

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	9CP0
Title	:	Crystal structure of the porcine astrovirus 4 capsid spike domain
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Deposited on	:	2024-07-17
Resolution	:	1.85 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.85 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	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m A}))$		
R_{free}	164625	3097 (1.86-1.86)		
Clashscore	180529	3359(1.86-1.86)		
Ramachandran outliers	177936	3335 (1.86-1.86)		
Sidechain outliers	177891	3335 (1.86-1.86)		
RSRZ outliers	164620	3097 (1.86-1.86)		

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 >=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 <=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				
			31%				
1	A	247	76%	17%	7%		
			25%				
1	В	247	74%	18%	8%		
			34%				
1	С	247	74%	17%	8%		
			22%				
1	D	247	74%	17%	8%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7411 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	D	227	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	221	1776	1138	295	339	4	0	0	U
1	C	227	Total	С	Ν	0	S	0	0	0
		221	1776	1138	295	339	4	0	0	U
1	П	227	Total	С	Ν	0	S	0	0	0
			1776	1138	295	339	4	0	0	0
1 A	220	Total	С	Ν	0	S	0	0	0	
	230	1800	1154	298	344	4	0	U	U	

• Molecule 1 is a protein called Spike protein.

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Ca 1 1	0	0
2	А	1	Total Ca 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
3	С	82	Total O 82 82	0	0
3	D	73	Total O 73 73	0	0
3	А	74	$\begin{array}{cc} \text{Total} & \text{O} \\ 74 & 74 \end{array}$	0	0



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: Spike protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	46.39Å 66.21Å 87.75Å	Depositor
a, b, c, α , β , γ	74.54° 81.67° 78.61°	Depositor
Bosolution(A)	39.78 - 1.85	Depositor
Resolution (A)	39.78 - 1.85	EDS
% Data completeness	95.8 (39.78-1.85)	Depositor
(in resolution range)	87.8 (39.78-1.85)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.63 (at 1.85 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.316 , 0.362	Depositor
n, n_{free}	0.316 , 0.361	DCC
R_{free} test set	78508 reflections $(2.47%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	11.2	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 33.1	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7411	wwPDB-VP
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 18.19% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: CA

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).

Mal	Chain	Bond	lengths	Bond angles		
IVI01	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/1847	0.57	0/2526	
1	В	0.31	0/1822	0.56	0/2489	
1	С	0.31	0/1822	0.56	0/2489	
1	D	0.31	0/1822	0.56	0/2489	
All	All	0.31	0/7313	0.56	0/9993	

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	А	1800	0	1760	34	0
1	В	1776	0	1734	33	0
1	С	1776	0	1735	30	0
1	D	1776	0	1735	31	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	74	0	0	6	0
3	В	52	0	0	2	0
3	C	82	0	0	2	0



Continuea from previous page								
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
3	D	73	0	0	0	0		
All	All	7411	0	6964	113	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 8.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:606:ARG:HD3	1:C:614:PRO:HB3	1.70	0.74
1:A:471:LEU:HD11	1:A:533:TRP:HZ2	1.56	0.69
1:B:562:MET:HB3	1:D:625:GLN:HE22	1.59	0.68
1:D:644:THR:HG21	1:A:439:LEU:HB2	1.76	0.66
1:A:577:SER:N	3:A:804:HOH:O	2.32	0.62
1:A:539:LYS:HG2	1:A:540:GLN:N	2.15	0.62
1:C:544:ARG:HD2	1:C:584:GLU:HB2	1.82	0.61
1:A:493:LEU:HB3	3:A:813:HOH:O	1.99	0.60
1:A:539:LYS:HD3	1:A:541:ILE:HD13	1.82	0.60
1:B:500:GLN:OE1	1:B:539:LYS:NZ	2.32	0.60
1:D:644:THR:HG21	1:A:439:LEU:H	1.65	0.60
1:C:606:ARG:HG2	1:C:616:TYR:CZ	2.37	0.59
1:C:459:ALA:HB2	1:C:608:PHE:CG	2.38	0.58
1:A:559:GLN:N	1:A:571:THR:O	2.29	0.58
1:D:630:GLU:OE1	1:D:630:GLU:N	2.19	0.57
1:D:509:ILE:HG21	1:D:541:ILE:HD11	1.87	0.56
1:B:602:PHE:N	1:B:618:SER:OG	2.39	0.56
1:A:433:LEU:HB2	1:A:436:GLU:HB2	1.87	0.56
1:B:433:LEU:CD1	1:B:475:LEU:HB2	2.36	0.56
1:A:486:ILE:HD12	1:A:491:ILE:HD11	1.88	0.56
1:A:455:VAL:HG21	1:A:471:LEU:HD13	1.89	0.55
1:A:552:GLN:HG3	1:A:579:LEU:HD23	1.88	0.54
1:D:579:LEU:HD13	1:D:621:GLN:HG3	1.90	0.54
1:A:493:LEU:HD22	1:A:494:PRO:HD2	1.90	0.53
1:B:455:VAL:HG21	1:B:471:LEU:HD12	1.91	0.53
1:B:501:LYS:NZ	1:B:503:GLY:O	2.39	0.53
1:D:488:ILE:HD11	1:D:513:TYR:HB3	1.91	0.53
1:D:631:PRO:HG2	1:A:435:GLY:HA2	1.89	0.53
1:A:443:THR:HG23	3:A:807:HOH:O	2.09	0.53
1:B:585:ARG:NH1	1:C:567:LEU:H	2.08	0.52
1:A:426:VAL:HG13	1:A:652:LEU:HD21	1.90	0.52
1:B:606:ARG:HH21	1:B:609:ASP:HB3	1.75	0.52



	louis page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:644:THR:HG21	1:C:439:LEU:HG	1.92	0.52	
1:B:544:ARG:HD2	1:B:584:GLU:HB2	1.92	0.51	
1:C:443:THR:HA	3:C:735:HOH:O	2.09	0.51	
1:D:567:LEU:H	1:A:585:ARG:NH1	2.08	0.50	
1:C:517:PHE:HE1	1:C:527:GLN:HB3	1.76	0.50	
1:D:464:GLN:HB3	1:D:607:GLU:HG3	1.94	0.50	
1:D:556:PHE:HA	1:D:573:GLY:O	2.12	0.49	
1:C:634:GLU:OE1	1:C:637:ASN:ND2	2.45	0.49	
1:B:449:ARG:NH2	3:B:809:HOH:O	2.46	0.49	
1:A:590:ASN:HB2	1:A:593:LYS:HG3	1.94	0.49	
1:D:430:SER:HB2	1:D:477:PRO:HA	1.95	0.48	
1:B:433:LEU:HD11	1:B:475:LEU:HB2	1.95	0.48	
1:A:471:LEU:HD11	1:A:533:TRP:CZ2	2.42	0.48	
1:C:430:SER:HB2	1:C:477:PRO:HA	1.94	0.48	
1:C:500:GLN:HG2	1:C:509:ILE:CG2	2.43	0.48	
1:A:500:GLN:HG2	1:A:509:ILE:CG2	2.44	0.48	
1:C:464:GLN:HB3	1:C:607:GLU:HG3	1.95	0.47	
1:D:645:ALA:HB1	1:A:429:TYR:HA	1.96	0.47	
1:D:606:ARG:HH12	1:D:609:ASP:HB3	1.77	0.47	
1:B:464:GLN:HB3	1:B:607:GLU:HG3	1.95	0.47	
1:C:542:ARG:NH1	1:C:584:GLU:OE1	2.45	0.47	
1:C:453:ALA:HA	1:C:501:LYS:O	2.15	0.47	
1:B:506:TYR:O	3:B:801:HOH:O	2.21	0.47	
1:D:520:ILE:HG21	1:D:556:PHE:CZ	2.49	0.46	
1:C:540:GLN:HA	1:C:540:GLN:OE1	2.15	0.46	
1:D:430:SER:OG	1:D:475:LEU:O	2.33	0.46	
1:D:552:GLN:HG3	1:D:579:LEU:HD12	1.96	0.46	
1:A:653:ASN:HB2	3:A:813:HOH:O	2.15	0.46	
1:D:563:SER:O	1:D:566:ASN:ND2	2.41	0.46	
1:D:645:ALA:HB2	1:A:648:LEU:HD13	1.96	0.46	
1:B:426:VAL:HG23	1:B:652:LEU:HD21	1.98	0.46	
1:B:487:ASP:HB3	1:B:490:VAL:HG22	1.97	0.46	
1:C:516:HIS:HB2	1:C:650:LEU:HA	1.99	0.45	
1:C:649:LYS:NZ	3:C:711:HOH:O	2.48	0.45	
1:A:501:LYS:NZ	3:A:809:HOH:O	2.40	0.45	
1:B:606:ARG:CZ	1:B:614:PRO:HB3	2.46	0.45	
1:C:520:ILE:HG22	1:C:629:TYR:HD2	1.82	0.44	
1:C:576:VAL:HB	1:C:624:THR:HA	1.99	0.44	
1:B:634:GLU:O	1:B:638:VAL:HG23	2.18	0.44	
1:C:473:GLU:HG2	1:C:595:TYR:CE1	2.52	0.44	
1:A:488:ILE:HD11	1:A:652:LEU:HD11	2.00	0.44	



	louis page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:530:THR:OG1	1:D:638:VAL:HG22	2.17	0.44	
1:D:481:GLN:HB2	1:D:486:ILE:HD13	1.99	0.44	
1:B:582:LEU:HD11	1:C:567:LEU:HD23	1.99	0.44	
1:C:648:LEU:HD12	1:C:648:LEU:HA	1.68	0.43	
1:B:439:LEU:HD12	1:B:439:LEU:HA	1.85	0.43	
1:A:531:VAL:HG22	1:A:597:SER:O	2.18	0.43	
1:A:537:ILE:HD12	1:A:538:SER:H	1.83	0.43	
1:D:542:ARG:NH1	1:D:584:GLU:OE1	2.48	0.43	
1:B:433:LEU:HD12	1:B:475:LEU:HB2	1.99	0.43	
1:C:517:PHE:HB3	1:C:614:PRO:HD2	1.99	0.43	
1:B:606:ARG:HB2	1:B:616:TYR:CZ	2.53	0.43	
1:D:517:PHE:HE1	1:D:527:GLN:HB3	1.83	0.43	
1:D:647:PRO:HG3	1:A:429:TYR:CD1	2.54	0.43	
1:D:590:ASN:HB2	1:D:593:LYS:HG3	2.01	0.43	
1:B:486:ILE:HD12	1:B:486:ILE:O	2.19	0.42	
1:B:512:VAL:HG22	1:B:533:TRP:HB3	2.01	0.42	
1:B:452:VAL:HB	1:B:544:ARG:HG2	2.01	0.42	
1:B:453:ALA:HA	1:B:501:LYS:O	2.19	0.42	
1:C:459:ALA:HB2	1:C:608:PHE:CD1	2.54	0.42	
1:A:556:PHE:HA	1:A:573:GLY:O	2.19	0.42	
1:B:429:TYR:HA	1:C:645:ALA:HB1	2.03	0.41	
1:A:439:LEU:HD23	1:A:439:LEU:HA	1.84	0.41	
1:B:473:GLU:HB2	1:B:595:TYR:CE1	2.55	0.41	
1:B:562:MET:O	1:D:625:GLN:NE2	2.54	0.41	
1:D:644:THR:CG2	1:A:439:LEU:H	2.31	0.41	
1:A:606:ARG:HH21	1:A:609:ASP:CG	2.24	0.41	
1:D:539:LYS:HE3	1:D:539:LYS:HB2	1.95	0.41	
1:A:553:PHE:N	3:A:804:HOH:O	2.48	0.41	
1:B:542:ARG:HA	1:B:586:GLN:OE1	2.20	0.41	
1:D:501:LYS:NZ	1:D:503:GLY:O	2.35	0.41	
1:D:606:ARG:HG3	1:D:616:TYR:CZ	2.56	0.41	
1:D:501:LYS:HD2	1:D:506:TYR:CZ	2.57	0.40	
1:B:458:GLN:HG3	1:B:459:ALA:N	2.37	0.40	
1:C:500:GLN:HE22	1:C:539:LYS:HE3	1.86	0.40	
1:C:524:ARG:NH2	1:C:626:GLN:OE1	2.54	0.40	
1:A:495:THR:HA	1:A:653:ASN:HD22	1.85	0.40	
1:B:498:ILE:HG21	1:B:533:TRP:CD2	2.56	0.40	
1:B:567:LEU:HD21	1:C:469:TYR:HB3	2.04	0.40	
1:C:471:LEU:HD23	1:C:471:LEU:HA	1.78	0.40	
1:C:651:HIS:CD2	1:C:651:HIS:N	2.89	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	Perce	ntiles
1	А	228/247~(92%)	$221 \ (97\%)$	7 (3%)	0	100	100
1	В	223/247~(90%)	219~(98%)	4(2%)	0	100	100
1	С	223/247~(90%)	214 (96%)	9~(4%)	0	100	100
1	D	223/247~(90%)	214 (96%)	9~(4%)	0	100	100
All	All	897/988~(91%)	868 (97%)	29(3%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	А	197/208~(95%)	195~(99%)	2(1%)	73	67
1	В	194/208~(93%)	194 (100%)	0	100	100
1	С	194/208~(93%)	192~(99%)	2(1%)	73	67
1	D	194/208~(93%)	192~(99%)	2 (1%)	73	67
All	All	779/832~(94%)	773~(99%)	6 (1%)	79	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	561	SER
1	С	586	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	D	597	SER
1	D	617	LEU
1	А	500	GLN
1	А	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	621	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	Z>2	2	$OWAB(Å^2)$	Q<0.9
1	А	230/247~(93%)	1.78	77~(33%)	1	1	6, 15, 24, 29	0
1	В	227/247~(91%)	1.63	62~(27%)	2	2	8, 15, 25, 35	0
1	С	227/247~(91%)	1.78	83~(36%)	1	1	6, 14, 23, 32	0
1	D	227/247~(91%)	1.63	54 (23%)	2	2	7, 14, 23, 29	0
All	All	911/988~(92%)	1.71	276 (30%)	1	1	6, 15, 24, 35	0

All (276) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	434	PHE	5.1
1	D	490	VAL	5.1
1	D	652	LEU	5.0
1	В	514	ALA	4.8
1	В	490	VAL	4.8
1	D	488	ILE	4.7
1	D	434	PHE	4.7
1	D	485	ILE	4.4
1	В	652	LEU	4.2
1	В	522	SER	4.1
1	С	488	ILE	4.1
1	С	654	ALA	4.0
1	А	434	PHE	4.0
1	С	490	VAL	4.0
1	А	435	GLY	4.0
1	А	571	THR	3.9
1	В	485	ILE	3.9
1	А	526	VAL	3.7
1	А	493	LEU	3.6
1	В	434	PHE	3.6
1	D	633	THR	3.6



Mol	Chain	Res	Type	RSRZ
1	А	633	THR	3.6
1	А	426	VAL	3.6
1	С	494	PRO	3.4
1	D	506	TYR	3.4
1	D	486	ILE	3.4
1	С	620	GLN	3.4
1	В	453	ALA	3.3
1	С	479	PHE	3.3
1	А	652	LEU	3.3
1	С	466	VAL	3.3
1	D	654	ALA	3.3
1	В	443	THR	3.3
1	D	431	PRO	3.2
1	А	461	GLY	3.2
1	А	453	ALA	3.2
1	В	624	THR	3.2
1	А	537	ILE	3.2
1	А	640	ALA	3.2
1	D	541	ILE	3.2
1	С	633	THR	3.1
1	А	611	TYR	3.1
1	С	603	ASN	3.1
1	В	460	VAL	3.1
1	А	478	VAL	3.1
1	С	495	THR	3.1
1	С	520	ILE	3.1
1	А	494	PRO	3.1
1	В	654	ALA	3.1
1	В	479	PHE	3.1
1	С	522	SER	3.1
1	А	475	LEU	3.1
1	А	648	LEU	3.1
1	С	455	VAL	3.1
1	В	630	GLU	3.0
1	В	525	PRO	3.0
1	А	488	ILE	3.0
1	С	506	TYR	3.0
1	С	496	TYR	3.0
1	С	523	SER	3.0
1	В	633	THR	3.0
1	В	440	TYR	3.0
1	А	429	TYR	3.0



Mol	Chain	Res	Type	RSRZ
1	А	567	LEU	3.0
1	А	631	PRO	2.9
1	В	488	ILE	2.9
1	D	517	PHE	2.9
1	А	471	LEU	2.9
1	В	475	LEU	2.9
1	А	650	LEU	2.9
1	В	435	GLY	2.9
1	С	555	PHE	2.9
1	А	639	GLY	2.9
1	D	456	CYS	2.9
1	С	471	LEU	2.8
1	А	524	ARG	2.8
1	A	560	LEU	2.8
1	В	625	GLN	2.8
1	D	482	ASN	2.8
1	D	437	PRO	2.8
1	D	631	PRO	2.8
1	А	479	PHE	2.8
1	А	632	THR	2.8
1	D	553	PHE	2.7
1	С	460	VAL	2.7
1	С	537	ILE	2.7
1	С	589	ILE	2.7
1	С	579	LEU	2.7
1	D	475	LEU	2.7
1	В	425	PRO	2.7
1	В	555	PHE	2.7
1	С	517	PHE	2.7
1	С	583	THR	2.7
1	С	574	LEU	2.7
1	С	611	TYR	2.7
1	А	608	PHE	2.7
1	D	617	LEU	2.7
1	В	557	ASN	2.6
1	С	429	TYR	2.6
1	С	571	THR	2.6
1	А	646	THR	2.6
1	С	601	ALA	2.6
1	С	475	LEU	2.6
1	С	648	LEU	2.6
1	В	563	SER	2.6



Mol	Chain	Res	Type	RSRZ
1	В	635	ALA	2.6
1	С	635	ALA	2.6
1	D	453	ALA	2.6
1	С	524	ARG	2.6
1	В	486	ILE	2.6
1	С	630	GLU	2.6
1	С	453	ALA	2.6
1	С	640	ALA	2.6
1	А	463	ALA	2.6
1	D	478	VAL	2.5
1	D	429	TYR	2.5
1	С	586	GLN	2.5
1	D	520	ILE	2.5
1	В	518	THR	2.5
1	В	517	PHE	2.5
1	В	638	VAL	2.5
1	С	478	VAL	2.5
1	С	638	VAL	2.5
1	D	526	VAL	2.5
1	А	490	VAL	2.5
1	D	614	PRO	2.5
1	С	561	SER	2.5
1	В	462	GLY	2.5
1	С	646	THR	2.5
1	А	609	ASP	2.5
1	А	513	TYR	2.5
1	В	554	LEU	2.5
1	С	485	ILE	2.5
1	С	489	THR	2.5
1	А	635	ALA	2.5
1	С	599	PHE	2.5
1	А	466	VAL	2.5
1	А	615	PHE	2.5
1	А	431	PRO	2.4
1	D	572	TYR	2.4
1	С	461	GLY	2.4
1	В	433	LEU	2.4
1	С	532	LEU	2.4
1	D	433	LEU	2.4
1	А	589	ILE	2.4
1	В	523	SER	2.4
1	А	451	PRO	2.4



Mol	Chain	Res	Type	RSRZ
1	А	455	VAL	2.4
1	В	461	GLY	2.4
1	D	632	THR	2.4
1	С	433	LEU	2.4
1	С	556	PHE	2.4
1	D	483	GLY	2.4
1	С	467	TYR	2.4
1	А	620	GLN	2.4
1	В	642	LEU	2.4
1	С	474	LEU	2.4
1	А	543	LEU	2.4
1	В	594	TRP	2.4
1	С	533	TRP	2.4
1	С	594	TRP	2.4
1	С	614	PRO	2.4
1	А	549	PRO	2.4
1	В	478	VAL	2.4
1	В	615	PHE	2.4
1	D	489	THR	2.4
1	А	506	TYR	2.4
1	С	628	ASN	2.3
1	А	606	ARG	2.3
1	D	471	LEU	2.3
1	С	498	ILE	2.3
1	А	515	ALA	2.3
1	С	528	TRP	2.3
1	D	630	GLU	2.3
1	D	642	LEU	2.3
1	D	494	PRO	2.3
1	В	548	THR	2.3
1	С	448	GLN	2.3
1	А	597	SER	2.3
1	В	622	ILE	2.3
1	D	438	ALA	2.3
1	А	613	ILE	2.3
1	В	526	VAL	2.3
1	С	608	PHE	2.3
1	D	555	PHE	2.3
1	D	474	LEU	2.3
1	А	574	LEU	2.3
1	D	435	GLY	2.2
1	D	646	THR	2.2



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Mol	Chain	Res	Type	RSRZ
1	А	583	THR	2.2
1	А	565	SER	2.2
1	С	642	LEU	2.2
1	В	611	TYR	2.2
1	В	498	ILE	2.2
1	В	520	ILE	2.2
1	С	435	GLY	2.2
1	А	491	ILE	2.2
1	В	631	PRO	2.2
1	D	583	THR	2.2
1	В	582	LEU	2.2
1	С	652	LEU	2.2
1	А	433	LEU	2.2
1	D	514	ALA	2.2
1	А	525	PRO	2.2
1	В	575	THR	2.2
1	В	646	THR	2.2
1	С	544	ARG	2.2
1	D	452	VAL	2.2
1	С	483	GLY	2.2
1	С	484	ASN	2.2
1	D	447	GLY	2.2
1	А	517	PHE	2.2
1	С	464	GLN	2.2
1	А	438	ALA	2.2
1	А	474	LEU	2.2
1	С	451	PRO	2.2
1	С	629	TYR	2.2
1	В	570	THR	2.1
1	А	432	SER	2.1
1	D	450	VAL	2.1
1	А	628	ASN	2.1
1	А	555	PHE	2.1
1	В	496	TYR	2.1
1	C	595	TYR	2.1
1	В	581	SER	2.1
1	С	432	SER	2.1
1	D	522	SER	2.1
1	С	503	GLY	2.1
1	A	564	GLY	2.1
1	D	460	VAL	2.1
1	А	459	ALA	2.1



Mol	Chain	Res	Type	RSRZ
1	А	425	PRO	2.1
1	В	533	TRP	2.1
1	А	594	TRP	2.1
1	С	513	TYR	2.1
1	D	498	ILE	2.1
1	А	541	ILE	2.1
1	В	571	THR	2.1
1	D	518	THR	2.1
1	А	522	SER	2.1
1	В	447	GLY	2.1
1	А	476	ASP	2.1
1	D	425	PRO	2.1
1	С	625	GLN	2.1
1	С	440	TYR	2.1
1	А	528	TRP	2.1
1	D	573	GLY	2.1
1	В	466	VAL	2.0
1	В	580	VAL	2.0
1	С	450	VAL	2.0
1	С	512	VAL	2.0
1	D	426	VAL	2.0
1	В	477	PRO	2.0
1	С	617	LEU	2.0
1	D	648	LEU	2.0
1	А	619	LEU	2.0
1	В	481	GLN	2.0
1	В	608	PHE	2.0
1	В	620	GLN	2.0
1	С	553	PHE	2.0
1	С	457	MET	2.0
1	А	504	SER	2.0
1	В	632	THR	2.0
1	С	575	THR	2.0
1	А	485	ILE	2.0
1	А	530	THR	2.0
1	А	469	TYR	2.0
1	А	496	TYR	2.0
1	А	483	GLY	2.0
1	С	515	ALA	2.0
1	D	588	GLU	2.0
1	С	631	PRO	2.0
1	В	474	LEU	2.0



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Mol	Chain	Res	Type	RSRZ
1	С	507	SER	2.0
1	D	560	LEU	2.0
1	А	523	SER	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)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CA	А	701	1/1	0.82	0.14	$15,\!15,\!15,\!15$	0
2	CA	В	701	1/1	0.86	0.15	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.

