



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:28 PM UTC

PDB ID : 3MTV / pdb_00003mtv
Title : The Crystal Structure of the PRRSV Nonstructural Protein Nsp1
Authors : Xue, F.; Sun, Y.N.; Yan, L.M.; Zhao, C.; Lou, Z.Y.; Rao, Z.H.
Deposited on : 2010-04-30
Resolution : 2.80 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

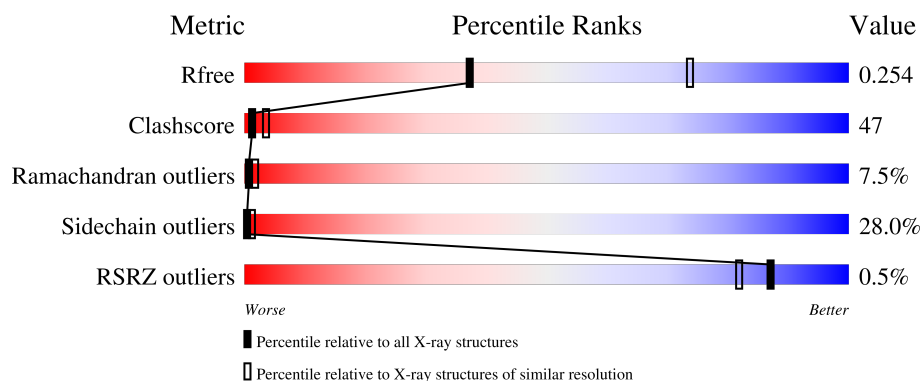
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	203	24% 36% 30% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1652 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 Papain-like cysteine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1632	1052	289	286	5			

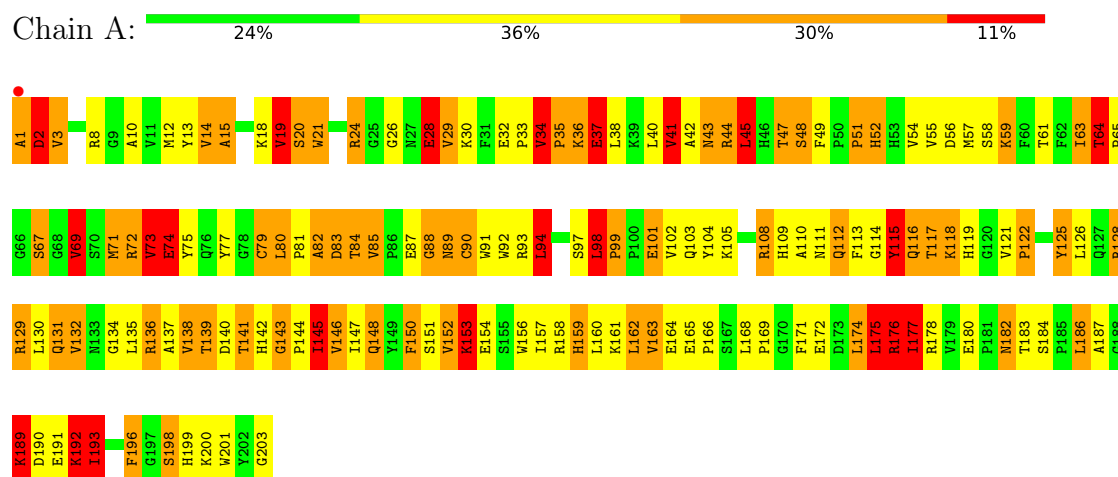
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		

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: Papain-like cysteine protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.89Å 100.89Å 81.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.91 – 2.80 31.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (31.91-2.80) 99.8 (31.91-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.201 , 0.261 0.208 , 0.254	Depositor DCC
R_{free} test set	521 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1652	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

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	2.10	48/1683 (2.9%)	2.28	88/2284 (3.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLY	C-O	8.50	1.33	1.23
1	A	176	ARG	CA-C	-8.10	1.42	1.52
1	A	129	ARG	CA-C	-8.05	1.42	1.53
1	A	82	ALA	CA-CB	-8.03	1.39	1.53
1	A	29	VAL	CA-CB	-7.96	1.44	1.54
1	A	110	ALA	CA-CB	-7.87	1.40	1.53
1	A	145	ILE	C-O	7.71	1.32	1.24
1	A	85	VAL	CA-CB	-7.51	1.48	1.55
1	A	51	PRO	C-O	-7.51	1.15	1.23
1	A	116	GLN	C-O	7.34	1.32	1.23
1	A	14	VAL	CA-CB	-7.25	1.44	1.54
1	A	19	VAL	CA-CB	-7.16	1.44	1.55
1	A	2	ASP	N-CA	7.13	1.55	1.46
1	A	77	TYR	CA-C	-6.66	1.44	1.52
1	A	52	HIS	CA-C	-6.63	1.43	1.52
1	A	102	VAL	N-CA	-6.58	1.38	1.46
1	A	193	ILE	CG1-CD1	6.53	1.77	1.51
1	A	150	PHE	CA-CB	-6.49	1.44	1.53
1	A	63	ILE	CA-CB	6.42	1.63	1.54
1	A	117	THR	CB-CG2	6.41	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	THR	CB-CG2	6.25	1.73	1.52
1	A	118	LYS	CA-C	-6.08	1.44	1.52
1	A	72	ARG	N-CA	-6.03	1.39	1.46
1	A	12	MET	CA-C	-5.95	1.45	1.52
1	A	41	VAL	CA-CB	-5.85	1.46	1.54
1	A	34	VAL	N-CA	-5.83	1.41	1.46
1	A	152	VAL	CA-CB	5.75	1.62	1.54
1	A	24	ARG	CZ-NH1	5.73	1.40	1.32
1	A	139	THR	N-CA	-5.66	1.39	1.46
1	A	105	LYS	CB-CG	5.51	1.69	1.52
1	A	1	ALA	N-CA	5.50	1.56	1.46
1	A	198	SER	C-O	5.48	1.30	1.23
1	A	129	ARG	CZ-NH1	5.48	1.40	1.32
1	A	104	TYR	C-O	-5.46	1.17	1.24
1	A	138	VAL	CA-C	-5.45	1.46	1.52
1	A	71	MET	C-O	-5.40	1.16	1.24
1	A	63	ILE	C-O	-5.40	1.17	1.24
1	A	45	LEU	C-O	-5.38	1.17	1.24
1	A	30	LYS	CA-C	-5.32	1.47	1.53
1	A	125	TYR	CA-C	-5.25	1.45	1.52
1	A	132	VAL	CA-C	-5.24	1.44	1.52
1	A	84	THR	N-CA	5.17	1.53	1.45
1	A	137	ALA	CA-C	-5.12	1.46	1.52
1	A	64	THR	CA-CB	5.11	1.62	1.53
1	A	21	TRP	C-O	-5.09	1.17	1.23
1	A	139	THR	CA-CB	-5.04	1.46	1.53
1	A	119	HIS	CA-C	-5.02	1.45	1.52
1	A	32	GLU	CD-OE2	5.01	1.34	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLY	CA-C-N	16.05	139.90	119.84
1	A	143	GLY	C-N-CA	16.05	139.90	119.84
1	A	85	VAL	N-CA-CB	-14.62	101.74	111.83
1	A	34	VAL	CA-C-N	14.55	138.03	119.84
1	A	34	VAL	C-N-CA	14.55	138.03	119.84
1	A	129	ARG	N-CA-C	-12.26	94.98	110.19
1	A	24	ARG	N-CA-C	-10.57	97.60	111.24
1	A	49	PHE	CA-C-N	-9.72	110.36	120.38
1	A	49	PHE	C-N-CA	-9.72	110.36	120.38
1	A	125	TYR	N-CA-C	-9.42	100.56	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLU	CA-C-N	-9.35	108.15	119.84
1	A	32	GLU	C-N-CA	-9.35	108.15	119.84
1	A	34	VAL	CB-CA-C	-8.11	103.40	110.94
1	A	175	LEU	N-CA-C	7.89	118.40	108.45
1	A	146	VAL	CB-CA-C	-7.70	100.37	110.84
1	A	99	PRO	CA-C-N	7.52	129.25	119.84
1	A	99	PRO	C-N-CA	7.52	129.25	119.84
1	A	14	VAL	CB-CA-C	-7.32	98.05	110.71
1	A	182	ASN	N-CA-C	-7.22	101.66	111.55
1	A	132	VAL	CB-CA-C	-7.20	95.42	111.77
1	A	115	TYR	N-CA-C	7.14	126.01	110.80
1	A	63	ILE	CA-C-N	-7.07	110.46	120.49
1	A	63	ILE	C-N-CA	-7.07	110.46	120.49
1	A	192	LYS	N-CA-C	7.07	120.18	109.23
1	A	3	VAL	N-CA-C	6.89	117.71	108.27
1	A	2	ASP	CB-CA-C	-6.67	99.25	109.99
1	A	61	THR	CB-CA-C	6.64	122.49	109.35
1	A	115	TYR	CA-CB-CG	-6.59	102.04	113.90
1	A	72	ARG	N-CA-C	6.55	118.83	108.67
1	A	14	VAL	N-CA-C	6.55	118.14	108.45
1	A	52	HIS	CA-C-N	-6.51	112.95	122.65
1	A	52	HIS	C-N-CA	-6.51	112.95	122.65
1	A	193	ILE	CB-CG1-CD1	6.48	127.41	113.80
1	A	159	HIS	CA-C-N	-6.48	111.94	122.82
1	A	159	HIS	C-N-CA	-6.48	111.94	122.82
1	A	198	SER	CA-C-N	-6.36	113.84	125.02
1	A	198	SER	C-N-CA	-6.36	113.84	125.02
1	A	145	ILE	CB-CA-C	-6.34	101.24	110.63
1	A	20	SER	CA-C-N	-6.34	112.17	122.82
1	A	20	SER	C-N-CA	-6.34	112.17	122.82
1	A	132	VAL	CG1-CB-CG2	-6.14	97.29	110.80
1	A	48	SER	N-CA-C	6.08	120.98	113.50
1	A	82	ALA	N-CA-C	6.05	119.49	111.75
1	A	74	GLU	CB-CA-C	-6.00	100.82	110.79
1	A	177	ILE	N-CA-C	5.96	115.80	108.53
1	A	67	SER	CA-C-O	5.88	124.99	118.52
1	A	134	GLY	CA-C-N	-5.88	112.24	122.64
1	A	134	GLY	C-N-CA	-5.88	112.24	122.64
1	A	28	GLU	CA-C-N	-5.85	113.61	121.80
1	A	28	GLU	C-N-CA	-5.85	113.61	121.80
1	A	98	LEU	CA-C-N	-5.83	115.46	119.66
1	A	98	LEU	C-N-CA	-5.83	115.46	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	CA-C-N	-5.82	110.43	121.54
1	A	129	ARG	C-N-CA	-5.82	110.43	121.54
1	A	98	LEU	N-CA-C	5.77	119.22	109.87
1	A	103	GLN	CA-C-N	-5.76	111.56	120.31
1	A	103	GLN	C-N-CA	-5.76	111.56	120.31
1	A	122	PRO	CA-C-N	-5.70	110.23	121.41
1	A	122	PRO	C-N-CA	-5.70	110.23	121.41
1	A	103	GLN	N-CA-C	-5.69	104.99	111.07
1	A	134	GLY	N-CA-C	-5.67	107.42	115.30
1	A	145	ILE	O-C-N	5.67	129.38	123.26
1	A	101	GLU	CB-CA-C	-5.63	101.79	110.81
1	A	153	LYS	CA-C-N	-5.63	113.64	122.65
1	A	153	LYS	C-N-CA	-5.63	113.64	122.65
1	A	153	LYS	N-CA-CB	5.57	119.90	110.49
1	A	10	ALA	N-CA-C	5.53	117.92	109.95
1	A	148	GLN	N-CA-C	5.53	118.08	109.52
1	A	90	CYS	N-CA-C	-5.52	106.62	113.19
1	A	2	ASP	O-C-N	-5.51	117.72	123.56
1	A	128	ARG	N-CA-C	-5.43	105.01	111.69
1	A	28	GLU	N-CA-C	-5.42	106.51	113.23
1	A	94	LEU	N-CA-C	5.36	119.30	112.34
1	A	196	PHE	N-CA-C	5.35	122.19	110.80
1	A	184	SER	N-CA-C	-5.34	103.42	108.22
1	A	88	GLY	N-CA-C	-5.33	107.69	115.63
1	A	69	VAL	N-CA-C	5.32	116.14	108.48
1	A	145	ILE	N-CA-C	5.27	115.48	108.11
1	A	131	GLN	CA-C-N	5.24	129.33	120.64
1	A	131	GLN	C-N-CA	5.24	129.33	120.64
1	A	101	GLU	N-CA-C	-5.18	104.90	111.11
1	A	115	TYR	CA-C-N	-5.09	114.68	122.21
1	A	115	TYR	C-N-CA	-5.09	114.68	122.21
1	A	49	PHE	N-CA-C	5.08	118.50	110.58
1	A	101	GLU	N-CA-CB	5.07	117.50	109.94
1	A	156	TRP	N-CA-C	5.07	119.19	113.15
1	A	79	CYS	CA-C-O	5.05	127.73	120.51
1	A	64	THR	CB-CA-C	5.03	117.32	109.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	74	GLU	Peptide

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	1632	0	1616	153	0
2	A	20	0	0	2	0
All	All	1652	0	1616	153	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 47.

All (153) 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:193:ILE:CD1	1:A:193:ILE:CG1	1.77	1.55
1:A:142:HIS:HA	1:A:176:ARG:NH2	1.63	1.14
1:A:139:THR:HA	1:A:177:ILE:HG22	1.47	0.96
1:A:130:LEU:C	1:A:130:LEU:HD23	1.92	0.95
1:A:142:HIS:HA	1:A:176:ARG:HH21	1.19	0.93
1:A:132:VAL:O	1:A:132:VAL:HG12	1.71	0.91
1:A:198:SER:O	1:A:199:HIS:HB2	1.76	0.85
1:A:129:ARG:O	1:A:130:LEU:HB3	1.77	0.85
1:A:115:TYR:N	1:A:115:TYR:CD2	2.38	0.83
1:A:192:LYS:CG	1:A:193:ILE:HD12	2.14	0.78
1:A:160:LEU:C	1:A:160:LEU:HD12	2.11	0.74
1:A:171:PHE:C	1:A:172:GLU:HG2	2.12	0.74
1:A:159:HIS:HD2	1:A:203:GLY:OXT	1.72	0.73
1:A:80:LEU:HD23	1:A:81:PRO:HD2	1.72	0.72
1:A:192:LYS:HG3	1:A:193:ILE:HD12	1.71	0.71
1:A:165:GLU:HB3	1:A:166:PRO:CD	2.19	0.71
1:A:186:LEU:HD12	1:A:187:ALA:N	2.07	0.70
1:A:115:TYR:HA	1:A:117:THR:HG22	1.74	0.69
1:A:150:PHE:O	1:A:151:SER:HB3	1.92	0.69
1:A:91:TRP:O	1:A:94:LEU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:131:GLN:N	2.08	0.68
1:A:129:ARG:O	1:A:130:LEU:CB	2.39	0.68
1:A:59:LYS:N	1:A:59:LYS:HD3	2.08	0.67
1:A:113:PHE:HB3	1:A:115:TYR:CE1	2.29	0.67
1:A:45:LEU:H	1:A:57:MET:HE1	1.59	0.67
1:A:139:THR:CA	1:A:177:ILE:HG22	2.24	0.66
1:A:139:THR:HG22	1:A:192:LYS:O	1.96	0.66
1:A:144:PRO:HD2	1:A:177:ILE:O	1.95	0.66
1:A:63:ILE:HD11	1:A:67:SER:O	1.96	0.65
1:A:84:THR:O	1:A:168:LEU:HD22	1.95	0.65
1:A:130:LEU:C	1:A:130:LEU:CD2	2.67	0.65
1:A:144:PRO:O	1:A:163:VAL:HG22	1.97	0.64
1:A:192:LYS:HG2	1:A:193:ILE:HD12	1.78	0.64
1:A:90:CYS:SG	1:A:203:GLY:C	2.81	0.63
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.81	0.63
1:A:142:HIS:CA	1:A:176:ARG:NH2	2.52	0.62
1:A:139:THR:O	1:A:139:THR:HG23	1.98	0.62
1:A:136:ARG:HB3	1:A:182:ASN:HB2	1.81	0.62
1:A:115:TYR:C	1:A:117:THR:H	2.07	0.61
1:A:130:LEU:CD2	1:A:131:GLN:N	2.64	0.61
1:A:132:VAL:O	1:A:132:VAL:CG1	2.43	0.60
1:A:168:LEU:HB3	1:A:169:PRO:HD2	1.84	0.60
1:A:82:ALA:O	1:A:84:THR:N	2.34	0.59
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.33	0.59
1:A:139:THR:HA	1:A:177:ILE:CG2	2.28	0.59
1:A:81:PRO:HG2	1:A:84:THR:HG21	1.84	0.59
1:A:58:SER:OG	1:A:59:LYS:HD3	2.03	0.58
1:A:111:ASN:HB2	1:A:116:GLN:NE2	2.18	0.58
1:A:35:PRO:O	1:A:37:GLU:N	2.36	0.57
1:A:14:VAL:HG12	1:A:15:ALA:N	2.19	0.57
1:A:117:THR:OG1	1:A:118:LYS:N	2.37	0.57
1:A:109:HIS:O	1:A:112:GLN:HB2	2.05	0.56
1:A:82:ALA:C	1:A:84:THR:H	2.14	0.56
1:A:36:LYS:C	1:A:38:LEU:H	2.14	0.55
1:A:82:ALA:O	1:A:83:ASP:C	2.48	0.55
1:A:153:LYS:H	1:A:153:LYS:HD3	1.71	0.55
1:A:165:GLU:HB3	1:A:166:PRO:HD2	1.89	0.55
1:A:44:ARG:HB3	1:A:57:MET:HE1	1.89	0.55
1:A:48:SER:HB2	1:A:80:LEU:HD12	1.88	0.55
1:A:128:ARG:C	1:A:129:ARG:O	2.38	0.54
1:A:115:TYR:HB3	1:A:121:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:HG3	1:A:89:ASN:ND2	2.23	0.54
1:A:111:ASN:HD22	1:A:116:GLN:HB2	1.74	0.53
1:A:165:GLU:CB	1:A:166:PRO:CD	2.85	0.53
1:A:140:ASP:OD1	1:A:142:HIS:N	2.37	0.53
1:A:139:THR:O	1:A:139:THR:CG2	2.56	0.53
1:A:178:ARG:NH1	1:A:180:GLU:OE1	2.41	0.53
1:A:43:ASN:O	1:A:47:THR:HB	2.09	0.52
1:A:113:PHE:CB	1:A:115:TYR:CD1	2.92	0.52
1:A:56:ASP:OD1	1:A:56:ASP:C	2.53	0.52
1:A:136:ARG:HD3	1:A:182:ASN:OD1	2.09	0.52
1:A:115:TYR:HB3	1:A:121:VAL:CG1	2.39	0.52
1:A:2:ASP:C	1:A:3:VAL:HG23	2.35	0.52
1:A:44:ARG:CB	1:A:57:MET:HE1	2.40	0.51
1:A:158:ARG:HB2	1:A:201:TRP:O	2.11	0.51
1:A:142:HIS:CA	1:A:176:ARG:HH21	2.07	0.51
1:A:168:LEU:HB3	1:A:169:PRO:CD	2.41	0.51
1:A:82:ALA:C	1:A:84:THR:N	2.69	0.51
1:A:113:PHE:HB2	1:A:115:TYR:CD1	2.46	0.51
1:A:69:VAL:O	1:A:80:LEU:HB2	2.09	0.50
1:A:51:PRO:HB2	1:A:52:HIS:CD2	2.47	0.50
1:A:33:PRO:O	1:A:35:PRO:HD3	2.11	0.50
1:A:186:LEU:HD12	1:A:187:ALA:H	1.74	0.50
1:A:153:LYS:HD3	1:A:153:LYS:N	2.27	0.50
1:A:87:GLU:HG3	1:A:89:ASN:HD21	1.77	0.49
1:A:140:ASP:OD1	1:A:140:ASP:C	2.54	0.49
1:A:115:TYR:C	1:A:117:THR:N	2.68	0.49
1:A:140:ASP:C	1:A:142:HIS:H	2.21	0.49
1:A:41:VAL:HG13	1:A:57:MET:HE2	1.95	0.48
1:A:43:ASN:HD22	1:A:43:ASN:H	1.61	0.48
1:A:18:LYS:C	1:A:19:VAL:HG23	2.38	0.48
1:A:84:THR:C	1:A:168:LEU:HD22	2.39	0.48
1:A:130:LEU:O	1:A:131:GLN:C	2.54	0.48
1:A:111:ASN:ND2	1:A:116:GLN:HB2	2.29	0.48
1:A:113:PHE:HB3	1:A:115:TYR:CD1	2.48	0.48
1:A:92:TRP:O	1:A:93:ARG:C	2.56	0.48
1:A:139:THR:HG22	1:A:192:LYS:H	1.78	0.47
1:A:72:ARG:O	1:A:73:VAL:C	2.58	0.47
1:A:38:LEU:C	1:A:40:LEU:N	2.71	0.47
1:A:153:LYS:H	1:A:153:LYS:CD	2.27	0.47
1:A:163:VAL:HG11	1:A:176:ARG:HH11	1.79	0.47
1:A:200:LYS:HA	1:A:200:LYS:HD2	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG23	1:A:57:MET:HG2	1.97	0.47
1:A:24:ARG:NE	2:A:214:HOH:O	2.36	0.47
1:A:74:GLU:HB2	1:A:75:TYR:HD1	1.80	0.46
1:A:81:PRO:HB2	1:A:84:THR:HG23	1.97	0.46
1:A:186:LEU:CD1	1:A:187:ALA:H	2.29	0.46
1:A:138:VAL:HG12	1:A:139:THR:N	2.30	0.46
1:A:45:LEU:CD2	1:A:45:LEU:C	2.87	0.46
1:A:114:GLY:O	1:A:116:GLN:N	2.43	0.46
1:A:168:LEU:CB	1:A:169:PRO:CD	2.93	0.46
1:A:140:ASP:O	1:A:142:HIS:N	2.49	0.46
1:A:186:LEU:CD1	1:A:187:ALA:N	2.79	0.45
1:A:98:LEU:HD21	1:A:135:LEU:HD11	1.99	0.45
1:A:192:LYS:HB2	1:A:192:LYS:HE2	1.40	0.45
1:A:28:GLU:HG2	1:A:29:VAL:N	2.27	0.45
1:A:175:LEU:HB2	1:A:176:ARG:H	1.37	0.45
1:A:115:TYR:CG	1:A:121:VAL:HG12	2.52	0.45
1:A:36:LYS:C	1:A:38:LEU:N	2.75	0.44
1:A:108:ARG:O	1:A:109:HIS:C	2.55	0.44
1:A:187:ALA:O	1:A:191:GLU:HG3	2.17	0.44
1:A:136:ARG:HB3	1:A:182:ASN:CB	2.48	0.44
1:A:160:LEU:H	1:A:160:LEU:HG	1.65	0.44
1:A:38:LEU:C	1:A:40:LEU:H	2.26	0.44
1:A:21:TRP:HB3	1:A:45:LEU:HD13	1.99	0.43
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.72	0.43
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.98	0.43
1:A:161:LYS:HE2	1:A:165:GLU:O	2.18	0.43
1:A:113:PHE:CB	1:A:115:TYR:CE1	2.98	0.43
1:A:115:TYR:CE2	1:A:122:PRO:HD3	2.53	0.43
1:A:34:VAL:HA	1:A:35:PRO:HD2	1.51	0.43
1:A:72:ARG:HB2	1:A:75:TYR:HB2	2.01	0.43
1:A:88:GLY:HA2	1:A:203:GLY:CA	2.48	0.43
1:A:40:LEU:HB3	1:A:41:VAL:H	1.56	0.42
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.74	0.42
1:A:81:PRO:HG2	1:A:84:THR:CG2	2.48	0.42
1:A:36:LYS:HE3	2:A:206:HOH:O	2.20	0.42
1:A:138:VAL:HG13	1:A:192:LYS:O	2.20	0.42
1:A:171:PHE:C	1:A:172:GLU:CG	2.87	0.42
1:A:89:ASN:C	1:A:91:TRP:H	2.28	0.42
1:A:63:ILE:HG13	1:A:64:THR:N	2.33	0.41
1:A:41:VAL:O	1:A:45:LEU:HB2	2.19	0.41
1:A:147:ILE:HD12	1:A:147:ILE:HG23	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLY:HA2	1:A:203:GLY:HA3	2.02	0.41
1:A:174:LEU:HB3	1:A:175:LEU:H	1.69	0.41
1:A:145:ILE:HD12	1:A:145:ILE:HG21	1.63	0.41
1:A:125:TYR:CD1	1:A:125:TYR:C	2.99	0.41
1:A:89:ASN:C	1:A:91:TRP:N	2.78	0.41
1:A:143:GLY:HA2	1:A:144:PRO:HD3	1.40	0.41
1:A:162:LEU:HD12	1:A:165:GLU:CD	2.46	0.41
1:A:1:ALA:HA	1:A:15:ALA:HB2	2.02	0.40
1:A:148:GLN:O	1:A:158:ARG:HA	2.20	0.40
1:A:168:LEU:HA	1:A:169:PRO:HD3	1.84	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	201/203 (99%)	159 (79%)	27 (13%)	15 (8%)	1 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	83	ASP
1	A	115	TYR
1	A	196	PHE
1	A	45	LEU
1	A	141	THR
1	A	15	ALA
1	A	35	PRO
1	A	37	GLU
1	A	43	ASN
1	A	44	ARG

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Mol	Chain	Res	Type
1	A	189	LYS
1	A	42	ALA
1	A	65	PRO
1	A	73	VAL

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	175/175 (100%)	126 (72%)	49 (28%)	0 1

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	8	ARG
1	A	13	TYR
1	A	19	VAL
1	A	20	SER
1	A	28	GLU
1	A	34	VAL
1	A	36	LYS
1	A	37	GLU
1	A	45	LEU
1	A	47	THR
1	A	54	VAL
1	A	59	LYS
1	A	64	THR
1	A	69	VAL
1	A	71	MET
1	A	73	VAL
1	A	79	CYS
1	A	80	LEU
1	A	85	VAL
1	A	89	ASN
1	A	94	LEU

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Mol	Chain	Res	Type
1	A	97	SER
1	A	98	LEU
1	A	101	GLU
1	A	108	ARG
1	A	112	GLN
1	A	126	LEU
1	A	136	ARG
1	A	141	THR
1	A	145	ILE
1	A	146	VAL
1	A	152	VAL
1	A	153	LYS
1	A	154	GLU
1	A	157	ILE
1	A	162	LEU
1	A	163	VAL
1	A	164	GLU
1	A	174	LEU
1	A	175	LEU
1	A	176	ARG
1	A	177	ILE
1	A	183	THR
1	A	186	LEU
1	A	189	LYS
1	A	190	ASP
1	A	192	LYS
1	A	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	46	HIS
1	A	52	HIS
1	A	76	GLN
1	A	89	ASN
1	A	111	ASN
1	A	119	HIS
1	A	159	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 [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, 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	203/203 (100%)	-0.31	1 (0%) 87 82	47, 66, 93, 117	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.