.03	0.40
1:A:551:PHE:CD1	1:A:553:TRP:CZ2	3.09	0.40
1:A:614:MET:CE	1:A:632:GLU:HG3	2.52	0.40
1:A:678:TRP:HA	5:A:1760:H4B:N1	2.37	0.40
1:A:711:TRP:CD1	1:A:712:ASN:ND2	2.90	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	403/419 (96%)	370 (92%)	31 (8%)	2 (0%)	34 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	406/419 (97%)	385 (95%)	21 (5%)	0	100	100
All	All	809/838 (96%)	755 (93%)	52 (6%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER
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	363/375 (97%)	352 (97%)	11 (3%)	48	60
1	B	366/375 (98%)	356 (97%)	10 (3%)	52	64
All	All	729/750 (97%)	708 (97%)	21 (3%)	50	62

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

Mol	Chain	Res	Type
1	A	336	MET
1	A	337	LEU
1	A	396	LEU
1	A	454	ASN
1	A	485	TYR
1	A	523	LEU
1	A	530	ASP
1	A	547	ARG
1	A	600	ASP
1	A	616	LEU
1	A	697	ASN
1	B	303	VAL
1	B	316	LEU
1	B	336	MET

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Mol	Chain	Res	Type
1	B	337	LEU
1	B	378	MET
1	B	454	ASN
1	B	523	LEU
1	B	540	LEU
1	B	547	ARG
1	B	697	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	407	HIS
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	548	HIS
1	A	628	GLN
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	B	377	HIS
1	B	425	GLN
1	B	440	ASN
1	B	451	ASN
1	B	454	ASN
1	B	527	ASN
1	B	548	HIS
1	B	634	ASN
1	B	664	ASN
1	B	697	ASN
1	B	712	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$
5	H4B	A	1760	-	13,18,18	2.27	4 (30%)	11,26,26	4.04	6 (54%)
6	PTU	A	1810	-	11,12,12	1.85	3 (27%)	12,14,14	2.14	1 (8%)
2	ACT	A	1860	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
4	HEM	A	750	1	30,50,50	2.89	10 (33%)	24,82,82	2.24	7 (29%)
5	H4B	B	2760	-	13,18,18	2.25	3 (23%)	11,26,26	4.06	6 (54%)
6	PTU	B	2810	-	11,12,12	1.89	4 (36%)	12,14,14	2.13	1 (8%)
2	ACT	B	2860	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-
4	HEM	B	750	1	30,50,50	2.78	9 (30%)	24,82,82	2.20	9 (37%)

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	H4B	A	1760	-	-	0/8/17/17	0/2/2/2
6	PTU	A	1810	-	-	0/6/7/7	0/1/1/1
2	ACT	A	1860	-	-	0/0/0/0	0/0/0/0
4	HEM	A	750	1	-	0/10/54/54	0/0/8/8
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2
6	PTU	B	2810	-	-	0/6/7/7	0/1/1/1
2	ACT	B	2860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/10/54/54	0/0/8/8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	C2D-C3D	-6.73	1.34	1.54
4	A	750	HEM	C3B-C4B	-6.56	1.46	1.51
4	A	750	HEM	C2D-C3D	-6.43	1.35	1.54
4	A	750	HEM	C3D-C4D	-6.26	1.43	1.51
4	B	750	HEM	C3D-C4D	-6.02	1.43	1.51
4	A	750	HEM	C3C-CAC	-5.80	1.40	1.51
4	B	750	HEM	C3B-CAB	-5.60	1.40	1.51
4	A	750	HEM	C3B-CAB	-5.14	1.41	1.51
4	B	750	HEM	C3C-CAC	-5.08	1.41	1.51
4	B	750	HEM	C2C-C1C	-4.59	1.43	1.52
4	A	750	HEM	C2C-C1C	-4.21	1.44	1.52
4	B	750	HEM	C3B-C4B	-3.55	1.48	1.51
6	B	2810	PTU	C1-N2	-2.59	1.38	1.42
6	A	1810	PTU	C1-N2	-2.41	1.38	1.42
4	A	750	HEM	C2B-C1B	-2.33	1.44	1.51
4	A	750	HEM	C2D-C1D	-2.06	1.45	1.51
5	A	1760	H4B	C8A-N1	2.08	1.38	1.34
6	B	2810	PTU	C2-C1	2.11	1.43	1.39
4	B	750	HEM	CHC-C1C	2.12	1.41	1.36
2	B	2860	ACT	CH3-C	2.25	1.51	1.48
6	A	1810	PTU	C3-C2	2.53	1.44	1.38
2	A	1860	ACT	CH3-C	2.57	1.52	1.48
6	B	2810	PTU	C3-C2	2.64	1.44	1.38
6	A	1810	PTU	C6-C1	3.06	1.45	1.39
6	B	2810	PTU	C6-C1	3.10	1.45	1.39
4	A	750	HEM	C1C-NC	3.11	1.39	1.36
4	A	750	HEM	C4C-NC	3.35	1.40	1.36
4	B	750	HEM	C4C-NC	3.38	1.40	1.36
5	B	2760	H4B	C4A-N5	3.66	1.46	1.38
5	A	1760	H4B	C4A-N5	3.86	1.47	1.38
5	B	2760	H4B	C6-N5	4.38	1.54	1.45
5	A	1760	H4B	C6-N5	4.58	1.54	1.45
5	A	1760	H4B	C4-N3	4.74	1.41	1.33
4	B	750	HEM	C1C-NC	4.83	1.42	1.36
5	B	2760	H4B	C4-N3	4.84	1.42	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1760	H4B	N3-C2-N1	-4.52	118.13	125.53
5	B	2760	H4B	N3-C2-N1	-4.41	118.31	125.53
4	A	750	HEM	CBA-CAA-C2A	-2.75	107.61	112.53
4	B	750	HEM	CBA-CAA-C2A	-2.05	108.85	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	C3B-C4B-CHC	2.05	126.04	123.16
4	A	750	HEM	CMD-C2D-C3D	2.59	125.80	114.35
4	B	750	HEM	CMD-C2D-C3D	2.60	125.83	114.35
4	B	750	HEM	CMA-C3A-C4A	2.86	133.09	128.36
4	B	750	HEM	C2D-C3D-C4D	2.87	106.36	101.50
5	A	1760	H4B	N2-C2-N1	2.96	122.11	117.20
4	A	750	HEM	CAD-C3D-C4D	3.16	123.62	112.47
5	B	2760	H4B	N2-C2-N1	3.27	122.61	117.20
5	B	2760	H4B	C2-N1-C8A	3.38	122.14	114.54
4	A	750	HEM	CMB-C2B-C3B	3.39	125.00	116.53
5	B	2760	H4B	C4A-C8A-N8	3.60	122.67	118.43
4	B	750	HEM	CAD-C3D-C4D	3.62	125.24	112.47
5	A	1760	H4B	C2-N1-C8A	3.70	122.86	114.54
5	A	1760	H4B	C4A-C8A-N8	4.01	123.15	118.43
4	B	750	HEM	CMB-C2B-C3B	4.05	126.65	116.53
4	B	750	HEM	CMC-C2C-C3C	4.10	126.76	116.53
4	A	750	HEM	CAD-C3D-C2D	4.58	126.39	113.22
4	A	750	HEM	C2D-C3D-C4D	4.92	109.84	101.50
4	B	750	HEM	CAD-C3D-C2D	5.18	128.11	113.22
4	A	750	HEM	CMC-C2C-C3C	5.19	129.48	116.53
5	B	2760	H4B	C4-N3-C2	6.43	124.86	115.94
5	A	1760	H4B	C4-N3-C2	6.58	125.07	115.94
6	B	2810	PTU	C1'-S-C	6.77	111.47	101.53
6	A	1810	PTU	C1'-S-C	6.80	111.50	101.53
5	A	1760	H4B	C4-C4A-C8A	8.57	122.32	114.56
5	B	2760	H4B	C4-C4A-C8A	9.03	122.73	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	H4B	1	0
4	B	750	HEM	2	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	407/419 (97%)	0.40	27 (6%) 22 21	24, 45, 80, 95	0
1	B	410/419 (97%)	0.07	11 (2%) 58 57	21, 39, 66, 84	0
All	All	817/838 (97%)	0.24	38 (4%) 35 34	21, 42, 76, 95	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	5.2
1	A	352	ASP	4.8
1	A	351	LYS	4.7
1	A	370	LYS	4.2
1	A	350	THR	3.8
1	A	388	ILE	3.8
1	B	348	VAL	3.8
1	B	350	THR	3.7
1	A	299	ARG	3.7
1	B	300	PHE	3.5
1	A	619	ARG	3.4
1	A	716	TRP	3.2
1	A	489	ASP	3.2
1	A	389	GLU	3.2
1	B	392	SER	3.1
1	A	322	LEU	3.0
1	B	619	ARG	2.9
1	A	715	VAL	2.9
1	A	355	PHE	2.9
1	B	667	ARG	2.8
1	A	392	SER	2.7
1	A	486	LYS	2.7
1	A	311	VAL	2.7
1	B	352	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	371	ARG	2.4
1	B	715	VAL	2.4
1	A	667	ARG	2.4
1	A	505	CYS	2.4
1	A	617	ASP	2.3
1	B	617	ASP	2.3
1	A	385	ASN	2.3
1	B	351	LYS	2.3
1	A	714	HIS	2.2
1	A	618	MET	2.2
1	B	620	LYS	2.1
1	A	507	GLN	2.1
1	A	469	LYS	2.1
1	A	533	LEU	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
2	ACT	A	1860	4/4	0.97	0.16	2.97	41,44,44,45	0
5	H4B	A	1760	17/17	0.95	0.17	1.13	22,27,33,36	0
4	HEM	A	750	43/43	0.98	0.17	0.67	21,29,34,37	0
6	PTU	A	1810	12/12	0.98	0.18	0.49	23,26,29,29	0
4	HEM	B	750	43/43	0.98	0.16	0.49	16,25,29,33	0
6	PTU	B	2810	12/12	0.96	0.17	0.31	23,27,29,30	0
5	H4B	B	2760	17/17	0.96	0.13	0.26	22,25,31,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	B	2860	4/4	0.99	0.11	-0.76	29,32,33,39	0
3	ZN	A	900	1/1	1.00	0.06	-2.34	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.