



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:04 AM UTC

PDB ID : 2QJ1 / pdb_00002qj1
Title : Crystal structure of infectious bursal disease virus VP1 polymerase incubated with an oligopeptide mimicking the VP3 C-terminus
Authors : Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguier, N.
Deposited on : 2007-07-06
Resolution : 3.48 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

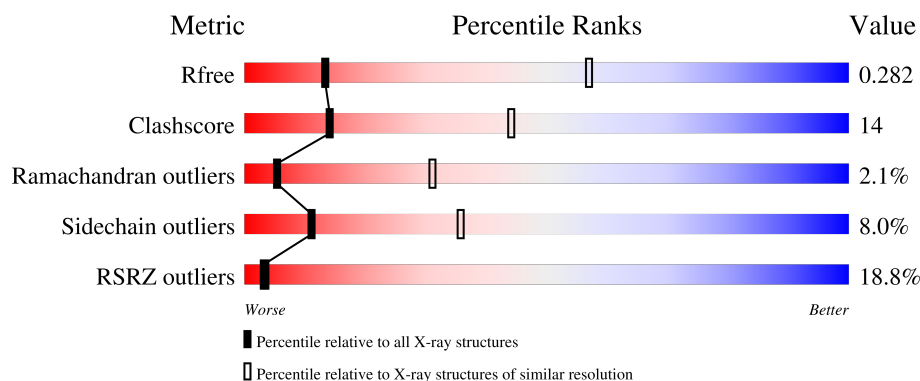
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	852	17% 61% 26% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5927 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 Infectious bursal disease virus VP1 polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	14	0	0
			5927	3793	1009	1103	22			

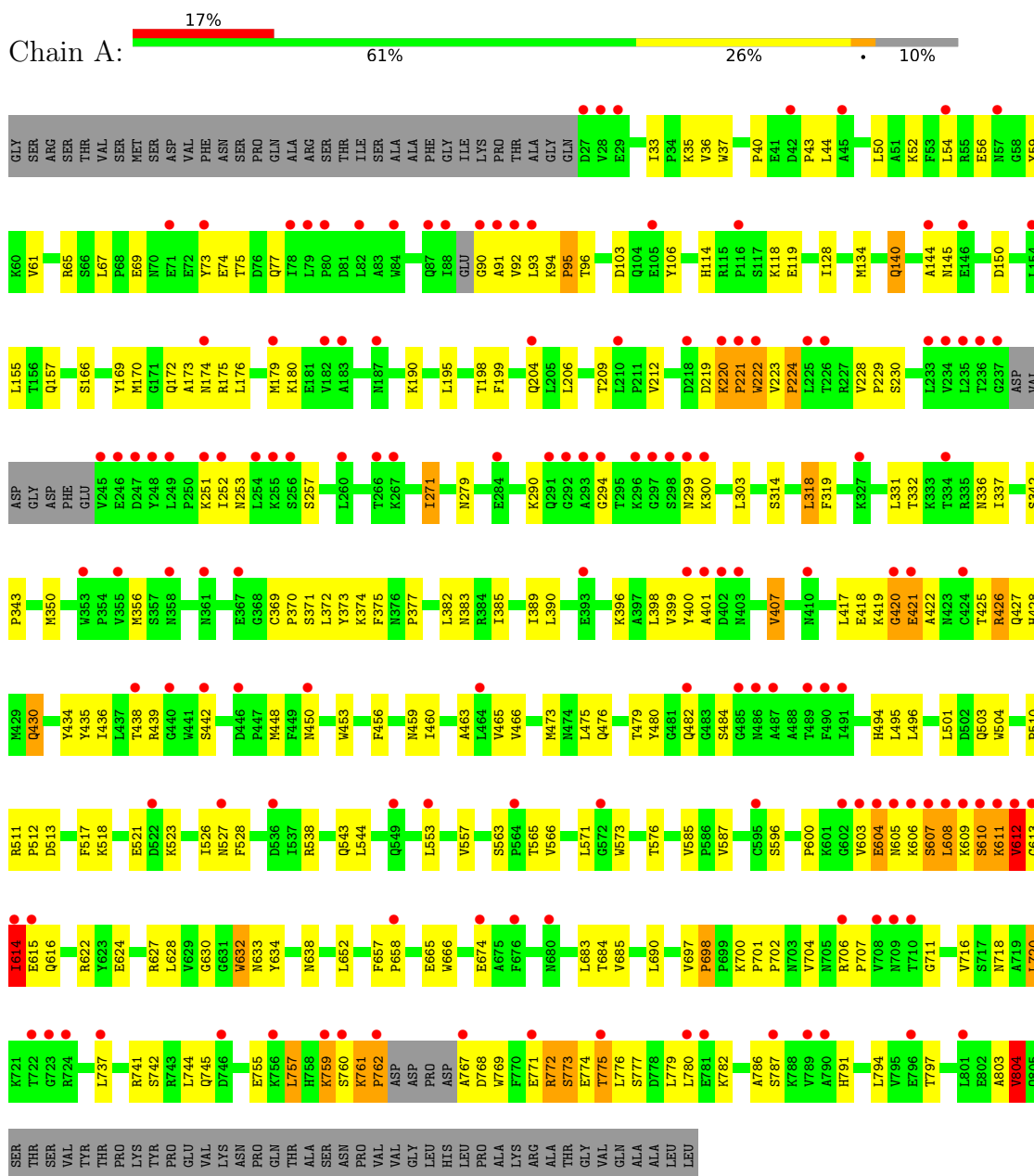
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q82629
A	-5	SER	-	expression tag	UNP Q82629
A	-4	ARG	-	expression tag	UNP Q82629
A	-3	SER	-	expression tag	UNP Q82629
A	-2	THR	-	expression tag	UNP Q82629
A	-1	VAL	-	expression tag	UNP Q82629
A	0	SER	-	expression tag	UNP Q82629
A	4	VAL	ILE	SEE REMARK 999	UNP Q82629

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: Infectious bursal disease virus VP1 polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.91Å 121.91Å 359.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.48 19.98 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.98-3.48) 95.8 (19.98-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.52Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.281 (Not available) , 0.282	Depositor DCC
R_{free} test set	1039 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

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	0.46	0/6066	1.06	24/8250 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	GLY	N-CA-C	-26.20	83.51	112.33
1	A	610	SER	CB-CA-C	-17.84	82.16	111.23
1	A	421	GLU	N-CA-CB	17.31	133.90	114.17
1	A	610	SER	N-CA-C	15.63	131.67	113.38
1	A	612	VAL	N-CA-CB	-13.64	88.73	111.23
1	A	93	LEU	N-CA-CB	-12.88	91.03	110.60
1	A	421	GLU	CB-CA-C	-12.86	91.55	110.06
1	A	222	TRP	CB-CA-C	-12.20	87.05	110.35
1	A	611	LYS	N-CA-CB	-11.91	90.35	110.49
1	A	422	ALA	N-CA-C	-10.88	100.27	114.31
1	A	611	LYS	N-CA-C	-10.54	88.34	110.80
1	A	804	VAL	N-CA-C	-9.35	89.89	109.34
1	A	768	ASP	N-CA-C	-8.96	91.71	110.80
1	A	767	ALA	N-CA-C	7.67	132.48	111.00
1	A	611	LYS	CB-CA-C	-7.54	95.41	110.42
1	A	762	PRO	N-CA-CB	6.75	110.42	103.00
1	A	144	ALA	N-CA-C	6.64	118.41	108.31
1	A	422	ALA	N-CA-CB	6.60	119.67	110.90
1	A	222	TRP	N-CA-C	6.57	126.43	113.29
1	A	604	GLU	N-CA-C	-6.25	97.50	110.80
1	A	93	LEU	N-CA-C	-5.86	101.51	109.95
1	A	634	TYR	CA-C-N	5.74	127.01	119.84
1	A	634	TYR	C-N-CA	5.74	127.01	119.84
1	A	144	ALA	CB-CA-C	-5.30	110.44	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5927	0	5873	168	0
All	All	5927	0	5873	168	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 (168) 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:92:VAL:O	1:A:271:ILE:HD11	1.17	1.26
1:A:92:VAL:O	1:A:271:ILE:CD1	1.82	1.26
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.24	1.02
1:A:221:PRO:O	1:A:222:TRP:HB2	1.67	0.91
1:A:421:GLU:HG2	1:A:484:SER:HA	1.53	0.90
1:A:613:GLY:O	1:A:614:ILE:C	2.15	0.90
1:A:611:LYS:O	1:A:657:PHE:CD1	2.24	0.89
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.55	0.88
1:A:610:SER:H	1:A:614:ILE:HG12	1.40	0.87
1:A:230:SER:HB2	1:A:279:ASN:HD21	1.44	0.83
1:A:737:LEU:HD11	1:A:769:TRP:HE1	1.45	0.81
1:A:609:LYS:CB	1:A:614:ILE:HD11	2.10	0.80
1:A:459:ASN:O	1:A:797:THR:HG21	1.82	0.79
1:A:229:PRO:HG3	1:A:350:MET:HE1	1.63	0.79
1:A:92:VAL:O	1:A:271:ILE:HD13	1.82	0.76
1:A:772:ARG:HA	1:A:775:THR:OG1	1.84	0.76
1:A:611:LYS:O	1:A:657:PHE:HD1	1.65	0.75
1:A:222:TRP:O	1:A:224:PRO:HD3	1.87	0.74
1:A:757:LEU:HD12	1:A:779:LEU:HD12	1.69	0.74
1:A:610:SER:N	1:A:614:ILE:HG12	2.03	0.73
1:A:220:LYS:CB	1:A:221:PRO:CD	2.67	0.72
1:A:737:LEU:HD21	1:A:769:TRP:HZ2	1.55	0.72
1:A:173:ALA:HA	1:A:176:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:O	1:A:657:PHE:CE1	2.44	0.70
1:A:69:GLU:HG2	1:A:106:TYR:HD1	1.56	0.70
1:A:75:THR:OG1	1:A:94:LYS:O	2.11	0.68
1:A:610:SER:O	1:A:612:VAL:N	2.27	0.68
1:A:606:LYS:C	1:A:608:LEU:H	2.01	0.68
1:A:419:LYS:C	1:A:420:GLY:O	2.25	0.67
1:A:303:LEU:HD21	1:A:744:LEU:HD22	1.75	0.67
1:A:511:ARG:HD3	1:A:513:ASP:OD1	1.95	0.66
1:A:706:ARG:HB2	1:A:707:PRO:HD2	1.77	0.66
1:A:504:TRP:CD1	1:A:510:PRO:HD2	2.31	0.66
1:A:757:LEU:CD1	1:A:776:LEU:HA	2.27	0.65
1:A:757:LEU:HD13	1:A:776:LEU:HA	1.79	0.64
1:A:611:LYS:CB	1:A:657:PHE:CE1	2.81	0.64
1:A:610:SER:H	1:A:614:ILE:CG1	2.10	0.63
1:A:565:THR:HG22	1:A:576:THR:HB	1.80	0.63
1:A:418:GLU:HB2	1:A:527:ASN:HB2	1.81	0.62
1:A:212:VAL:HG12	1:A:356:MET:HE1	1.83	0.61
1:A:157:GLN:HA	1:A:157:GLN:HE21	1.65	0.61
1:A:172:GLN:HB3	1:A:336:ASN:HD21	1.66	0.61
1:A:140:GLN:HA	1:A:140:GLN:NE2	2.06	0.61
1:A:50:LEU:HD22	1:A:473:MET:HE3	1.83	0.61
1:A:614:ILE:HG22	1:A:615:GLU:N	2.14	0.60
1:A:425:THR:H	1:A:428:HIS:HD2	1.48	0.60
1:A:761:LYS:O	1:A:762:PRO:CB	2.50	0.59
1:A:737:LEU:HD11	1:A:769:TRP:NE1	2.15	0.58
1:A:373:TYR:HA	1:A:400:TYR:CE2	2.38	0.58
1:A:33:ILE:HG23	1:A:128:ILE:HD12	1.86	0.57
1:A:616:GLN:HB2	1:A:652:LEU:HD21	1.87	0.57
1:A:772:ARG:CA	1:A:775:THR:OG1	2.51	0.56
1:A:170:MET:O	1:A:174:ASN:HB2	2.06	0.56
1:A:220:LYS:CB	1:A:221:PRO:HD3	2.35	0.56
1:A:157:GLN:HA	1:A:157:GLN:NE2	2.21	0.55
1:A:375:PHE:HD2	1:A:571:LEU:HD12	1.72	0.55
1:A:606:LYS:C	1:A:608:LEU:N	2.65	0.55
1:A:456:PHE:HA	1:A:460:ILE:HB	1.89	0.54
1:A:612:VAL:O	1:A:657:PHE:HB2	2.06	0.54
1:A:606:LYS:O	1:A:608:LEU:N	2.41	0.54
1:A:435:TYR:CE2	1:A:439:ARG:HD2	2.42	0.54
1:A:418:GLU:O	1:A:419:LYS:C	2.51	0.54
1:A:209:THR:O	1:A:371:SER:HB2	2.08	0.54
1:A:420:GLY:O	1:A:421:GLU:OE1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:O	1:A:612:VAL:C	2.52	0.53
1:A:90:GLY:N	1:A:251:LYS:HE3	2.23	0.53
1:A:37:TRP:CZ2	1:A:40:PRO:HD3	2.44	0.53
1:A:613:GLY:O	1:A:616:GLN:N	2.41	0.53
1:A:94:LYS:O	1:A:96:THR:N	2.42	0.52
1:A:609:LYS:O	1:A:610:SER:CB	2.57	0.52
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.91	0.52
1:A:35:LYS:HG2	1:A:36:VAL:N	2.25	0.52
1:A:417:LEU:HD23	1:A:528:PHE:HB3	1.92	0.52
1:A:426:ARG:HD3	1:A:463:ALA:HA	1.91	0.52
1:A:52:LYS:O	1:A:56:GLU:HB2	2.10	0.52
1:A:773:SER:OG	1:A:774:GLU:N	2.43	0.51
1:A:613:GLY:O	1:A:615:GLU:N	2.43	0.51
1:A:140:GLN:HE21	1:A:140:GLN:CA	2.06	0.51
1:A:94:LYS:O	1:A:95:PRO:C	2.54	0.50
1:A:426:ARG:HG2	1:A:466:VAL:HB	1.94	0.50
1:A:803:ALA:O	1:A:804:VAL:C	2.53	0.50
1:A:319:PHE:HB3	1:A:337:ILE:HB	1.93	0.50
1:A:170:MET:HG3	1:A:331:LEU:O	2.11	0.50
1:A:221:PRO:O	1:A:222:TRP:CB	2.50	0.50
1:A:627:ARG:HD2	1:A:638:ASN:OD1	2.11	0.50
1:A:742:SER:HA	1:A:787:SER:H	1.77	0.50
1:A:356:MET:HE3	1:A:436:ILE:HD12	1.95	0.49
1:A:521:GLU:HB2	1:A:526:ILE:O	2.12	0.49
1:A:780:LEU:HB3	1:A:786:ALA:HB2	1.95	0.49
1:A:600:PRO:CB	1:A:622:ARG:HD2	2.37	0.49
1:A:91:ALA:O	1:A:92:VAL:C	2.55	0.48
1:A:43:PRO:HB2	1:A:170:MET:HE2	1.93	0.48
1:A:180:LYS:HG3	1:A:480:TYR:CZ	2.47	0.48
1:A:544:LEU:HD21	1:A:566:VAL:HG23	1.94	0.48
1:A:604:GLU:O	1:A:605:ASN:C	2.56	0.48
1:A:212:VAL:CG1	1:A:356:MET:HE1	2.42	0.48
1:A:624:GLU:HB3	1:A:683:LEU:HD22	1.94	0.48
1:A:419:LYS:O	1:A:420:GLY:C	2.56	0.48
1:A:518:LYS:O	1:A:521:GLU:HG2	2.14	0.48
1:A:803:ALA:C	1:A:804:VAL:O	2.50	0.48
1:A:587:VAL:HG22	1:A:632:TRP:CZ2	2.49	0.47
1:A:421:GLU:O	1:A:482:GLN:O	2.33	0.47
1:A:114:HIS:HA	1:A:166:SER:HB2	1.97	0.47
1:A:228:VAL:HB	1:A:229:PRO:HD2	1.97	0.47
1:A:553:LEU:HD13	1:A:585:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLU:O	1:A:775:THR:OG1	2.33	0.47
1:A:65:ARG:H	1:A:476:GLN:HE22	1.63	0.46
1:A:43:PRO:HD2	1:A:170:MET:HB2	1.98	0.46
1:A:611:LYS:C	1:A:657:PHE:HD1	2.22	0.46
1:A:607:SER:O	1:A:608:LEU:C	2.59	0.46
1:A:611:LYS:CB	1:A:657:PHE:HE1	2.29	0.46
1:A:373:TYR:CE2	1:A:374:LYS:HG3	2.51	0.46
1:A:174:ASN:HD22	1:A:332:THR:HA	1.81	0.45
1:A:603:VAL:O	1:A:604:GLU:C	2.57	0.45
1:A:755:GLU:O	1:A:759:LYS:HG2	2.16	0.45
1:A:50:LEU:HD23	1:A:475:LEU:HD12	1.97	0.45
1:A:303:LEU:HD22	1:A:745:GLN:HG2	1.97	0.45
1:A:418:GLU:HB2	1:A:527:ASN:CB	2.46	0.45
1:A:628:LEU:HD13	1:A:685:VAL:HG22	1.99	0.45
1:A:176:LEU:HD11	1:A:318:LEU:HD11	1.99	0.45
1:A:74:GLU:HA	1:A:96:THR:HG22	1.99	0.44
1:A:230:SER:HB2	1:A:279:ASN:ND2	2.23	0.44
1:A:206:LEU:HD11	1:A:495:LEU:HD12	2.00	0.44
1:A:372:LEU:O	1:A:375:PHE:HB3	2.17	0.44
1:A:434:TYR:CZ	1:A:438:THR:HG21	2.53	0.44
1:A:512:PRO:HA	1:A:517:PHE:CG	2.53	0.44
1:A:169:TYR:CD1	1:A:473:MET:HE2	2.53	0.43
1:A:299:ASN:C	1:A:745:GLN:HE22	2.26	0.43
1:A:134:MET:SD	1:A:155:LEU:HD22	2.58	0.43
1:A:701:PRO:HA	1:A:702:PRO:HD3	1.88	0.43
1:A:94:LYS:C	1:A:96:THR:N	2.76	0.43
1:A:176:LEU:HD21	1:A:318:LEU:HD11	2.01	0.43
1:A:610:SER:HA	1:A:614:ILE:HG12	2.01	0.43
1:A:716:VAL:O	1:A:720:LEU:HB2	2.18	0.43
1:A:175:ARG:O	1:A:179:MET:HG3	2.19	0.42
1:A:198:THR:O	1:A:199:PHE:C	2.62	0.42
1:A:613:GLY:HA3	1:A:652:LEU:CD2	2.49	0.42
1:A:737:LEU:CD2	1:A:769:TRP:HZ2	2.29	0.42
1:A:342:SER:OG	1:A:343:PRO:HD3	2.20	0.42
1:A:73:TYR:CE1	1:A:77:GLN:HG2	2.55	0.42
1:A:190:LYS:HD3	1:A:195:LEU:HD21	2.00	0.42
1:A:369:CYS:HA	1:A:370:PRO:HD3	1.91	0.42
1:A:563:SER:HB3	1:A:633:ASN:OD1	2.20	0.42
1:A:627:ARG:HB3	1:A:685:VAL:HG11	2.00	0.42
1:A:390:LEU:HA	1:A:538:ARG:HG2	2.00	0.42
1:A:396:LYS:HG3	1:A:407:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PRO:HG3	1:A:573:TRP:CE2	2.54	0.42
1:A:54:LEU:HB3	1:A:59:TYR:HB3	2.02	0.42
1:A:401:ALA:H	1:A:494:HIS:CD2	2.38	0.41
1:A:385:ILE:O	1:A:389:ILE:HG13	2.20	0.41
1:A:40:PRO:HB2	1:A:331:LEU:HD21	2.01	0.41
1:A:118:LYS:HG3	1:A:119:GLU:N	2.35	0.41
1:A:425:THR:H	1:A:428:HIS:CD2	2.34	0.41
1:A:179:MET:HG2	1:A:419:LYS:HG2	2.02	0.41
1:A:438:THR:O	1:A:442:SER:HB2	2.20	0.41
1:A:779:LEU:HD23	1:A:782:LYS:HD3	2.01	0.41
1:A:657:PHE:HA	1:A:658:PRO:HD3	1.90	0.41
1:A:607:SER:C	1:A:609:LYS:N	2.78	0.41
1:A:697:VAL:HA	1:A:698:PRO:HD2	1.81	0.41
1:A:75:THR:C	1:A:77:GLN:H	2.29	0.41
1:A:666:TRP:CE2	1:A:683:LEU:HG	2.56	0.40
1:A:44:LEU:HD12	1:A:170:MET:HA	2.03	0.40
1:A:350:MET:HE3	1:A:453:TRP:HH2	1.85	0.40
1:A:373:TYR:HA	1:A:400:TYR:HE2	1.82	0.40
1:A:400:TYR:O	1:A:401:ALA:C	2.65	0.40
1:A:450:ASN:HD22	1:A:453:TRP:HD1	1.69	0.40
1:A:607:SER:O	1:A:609:LYS:N	2.54	0.40
1:A:382:LEU:O	1:A:383:ASN:C	2.64	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	759/852 (89%)	675 (89%)	68 (9%)	16 (2%)	5	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	220	LYS
1	A	221	PRO
1	A	612	VAL
1	A	614	ILE
1	A	224	PRO
1	A	804	VAL
1	A	607	SER
1	A	630	GLY
1	A	761	LYS
1	A	608	LEU
1	A	95	PRO
1	A	632	TRP
1	A	711	GLY
1	A	698	PRO
1	A	294	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	627/730 (86%)	577 (92%)	50 (8%)	11	36

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	67	LEU
1	A	103	ASP
1	A	140	GLN
1	A	145	ASN
1	A	150	ASP
1	A	204	GLN
1	A	223	VAL
1	A	252	ILE
1	A	253	ASN
1	A	257	SER

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Mol	Chain	Res	Type
1	A	271	ILE
1	A	290	LYS
1	A	300	LYS
1	A	314	SER
1	A	318	LEU
1	A	398	LEU
1	A	399	VAL
1	A	407	VAL
1	A	426	ARG
1	A	430	GLN
1	A	448	MET
1	A	465	VAL
1	A	479	THR
1	A	496	LEU
1	A	501	LEU
1	A	503	GLN
1	A	523	LYS
1	A	543	GLN
1	A	557	VAL
1	A	596	SER
1	A	614	ILE
1	A	665	GLU
1	A	674	GLU
1	A	684	THR
1	A	690	LEU
1	A	700	LYS
1	A	704	VAL
1	A	718	ASN
1	A	720	LEU
1	A	741	ARG
1	A	757	LEU
1	A	759	LYS
1	A	760	SER
1	A	772	ARG
1	A	773	SER
1	A	775	THR
1	A	777	SER
1	A	791	HIS
1	A	794	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	145	ASN
1	A	157	GLN
1	A	172	GLN
1	A	204	GLN
1	A	279	ASN
1	A	291	GLN
1	A	299	ASN
1	A	336	ASN
1	A	358	ASN
1	A	423	ASN
1	A	428	HIS
1	A	430	GLN
1	A	450	ASN
1	A	451	GLN
1	A	476	GLN
1	A	494	HIS
1	A	503	GLN
1	A	543	GLN
1	A	549	GLN
1	A	643	ASN
1	A	651	HIS

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](#)

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, 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	764/852 (89%)	1.18	144 (18%) 3 3	20, 74, 103, 123	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	VAL	9.0
1	A	610	SER	8.2
1	A	611	LYS	8.2
1	A	609	LYS	6.8
1	A	234	VAL	6.7
1	A	245	VAL	6.3
1	A	235	LEU	6.3
1	A	604	GLU	6.2
1	A	486	ASN	6.2
1	A	233	LEU	6.2
1	A	220	LYS	5.8
1	A	603	VAL	5.7
1	A	358	ASN	5.3
1	A	292	GLY	5.0
1	A	226	THR	5.0
1	A	487	ALA	4.8
1	A	402	ASP	4.8
1	A	246	GLU	4.8
1	A	293	ALA	4.7
1	A	92	VAL	4.7
1	A	605	ASN	4.5
1	A	353	TRP	4.5
1	A	710	THR	4.4
1	A	367	GLU	4.4
1	A	28	VAL	4.4
1	A	91	ALA	4.3
1	A	446	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	608	LEU	4.1
1	A	182	VAL	4.0
1	A	607	SER	4.0
1	A	403	ASN	3.9
1	A	105	GLU	3.9
1	A	248	TYR	3.8
1	A	549	GLN	3.8
1	A	674	GLU	3.8
1	A	221	PRO	3.8
1	A	87	GLN	3.8
1	A	225	LEU	3.7
1	A	489	THR	3.7
1	A	174	ASN	3.6
1	A	71	GLU	3.6
1	A	187	ASN	3.6
1	A	424	CYS	3.6
1	A	775	THR	3.6
1	A	93	LEU	3.5
1	A	522	ASP	3.5
1	A	183	ALA	3.5
1	A	267	LYS	3.4
1	A	254	LEU	3.4
1	A	767	ALA	3.3
1	A	291	GLN	3.3
1	A	420	GLY	3.2
1	A	297	GLY	3.2
1	A	756	LYS	3.1
1	A	708	VAL	3.1
1	A	255	LYS	3.1
1	A	796	GLU	3.1
1	A	80	PRO	3.1
1	A	361	ASN	3.1
1	A	723	GLY	3.1
1	A	79	LEU	3.0
1	A	485	GLY	3.0
1	A	602	GLY	3.0
1	A	88	ILE	3.0
1	A	116	PRO	3.0
1	A	401	ALA	3.0
1	A	680	ASN	3.0
1	A	572	GLY	2.9
1	A	144	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	421	GLU	2.8
1	A	801	LEU	2.8
1	A	790	ALA	2.8
1	A	237	GLY	2.7
1	A	251	LYS	2.7
1	A	491	ILE	2.7
1	A	247	ASP	2.7
1	A	146	GLU	2.6
1	A	393	GLU	2.6
1	A	256	SER	2.6
1	A	73	TYR	2.6
1	A	400	TYR	2.6
1	A	759	LYS	2.6
1	A	298	SER	2.6
1	A	760	SER	2.6
1	A	355	VAL	2.6
1	A	90	GLY	2.5
1	A	490	PHE	2.5
1	A	218	ASP	2.5
1	A	482	GLN	2.5
1	A	746	ASP	2.5
1	A	210	LEU	2.4
1	A	45	ALA	2.4
1	A	204	GLN	2.4
1	A	606	LYS	2.4
1	A	29	GLU	2.4
1	A	464	LEU	2.4
1	A	27	ASP	2.4
1	A	327	LYS	2.3
1	A	249	LEU	2.3
1	A	284	GLU	2.3
1	A	709	ASN	2.3
1	A	440	GLY	2.3
1	A	438	THR	2.3
1	A	442	SER	2.3
1	A	299	ASN	2.3
1	A	789	VAL	2.3
1	A	564	PRO	2.3
1	A	294	GLY	2.3
1	A	57	ASN	2.3
1	A	527	ASN	2.2
1	A	553	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	724	ARG	2.2
1	A	450	ASN	2.2
1	A	300	LYS	2.2
1	A	236	THR	2.2
1	A	410	ASN	2.2
1	A	737	LEU	2.2
1	A	780	LEU	2.2
1	A	595	CYS	2.2
1	A	676	PHE	2.2
1	A	260	LEU	2.2
1	A	615	GLU	2.2
1	A	781	GLU	2.2
1	A	787	SER	2.1
1	A	771	GLU	2.1
1	A	266	THR	2.1
1	A	334	THR	2.1
1	A	42	ASP	2.1
1	A	78	ILE	2.1
1	A	222	TRP	2.1
1	A	722	THR	2.1
1	A	762	PRO	2.1
1	A	296	LYS	2.1
1	A	706	ARG	2.1
1	A	54	LEU	2.0
1	A	82	LEU	2.0
1	A	154	LEU	2.0
1	A	613	GLY	2.0
1	A	614	ILE	2.0
1	A	84	TRP	2.0
1	A	179	MET	2.0
1	A	536	ASP	2.0
1	A	658	PRO	2.0
1	A	252	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.