



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 10:05 AM EST

PDB ID : 8UFN  
Title : Crystal Structure of neuronal HAstV VA1 capsid spike domain at 2.73 Å resolution  
Authors : Ghosh, A.; Delgado-Cunningham, K.; DuBois, R.M.  
Deposited on : 2023-10-04  
Resolution : 2.73 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

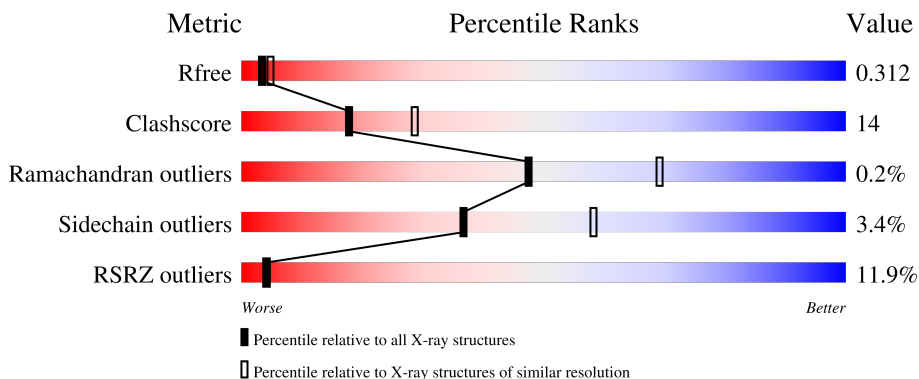
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	304	
1	B	304	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4265 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 Capsid polyprotein VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2140	1369	365	397	9	0	0	0
1	B	267	2125	1360	360	396	9	0	0	0

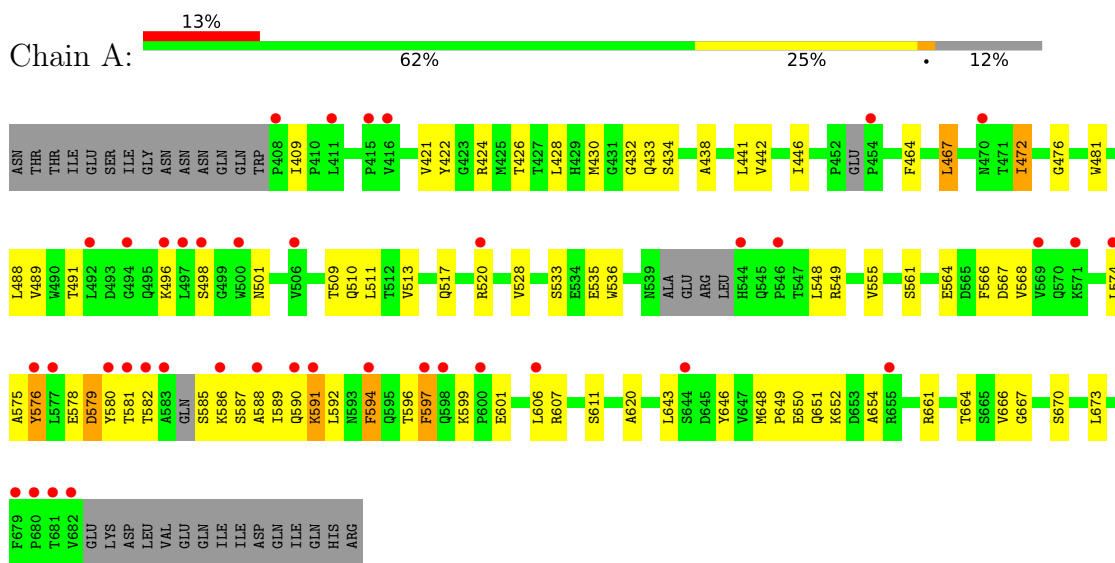
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	650	GLU	GLN	conflict	UNP D7P3D4
B	650	GLU	GLN	conflict	UNP D7P3D4

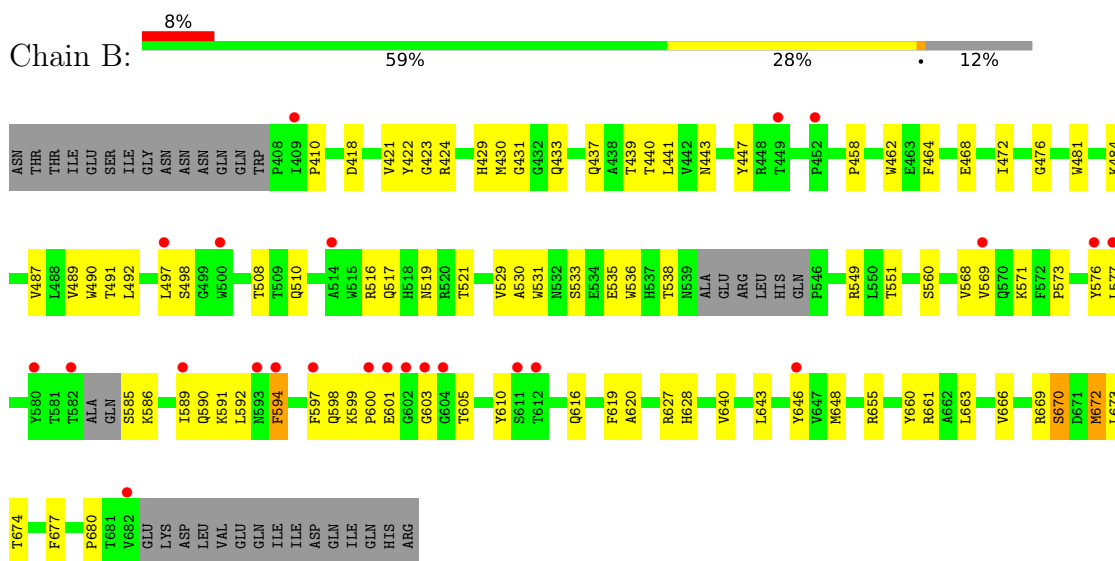
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Capsid polyprotein VP90



- Molecule 1: Capsid polyprotein VP90



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.20Å 86.31Å 108.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.73 46.04 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.04-2.73) 88.7 (46.04-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.269 , 0.312 0.269 , 0.312	Depositor DCC
$R_{free}$ test set	1595 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.830	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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](#)

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	0.27	0/2202	0.53	0/3002
1	B	0.25	0/2187	0.50	0/2983
All	All	0.26	0/4389	0.51	0/5985

There are no bond length outliers.

There are no bond angle outliers.

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	2140	0	2060	65	0
1	B	2125	0	2047	74	0
All	All	4265	0	4107	114	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 14.

All (114) 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:432:GLY:HA2	1:B:591:LYS:HG2	1.67	0.76
1:A:434:SER:OG	1:A:607:ARG:NH1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:LYS:HG2	1:B:598:GLN:HG3	1.69	0.74
1:B:571:LYS:HE3	1:B:643:LEU:HB2	1.69	0.73
1:A:496:LYS:HG2	1:B:410:PRO:HA	1.71	0.73
1:A:424:ARG:HH22	1:B:655:ARG:HG2	1.53	0.73
1:A:491:THR:HG23	1:A:498:SER:HB2	1.73	0.70
1:A:601:GLU:HG3	1:B:591:LYS:NZ	2.09	0.67
1:A:666:VAL:HB	1:B:594:PHE:HE1	1.59	0.67
1:A:596:THR:HG21	1:A:643:LEU:HD13	1.75	0.66
1:A:651:GLN:HG2	1:B:439:THR:HG22	1.80	0.64
1:A:446:ILE:HG23	1:A:568:VAL:HG21	1.81	0.62
1:B:517:GLN:O	1:B:519:ASN:N	2.31	0.62
1:A:589:ILE:HD11	1:B:441:LEU:HD22	1.83	0.61
1:B:424:ARG:HD2	1:B:670:SER:HB2	1.82	0.61
1:A:535:GLU:HB2	1:A:549:ARG:HG2	1.84	0.59
1:B:535:GLU:HB3	1:B:549:ARG:HG2	1.83	0.59
1:A:464:PHE:HB2	1:A:476:GLY:HA3	1.85	0.58
1:A:509:THR:HG23	1:A:511:LEU:H	1.68	0.58
1:A:409:ILE:HB	1:B:497:LEU:HB3	1.84	0.58
1:A:517:GLN:HB2	1:A:520:ARG:HG3	1.85	0.58
1:B:421:VAL:HG22	1:B:489:VAL:HG22	1.87	0.57
1:A:441:LEU:HD11	1:B:589:ILE:HG12	1.85	0.57
1:A:576:TYR:HB3	1:A:590:GLN:HB2	1.87	0.57
1:B:569:VAL:HG22	1:B:598:GLN:HG2	1.86	0.57
1:B:508:THR:HG22	1:B:529:VAL:HG22	1.87	0.56
1:B:661:ARG:O	1:B:661:ARG:NH1	2.37	0.56
1:B:418:ASP:O	1:B:491:THR:OG1	2.22	0.56
1:B:431:GLY:O	1:B:441:LEU:HD12	2.06	0.56
1:A:426:THR:HG23	1:A:670:SER:HB2	1.89	0.55
1:B:576:TYR:HD2	1:B:590:GLN:HG3	1.72	0.55
1:B:484:LYS:HE3	1:B:619:PHE:HE1	1.73	0.54
1:B:533:SER:HB2	1:B:551:THR:HG23	1.87	0.54
1:A:601:GLU:HG3	1:B:591:LYS:HZ2	1.71	0.54
1:B:516:ARG:HG3	1:B:521:THR:HG22	1.91	0.53
1:A:430:MET:HE1	1:A:442:VAL:HG23	1.90	0.53
1:A:664:THR:OG1	1:A:666:VAL:O	2.27	0.52
1:B:468:GLU:O	1:B:510:GLN:NE2	2.32	0.52
1:A:589:ILE:HB	1:B:599:LYS:HD2	1.92	0.52
1:A:666:VAL:HB	1:B:594:PHE:CE1	2.43	0.52
1:A:589:ILE:HB	1:B:599:LYS:HB3	1.92	0.51
1:B:585:SER:O	1:B:585:SER:OG	2.28	0.51
1:A:578:GLU:HB2	1:A:588:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLY:HA3	1:B:487:VAL:HG12	1.94	0.50
1:A:441:LEU:HD12	1:A:606:LEU:HD21	1.93	0.50
1:B:458:PRO:HB2	1:B:472:ILE:HD11	1.94	0.50
1:B:673:LEU:HD12	1:B:674:THR:H	1.77	0.49
1:A:513:VAL:HG21	1:A:555:VAL:HG11	1.93	0.49
1:A:509:THR:HG22	1:A:528:VAL:O	2.12	0.49
1:A:467:LEU:HD23	1:A:472:ILE:H	1.77	0.49
1:B:443:ASN:HD22	1:B:573:PRO:HG2	1.78	0.49
1:A:548:LEU:HD12	1:A:646:TYR:CD2	2.48	0.48
1:A:488:LEU:HD11	1:B:492:LEU:HD11	1.95	0.48
1:A:580:TYR:HA	1:A:587:SER:OG	2.13	0.48
1:A:667:GLY:HA2	1:B:663:LEU:HD13	1.95	0.48
1:B:586:LYS:HB2	1:B:586:LYS:HE2	1.65	0.48
1:A:567:ASP:HA	1:A:607:ARG:HA	1.95	0.48
1:A:533:SER:HB3	1:A:549:ARG:HH21	1.79	0.48
1:B:464:PHE:HB2	1:B:476:GLY:HA3	1.96	0.48
1:B:429:HIS:HB3	1:B:610:TYR:CD1	2.48	0.47
1:B:591:LYS:N	1:B:591:LYS:HD3	2.30	0.47
1:B:568:VAL:C	1:B:605:THR:HB	2.36	0.47
1:A:574:LEU:HG	1:A:575:ALA:O	2.14	0.47
1:A:587:SER:O	1:B:600:PRO:HD2	2.15	0.47
1:A:594:PHE:CE1	1:B:666:VAL:HB	2.50	0.46
1:B:430:MET:HE3	1:B:669:ARG:HA	1.96	0.46
1:B:531:TRP:HH2	1:B:680:PRO:HG3	1.80	0.46
1:A:599:LYS:HB3	1:B:589:ILE:HG21	1.98	0.46
1:A:442:VAL:HG13	1:A:661:ARG:HH21	1.81	0.46
1:A:661:ARG:HD2	1:B:660:TYR:CD2	2.51	0.46
1:A:433:GLN:HB3	1:B:591:LYS:HE3	1.96	0.46
1:A:421:VAL:HG22	1:A:489:VAL:HG22	1.98	0.46
1:A:432:GLY:HA3	1:A:438:ALA:HB2	1.96	0.46
1:A:592:LEU:HD12	1:B:439:THR:OG1	2.16	0.45
1:B:576:TYR:HD2	1:B:590:GLN:CG	2.29	0.45
1:A:428:LEU:HD23	1:A:428:LEU:HA	1.72	0.45
1:A:428:LEU:HD12	1:A:464:PHE:HZ	1.81	0.45
1:B:530:ALA:CB	1:B:677:PHE:HB3	2.47	0.45
1:A:654:ALA:N	1:B:670:SER:O	2.47	0.45
1:B:441:LEU:HD23	1:B:666:VAL:HG12	1.99	0.45
1:B:603:GLY:C	1:B:605:THR:H	2.21	0.44
1:A:489:VAL:HB	1:A:501:ASN:O	2.17	0.44
1:B:560:SER:OG	1:B:616:GLN:N	2.49	0.44
1:B:538:THR:OG1	1:B:627:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:HD22	1:A:597:PHE:CD1	2.53	0.44
1:A:594:PHE:CE1	1:B:440:THR:HB	2.53	0.44
1:A:422:TYR:HD2	1:A:488:LEU:HD12	1.83	0.43
1:B:433:GLN:OE1	1:B:601:GLU:HG3	2.18	0.43
1:A:536:TRP:CE2	1:A:652:LYS:HB2	2.54	0.43
1:B:430:MET:CE	1:B:669:ARG:HA	2.48	0.43
1:A:564:GLU:O	1:A:566:PHE:HD1	2.02	0.42
1:A:581:THR:HG22	1:A:585:SER:HA	2.00	0.42
1:B:422:TYR:HB3	1:B:490:TRP:HZ3	1.85	0.42
1:B:538:THR:OG1	1:B:538:THR:O	2.30	0.42
1:A:579:ASP:O	1:A:587:SER:HA	2.19	0.42
1:B:592:LEU:O	1:B:648:MET:N	2.36	0.42
1:B:530:ALA:HB3	1:B:677:PHE:HB3	2.01	0.42
1:A:536:TRP:CD2	1:A:648:MET:HE2	2.55	0.41
1:A:601:GLU:HG3	1:B:591:LYS:HZ3	1.81	0.41
1:A:581:THR:N	1:A:586:LYS:O	2.54	0.41
1:B:481:TRP:HA	1:B:620:ALA:HA	2.02	0.41
1:A:481:TRP:HA	1:A:620:ALA:HA	2.02	0.41
1:B:536:TRP:NE1	1:B:648:MET:HB3	2.35	0.41
1:A:592:LEU:HD11	1:A:649:PRO:HA	2.03	0.41
1:B:422:TYR:CE1	1:B:672:MET:HB3	2.55	0.41
1:B:491:THR:HG23	1:B:498:SER:OG	2.20	0.41
1:A:582:THR:HA	1:A:585:SER:OG	2.21	0.41
1:B:643:LEU:HA	1:B:646:TYR:OH	2.21	0.41
1:B:490:TRP:HB2	1:B:497:LEU:HD11	2.03	0.41
1:B:447:TYR:HB2	1:B:462:TRP:CZ3	2.56	0.40
1:A:599:LYS:HE3	1:B:577:LEU:HD21	2.03	0.40
1:B:628:HIS:HB3	1:B:640:VAL:HG22	2.04	0.40
1:A:591:LYS:H	1:A:591:LYS:HG3	1.49	0.40
1:B:591:LYS:HE2	1:B:591:LYS:HB2	1.76	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	261/304 (86%)	239 (92%)	21 (8%)	1 (0%)	34	55
1	B	261/304 (86%)	233 (89%)	28 (11%)	0	100	100
All	All	522/608 (86%)	472 (90%)	49 (9%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ILE

### 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	233/266 (88%)	222 (95%)	11 (5%)	26	45
1	B	232/266 (87%)	227 (98%)	5 (2%)	52	71
All	All	465/532 (87%)	449 (97%)	16 (3%)	37	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	LEU
1	A	510	GLN
1	A	561	SER
1	A	576	TYR
1	A	579	ASP
1	A	591	LYS
1	A	594	PHE
1	A	597	PHE
1	A	611	SER
1	A	650	GLU
1	A	673	LEU
1	B	437	GLN

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Mol	Chain	Res	Type
1	B	594	PHE
1	B	597	PHE
1	B	670	SER
1	B	672	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	ASN
1	A	595	GLN
1	B	595	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	269/304 (88%)	0.92	40 (14%) <b>2</b>   <b>2</b>	27, 44, 65, 83	0
1	B	267/304 (87%)	0.86	24 (8%) <b>9</b>   <b>10</b>	29, 42, 64, 87	0
All	All	536/608 (88%)	0.89	64 (11%) <b>4</b>   <b>4</b>	27, 43, 65, 87	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	603	GLY	5.5
1	B	602	GLY	5.4
1	B	449	THR	5.1
1	A	583	ALA	5.0
1	B	682	VAL	4.7
1	A	600	PRO	4.4
1	B	452	PRO	4.2
1	A	576	TYR	3.7
1	B	597	PHE	3.6
1	A	588	ALA	3.5
1	A	580	TYR	3.4
1	B	582	THR	3.3
1	A	500	TRP	3.3
1	B	569	VAL	3.2
1	A	594	PHE	3.2
1	A	416	VAL	3.2
1	A	581	THR	3.2
1	A	492	LEU	3.2
1	B	589	ILE	3.2
1	A	606	LEU	3.2
1	A	590	GLN	3.2
1	A	597	PHE	3.1
1	A	582	THR	3.0
1	B	593	ASN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	577	LEU	2.9
1	A	681	THR	2.9
1	A	574	LEU	2.8
1	B	577	LEU	2.8
1	A	571	LYS	2.8
1	A	682	VAL	2.8
1	A	496	LYS	2.8
1	B	497	LEU	2.8
1	A	655	ARG	2.8
1	A	591	LYS	2.7
1	B	600	PRO	2.7
1	B	601	GLU	2.6
1	A	415	PRO	2.6
1	B	580	TYR	2.5
1	B	594	PHE	2.5
1	A	598	GLN	2.5
1	A	569	VAL	2.5
1	B	500	TRP	2.5
1	B	604	GLY	2.4
1	A	454	PRO	2.4
1	B	576	TYR	2.4
1	A	644	SER	2.4
1	B	612	THR	2.3
1	A	680	PRO	2.3
1	B	514	ALA	2.3
1	A	506	VAL	2.3
1	B	611	SER	2.3
1	A	498	SER	2.2
1	A	408	PRO	2.2
1	A	544	HIS	2.1
1	A	586	LYS	2.1
1	B	646	TYR	2.1
1	A	546	PRO	2.1
1	A	411	LEU	2.1
1	A	494	GLY	2.1
1	A	679	PHE	2.1
1	A	497	LEU	2.1
1	B	409	ILE	2.0
1	A	520	ARG	2.0
1	A	470	ASN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.