



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2025 – 08:25 PM JST

PDB ID : 9KZ3 / pdb_00009kz3
Title : PEDV 3CLpro mutant (C144A) in complex with nsp8|9 peptide substrate
Authors : Zhang, Y.; Zhang, D.; Zhang, Z.T.; Shi, Y.J.; Peng, G.Q.
Deposited on : 2024-12-09
Resolution : 1.93 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.47

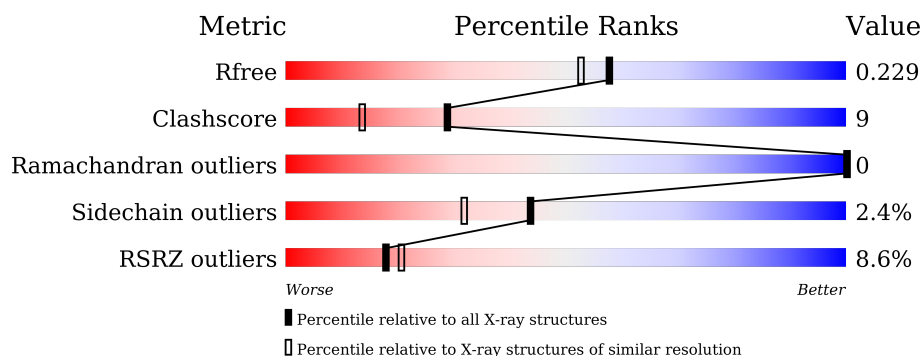
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	310	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div> </div>
1	B	310	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
2	C	6	<div> <div>17%</div> <div> <div></div> <div>50%</div> <div>17%</div> <div>17%</div> <div>17%</div> </div> </div>
3	D	6	<div> <div>17%</div> <div> <div>67%</div> <div>50%</div> <div>17%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4859 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 ORF1ab polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2265	1431	391	428	15			
1	B	295	Total	C	N	O	S	0	0	0
			2248	1420	389	424	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A023J7B5
A	144	ALA	CYS	engineered mutation	UNP A0A023J7B5
A	300	LEU	-	expression tag	UNP A0A023J7B5
A	301	GLU	-	expression tag	UNP A0A023J7B5
A	302	HIS	-	expression tag	UNP A0A023J7B5
A	303	HIS	-	expression tag	UNP A0A023J7B5
A	304	HIS	-	expression tag	UNP A0A023J7B5
A	305	HIS	-	expression tag	UNP A0A023J7B5
A	306	HIS	-	expression tag	UNP A0A023J7B5
A	307	HIS	-	expression tag	UNP A0A023J7B5
A	308	HIS	-	expression tag	UNP A0A023J7B5
A	309	HIS	-	expression tag	UNP A0A023J7B5
B	0	MET	-	initiating methionine	UNP A0A023J7B5
B	144	ALA	CYS	engineered mutation	UNP A0A023J7B5
B	300	LEU	-	expression tag	UNP A0A023J7B5
B	301	GLU	-	expression tag	UNP A0A023J7B5
B	302	HIS	-	expression tag	UNP A0A023J7B5
B	303	HIS	-	expression tag	UNP A0A023J7B5
B	304	HIS	-	expression tag	UNP A0A023J7B5
B	305	HIS	-	expression tag	UNP A0A023J7B5
B	306	HIS	-	expression tag	UNP A0A023J7B5
B	307	HIS	-	expression tag	UNP A0A023J7B5
B	308	HIS	-	expression tag	UNP A0A023J7B5
B	309	HIS	-	expression tag	UNP A0A023J7B5

- Molecule 2 is a protein called Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			41	28	7	6			

- Molecule 3 is a protein called Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			41	28	7	6			

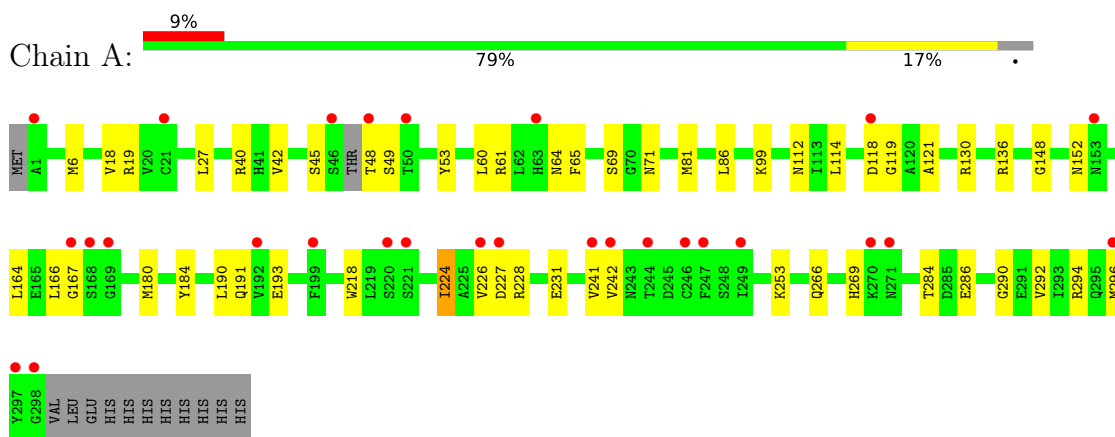
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	134	Total	O	0	0
			134	134		
4	C	3	Total	O	0	0
			3	3		
4	D	4	Total	O	0	0
			4	4		

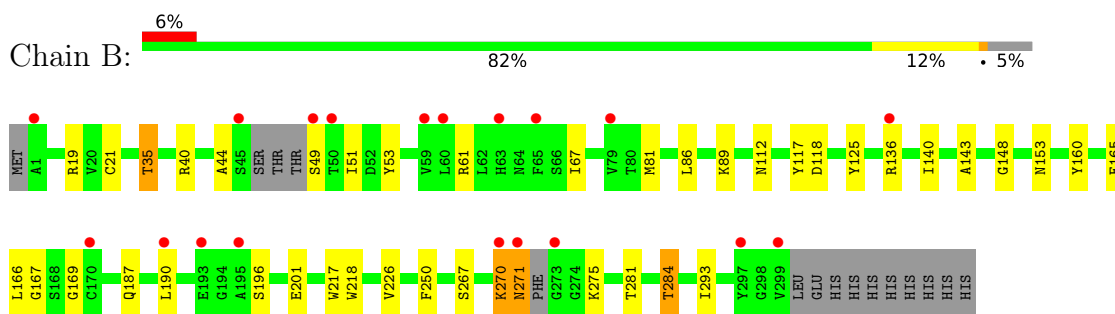
3 Residue-property plots [i](#)

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.

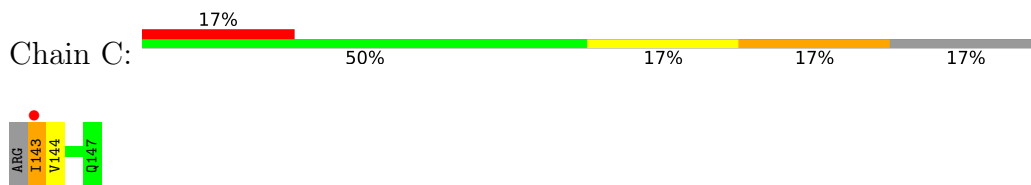
- Molecule 1: ORF1ab polyprotein



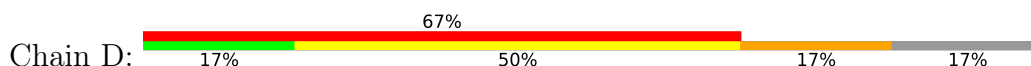
- Molecule 1: ORF1ab polyprotein

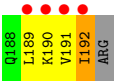


- Molecule 2: Replicase polyprotein 1a



- Molecule 3: Replicase polyprotein 1a





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.87Å 92.38Å 58.09Å 90.00° 100.07° 90.00°	Depositor
Resolution (Å)	35.94 – 1.93 35.94 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.94-1.93) 97.6 (35.94-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.214 , 0.226 0.216 , 0.229	Depositor DCC
R_{free} test set	2103 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4859	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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	0.38	0/2311	0.61	0/3136
1	B	0.39	0/2292	0.61	0/3109
2	C	0.80	0/40	1.21	0/52
3	D	0.80	0/40	1.55	0/52
All	All	0.39	0/4683	0.63	0/6349

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	2265	0	2213	40	0
1	B	2248	0	2200	37	0
2	C	41	0	51	3	0
3	D	41	0	51	7	0
4	A	123	0	0	5	0
4	B	134	0	0	13	0
4	C	3	0	0	1	0
4	D	4	0	0	0	0
All	All	4859	0	4515	78	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 9.

All (78) 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:B:196:SER:HA	4:B:403:HOH:O	1.67	0.94
1:B:61:ARG:HD3	4:B:401:HOH:O	1.70	0.90
1:A:61:ARG:HB2	1:A:64:ASN:HD22	1.40	0.86
1:B:35:THR:HG23	4:B:471:HOH:O	1.87	0.74
1:B:281:THR:O	1:B:284:THR:HG22	1.90	0.72
1:B:166:LEU:HD23	3:D:191:VAL:HG21	1.74	0.69
1:A:136:ARG:NH2	1:A:286:GLU:OE1	2.27	0.67
1:A:167:GLY:HA3	2:C:143:ILE:HD12	1.75	0.67
3:D:191:VAL:O	3:D:192:ILE:C	2.38	0.67
1:A:61:ARG:HB2	1:A:64:ASN:ND2	2.07	0.67
1:A:130:ARG:NH2	1:A:136:ARG:HB2	2.14	0.63
1:B:19:ARG:HD2	4:B:438:HOH:O	1.97	0.63
1:B:217:TRP:CE2	1:B:275:LYS:HD3	2.34	0.63
1:B:19:ARG:HD3	1:B:21:CYS:SG	2.40	0.61
1:A:284:THR:OG1	1:A:286:GLU:HG2	2.00	0.61
1:A:53:TYR:HB3	1:A:81:MET:HE1	1.83	0.60
1:B:217:TRP:CD2	1:B:275:LYS:HD3	2.37	0.60
1:B:166:LEU:HD23	3:D:191:VAL:CG2	2.32	0.58
1:B:136:ARG:HD2	4:B:481:HOH:O	2.03	0.58
1:A:190:LEU:HA	2:C:143:ILE:HG12	1.89	0.55
1:B:49:SER:N	4:B:407:HOH:O	2.40	0.54
1:A:40:ARG:HA	1:A:86:LEU:HG	1.89	0.54
2:C:143:ILE:HG13	2:C:144:VAL:N	2.22	0.54
1:A:48:THR:OG1	1:A:49:SER:N	2.38	0.53
1:B:169:GLY:HA3	4:B:408:HOH:O	2.07	0.53
1:A:290:GLY:O	1:A:294:ARG:HG3	2.09	0.53
1:B:201:GLU:HG3	4:B:470:HOH:O	2.09	0.52
1:B:267:SER:HB2	4:B:424:HOH:O	2.09	0.52
1:B:44:ALA:HB1	1:B:51:ILE:HD13	1.92	0.51
1:A:71:ASN:OD1	1:A:71:ASN:N	2.42	0.51
1:B:148:GLY:HA3	1:B:160:TYR:HB3	1.91	0.50
1:B:218:TRP:CD1	1:B:218:TRP:H	2.29	0.50
1:B:117:TYR:CE1	1:B:143:ALA:HB2	2.48	0.49
1:B:89:LYS:HG3	4:B:532:HOH:O	2.13	0.48
1:A:224:ILE:HD12	1:A:266:GLN:HE22	1.78	0.48
1:B:166:LEU:HA	3:D:191:VAL:CG2	2.43	0.48
1:B:270:LYS:HA	1:B:270:LYS:HD2	1.55	0.48
1:B:165:GLU:O	3:D:190:LYS:HD2	2.15	0.47
1:B:226:VAL:HG23	4:B:445:HOH:O	2.14	0.47
1:A:18:VAL:HG12	1:A:69:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:OD1	1:A:228:ARG:N	2.45	0.46
1:A:152:ASN:HB2	4:A:409:HOH:O	2.15	0.46
1:B:217:TRP:CH2	1:B:275:LYS:HB3	2.51	0.46
1:A:226:VAL:HG13	1:A:241:VAL:HG23	1.98	0.46
1:B:153:ASN:N	4:B:412:HOH:O	2.50	0.45
1:A:27:LEU:HD11	1:A:42:VAL:HB	1.97	0.45
1:A:19:ARG:HB2	1:A:119:GLY:HA3	1.98	0.45
1:A:253:LYS:HA	1:A:253:LYS:HE2	1.99	0.45
1:B:19:ARG:O	1:B:67:ILE:HA	2.18	0.45
1:A:152:ASN:HA	4:A:473:HOH:O	2.18	0.44
1:A:99:LYS:HE2	1:A:99:LYS:HB2	1.59	0.44
1:A:227:ASP:O	1:A:231:GLU:HG3	2.18	0.44
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.82	0.44
1:B:19:ARG:NH2	1:B:118:ASP:HB3	2.33	0.43
1:B:167:GLY:HA2	3:D:190:LYS:NZ	2.34	0.43
1:A:164:LEU:HD12	1:A:164:LEU:C	2.44	0.43
1:A:40:ARG:HH11	1:A:81:MET:HE3	1.83	0.43
1:A:166:LEU:HD13	1:A:193:GLU:HB3	2.01	0.43
1:B:112:ASN:O	1:B:148:GLY:HA2	2.19	0.42
1:B:250:PHE:CZ	1:B:293:ILE:HG13	2.54	0.42
1:B:271:ASN:HD22	1:B:271:ASN:HA	1.65	0.42
1:B:187:GLN:O	3:D:191:VAL:HG12	2.19	0.42
1:A:6:MET:HE1	4:B:442:HOH:O	2.18	0.42
1:A:292:VAL:O	1:A:296:MET:HG2	2.20	0.42
1:A:136:ARG:NE	4:A:406:HOH:O	2.50	0.42
1:B:53:TYR:HB3	1:B:81:MET:HE1	2.02	0.42
1:B:40:ARG:HA	1:B:86:LEU:HG	2.02	0.42
1:A:269:HIS:HE1	4:A:405:HOH:O	2.03	0.42
1:A:180:MET:HG2	1:A:184:TYR:O	2.19	0.41
1:A:114:LEU:HD11	1:A:121:ALA:HB1	2.01	0.41
1:A:152:ASN:ND2	4:A:409:HOH:O	2.53	0.41
1:A:6:MET:HE2	1:B:125:TYR:CE1	2.55	0.41
1:A:112:ASN:O	1:A:148:GLY:HA2	2.21	0.40
1:A:218:TRP:CD1	1:A:218:TRP:H	2.39	0.40
1:A:19:ARG:NE	1:A:118:ASP:OD1	2.54	0.40
1:A:60:LEU:HD21	1:A:65:PHE:HE2	1.86	0.40
1:A:167:GLY:HA2	4:C:201:HOH:O	2.21	0.40
1:B:117:TYR:CE1	1:B:140:ILE:HG12	2.57	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	293/310 (94%)	286 (98%)	7 (2%)	0	100	100
1	B	289/310 (93%)	286 (99%)	3 (1%)	0	100	100
2	C	3/6 (50%)	3 (100%)	0	0	100	100
3	D	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	588/632 (93%)	577 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	243/256 (95%)	239 (98%)	4 (2%)	58	49
1	B	241/256 (94%)	236 (98%)	5 (2%)	48	36
2	C	5/6 (83%)	4 (80%)	1 (20%)	1	0
3	D	5/6 (83%)	3 (60%)	2 (40%)	0	0
All	All	494/524 (94%)	482 (98%)	12 (2%)	44	32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	224	ILE
1	A	242	VAL
1	B	35	THR
1	B	190	LEU
1	B	270	LYS
1	B	271	ASN
1	B	284	THR
2	C	143	ILE
3	D	189	LEU
3	D	192	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	64	ASN
1	A	92	GLN
1	A	152	ASN
1	A	243	ASN
1	A	266	GLN
1	B	236	ASN
1	B	243	ASN
1	B	276	GLN

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 ⓘ

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	297/310 (95%)	0.65	28 (9%) 15 18	15, 30, 51, 68	0
1	B	295/310 (95%)	0.49	19 (6%) 27 29	16, 28, 45, 62	0
2	C	5/6 (83%)	1.05	1 (20%) 3 3	26, 28, 34, 42	0
3	D	5/6 (83%)	3.14	4 (80%) 0 0	35, 36, 45, 51	0
All	All	602/632 (95%)	0.59	52 (8%) 18 21	15, 30, 49, 68	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	4.7
2	C	143	ILE	4.4
3	D	191	VAL	4.3
1	A	48	THR	4.2
3	D	192	ILE	4.0
3	D	189	LEU	4.0
1	B	271	ASN	4.0
1	A	242	VAL	4.0
1	B	299	VAL	3.9
1	A	192	VAL	3.5
1	B	270	LYS	3.4
1	A	244	THR	3.4
1	A	21	CYS	3.3
1	A	249	ILE	3.2
1	A	271	ASN	3.1
1	B	45	SER	3.0
1	B	49	SER	3.0
1	B	60	LEU	3.0
1	A	298	GLY	2.9
1	B	170	CYS	2.9
1	B	190	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	199	PHE	2.6
1	B	297	TYR	2.6
1	A	246	CYS	2.6
1	A	63	HIS	2.5
1	A	46	SER	2.5
1	B	65	PHE	2.5
1	A	226	VAL	2.4
1	B	273	GLY	2.4
1	B	59	VAL	2.3
1	B	79	VAL	2.3
1	B	63	HIS	2.3
1	B	136	ARG	2.3
1	A	50	THR	2.3
1	A	270	LYS	2.3
1	A	220	SER	2.2
1	B	195	ALA	2.2
1	A	297	TYR	2.2
1	A	118	ASP	2.1
1	A	168	SER	2.1
1	A	221	SER	2.1
1	A	169	GLY	2.1
1	A	1	ALA	2.1
1	A	227	ASP	2.1
1	B	1	ALA	2.1
1	A	153	ASN	2.1
1	A	167	GLY	2.1
1	A	247	PHE	2.0
1	B	193	GLU	2.0
1	B	50	THR	2.0
3	D	190	LYS	2.0
1	A	296	MET	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.