



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:14 AM UTC

PDB ID : 9CP0 / pdb_00009cp0
Title : Crystal structure of the porcine astrovirus 4 capsid spike domain
Authors : Haley, D.J.; DuBois, R.M.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

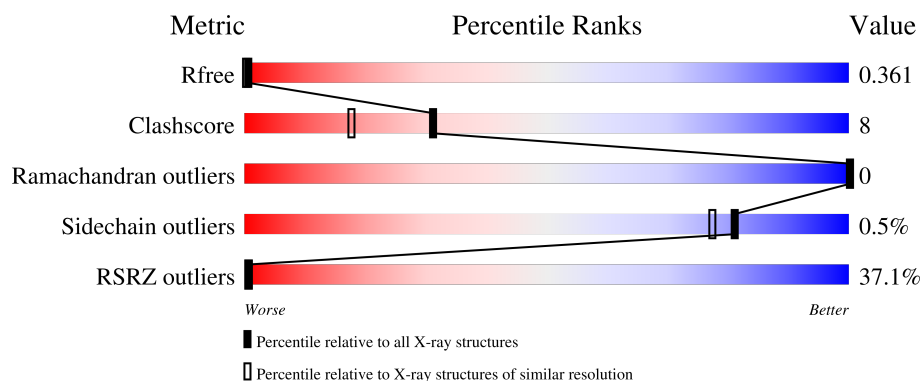
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 $\leq 5\%$. 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	247	39% 76% 17% 7%
1	B	247	31% 73% 19% 8%
1	C	247	39% 75% 16% 8%
1	D	247	28% 74% 18% 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.

- Molecule 1 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	227	Total	C	N	O	S	0	0	0
			1776	1138	295	339	4			
1	C	227	Total	C	N	O	S	0	0	0
			1776	1138	295	339	4			
1	D	227	Total	C	N	O	S	0	0	0
			1776	1138	295	339	4			
1	A	230	Total	C	N	O	S	0	0	0
			1800	1154	298	344	4			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

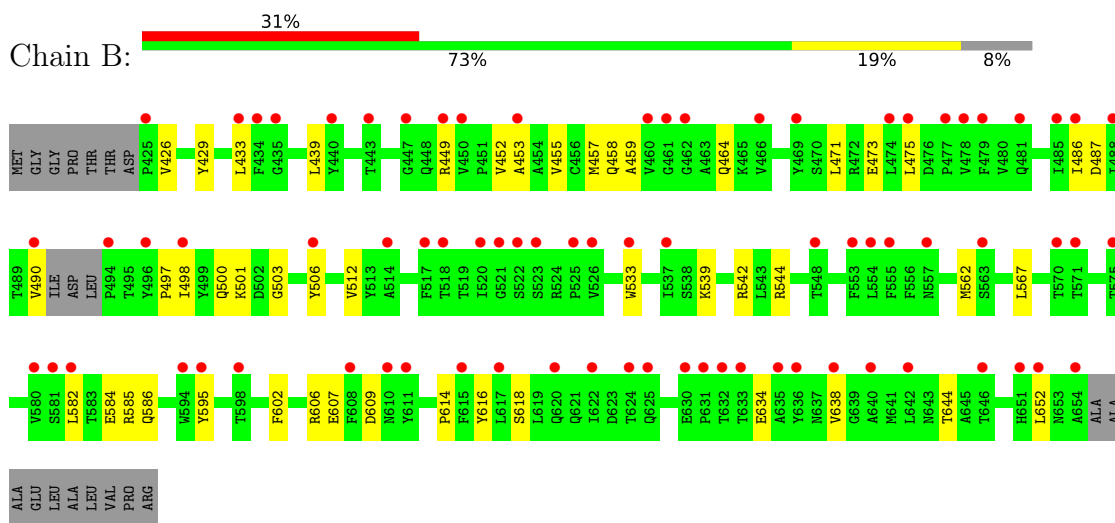
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	52	Total	O	0	0
			52	52		
3	C	82	Total	O	0	0
			82	82		
3	D	73	Total	O	0	0
			73	73		
3	A	74	Total	O	0	0
			74	74		

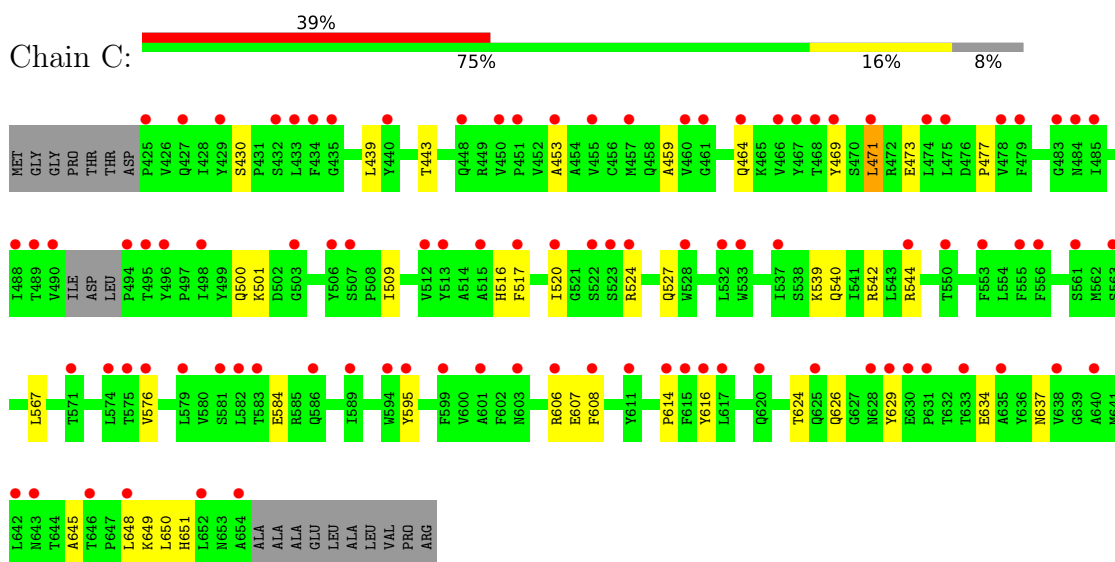
3 Residue-property plots

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

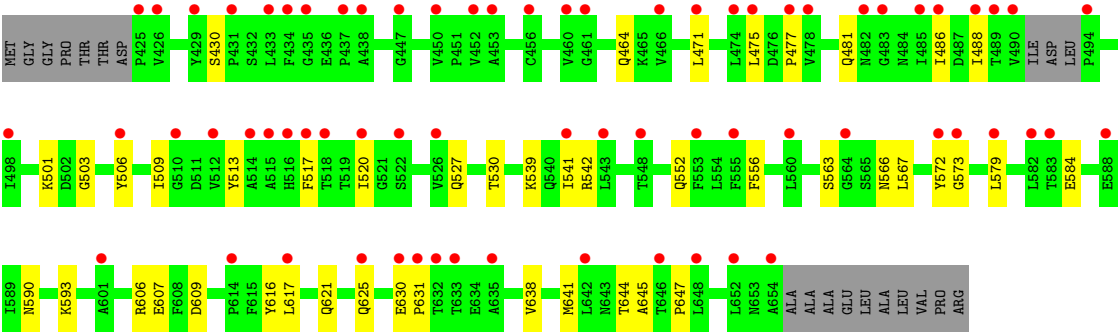


• Molecule 1: Spike protein

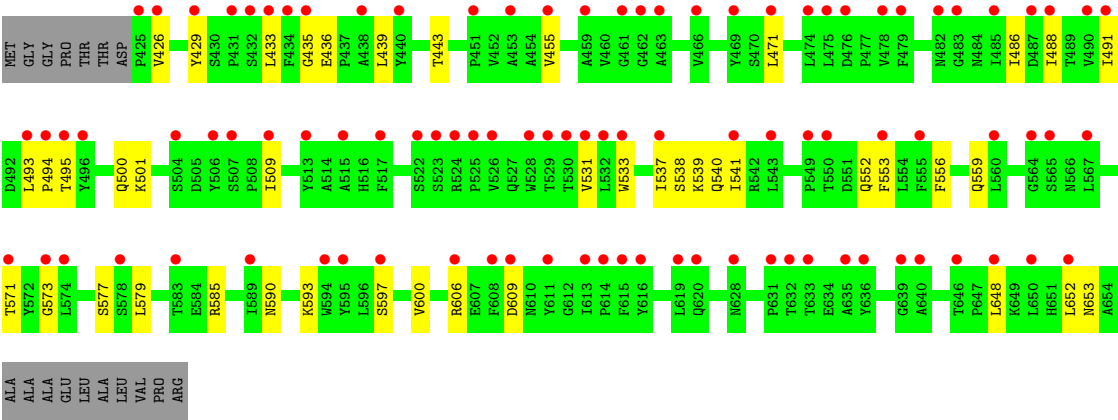
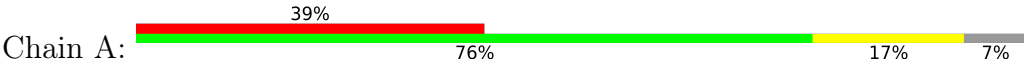


• Molecule 1: Spike protein





● Molecule 1: Spike protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.39Å 66.21Å 87.75Å 74.54° 81.67° 78.61°	Depositor
Resolution (Å)	39.78 – 1.85 39.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.78-1.85) 87.8 (39.78-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.316 , 0.362 0.316 , 0.361	Depositor DCC
R_{free} test set	2000 reflections (2.48%)	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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/1847	0.42	0/2526
1	B	0.25	0/1822	0.44	0/2489
1	C	0.21	0/1822	0.41	0/2489
1	D	0.24	0/1822	0.43	0/2489
All	All	0.23	0/7313	0.42	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	A	1800	0	1760	34	0
1	B	1776	0	1734	35	0
1	C	1776	0	1735	30	0
1	D	1776	0	1735	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	74	0	0	6	0
3	B	52	0	0	2	0
3	C	82	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	73	0	0	0	0
All	All	7411	0	6964	116	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 (116) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:572:TYR:HB2	1:D:641:MET:HE2	1.91	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:D:501:LYS:NZ	1:D:503:GLY:O	2.35	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:A:606:ARG:HH21	1:A:609:ASP:CG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:457:MET:HE1	1:B:497:PRO:O	2.18	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:B:486:ILE:HD12	1:B:486:ILE:C	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Percentiles	
1	A	228/247 (92%)	221 (97%)	7 (3%)	0	100	100
1	B	223/247 (90%)	219 (98%)	4 (2%)	0	100	100
1	C	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	Percentiles	
1	A	197/208 (95%)	196 (100%)	1 (0%)	81	77
1	B	194/208 (93%)	194 (100%)	0	100	100
1	C	194/208 (93%)	193 (100%)	1 (0%)	81	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	194/208 (93%)	192 (99%)	2 (1%)	68	60
All	All	779/832 (94%)	775 (100%)	4 (0%)	81	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	471	LEU
1	D	471	LEU
1	D	617	LEU
1	A	600	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	481	GLN
1	B	484	ASN
1	B	625	GLN
1	D	482	ASN
1	D	625	GLN
1	A	590	ASN
1	A	651	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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, 95th 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 ²)	Q<0.9
1	A	230/247 (93%)	1.92	96 (41%) 0 0	6, 15, 24, 29	0
1	B	227/247 (91%)	1.77	77 (33%) 1 1	8, 15, 25, 35	0
1	C	227/247 (91%)	1.91	96 (42%) 0 0	6, 14, 23, 32	0
1	D	227/247 (91%)	1.77	69 (30%) 1 1	7, 14, 23, 29	0
All	All	911/988 (92%)	1.84	338 (37%) 1 0	6, 15, 24, 35	0

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	PHE	5.4
1	D	490	VAL	5.4
1	D	652	LEU	5.2
1	B	514	ALA	5.1
1	B	490	VAL	5.0
1	D	488	ILE	5.0
1	D	434	PHE	4.9
1	D	485	ILE	4.6
1	B	652	LEU	4.4
1	B	522	SER	4.3
1	C	488	ILE	4.3
1	C	654	ALA	4.3
1	A	435	GLY	4.2
1	A	434	PHE	4.2
1	C	490	VAL	4.1
1	B	485	ILE	4.1
1	A	571	THR	4.1
1	A	526	VAL	3.9
1	A	493	LEU	3.8
1	B	434	PHE	3.8
1	D	633	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	633	THR	3.8
1	A	426	VAL	3.8
1	D	486	ILE	3.7
1	C	494	PRO	3.6
1	D	506	TYR	3.6
1	B	453	ALA	3.5
1	A	652	LEU	3.6
1	C	479	PHE	3.5
1	D	654	ALA	3.5
1	C	620	GLN	3.5
1	C	466	VAL	3.5
1	A	461	GLY	3.4
1	A	640	ALA	3.4
1	D	431	PRO	3.4
1	A	453	ALA	3.4
1	B	443	THR	3.4
1	A	537	ILE	3.4
1	B	624	THR	3.4
1	D	541	ILE	3.3
1	C	633	THR	3.3
1	A	611	TYR	3.3
1	A	478	VAL	3.3
1	B	460	VAL	3.3
1	B	654	ALA	3.3
1	A	475	LEU	3.3
1	A	648	LEU	3.3
1	C	506	TYR	3.2
1	C	455	VAL	3.2
1	A	494	PRO	3.2
1	B	479	PHE	3.2
1	C	603	ASN	3.2
1	C	520	ILE	3.2
1	A	488	ILE	3.2
1	C	495	THR	3.2
1	C	522	SER	3.2
1	C	496	TYR	3.2
1	B	525	PRO	3.2
1	B	440	TYR	3.1
1	A	567	LEU	3.1
1	B	630	GLU	3.1
1	A	631	PRO	3.1
1	A	429	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	471	LEU	3.1
1	D	517	PHE	3.1
1	B	633	THR	3.1
1	C	523	SER	3.1
1	B	435	GLY	3.1
1	B	488	ILE	3.1
1	A	639	GLY	3.1
1	B	475	LEU	3.1
1	A	650	LEU	3.1
1	C	555	PHE	3.0
1	D	456	CYS	3.0
1	D	437	PRO	3.0
1	C	471	LEU	3.0
1	A	560	LEU	3.0
1	B	625	GLN	3.0
1	A	479	PHE	3.0
1	D	482	ASN	3.0
1	D	475	LEU	2.9
1	A	524	ARG	2.9
1	D	631	PRO	2.9
1	C	537	ILE	2.9
1	A	632	THR	2.9
1	D	553	PHE	2.9
1	C	589	ILE	2.9
1	C	574	LEU	2.9
1	C	579	LEU	2.9
1	B	425	PRO	2.9
1	C	453	ALA	2.9
1	C	460	VAL	2.8
1	C	611	TYR	2.8
1	B	555	PHE	2.8
1	C	517	PHE	2.8
1	A	608	PHE	2.8
1	D	617	LEU	2.8
1	C	429	TYR	2.8
1	D	453	ALA	2.8
1	C	571	THR	2.8
1	C	583	THR	2.8
1	A	646	THR	2.8
1	B	635	ALA	2.8
1	C	601	ALA	2.8
1	C	635	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	557	ASN	2.8
1	C	475	LEU	2.8
1	C	648	LEU	2.8
1	B	486	ILE	2.8
1	D	478	VAL	2.8
1	C	640	ALA	2.7
1	A	463	ALA	2.7
1	C	478	VAL	2.7
1	D	614	PRO	2.7
1	B	563	SER	2.7
1	C	524	ARG	2.7
1	B	638	VAL	2.7
1	C	638	VAL	2.7
1	D	526	VAL	2.7
1	B	462	GLY	2.7
1	B	518	THR	2.7
1	C	646	THR	2.7
1	D	433	LEU	2.7
1	C	485	ILE	2.7
1	D	520	ILE	2.7
1	A	490	VAL	2.7
1	A	635	ALA	2.6
1	D	429	TYR	2.6
1	A	513	TYR	2.6
1	B	517	PHE	2.6
1	C	561	SER	2.6
1	C	461	GLY	2.6
1	A	466	VAL	2.6
1	C	586	GLN	2.6
1	C	630	GLU	2.6
1	D	572	TYR	2.6
1	C	599	PHE	2.6
1	A	615	PHE	2.6
1	A	431	PRO	2.6
1	B	433	LEU	2.6
1	B	554	LEU	2.6
1	A	589	ILE	2.6
1	A	455	VAL	2.6
1	C	489	THR	2.6
1	C	467	TYR	2.6
1	A	451	PRO	2.6
1	B	594	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	533	TRP	2.6
1	C	594	TRP	2.6
1	C	433	LEU	2.6
1	C	532	LEU	2.6
1	A	609	ASP	2.6
1	B	461	GLY	2.6
1	A	515	ALA	2.6
1	B	523	SER	2.6
1	D	632	THR	2.6
1	A	506	TYR	2.5
1	B	642	LEU	2.5
1	C	474	LEU	2.5
1	A	543	LEU	2.5
1	B	478	VAL	2.5
1	A	549	PRO	2.5
1	B	615	PHE	2.5
1	C	556	PHE	2.5
1	D	471	LEU	2.5
1	D	483	GLY	2.5
1	C	498	ILE	2.5
1	D	489	THR	2.5
1	A	620	GLN	2.5
1	C	614	PRO	2.5
1	C	628	ASN	2.5
1	B	622	ILE	2.5
1	C	528	TRP	2.5
1	D	494	PRO	2.5
1	A	606	ARG	2.4
1	D	642	LEU	2.4
1	A	613	ILE	2.4
1	D	438	ALA	2.4
1	B	526	VAL	2.4
1	D	435	GLY	2.4
1	D	630	GLU	2.4
1	D	474	LEU	2.4
1	A	597	SER	2.4
1	C	608	PHE	2.4
1	B	548	THR	2.4
1	A	583	THR	2.4
1	D	452	VAL	2.4
1	C	448	GLN	2.4
1	C	435	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	642	LEU	2.4
1	C	652	LEU	2.4
1	A	574	LEU	2.4
1	B	611	TYR	2.4
1	D	555	PHE	2.4
1	D	583	THR	2.4
1	D	646	THR	2.4
1	B	498	ILE	2.4
1	B	520	ILE	2.4
1	A	491	ILE	2.4
1	D	514	ALA	2.4
1	B	631	PRO	2.4
1	C	483	GLY	2.4
1	A	433	LEU	2.3
1	A	438	ALA	2.3
1	C	451	PRO	2.3
1	D	447	GLY	2.3
1	D	450	VAL	2.3
1	A	565	SER	2.3
1	A	474	LEU	2.3
1	B	570	THR	2.3
1	B	575	THR	2.3
1	B	646	THR	2.3
1	A	517	PHE	2.3
1	A	459	ALA	2.3
1	A	525	PRO	2.3
1	C	464	GLN	2.3
1	B	533	TRP	2.3
1	B	582	LEU	2.3
1	A	594	TRP	2.3
1	C	484	ASN	2.3
1	B	496	TYR	2.3
1	C	513	TYR	2.3
1	C	595	TYR	2.3
1	C	629	TYR	2.3
1	A	425	PRO	2.3
1	C	503	GLY	2.3
1	A	564	GLY	2.3
1	C	432	SER	2.3
1	A	432	SER	2.3
1	D	460	VAL	2.3
1	D	518	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	544	ARG	2.2
1	A	528	TRP	2.2
1	B	447	GLY	2.2
1	B	581	SER	2.2
1	D	522	SER	2.2
1	A	541	ILE	2.2
1	B	580	VAL	2.2
1	A	628	ASN	2.2
1	B	571	THR	2.2
1	D	573	GLY	2.2
1	A	476	ASP	2.2
1	A	522	SER	2.2
1	A	496	TYR	2.2
1	A	555	PHE	2.2
1	D	498	ILE	2.2
1	B	466	VAL	2.2
1	C	512	VAL	2.2
1	A	530	THR	2.2
1	C	617	LEU	2.2
1	C	625	GLN	2.2
1	D	648	LEU	2.2
1	A	619	LEU	2.2
1	A	483	GLY	2.2
1	B	477	PRO	2.2
1	D	425	PRO	2.2
1	C	515	ALA	2.2
1	B	595	TYR	2.2
1	B	608	PHE	2.2
1	C	440	TYR	2.2
1	C	553	PHE	2.2
1	A	469	TYR	2.2
1	A	485	ILE	2.2
1	C	457	MET	2.2
1	B	620	GLN	2.2
1	C	450	VAL	2.2
1	D	426	VAL	2.2
1	A	504	SER	2.2
1	B	474	LEU	2.2
1	D	564	GLY	2.2
1	A	462	GLY	2.2
1	A	573	GLY	2.2
1	C	631	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	469	TYR	2.1
1	B	632	THR	2.1
1	C	575	THR	2.1
1	A	523	SER	2.1
1	D	461	GLY	2.1
1	B	617	LEU	2.1
1	C	425	PRO	2.1
1	D	560	LEU	2.1
1	D	582	LEU	2.1
1	B	651	HIS	2.1
1	B	640	ALA	2.1
1	B	481	GLN	2.1
1	B	553	PHE	2.1
1	B	636	TYR	2.1
1	A	509	ILE	2.1
1	A	595	TYR	2.1
1	A	616	TYR	2.1
1	C	581	SER	2.1
1	D	588	GLU	2.1
1	D	477	PRO	2.1
1	D	516	HIS	2.1
1	D	601	ALA	2.1
1	D	625	GLN	2.1
1	B	537	ILE	2.1
1	A	487	ASP	2.1
1	C	507	SER	2.1
1	A	507	SER	2.1
1	D	548	THR	2.1
1	B	610	ASN	2.1
1	C	576	VAL	2.1
1	D	466	VAL	2.1
1	D	512	VAL	2.1
1	A	531	VAL	2.1
1	A	533	TRP	2.1
1	B	494	PRO	2.1
1	A	614	PRO	2.1
1	D	543	LEU	2.1
1	D	579	LEU	2.1
1	C	615	PHE	2.0
1	A	578	SER	2.0
1	B	506	TYR	2.0
1	C	616	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	440	TYR	2.0
1	B	598	THR	2.0
1	C	550	THR	2.0
1	A	495	THR	2.0
1	A	529	THR	2.0
1	C	643	ASN	2.0
1	A	482	ASN	2.0
1	B	450	VAL	2.0
1	C	582	LEU	2.0
1	A	532	LEU	2.0
1	B	449	ARG	2.0
1	C	606	ARG	2.0
1	D	515	ALA	2.0
1	D	635	ALA	2.0
1	C	563	SER	2.0
1	A	553	PHE	2.0
1	B	521	GLY	2.0
1	C	427	GLN	2.0
1	C	468	THR	2.0
1	D	510	GLY	2.0
1	A	550	THR	2.0
1	B	469	TYR	2.0
1	A	636	TYR	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 oligosaccharides 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, 95th 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	701	1/1	0.78	0.14	15,15,15,15	0
2	CA	B	701	1/1	0.83	0.15	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.