



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:41 AM GMT

PDB ID : 3MTV
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

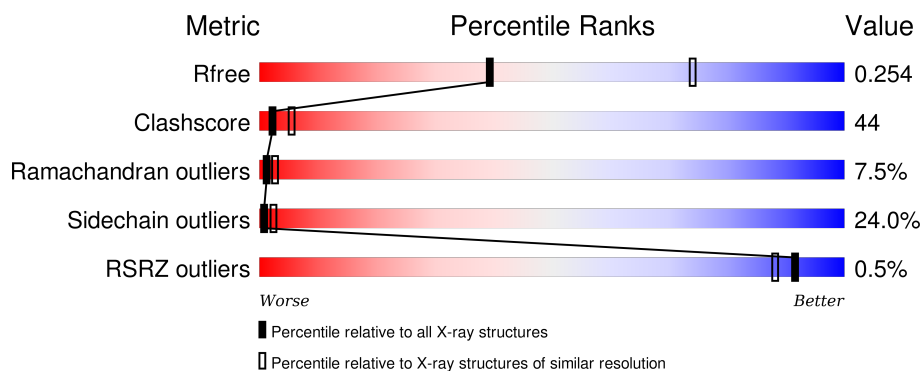
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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			

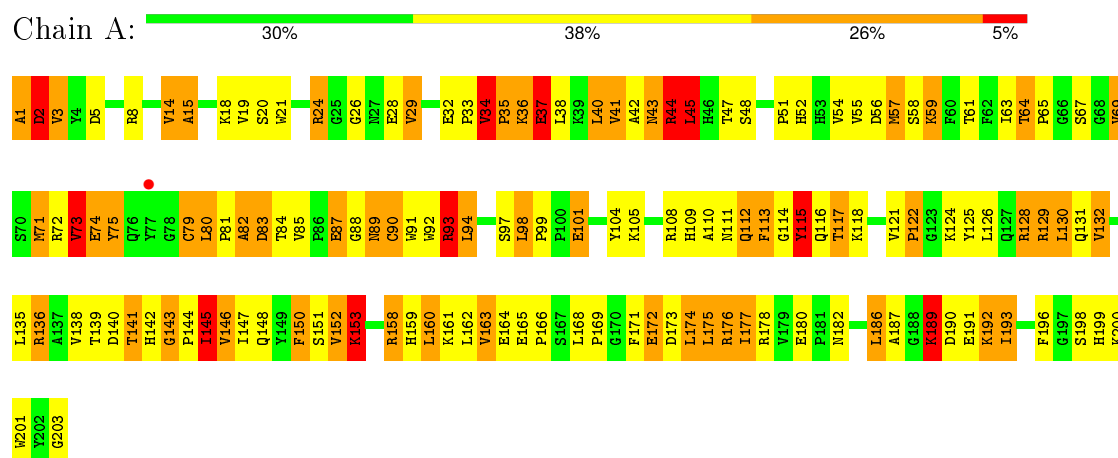
- Molecule 2 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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) 99.9 (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 0.203 , 0.254	Depositor DCC
R_{free} test set	521 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 10839 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.79	27/1683 (1.6%)	1.72	36/2284 (1.6%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	8.38	1.34	1.25
1	A	32	GLU	CD-OE1	8.36	1.34	1.25
1	A	75	TYR	CD1-CE1	7.68	1.50	1.39
1	A	104	TYR	CD2-CE2	7.64	1.50	1.39
1	A	172	GLU	CD-OE2	6.94	1.33	1.25
1	A	90	CYS	CB-SG	6.47	1.93	1.82
1	A	117	THR	CB-CG2	6.47	1.73	1.52
1	A	115	TYR	CE1-CZ	6.44	1.47	1.38
1	A	61	THR	CB-CG2	6.31	1.73	1.52
1	A	113	PHE	CD2-CE2	6.17	1.51	1.39
1	A	26	GLY	C-O	6.15	1.33	1.23
1	A	105	LYS	CB-CG	6.08	1.69	1.52
1	A	132	VAL	CB-CG2	-6.03	1.40	1.52
1	A	82	ALA	CA-CB	-6.00	1.39	1.52
1	A	24	ARG	CZ-NH1	5.94	1.40	1.33
1	A	3	VAL	CB-CG2	-5.82	1.40	1.52
1	A	110	ALA	CA-CB	-5.82	1.40	1.52
1	A	87	GLU	CD-OE1	5.80	1.32	1.25
1	A	150	PHE	CB-CG	-5.79	1.41	1.51
1	A	129	ARG	CZ-NH1	5.67	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLU	CD-OE1	5.65	1.31	1.25
1	A	124	LYS	CD-CE	5.65	1.65	1.51
1	A	87	GLU	CG-CD	5.37	1.60	1.51
1	A	125	TYR	CD2-CE2	5.33	1.47	1.39
1	A	115	TYR	CB-CG	-5.20	1.43	1.51
1	A	1	ALA	N-CA	5.18	1.56	1.46
1	A	14	VAL	CA-CB	-5.01	1.44	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	44	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	132	VAL	CG1-CB-CG2	-8.51	97.29	110.90
1	A	132	VAL	CB-CA-C	-8.41	95.42	111.40
1	A	128	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	24	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	173	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	24	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	130	LEU	CB-CG-CD1	7.25	123.33	111.00
1	A	14	VAL	CB-CA-C	-7.03	98.05	111.40
1	A	160	LEU	CA-CB-CG	-6.99	99.23	115.30
1	A	115	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	A	152	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	A	173	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	79	CYS	CA-CB-SG	6.30	125.35	114.00
1	A	40	LEU	CA-CB-CG	-6.02	101.46	115.30
1	A	115	TYR	CA-CB-CG	-5.98	102.04	113.40
1	A	129	ARG	N-CA-C	-5.93	94.98	111.00
1	A	143	GLY	C-N-CD	-5.87	107.68	120.60
1	A	146	VAL	CB-CA-C	-5.81	100.37	111.40
1	A	122	PRO	C-N-CA	-5.75	110.23	122.30
1	A	32	GLU	OE1-CD-OE2	5.65	130.09	123.30
1	A	2	ASP	CB-CA-C	-5.58	99.25	110.40
1	A	115	TYR	N-CA-C	5.56	126.01	111.00
1	A	129	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	57	MET	CG-SD-CE	5.49	108.98	100.20
1	A	162	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	A	93	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	145	ILE	CG1-CB-CG2	-5.39	99.54	111.40
1	A	44	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	145	ILE	CB-CA-C	-5.18	101.24	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LYS	N-CA-CB	5.17	119.90	110.60
1	A	34	VAL	C-N-CD	-5.14	109.29	120.60
1	A	2	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	29	VAL	CA-CB-CG1	-5.06	103.31	110.90
1	A	5	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	LYS	Peptide
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	144	0
2	A	20	0	0	2	0
All	All	1652	0	1616	144	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 44.

All (144) 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:CG1	1:A:193:ILE:CD1	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: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:130:LEU:HD23	1:A:130:LEU:C	1.92	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:44:ARG:HB3	1:A:57:MET:HE1	1.71	0.71
1:A:171:PHE:C	1:A:172:GLU:HG2	2.12	0.71
1:A:186:LEU:HD12	1:A:187:ALA:N	2.07	0.70
1:A:160:LEU:C	1:A:160:LEU:HD12	2.11	0.69
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
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:113:PHE:HB3	1:A:115:TYR:CE1	2.29	0.67
1:A:59:LYS:HD3	1:A:59:LYS:N	2.08	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: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:130:LEU:CD2	1:A:130:LEU:C	2.67	0.63
1:A:44:ARG:CB	1:A:57:MET:HE1	2.28	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:HG23	1:A:139:THR:O	1.98	0.62
1:A:136:ARG:HB3	1:A:182:ASN:HB2	1.81	0.62
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:90:CYS:SG	1:A:203:GLY:C	2.81	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:128:ARG:C	1:A:129:ARG:O	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:O	1:A:37:GLU:N	2.36	0.57
1:A:117:THR:OG1	1:A:118:LYS:N	2.37	0.57
1:A:14:VAL:HG12	1:A:15:ALA:N	2.19	0.57
1:A:115:TYR:C	1:A:117:THR:H	2.07	0.56
1:A:109:HIS:O	1:A:112:GLN:HB2	2.05	0.56
1:A:165:GLU:HB3	1:A:166:PRO:HD2	1.89	0.55
1:A:153:LYS:H	1:A:153:LYS:HD3	1.71	0.55
1:A:48:SER:HB2	1:A:80:LEU:HD12	1.88	0.55
1:A:115:TYR:HB3	1:A:121:VAL:HG12	1.90	0.54
1:A:87:GLU:HG3	1:A:89:ASN:ND2	2.23	0.54
1:A:165:GLU:CB	1:A:166:PRO:CD	2.85	0.53
1:A:111:ASN:HD22	1:A:116:GLN:HB2	1.74	0.53
1:A:140:ASP:OD1	1:A:142:HIS:N	2.37	0.53
1:A:139:THR:CG2	1:A:139:THR:O	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: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: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:82:ALA:C	1:A:84:THR:H	2.14	0.51
1:A:168:LEU:HB3	1:A:169:PRO:CD	2.41	0.51
1:A:113:PHE:HB2	1:A:115:TYR:CD1	2.46	0.51
1:A:82:ALA:O	1:A:83:ASP:C	2.48	0.51
1:A:36:LYS:C	1:A:38:LEU:H	2.14	0.50
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:186:LEU:HD12	1:A:187:ALA:H	1.74	0.50
1:A:33:PRO:O	1:A:35:PRO:HD3	2.11	0.50
1:A:153:LYS:N	1:A:153:LYS:HD3	2.27	0.50
1:A:87:GLU:HG3	1:A:89:ASN:HD21	1.77	0.49
1:A:43:ASN:H	1:A:43:ASN:HD22	1.61	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:56:ASP:C	1:A:56:ASP:OD1	2.53	0.47
1:A:139:THR:HG22	1:A:192:LYS:H	1.78	0.47
1:A:28:GLU:HG2	1:A:29:VAL:N	2.27	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:2:ASP:C	1:A:3:VAL:HG23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HA	1:A:200:LYS:HD2	1.68	0.47
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:82:ALA:C	1:A:84:THR:N	2.69	0.46
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: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:192:LYS:HE2	1:A:192:LYS:HB2	1.40	0.45
1:A:98:LEU:HD21	1:A:135:LEU:HD11	1.99	0.45
1:A:115:TYR:C	1:A:117:THR:N	2.68	0.45
1:A:140:ASP:C	1:A:140:ASP:OD1	2.54	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:140:ASP:C	1:A:142:HIS:H	2.21	0.44
1:A:187:ALA:O	1:A:191:GLU:HG3	2.17	0.44
1:A:160:LEU:HG	1:A:160:LEU:H	1.65	0.44
1:A:136:ARG:HB3	1:A:182:ASN:CB	2.48	0.44
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.98	0.43
1:A:40:LEU:HA	1:A:40:LEU:HD12	1.72	0.43
1:A:21:TRP:HB3	1:A:45:LEU:HD13	1.99	0.43
1:A:161:LYS:HE2	1:A:165:GLU:O	2.18	0.43
1:A:18:LYS:C	1:A:19:VAL:HG23	2.38	0.43
1:A:130:LEU:O	1:A:131:GLN:C	2.54	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:92:TRP:O	1:A:93:ARG:C	2.56	0.43
1:A:72:ARG:HB2	1:A:75:TYR:HB2	2.01	0.43
1:A:71:MET:HB3	1:A:71:MET:HE3	1.93	0.43
1:A:88:GLY:HA2	1:A:203:GLY:CA	2.48	0.43
1:A:72:ARG:O	1:A:73:VAL:C	2.58	0.43
1:A:38:LEU:C	1:A:40:LEU:N	2.71	0.42
1:A:40:LEU:HB3	1:A:41:VAL:H	1.56	0.42
1:A:81:PRO:HG2	1:A:84:THR:CG2	2.48	0.42
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.74	0.42
1:A:84:THR:C	1:A:168:LEU:HD22	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:45:LEU:C	1:A:45:LEU:CD2	2.87	0.41
1:A:147:ILE:HD12	1:A:147:ILE:HG23	1.71	0.41
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:HG21	1:A:145:ILE:HD12	1.63	0.41
1:A:143:GLY:HA2	1:A:144:PRO:HD3	1.40	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 3

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

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Mol	Chain	Res	Type
1	A	37	GLU
1	A	43	ASN
1	A	44	ARG
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%)	133 (76%)	42 (24%)	1 2

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	8	ARG
1	A	20	SER
1	A	34	VAL
1	A	36	LYS
1	A	37	GLU
1	A	45	LEU
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	93	ARG
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	163	VAL
1	A	164	GLU
1	A	174	LEU
1	A	175	LEU
1	A	176	ARG
1	A	177	ILE
1	A	186	LEU
1	A	189	LYS
1	A	190	ASP
1	A	192	LYS
1	A	193	ILE

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	HIS
1	A	89	ASN
1	A	111	ASN
1	A	119	HIS
1	A	133	ASN
1	A	159	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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%)	-0.53	1 (0%) 91 88	47, 66, 93, 117	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	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 carbohydrates 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.