



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:42 AM UTC

PDB ID : 9RN6 / pdb_00009rn6
Title : Crystal structure of a protein mimic of SARS-CoV-2 spike's HR1 domain in complex with two nanobodies bound to different epitopes
Authors : Camara-Artigas, A.; Conejero-Lara, F.; Polo-Megias, D.; Salinas-Garcia, M.C.; Gavira, J.A.
Deposited on : 2025-06-19
Resolution : 2.40 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

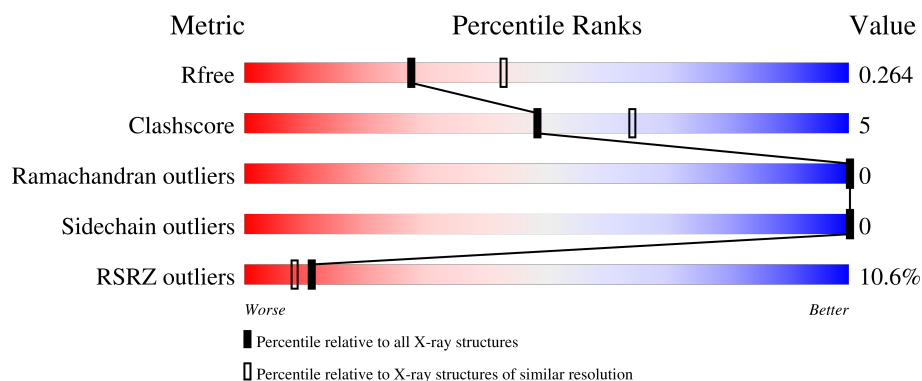
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	241	
2	B	123	
3	C	138	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6959 atoms, of which 3455 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 S2',Chimeric protein mimic of SARS-CoV-2 Spike HR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	H	N	O	0	0	0
			3290	998	1671	288	333			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0DTC2
A	2	ASP	-	expression tag	UNP P0DTC2
A	14	LYS	GLN	engineered mutation	UNP P0DTC2
A	32	GLU	ALA	engineered mutation	UNP P0DTC2
A	39	GLU	VAL	engineered mutation	UNP P0DTC2
A	46	ASP	ALA	engineered mutation	UNP P0DTC2
A	60	ARG	ALA	engineered mutation	UNP P0DTC2
A	64	GLU	VAL	engineered mutation	UNP P0DTC2
A	75	GLY	VAL	engineered mutation	UNP P0DTC2
A	77	PRO	-	linker	UNP P0DTC2
A	78	ALA	-	linker	UNP P0DTC2
A	79	LYS	-	linker	UNP P0DTC2
A	80	ASP	-	linker	UNP P0DTC2
A	81	LEU	-	linker	UNP P0DTC2
A	82	ARG	-	linker	UNP P0DTC2
A	83	SER	-	linker	UNP P0DTC2
A	84	ASP	-	linker	UNP P0DTC2
A	85	ILE	-	linker	UNP P0DTC2
A	86	ASP	-	linker	UNP P0DTC2
A	87	ASN	-	linker	UNP P0DTC2
A	88	LEU	-	linker	UNP P0DTC2
A	89	GLU	-	linker	UNP P0DTC2
A	90	SER	-	linker	UNP P0DTC2
A	91	LYS	-	linker	UNP P0DTC2
A	92	ILE	-	linker	UNP P0DTC2
A	93	ALA	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	94	GLY	-	linker	UNP P0DTC2
A	95	PHE	-	linker	UNP P0DTC2
A	96	ASN	-	linker	UNP P0DTC2
A	97	SER	-	linker	UNP P0DTC2
A	98	SER	-	linker	UNP P0DTC2
A	99	LEU	-	linker	UNP P0DTC2
A	100	GLN	-	linker	UNP P0DTC2
A	101	LYS	-	linker	UNP P0DTC2
A	102	VAL	-	linker	UNP P0DTC2
A	103	LEU	-	linker	UNP P0DTC2
A	104	THR	-	linker	UNP P0DTC2
A	105	ASN	-	linker	UNP P0DTC2
A	106	LEU	-	linker	UNP P0DTC2
A	107	ALA	-	linker	UNP P0DTC2
A	108	GLN	-	linker	UNP P0DTC2
A	109	LYS	-	linker	UNP P0DTC2
A	110	ASN	-	linker	UNP P0DTC2
A	111	GLN	-	linker	UNP P0DTC2
A	112	ASN	-	linker	UNP P0DTC2
A	113	VAL	-	linker	UNP P0DTC2
A	114	GLU	-	linker	UNP P0DTC2
A	115	ASP	-	linker	UNP P0DTC2
A	116	LYS	-	linker	UNP P0DTC2
A	117	LEU	-	linker	UNP P0DTC2
A	118	LYS	-	linker	UNP P0DTC2
A	119	GLY	-	linker	UNP P0DTC2
A	120	LEU	-	linker	UNP P0DTC2
A	121	GLU	-	linker	UNP P0DTC2
A	122	SER	-	linker	UNP P0DTC2
A	123	ARG	-	linker	UNP P0DTC2
A	124	THR	-	linker	UNP P0DTC2
A	125	SER	-	linker	UNP P0DTC2
A	126	SER	-	linker	UNP P0DTC2
A	127	LEU	-	linker	UNP P0DTC2
A	128	GLU	-	linker	UNP P0DTC2
A	129	LYS	-	linker	UNP P0DTC2
A	130	GLN	-	linker	UNP P0DTC2
A	131	ILE	-	linker	UNP P0DTC2
A	132	LYS	-	linker	UNP P0DTC2
A	133	GLY	-	linker	UNP P0DTC2
A	134	ILE	-	linker	UNP P0DTC2
A	135	ALA	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	-	linker	UNP P0DTC2
A	137	ASN	-	linker	UNP P0DTC2
A	138	PHE	-	linker	UNP P0DTC2
A	139	GLN	-	linker	UNP P0DTC2
A	140	ASN	-	linker	UNP P0DTC2
A	141	GLU	-	linker	UNP P0DTC2
A	142	ILE	-	linker	UNP P0DTC2
A	143	LEU	-	linker	UNP P0DTC2
A	144	LYS	-	linker	UNP P0DTC2
A	145	GLN	-	linker	UNP P0DTC2
A	146	ARG	-	linker	UNP P0DTC2
A	147	GLU	-	linker	UNP P0DTC2
A	148	TYR	-	linker	UNP P0DTC2
A	149	LEU	-	linker	UNP P0DTC2
A	150	VAL	-	linker	UNP P0DTC2
A	151	ASN	-	linker	UNP P0DTC2
A	152	LYS	-	linker	UNP P0DTC2
A	153	GLY	-	linker	UNP P0DTC2
A	154	SER	-	linker	UNP P0DTC2
A	155	GLY	-	linker	UNP P0DTC2
A	156	ASN	-	linker	UNP P0DTC2
A	166	GLU	ALA	engineered mutation	UNP P0DTC2
A	184	LYS	ALA	engineered mutation	UNP P0DTC2
A	191	LYS	GLN	engineered mutation	UNP P0DTC2
A	198	LYS	ALA	engineered mutation	UNP P0DTC2
A	223	LYS	LEU	engineered mutation	UNP P0DTC2
A	231	GLY	-	expression tag	UNP P0DTC2
A	232	GLY	-	expression tag	UNP P0DTC2
A	233	GLY	-	expression tag	UNP P0DTC2
A	234	GLY	-	expression tag	UNP P0DTC2
A	235	SER	-	expression tag	UNP P0DTC2
A	236	HIS	-	expression tag	UNP P0DTC2
A	237	HIS	-	expression tag	UNP P0DTC2
A	238	HIS	-	expression tag	UNP P0DTC2
A	239	HIS	-	expression tag	UNP P0DTC2
A	240	HIS	-	expression tag	UNP P0DTC2
A	241	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody NB278.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	121	Total	C	H	N	O	S	0	0	0
			1819	582	881	172	180	4			

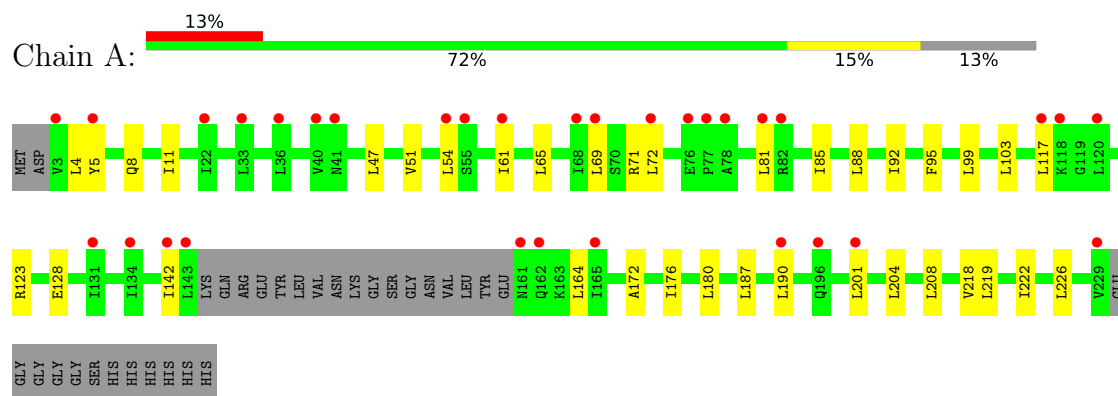
- Molecule 3 is a protein called Nanobody NB184.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	123	Total	C	H	N	O	S	0	0	0
			1850	595	903	164	185	3			

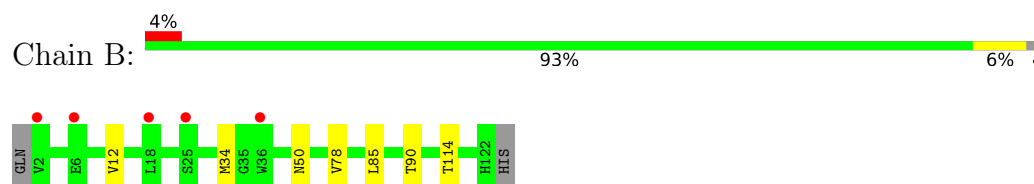
3 Residue-property plots [i](#)

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.

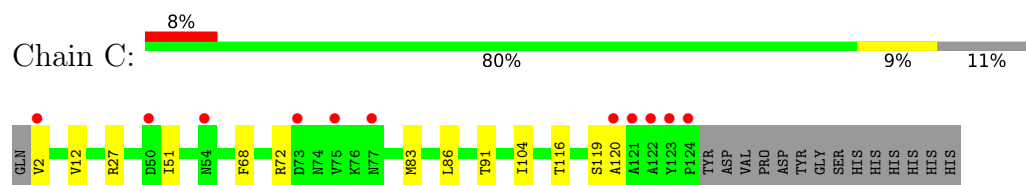
- Molecule 1: Spike protein S2',Chimeric protein mimic of SARS-CoV-2 Spike HR1



- Molecule 2: Nanobody NB278



- Molecule 3: Nanobody NB184



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	47.56Å 67.34Å 230.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-2.40) 99.7 (19.99-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.247 , 0.263 0.251 , 0.264	Depositor DCC
R_{free} test set	1434 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6959	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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	0.22	0/1625	0.41	0/2177
2	B	0.26	0/961	0.42	0/1302
3	C	0.38	0/970	0.52	0/1318
All	All	0.28	0/3556	0.45	0/4797

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	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
3	C	72	ARG	Sidechain

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	1619	1671	1670	26	0
2	B	938	881	881	5	0
3	C	947	903	902	8	0
All	All	3504	3455	3453	38	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 5.

All (38) 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:117:LEU:HD11	1:A:190:LEU:HD22	1.74	0.69
1:A:117:LEU:HD21	1:A:190:LEU:HD21	1.78	0.66
1:A:4:LEU:HD13	1:A:8:GLN:OE1	1.96	0.64
1:A:88:LEU:HD13	1:A:92:ILE:HD13	1.79	0.64
3:C:91:THR:HG23	3:C:116:THR:HA	1.78	0.64
1:A:69:LEU:HD21	1:A:222:ILE:HG12	1.80	0.64
1:A:54:LEU:HD22	1:A:208:LEU:HD21	1.81	0.63
1:A:51:VAL:HA	1:A:54:LEU:HD12	1.84	0.58
1:A:61:ILE:HD13	1:A:92:ILE:HG13	1.86	0.57
1:A:128:GLU:HG2	1:A:180:LEU:HD21	1.88	0.56
1:A:47:LEU:HD13	1:A:201:LEU:HD23	1.87	0.56
1:A:103:LEU:HD21	1:A:204:LEU:HD23	1.89	0.54
1:A:218:VAL:HG23	2:B:50:ASN:HD21	1.73	0.53
1:A:5:TYR:CE1	1:A:164:LEU:HD23	2.43	0.53
1:A:65:LEU:HD21	1:A:219:LEU:HD21	1.90	0.52
1:A:95:PHE:CZ	1:A:99:LEU:HD11	2.45	0.51
2:B:34:MET:SD	2:B:78:VAL:HG11	2.51	0.51
1:A:117:LEU:HD11	1:A:190:LEU:CD2	2.40	0.50
2:B:12:VAL:HG11	2:B:85:LEU:HD13	1.96	0.47
1:A:47:LEU:HD13	1:A:201:LEU:CD2	2.44	0.47
1:A:187:LEU:HD23	1:A:187:LEU:C	2.41	0.46
2:B:90:THR:HG23	2:B:114:THR:HA	1.97	0.46
3:C:51:ILE:HG23	3:C:51:ILE:O	2.16	0.46
2:B:34:MET:HE2	2:B:34:MET:HB2	1.89	0.46
3:C:104:ILE:HD12	3:C:104:ILE:C	2.41	0.46
1:A:85:ILE:HD11	1:A:222:ILE:CG2	2.46	0.45
1:A:71:ARG:HB2	1:A:81:LEU:HD21	1.97	0.45
1:A:54:LEU:CD2	1:A:208:LEU:HD21	2.45	0.44
1:A:117:LEU:HD21	1:A:190:LEU:CD2	2.46	0.44
1:A:72:LEU:HD21	1:A:226:LEU:CD2	2.49	0.43
3:C:12:VAL:HG21	3:C:86:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:O	1:A:176:ILE:HD12	2.19	0.42
3:C:68:PHE:CZ	3:C:83:MET:HG2	2.55	0.41
1:A:85:ILE:HD11	1:A:222:ILE:HG21	2.02	0.41
3:C:2:VAL:HG23	3:C:27:ARG:NE	2.36	0.41
1:A:11:ILE:HG21	1:A:142:ILE:CD1	2.51	0.41
3:C:68:PHE:CE2	3:C:83:MET:HG2	2.56	0.40
3:C:119:SER:O	3:C:120:ALA:HB3	2.20	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	206/241 (86%)	206 (100%)	0	0	100	100
2	B	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
3	C	121/138 (88%)	116 (96%)	5 (4%)	0	100	100
All	All	446/502 (89%)	440 (99%)	6 (1%)	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	188/213 (88%)	188 (100%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	100	100
3	C	100/114 (88%)	100 (100%)	0	100	100
All	All	386/427 (90%)	386 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	207	GLN
2	B	3	GLN
2	B	50	ASN

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	210/241 (87%)	0.97	32 (15%) 5 4	64, 96, 133, 154	0
2	B	121/123 (98%)	0.48	5 (4%) 41 37	60, 76, 106, 117	0
3	C	123/138 (89%)	0.77	11 (8%) 15 12	55, 79, 126, 151	0
All	All	454/502 (90%)	0.79	48 (10%) 11 8	55, 85, 127, 154	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	121	ALA	5.5
1	A	5	TYR	5.4
1	A	143	LEU	5.4
3	C	77	ASN	5.1
1	A	81	LEU	4.8
3	C	122	ALA	4.7
3	C	124	PRO	4.4
3	C	120	ALA	4.4
3	C	2	VAL	4.2
1	A	77	PRO	3.7
1	A	120	LEU	3.5
1	A	33	LEU	3.4
1	A	131	ILE	3.3
1	A	69	LEU	3.2
3	C	123	TYR	3.1
3	C	50	ASP	3.1
2	B	18	LEU	3.0
1	A	229	VAL	3.0
1	A	190	LEU	2.9
1	A	117	LEU	2.9
2	B	2	VAL	2.8
1	A	61	ILE	2.7
1	A	3	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	2.7
1	A	68	ILE	2.7
1	A	165	ILE	2.7
3	C	54	ASN	2.7
1	A	161	ASN	2.5
1	A	142	ILE	2.4
2	B	25	SER	2.4
1	A	55	SER	2.4
1	A	40	VAL	2.3
3	C	75	VAL	2.3
1	A	72	LEU	2.3
3	C	73	ASP	2.3
1	A	54	LEU	2.2
1	A	134	ILE	2.2
2	B	6	GLU	2.2
1	A	118	LYS	2.1
1	A	196	GLN	2.1
1	A	78	ALA	2.1
1	A	41	ASN	2.1
2	B	36	TRP	2.1
1	A	76	GLU	2.1
1	A	82	ARG	2.0
1	A	201	LEU	2.0
1	A	162	GLN	2.0
1	A	22	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.