



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:55 am GMT

PDB ID : 1K2S  
Title : Structure of rat brain nNOS heme domain complexed with NG-allyl-L-arginine  
Authors : Li, H.; Martasek, P.; Masters, B.S.S.; Poulos, T.L.; Raman, C.S.  
Deposited on : 2001-09-28  
Resolution : 2.55 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 : trunk28620  
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) : recalc28949

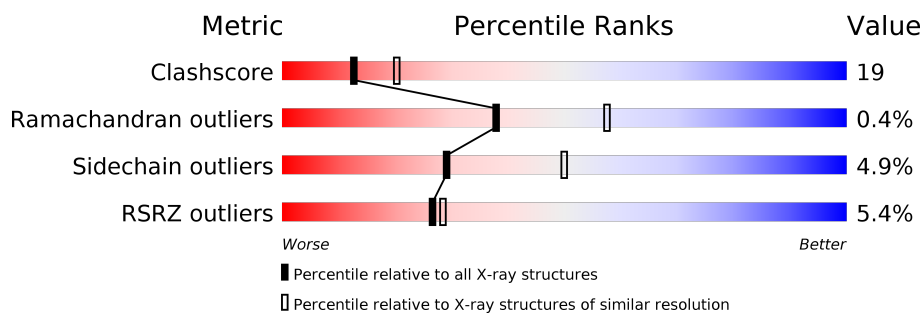
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	419	
1	B	419	

## 2 Entry composition [i](#)

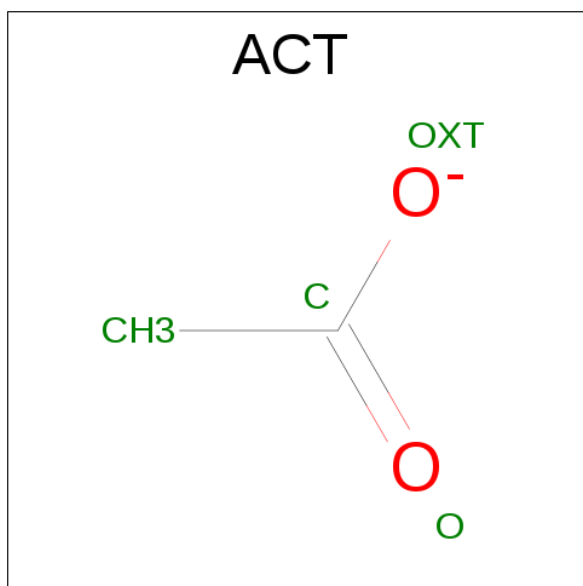
There are 7 unique types of molecules in this entry. The entry contains 7008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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:  $C_2H_3O_2$ ).

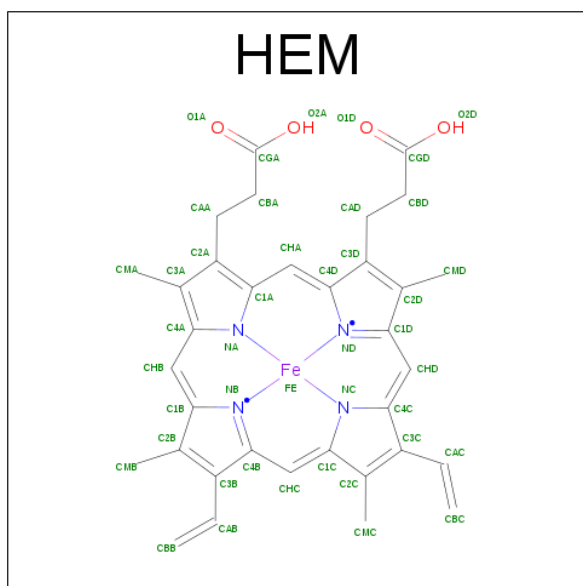


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

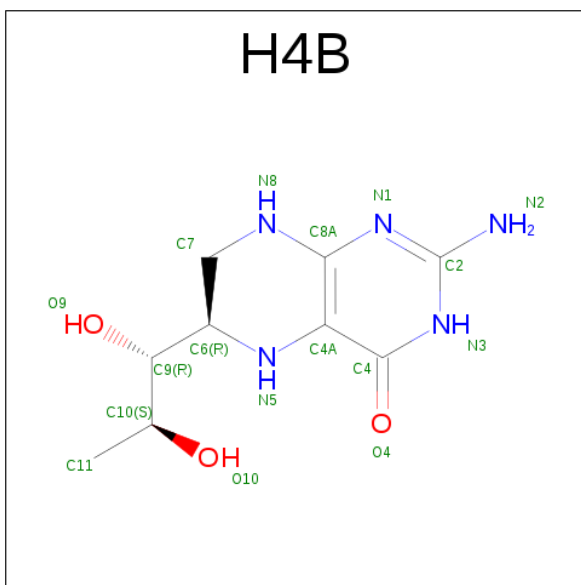
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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



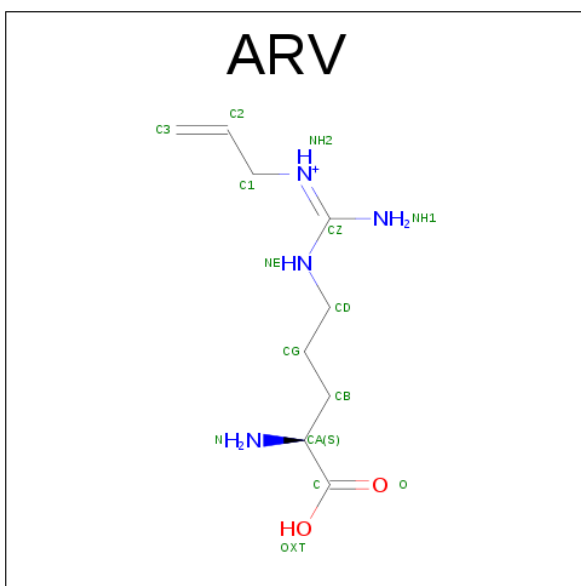
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
4	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- 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 5-N-ALLYL-ARGININE (three-letter code: ARV) (formula:  $C_9H_{19}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	9	4	2		
6	B	1	Total	C	N	O	0	0
			15	9	4	2		

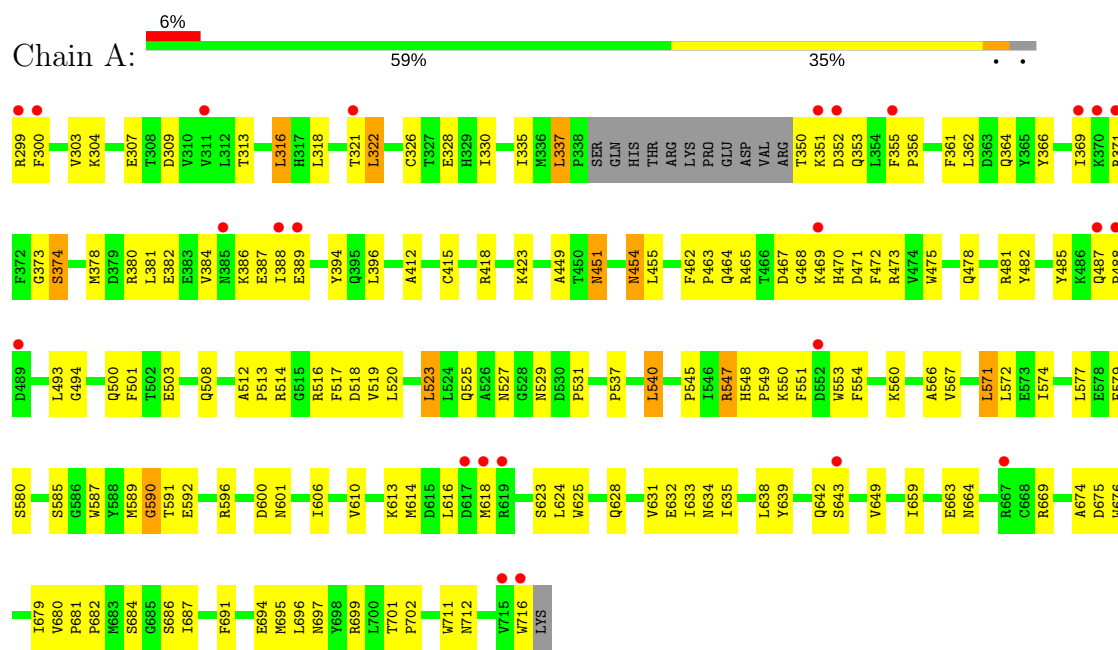
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	92	Total 92	O 92	0	0
7	B	103	Total 103	O 103	0	0

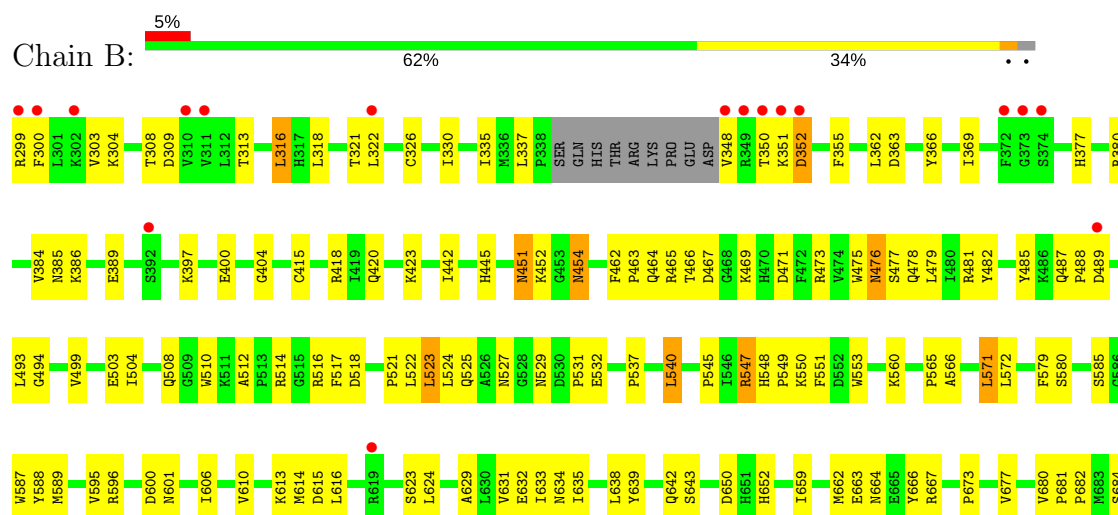
### 3 Residue-property plots

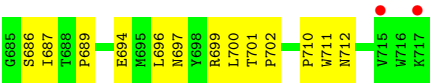
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



#### • 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, $\alpha$ , $\beta$ , $\gamma$	51.73Å 111.03Å 165.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.55 29.61 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.61-2.55) 88.4 (29.61-2.55)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.286 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.999	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.3	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	0.93	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, H4B, ARV, 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	0.37	0/3406	0.65	1/4621 (0.0%)
1	B	0.39	0/3434	0.64	2/4656 (0.0%)
All	All	0.38	0/6840	0.64	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	A	326	CYS	CA-CB-SG	7.00	126.60	114.00
1	B	326	CYS	CA-CB-SG	6.85	126.33	114.00
1	B	589	MET	N-CA-C	-5.20	96.97	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	136	0
1	B	3341	0	3256	121	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	3	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	15	0	18	6	0
6	B	15	0	18	3	0
7	A	92	0	0	7	0
7	B	103	0	0	6	0
All	All	7008	0	6609	249	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 19.

All (249) 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:523:LEU:HD22	1:B:531:PRO:HB2	1.30	1.11
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.41	1.00
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.51	0.92
1:A:299:ARG:HB3	1:A:318:LEU:HD21	1.53	0.91
1:B:465:ARG:HG3	1:B:471:ASP:OD1	1.74	0.88
1:B:571:LEU:HD12	1:B:572:LEU:N	1.94	0.80
4:B:750:HEM:HMC2	4:B:750:HEM:HBC2	1.65	0.78
1:A:396:LEU:HD13	1:A:577:LEU:HD12	1.67	0.75
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.67	0.75
1:B:587:TRP:H	4:B:750:HEM:HAB	1.53	0.73
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.23	0.73
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.04	0.73
1:A:635:ILE:HD11	1:B:624:LEU:HB2	1.71	0.73
1:A:624:LEU:HB2	1:B:635:ILE:HD11	1.71	0.73
1:B:348:VAL:O	1:B:348:VAL:CG1	2.36	0.73
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.23	0.73
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.05	0.71
1:B:523:LEU:CD2	1:B:531:PRO:HB2	2.17	0.68
1:A:585:SER:HA	6:A:1780:ARV:HC32	1.76	0.68
1:B:585:SER:HA	6:B:2780:ARV:HC32	1.76	0.67
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.77	0.67
1:A:374:SER:HB2	7:A:130:HOH:O	1.96	0.66
1:A:624:LEU:HB2	1:B:635:ILE:CD1	2.26	0.66
6:B:2780:ARV:HC12	6:B:2780:ARV:CD	2.26	0.66
1:A:635:ILE:CD1	1:B:624:LEU:HB2	2.26	0.66
1:B:489:ASP:HB2	7:B:18:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1780:ARV:CD	6:A:1780:ARV:HC12	2.26	0.65
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.31	0.65
1:A:299:ARG:CB	1:A:318:LEU:HD21	2.25	0.63
1:B:596:ARG:O	1:B:600:ASP:HB2	1.98	0.63
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.81	0.62
1:B:348:VAL:O	1:B:348:VAL:HG12	1.99	0.62
1:B:452:LYS:HB2	7:B:78:HOH:O	2.00	0.62
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.82	0.61
1:A:711:TRP:CD1	1:A:712:ASN:ND2	2.69	0.60
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.66	0.60
1:A:493:LEU:HD12	1:A:494:GLY:H	1.66	0.60
1:A:493:LEU:HD12	1:A:494:GLY:N	2.16	0.60
1:A:396:LEU:HD21	1:A:574:ILE:HG21	1.82	0.60
1:B:299:ARG:CB	1:B:318:LEU:HD21	2.30	0.59
1:A:304:LYS:O	1:A:694:GLU:HG3	2.01	0.59
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.16	0.59
1:B:610:VAL:O	1:B:614:MET:HG3	2.02	0.59
1:B:664:ASN:O	1:B:667:ARG:HG2	2.03	0.59
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.84	0.59
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.85	0.59
1:A:465:ARG:HG3	1:A:471:ASP:OD1	2.02	0.59
1:B:571:LEU:HD12	1:B:571:LEU:C	2.23	0.59
1:B:350:THR:HG22	1:B:351:LYS:N	2.19	0.58
1:B:303:VAL:HG13	1:B:694:GLU:HB2	1.85	0.58
1:A:396:LEU:HD21	1:A:574:ILE:CG2	2.34	0.58
1:A:684:SER:O	1:A:687:ILE:HG12	2.03	0.58
1:B:631:VAL:O	1:B:635:ILE:HG12	2.04	0.58
1:A:537:PRO:HB2	1:A:540:LEU:HD22	1.84	0.58
1:A:396:LEU:HD13	1:A:577:LEU:CD1	2.34	0.57
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.87	0.57
1:B:467:ASP:OD2	1:B:469:LYS:HB2	2.05	0.57
1:A:571:LEU:HD12	1:A:572:LEU:N	2.20	0.56
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.35	0.56
1:A:596:ARG:O	1:A:600:ASP:HB2	2.05	0.56
1:A:701:THR:HA	1:A:702:PRO:C	2.26	0.56
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.69	0.56
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.41	0.55
1:A:451:ASN:HB3	1:A:454:ASN:O	2.06	0.55
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.88	0.55
1:A:355:PHE:N	1:A:356:PRO:HD2	2.21	0.55
1:A:386:LYS:O	1:A:389:GLU:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ILE:HD11	1:A:633:ILE:HD13	1.87	0.55
1:B:363:ASP:HA	1:B:377:HIS:HE1	1.71	0.54
1:A:589:MET:HA	1:A:649:VAL:O	2.07	0.54
1:A:500:GLN:OE1	1:A:711:TRP:NE1	2.41	0.54
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.88	0.54
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.90	0.54
1:A:548:HIS:HD2	1:A:550:LYS:H	1.56	0.54
1:A:631:VAL:O	1:A:635:ILE:HG12	2.08	0.54
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.43	0.54
1:B:525:GLN:HG3	1:B:529:ASN:O	2.08	0.53
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.43	0.53
1:A:381:LEU:HG	7:A:149:HOH:O	2.08	0.53
1:A:686:SER:OG	1:B:682:PRO:HB2	2.09	0.53
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.43	0.53
1:A:485:TYR:HB3	1:A:514:ARG:NH1	2.24	0.53
1:A:638:LEU:O	1:A:642:GLN:HG3	2.08	0.53
1:B:476:ASN:HB3	7:B:71:HOH:O	2.08	0.53
1:A:380:ARG:O	1:A:384:VAL:HG23	2.09	0.53
1:A:350:THR:HB	1:A:353:GLN:HG3	1.91	0.52
1:A:659:ILE:O	1:A:663:GLU:HG3	2.10	0.52
1:B:701:THR:HA	1:B:702:PRO:C	2.28	0.52
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.91	0.52
1:A:675:ASP:O	1:A:679:ILE:HG12	2.10	0.52
1:A:682:PRO:HB2	1:B:686:SER:OG	2.10	0.52
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.91	0.52
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.39	0.52
1:A:374:SER:O	1:A:378:MET:HG2	2.09	0.52
1:A:711:TRP:HD1	1:A:712:ASN:ND2	2.08	0.52
1:B:473:ARG:NH2	1:B:710:PRO:HD3	2.25	0.52
1:A:567:VAL:HG23	6:A:1780:ARV:HC31	1.91	0.51
1:A:478:GLN:HA	1:A:566:ALA:O	2.09	0.51
1:B:300:PHE:HD2	1:B:313:THR:HG21	1.75	0.51
1:B:451:ASN:HB3	1:B:454:ASN:O	2.10	0.51
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.75	0.51
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.45	0.51
1:A:686:SER:HA	1:A:691:PHE:CG	2.45	0.51
1:B:537:PRO:HB2	1:B:540:LEU:HD22	1.92	0.51
1:A:517:PHE:HB2	1:A:560:LYS:HE2	1.92	0.51
1:B:638:LEU:O	1:B:642:GLN:HG3	2.11	0.51
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.10	0.51
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:HG3	7:A:146:HOH:O	2.10	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.42	0.50
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.28	0.50
1:B:493:LEU:HD12	1:B:494:GLY:N	2.27	0.50
1:A:300:PHE:HD2	1:A:313:THR:HG21	1.77	0.50
1:A:571:LEU:HD12	1:A:571:LEU:C	2.33	0.50
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.41	0.50
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.94	0.49
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.93	0.49
6:B:2780:ARV:HD2	6:B:2780:ARV:HC12	1.93	0.49
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.95	0.49
1:A:525:GLN:HG3	1:A:529:ASN:O	2.12	0.49
1:B:485:TYR:CE2	1:B:512:ALA:HB1	2.47	0.49
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.47	0.49
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.95	0.49
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.95	0.49
1:B:420:GLN:HB3	7:B:69:HOH:O	2.13	0.49
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.95	0.49
1:A:467:ASP:OD1	1:A:470:HIS:ND1	2.45	0.48
1:A:316:LEU:HD11	1:A:669:ARG:HD3	1.95	0.48
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.47	0.48
1:B:442:ILE:HG23	1:B:479:LEU:HD13	1.95	0.48
1:B:445:HIS:HE1	1:B:585:SER:OG	1.96	0.48
1:A:353:GLN:O	1:A:356:PRO:HG2	2.13	0.48
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.95	0.48
1:A:373:GLY:O	1:A:374:SER:O	2.31	0.48
1:A:482:TYR:HA	1:A:518:ASP:O	2.13	0.48
1:B:629:ALA:O	1:B:633:ILE:HG13	2.14	0.48
1:A:468:GLY:HA2	1:A:471:ASP:OD1	2.14	0.48
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.95	0.48
1:B:366:TYR:CD2	1:B:369:ILE:HD11	2.48	0.48
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.44	0.47
1:B:659:ILE:HG13	1:B:689:PRO:HB2	1.95	0.47
1:A:361:PHE:O	1:A:364:GLN:HB2	2.13	0.47
1:A:606:ILE:O	1:A:610:VAL:HG23	2.15	0.47
1:B:415:CYS:HB3	1:B:418:ARG:HG3	1.95	0.47
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.78	0.47
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.79	0.47
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.97	0.47
1:B:615:ASP:HA	7:B:131:HOH:O	2.14	0.47
1:B:547:ARG:NH2	1:B:643:SER:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:TRP:CE3	1:B:613:LYS:HD3	2.49	0.47
1:A:635:ILE:HD12	1:B:623:SER:O	2.14	0.47
1:A:382:GLU:HG3	7:A:135:HOH:O	2.15	0.47
1:A:547:ARG:NH2	1:A:643:SER:HB2	2.30	0.47
1:B:523:LEU:HA	1:B:532:GLU:O	2.15	0.47
1:A:519:VAL:HG23	7:A:8:HOH:O	2.14	0.46
1:B:380:ARG:O	1:B:384:VAL:HG23	2.14	0.46
1:B:493:LEU:HD12	1:B:494:GLY:H	1.80	0.46
1:A:415:CYS:HB3	1:A:418:ARG:HG3	1.97	0.46
1:B:350:THR:HG22	1:B:351:LYS:H	1.79	0.46
1:B:632:GLU:O	1:B:635:ILE:HB	2.15	0.46
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.50	0.46
1:A:350:THR:HG22	1:A:351:LYS:N	2.30	0.46
1:A:548:HIS:CD2	1:A:550:LYS:H	2.33	0.45
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.97	0.45
1:B:350:THR:CG2	1:B:352:ASP:OD1	2.65	0.45
1:B:524:LEU:O	1:B:531:PRO:HA	2.16	0.45
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.52	0.45
1:B:350:THR:HG21	1:B:352:ASP:OD1	2.16	0.45
1:B:516:ARG:HD3	1:B:517:PHE:CE1	2.51	0.45
1:A:384:VAL:O	1:A:388:ILE:HG13	2.16	0.45
1:A:500:GLN:O	1:A:503:GLU:HB2	2.17	0.45
1:B:537:PRO:O	1:B:540:LEU:HB2	2.17	0.45
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.52	0.44
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.81	0.44
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.31	0.44
1:A:591:THR:HA	1:A:634:ASN:HD21	1.82	0.44
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.99	0.44
1:B:466:THR:OG1	1:B:467:ASP:N	2.49	0.44
1:A:623:SER:O	1:B:635:ILE:CD1	2.64	0.44
1:A:396:LEU:CD1	1:A:577:LEU:HD12	2.44	0.44
1:B:684:SER:O	1:B:687:ILE:HG12	2.17	0.44
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.48	0.44
1:B:548:HIS:CD2	1:B:550:LYS:H	2.35	0.44
1:A:462:PHE:HB3	1:A:463:PRO:HD2	1.98	0.44
1:B:610:VAL:HG21	1:B:633:ILE:CD1	2.48	0.44
1:A:610:VAL:O	1:A:614:MET:HG3	2.17	0.44
1:B:478:GLN:HA	1:B:566:ALA:O	2.18	0.44
1:A:596:ARG:HH12	5:A:1760:H4B:C4	2.31	0.44
1:A:454:ASN:HD22	1:A:454:ASN:C	2.21	0.44
1:A:508:GLN:HE22	1:A:716:TRP:HZ3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:VAL:O	1:B:503:GLU:HG3	2.18	0.44
1:B:711:TRP:CD1	1:B:712:ASN:ND2	2.86	0.44
1:A:473:ARG:HD3	1:A:580:SER:HB2	2.00	0.43
1:A:606:ILE:CD1	1:A:633:ILE:HD13	2.48	0.43
1:B:545:PRO:HG2	1:B:547:ARG:HH11	1.83	0.43
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.89	0.43
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.53	0.43
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.54	0.43
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.48	0.43
1:B:504:ILE:O	1:B:508:GLN:HB2	2.17	0.43
1:B:587:TRP:N	4:B:750:HEM:HAB	2.27	0.43
1:B:473:ARG:CD	1:B:580:SER:HB2	2.49	0.43
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.82	0.43
1:B:548:HIS:HB3	1:B:551:PHE:HB2	2.01	0.43
1:A:465:ARG:CZ	7:A:11:HOH:O	2.66	0.42
1:B:304:LYS:O	1:B:694:GLU:HG3	2.19	0.42
1:B:523:LEU:HD23	1:B:532:GLU:O	2.19	0.42
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.54	0.42
1:B:348:VAL:O	1:B:348:VAL:HG13	2.15	0.42
1:A:548:HIS:HB2	1:A:554:PHE:CG	2.55	0.42
1:B:517:PHE:HB2	1:B:560:LYS:HE2	2.01	0.42
1:B:650:ASP:OD2	1:B:652:HIS:HB2	2.18	0.42
6:A:1780:ARV:HD3	6:A:1780:ARV:HC12	2.02	0.42
1:A:449:ALA:O	1:A:455:LEU:HA	2.20	0.42
1:B:614:MET:HE3	1:B:632:GLU:HG3	2.00	0.42
1:A:592:GLU:OE2	6:A:1780:ARV:NH1	2.52	0.42
1:B:303:VAL:CG1	1:B:694:GLU:O	2.68	0.42
1:B:673:PRO:HA	1:B:696:LEU:O	2.20	0.42
1:A:590:GLY:HA3	7:A:16:HOH:O	2.18	0.42
1:A:337:LEU:HD12	1:A:337:LEU:O	2.21	0.41
1:A:485:TYR:HB3	1:A:514:ARG:HH12	1.84	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.41
4:A:750:HEM:CMC	4:A:750:HEM:HBC2	2.45	0.41
6:A:1780:ARV:HD2	6:A:1780:ARV:HC12	2.00	0.41
1:B:482:TYR:HA	1:B:518:ASP:O	2.20	0.41
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.20	0.41
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.51	0.41
1:A:494:GLY:HA2	1:A:516:ARG:O	2.21	0.41
1:B:508:GLN:HG3	7:B:22:HOH:O	2.20	0.41
1:B:659:ILE:O	1:B:663:GLU:HG3	2.21	0.41
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLY:HA2	1:B:702:PRO:HG2	2.03	0.41
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.41
1:B:701:THR:HA	1:B:702:PRO:O	2.21	0.41
1:A:330:ILE:CD1	1:B:696:LEU:HD22	2.50	0.41
1:A:299:ARG:C	1:A:300:PHE:CD1	2.94	0.41
1:B:397:LYS:HB2	1:B:400:GLU:HG3	2.03	0.41
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.56	0.40
1:B:308:THR:O	1:B:309:ASP:HB2	2.21	0.40
1:A:537:PRO:O	1:A:540:LEU:HB2	2.22	0.40
1:B:662:MET:O	1:B:666:TYR:HD1	2.05	0.40
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.88	0.40
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.02	0.40
1:B:386:LYS:O	1:B:389:GLU:HB3	2.22	0.40
1:B:442:ILE:HG21	1:B:522:LEU:HD11	2.03	0.40
1:A:635:ILE:HD13	1:B:624:LEU:HG	2.02	0.40
1:A:454:ASN:C	1:A:454:ASN:ND2	2.75	0.40
1:B:316:LEU:HD22	1:B:700:LEU:HD11	2.04	0.40
1:B:487:GLN:HB3	1:B:488:PRO:HD2	2.03	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	403/419 (96%)	358 (89%)	42 (10%)	3 (1%)	25	42
1	B	406/419 (97%)	372 (92%)	34 (8%)	0	100	100
All	All	809/838 (96%)	730 (90%)	76 (9%)	3 (0%)	38	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER
1	A	412	ALA
1	A	590	GLY

### 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%)	344 (95%)	19 (5%)	27	47
1	B	366/375 (98%)	349 (95%)	17 (5%)	31	52
All	All	729/750 (97%)	693 (95%)	36 (5%)	29	50

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	A	316	LEU
1	A	321	THR
1	A	322	LEU
1	A	328	GLU
1	A	337	LEU
1	A	352	ASP
1	A	423	LYS
1	A	451	ASN
1	A	454	ASN
1	A	523	LEU
1	A	527	ASN
1	A	540	LEU
1	A	547	ARG
1	A	571	LEU
1	A	601	ASN
1	A	616	LEU
1	A	664	ASN
1	A	697	ASN
1	B	316	LEU
1	B	321	THR

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Mol	Chain	Res	Type
1	B	337	LEU
1	B	352	ASP
1	B	423	LYS
1	B	451	ASN
1	B	454	ASN
1	B	476	ASN
1	B	477	SER
1	B	523	LEU
1	B	527	ASN
1	B	540	LEU
1	B	547	ARG
1	B	571	LEU
1	B	601	ASN
1	B	616	LEU
1	B	697	ASN

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
1	A	451	ASN
1	A	454	ASN
1	A	487	GLN
1	A	548	HIS
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	A	714	HIS
1	B	445	HIS
1	B	451	ASN
1	B	454	ASN
1	B	487	GLN
1	B	548	HIS
1	B	634	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 [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$
5	H4B	A	1760	-	14,18,18	2.41	4 (28%)	12,26,26	3.88	7 (58%)
6	ARV	A	1780	-	7,14,14	1.77	2 (28%)	4,16,16	1.45	1 (25%)
2	ACT	A	1860	-	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
4	HEM	A	750	1	28,50,50	1.66	6 (21%)	17,82,82	1.62	4 (23%)
5	H4B	B	2760	-	14,18,18	2.19	4 (28%)	12,26,26	4.01	8 (66%)
6	ARV	B	2780	-	7,14,14	1.70	2 (28%)	4,16,16	1.45	1 (25%)
2	ACT	B	2860	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
4	HEM	B	750	1	28,50,50	1.90	7 (25%)	17,82,82	1.85	5 (29%)

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	ARV	A	1780	-	-	0/9/15/15	0/0/0/0
2	ACT	A	1860	-	-	0/0/0/0	0/0/0/0
4	HEM	A	750	1	-	0/6/54/54	0/0/8/8
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ARV	B	2780	-	-	0/9/15/15	0/0/0/0
2	ACT	B	2860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	750	1	-	0/6/54/54	0/0/8/8

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	C3B-C2B	-4.31	1.34	1.40
4	B	750	HEM	C3B-CAB	-4.14	1.39	1.47
4	A	750	HEM	C3C-CAC	-4.13	1.39	1.47
4	A	750	HEM	C3B-CAB	-3.35	1.41	1.47
4	B	750	HEM	C3C-CAC	-3.34	1.41	1.47
4	B	750	HEM	C3C-C2C	-3.09	1.36	1.40
4	A	750	HEM	C3C-C2C	-2.96	1.36	1.40
4	A	750	HEM	C3B-C2B	-2.92	1.36	1.40
6	A	1780	ARV	CZ-NH1	-2.56	1.28	1.34
6	B	2780	ARV	CZ-NH1	-2.08	1.29	1.34
4	B	750	HEM	C1D-ND	2.01	1.40	1.36
4	A	750	HEM	C4B-NB	2.19	1.40	1.36
4	A	750	HEM	C1D-ND	2.31	1.41	1.36
2	B	2860	ACT	CH3-C	2.37	1.51	1.48
5	B	2760	H4B	C8A-N1	2.38	1.38	1.34
5	A	1760	H4B	C8A-N1	2.70	1.39	1.34
4	B	750	HEM	C4C-NC	3.06	1.40	1.36
6	A	1780	ARV	CZ-NH2	3.20	1.33	1.28
2	A	1860	ACT	CH3-C	3.44	1.53	1.48
5	B	2760	H4B	C4A-N5	3.49	1.45	1.37
6	B	2780	ARV	CZ-NH2	3.57	1.33	1.28
4	B	750	HEM	C1B-NB	3.91	1.41	1.36
5	B	2760	H4B	C6-N5	4.03	1.53	1.45
5	A	1760	H4B	C4A-N5	4.38	1.47	1.37
5	A	1760	H4B	C6-N5	4.44	1.54	1.45
5	B	2760	H4B	C4-N3	5.40	1.42	1.33
5	A	1760	H4B	C4-N3	5.41	1.42	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1760	H4B	N3-C2-N1	-4.55	118.06	125.45
5	B	2760	H4B	N3-C2-N1	-4.34	118.41	125.45
4	A	750	HEM	C1D-C2D-C3D	-4.17	104.09	107.00
5	B	2760	H4B	C4A-C4-N3	-3.61	113.31	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-3.56	105.68	112.48
5	A	1760	H4B	C4A-C4-N3	-3.55	113.47	123.91
4	B	750	HEM	C1D-C2D-C3D	-3.34	104.67	107.00
4	A	750	HEM	C4C-C3C-C2C	-2.73	104.99	106.90
5	A	1760	H4B	C4A-N5-C6	-2.72	113.75	121.16
5	B	2760	H4B	C4A-N5-C6	-2.64	113.97	121.16
4	B	750	HEM	C4C-C3C-C2C	-2.36	105.25	106.90
4	A	750	HEM	CBA-CAA-C2A	-2.32	108.06	112.48
4	B	750	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
6	B	2780	ARV	NH1-CZ-NH2	-2.13	114.73	122.92
6	A	1780	ARV	NH1-CZ-NH2	-2.07	114.95	122.92
4	B	750	HEM	CMC-C2C-C3C	2.08	128.75	124.89
4	A	750	HEM	C4A-C3A-C2A	2.13	108.48	107.00
5	B	2760	H4B	O9-C9-C6	2.17	114.18	108.98
5	B	2760	H4B	N2-C2-N1	3.06	122.13	117.24
5	A	1760	H4B	N2-C2-N1	3.11	122.21	117.24
5	B	2760	H4B	C2-N1-C8A	3.35	122.06	114.51
5	A	1760	H4B	C2-N1-C8A	3.58	122.58	114.51
5	B	2760	H4B	C4-N3-C2	6.12	124.87	116.06
5	A	1760	H4B	C4-N3-C2	6.28	125.09	116.06
5	A	1760	H4B	C4-C4A-C8A	8.39	122.16	114.56
5	B	2760	H4B	C4-C4A-C8A	9.34	123.02	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	H4B	1	0
6	A	1780	ARV	6	0
4	A	750	HEM	2	0
6	B	2780	ARV	3	0
4	B	750	HEM	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	407/419 (97%)	0.46	25 (6%) 22 23	24, 51, 85, 102	0
1	B	410/419 (97%)	0.29	19 (4%) 33 36	21, 48, 78, 101	0
All	All	817/838 (97%)	0.37	44 (5%) 26 28	21, 49, 82, 102	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	6.3
1	A	715	VAL	5.5
1	A	619	ARG	4.3
1	B	392	SER	4.1
1	A	299	ARG	3.7
1	A	351	LYS	3.6
1	B	348	VAL	3.6
1	A	321	THR	3.3
1	A	352	ASP	3.2
1	A	370	LYS	3.2
1	B	352	ASP	3.2
1	B	350	THR	3.2
1	A	311	VAL	3.1
1	B	351	LYS	3.1
1	B	715	VAL	2.9
1	A	371	ARG	2.9
1	A	487	GLN	2.9
1	B	300	PHE	2.9
1	A	355	PHE	2.9
1	A	716	TRP	2.8
1	B	299	ARG	2.8
1	A	667	ARG	2.8
1	B	322	LEU	2.8
1	A	389	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	2.7
1	B	374	SER	2.6
1	B	373	GLY	2.6
1	B	717	LYS	2.6
1	A	385	ASN	2.5
1	A	618	MET	2.5
1	B	311	VAL	2.5
1	B	349	ARG	2.5
1	B	372	PHE	2.5
1	A	388	ILE	2.4
1	A	369	ILE	2.2
1	B	302	LYS	2.2
1	B	310	VAL	2.2
1	A	617	ASP	2.2
1	A	489	ASP	2.2
1	A	643	SER	2.1
1	A	552	ASP	2.1
1	B	489	ASP	2.1
1	A	300	PHE	2.0
1	B	619	ARG	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
6	ARV	B	2780	15/15	0.95	0.25	1.78	34,41,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ARV	A	1780	15/15	0.95	0.24	1.59	26,35,41,42	0
4	HEM	A	750	43/43	0.96	0.21	1.01	20,34,43,45	0
5	H4B	B	2760	17/17	0.95	0.18	0.95	29,35,43,45	0
5	H4B	A	1760	17/17	0.95	0.18	0.56	24,34,41,41	0
4	HEM	B	750	43/43	0.97	0.19	0.55	10,29,39,41	0
2	ACT	A	1860	4/4	0.96	0.16	0.09	48,54,55,58	0
2	ACT	B	2860	4/4	0.98	0.12	-0.86	35,39,40,44	0
3	ZN	A	900	1/1	0.99	0.08	-2.11	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.