



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:34 PM UTC

PDB ID : 9K6J / pdb_00009k6j
Title : Crystal structure of SARS-CoV-2 WT RBD bound with P5-1C8 Fab
Authors : Lv, N.N.; Yang, R.Y.
Deposited on : 2024-10-22
Resolution : 2.39 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
Mogul : 2022.3.0, CSD as543be (2022)
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

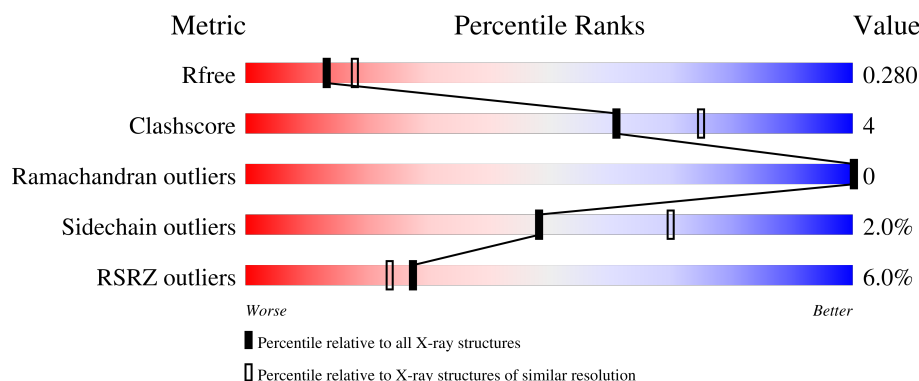
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

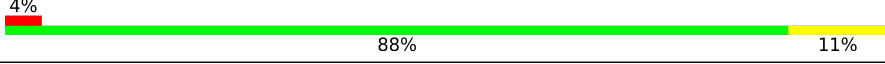
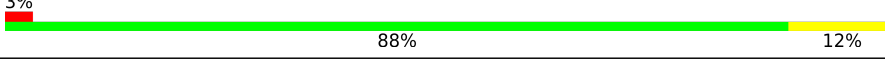
The reported resolution of this entry is 2.39 Å.

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	C	271	
2	A	217	
3	B	211	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4782 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	181	Total	C	N	O	S	0	0	0
			1412	907	238	260	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	300	MET	-	initiating methionine	UNP P0DTC2
C	301	GLY	-	expression tag	UNP P0DTC2
C	302	TRP	-	expression tag	UNP P0DTC2
C	303	SER	-	expression tag	UNP P0DTC2
C	304	CYS	-	expression tag	UNP P0DTC2
C	305	ILE	-	expression tag	UNP P0DTC2
C	306	ILE	-	expression tag	UNP P0DTC2
C	307	LEU	-	expression tag	UNP P0DTC2
C	308	PHE	-	expression tag	UNP P0DTC2
C	309	LEU	-	expression tag	UNP P0DTC2
C	310	VAL	-	expression tag	UNP P0DTC2
C	311	ALA	-	expression tag	UNP P0DTC2
C	312	THR	-	expression tag	UNP P0DTC2
C	313	ALA	-	expression tag	UNP P0DTC2
C	314	THR	-	expression tag	UNP P0DTC2
C	315	GLY	-	expression tag	UNP P0DTC2
C	316	VAL	-	expression tag	UNP P0DTC2
C	317	HIS	-	expression tag	UNP P0DTC2
C	318	SER	-	expression tag	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
C	540	HIS	-	expression tag	UNP P0DTC2
C	541	HIS	-	expression tag	UNP P0DTC2
C	542	HIS	-	expression tag	UNP P0DTC2
C	543	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	544	HIS	-	expression tag	UNP P0DTC2
C	545	GLN	-	expression tag	UNP P0DTC2
C	546	PRO	-	expression tag	UNP P0DTC2
C	547	ARG	-	expression tag	UNP P0DTC2
C	548	PHE	-	expression tag	UNP P0DTC2
C	549	ALA	-	expression tag	UNP P0DTC2
C	550	ALA	-	expression tag	UNP P0DTC2
C	551	ALA	-	expression tag	UNP P0DTC2
C	552	ALA	-	expression tag	UNP P0DTC2
C	553	SER	-	expression tag	UNP P0DTC2
C	554	SER	-	expression tag	UNP P0DTC2
C	555	ALA	-	expression tag	UNP P0DTC2
C	556	GLY	-	expression tag	UNP P0DTC2
C	557	LEU	-	expression tag	UNP P0DTC2
C	558	ASN	-	expression tag	UNP P0DTC2
C	559	ASP	-	expression tag	UNP P0DTC2
C	560	ILE	-	expression tag	UNP P0DTC2
C	561	PHE	-	expression tag	UNP P0DTC2
C	562	GLU	-	expression tag	UNP P0DTC2
C	563	ALA	-	expression tag	UNP P0DTC2
C	564	GLN	-	expression tag	UNP P0DTC2
C	565	LYS	-	expression tag	UNP P0DTC2
C	566	ILE	-	expression tag	UNP P0DTC2
C	567	GLU	-	expression tag	UNP P0DTC2
C	568	TRP	-	expression tag	UNP P0DTC2
C	569	HIS	-	expression tag	UNP P0DTC2
C	570	GLU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called H chain of P5-1C8 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	213	Total	C	N	O	S	0	0	0
			1587	1005	264	312	6			

- Molecule 3 is a protein called L chain of P5-1C8 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	211	Total	C	N	O	S	0	0	0
			1612	1010	274	324	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

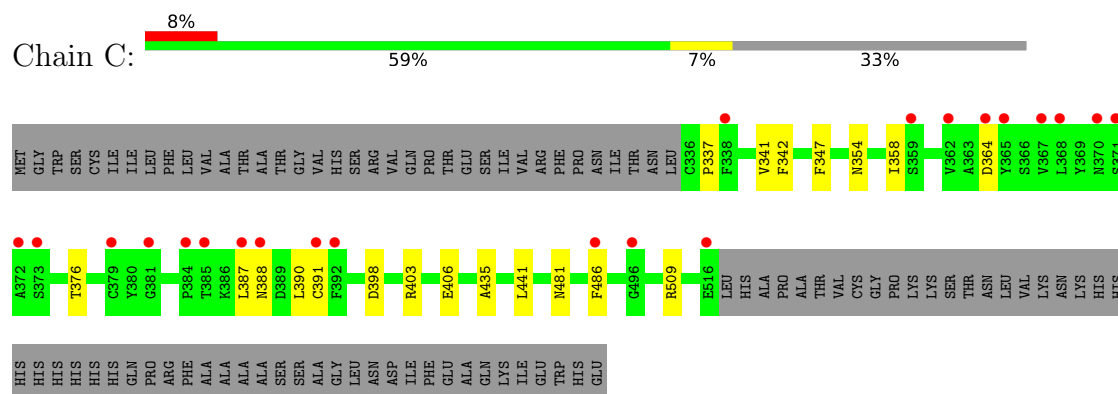
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	42	Total	O	0	0
			42	42		
5	A	57	Total	O	0	0
			57	57		
5	B	58	Total	O	0	0
			58	58		

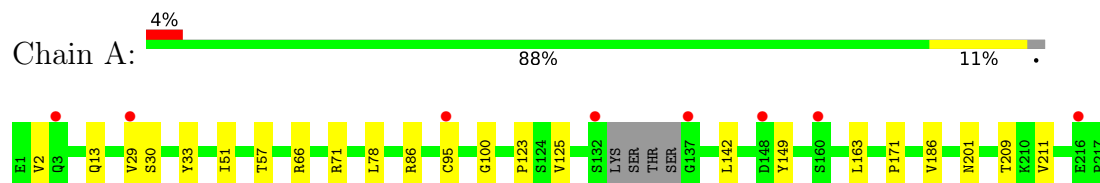
3 Residue-property plots [i](#)

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.

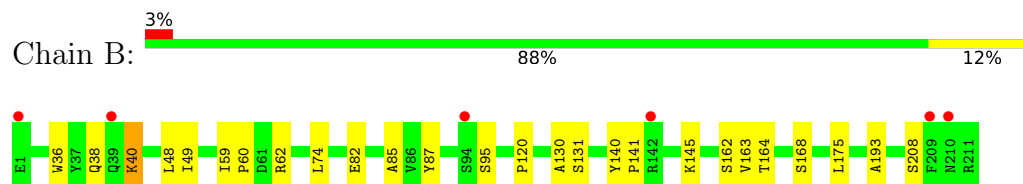
• Molecule 1: Spike protein S1



• Molecule 2: H chain of P5-1C8 Fab



• Molecule 3: L chain of P5-1C8 Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 115.09Å 144.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.44 – 2.39 53.44 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.2 (53.44-2.39) 91.2 (53.44-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.236 , 0.283 0.235 , 0.280	Depositor DCC
R_{free} test set	1686 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4782	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	C	0.24	0/1452	0.45	0/1976
2	A	0.28	0/1625	0.43	0/2217
3	B	0.35	0/1647	0.55	1/2236 (0.0%)
All	All	0.30	0/4724	0.48	1/6429 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	164	THR	N-CA-C	5.65	118.42	110.23

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	C	1412	0	1309	10	0
2	A	1587	0	1530	12	0
3	B	1612	0	1573	19	0
4	C	14	0	13	1	0
5	A	57	0	0	0	0
5	B	58	0	0	0	0
5	C	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4782	0	4425	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 4.

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)
3:B:38:GLN:HB2	3:B:48:LEU:HD11	1.72	0.71
3:B:163:VAL:HG22	3:B:175:LEU:HD12	1.84	0.60
2:A:51:ILE:HD13	2:A:57:THR:HG22	1.88	0.55
1:C:387:LEU:HA	1:C:390:LEU:HD23	1.89	0.54
3:B:60:PRO:HB2	3:B:62:ARG:HG2	1.91	0.53
2:A:163:LEU:HD21	2:A:186:VAL:HG21	1.89	0.52
3:B:48:LEU:HA	3:B:59:ILE:HG13	1.91	0.52
1:C:364:ASP:HA	1:C:388:ASN:HD21	1.74	0.52
2:A:29:VAL:HG21	2:A:78:LEU:HB2	1.92	0.52
1:C:486:PHE:CZ	2:A:2:VAL:HG21	2.45	0.52
3:B:36:TRP:HB2	3:B:49:ILE:HB	1.94	0.50
3:B:38:GLN:CB	3:B:48:LEU:HD11	2.41	0.50
1:C:337:PRO:HD2	1:C:358:ILE:HD12	1.95	0.49
3:B:38:GLN:HB3	3:B:48:LEU:HD21	1.93	0.49
1:C:342:PHE:HB2	4:C:601:NAG:H82	1.94	0.48
3:B:193:ALA:HB2	3:B:208:SER:HB3	1.95	0.48
1:C:376:THR:HB	1:C:435:ALA:HB3	1.96	0.47
1:C:347:PHE:CD2	1:C:509:ARG:HG2	2.50	0.47
2:A:13:GLN:H	2:A:13:GLN:CD	2.23	0.47
3:B:120:PRO:HG3	3:B:130:ALA:HB1	1.96	0.47
3:B:82:GLU:OE2	3:B:168:SER:HB3	2.17	0.45
2:A:171:PRO:HD2	3:B:162:SER:OG	2.16	0.45
3:B:36:TRP:CE2	3:B:74:LEU:HB2	2.52	0.44
1:C:403:ARG:HB2	1:C:406:GLU:HG3	1.99	0.44
1:C:486:PHE:HZ	2:A:2:VAL:HG21	1.82	0.44
2:A:33:TYR:CG	2:A:100:GLY:HA2	2.51	0.44
2:A:30:SER:HA	2:A:71:ARG:HD2	1.99	0.43
3:B:140:TYR:CG	3:B:141:PRO:HA	2.53	0.43
3:B:40:LYS:HD2	3:B:85:ALA:HB2	2.01	0.42
3:B:145:LYS:HE3	3:B:145:LYS:HB2	1.78	0.42
1:C:354:ASN:O	1:C:398:ASP:HA	2.19	0.42
2:A:125:VAL:HB	2:A:211:VAL:HG11	2.02	0.42
3:B:163:VAL:CG2	3:B:175:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:PRO:HB3	2:A:149:TYR:HB3	2.02	0.41
2:A:66:ARG:HD3	2:A:86:ARG:NH2	2.36	0.41
3:B:140:TYR:CD1	3:B:141:PRO:HA	2.56	0.41
3:B:38:GLN:HB2	3:B:87:TYR:CE2	2.57	0.40
3:B:120:PRO:HB3	3:B:131:SER:H	1.85	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	C	179/271 (66%)	170 (95%)	9 (5%)	0	100	100
2	A	209/217 (96%)	205 (98%)	4 (2%)	0	100	100
3	B	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
All	All	597/699 (85%)	579 (97%)	18 (3%)	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	C	147/233 (63%)	143 (97%)	4 (3%)	39	62
2	A	174/182 (96%)	170 (98%)	4 (2%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	181/182 (100%)	179 (99%)	2 (1%)	65	82
All	All	502/597 (84%)	492 (98%)	10 (2%)	48	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	341	VAL
1	C	391	CYS
1	C	441	LEU
1	C	481	ASN
2	A	95	CYS
2	A	142	LEU
2	A	201	ASN
2	A	209	THR
3	B	40	LYS
3	B	95	SER

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

Mol	Chain	Res	Type
1	C	394	ASN
2	A	3	GLN
2	A	196	GLN
3	B	147	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 [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	C	601	1	14,14,15	0.43	0	17,19,21	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	1	0

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	C	181/271 (66%)	0.64	22 (12%) 8 6	13, 25, 59, 98	0
2	A	213/217 (98%)	0.37	8 (3%) 44 40	12, 23, 45, 74	0
3	B	211/211 (100%)	0.25	6 (2%) 55 51	11, 21, 38, 53	0
All	All	605/699 (86%)	0.41	36 (5%) 27 24	11, 23, 50, 98	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	496	GLY	5.3
2	A	132	SER	4.8
1	C	371	SER	4.5
1	C	385	THR	4.5
2	A	137	GLY	4.1
1	C	372	ALA	4.1
2	A	148	ASP	4.0
1	C	381	GLY	3.3
1	C	516	GLU	3.3
1	C	365	TYR	3.3
1	C	370	ASN	3.2
1	C	392	PHE	3.2
1	C	486	PHE	3.2
3	B	1	GLU	3.0
1	C	367	VAL	2.9
3	B	39	GLN	2.9
1	C	362	VAL	2.9
1	C	387	LEU	2.8
1	C	368	LEU	2.5
1	C	388	ASN	2.5
1	C	359	SER	2.4
1	C	364	ASP	2.4
3	B	209	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	160	SER	2.4
3	B	94	SER	2.4
2	A	3	GLN	2.2
1	C	338	PHE	2.2
2	A	29	VAL	2.2
1	C	379	CYS	2.2
2	A	95	CYS	2.2
3	B	210	ASN	2.1
2	A	216	GLU	2.1
1	C	373	SER	2.1
3	B	142	ARG	2.1
1	C	384	PRO	2.1
1	C	391	CYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	601	14/15	0.78	0.16	36,59,75,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.