



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 9SSM / pdb_00009ssm
Title : Crystal structure of 084-7D Fab bound to SARS-CoV-2 Beta RBD
Authors : Ayres, F.; Moyo-Gwete, T.; Wibmer, C.K.
Deposited on : 2025-09-26
Resolution : 2.70 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

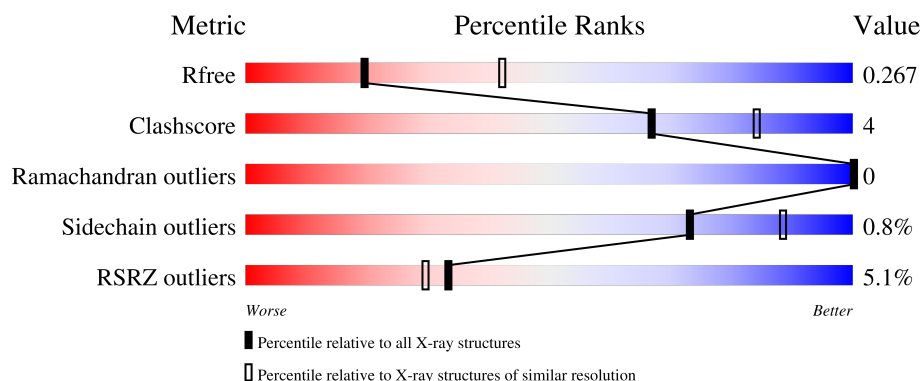
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	H	230	<div> <div>10%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
2	K	214	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
3	R	249	<div> <div>10%</div> <div>71%</div> <div>6%</div> <div>23%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9014 atoms, of which 4297 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 084-7D Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	221	Total	C	H	N	O	S	0	1	0
			3061	996	1482	264	313	6			

- Molecule 2 is a protein called 084-7D Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	K	214	Total	C	H	N	O	S	0	2	0
			3145	1009	1526	269	335	6			

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	R	191	Total	C	H	N	O	S	0	0	0
			2717	925	1277	237	270	8			

There are 28 discrepancies between the modelled and reference sequences:

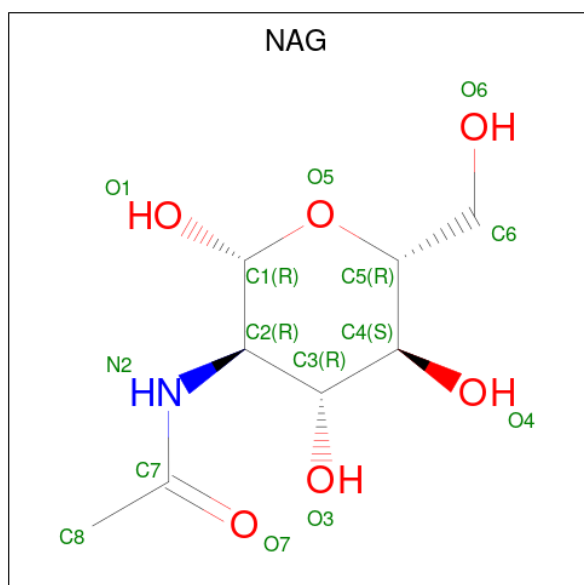
Chain	Residue	Modelled	Actual	Comment	Reference
R	542	GLY	-	expression tag	UNP A0A8A5XRG7
R	543	GLY	-	expression tag	UNP A0A8A5XRG7
R	544	PRO	-	expression tag	UNP A0A8A5XRG7
R	545	GLY	-	expression tag	UNP A0A8A5XRG7
R	546	HIS	-	expression tag	UNP A0A8A5XRG7
R	547	HIS	-	expression tag	UNP A0A8A5XRG7
R	548	HIS	-	expression tag	UNP A0A8A5XRG7
R	549	HIS	-	expression tag	UNP A0A8A5XRG7
R	550	HIS	-	expression tag	UNP A0A8A5XRG7
R	551	HIS	-	expression tag	UNP A0A8A5XRG7
R	552	HIS	-	expression tag	UNP A0A8A5XRG7
R	553	HIS	-	expression tag	UNP A0A8A5XRG7
R	554	GLY	-	expression tag	UNP A0A8A5XRG7
R	555	GLY	-	expression tag	UNP A0A8A5XRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	556	LEU	-	expression tag	UNP A0A8A5XRG7
R	557	ASN	-	expression tag	UNP A0A8A5XRG7
R	558	ASP	-	expression tag	UNP A0A8A5XRG7
R	559	ILE	-	expression tag	UNP A0A8A5XRG7
R	560	PHE	-	expression tag	UNP A0A8A5XRG7
R	561	GLU	-	expression tag	UNP A0A8A5XRG7
R	562	ALA	-	expression tag	UNP A0A8A5XRG7
R	563	GLN	-	expression tag	UNP A0A8A5XRG7
R	564	LYS	-	expression tag	UNP A0A8A5XRG7
R	565	ILE	-	expression tag	UNP A0A8A5XRG7
R	566	GLU	-	expression tag	UNP A0A8A5XRG7
R	567	TRP	-	expression tag	UNP A0A8A5XRG7
R	568	HIS	-	expression tag	UNP A0A8A5XRG7
R	569	GLU	-	expression tag	UNP A0A8A5XRG7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	R	1	Total	C	H	N	O	0	0
			26	8	12	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	24	Total	O	0	0
			24	24		

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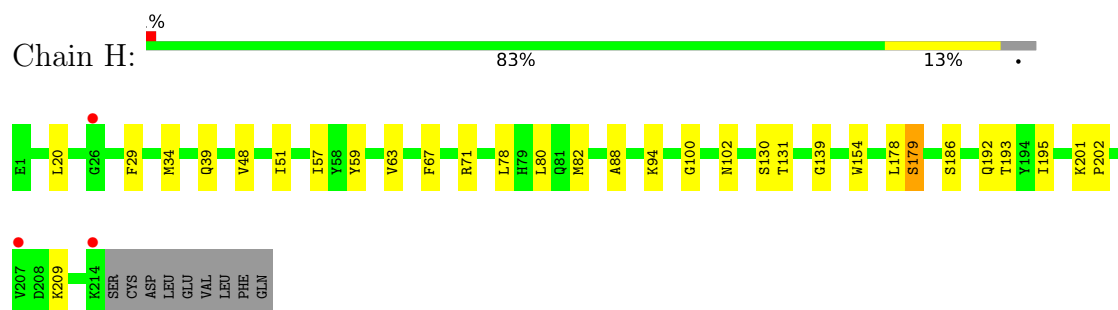
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	22	Total	O	0	0
			22	22		
5	R	19	Total	O	0	0
			19	19		

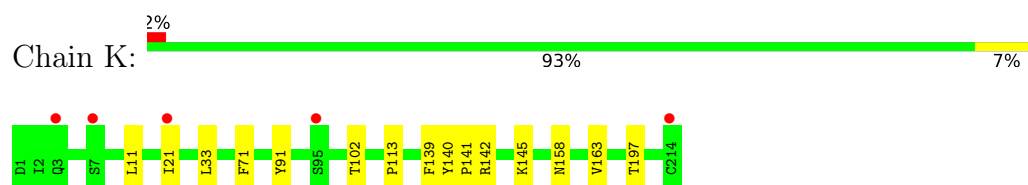
3 Residue-property plots [i](#)

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.

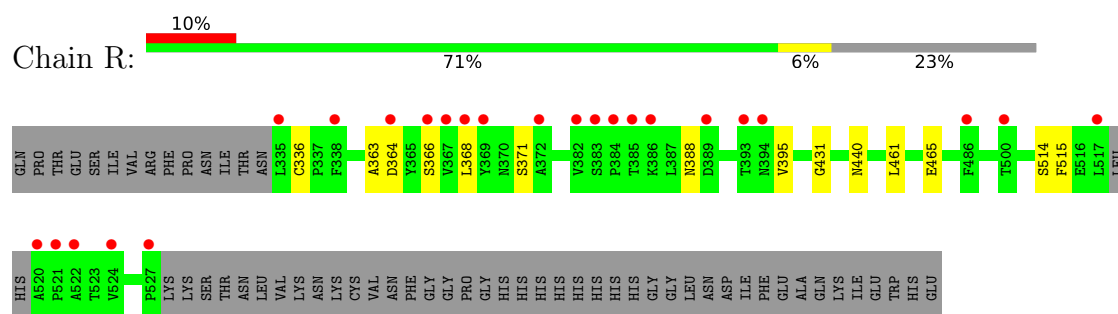
- Molecule 1: 084-7D Fab Heavy Chain



- Molecule 2: 084-7D Fab Light Chain



- Molecule 3: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.45Å 84.37Å 126.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.70) 89.3 (50.00-2.70)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.223 , 0.269 0.222 , 0.267	Depositor DCC
R_{free} test set	1223 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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

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	H	0.27	0/1627	0.45	0/2228
2	K	0.28	0/1654	0.45	0/2253
3	R	0.28	0/1482	0.43	0/2026
All	All	0.28	0/4763	0.44	0/6507

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

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	H	1579	1482	1469	18	0
2	K	1619	1526	1524	8	0
3	R	1440	1277	1264	8	0
4	R	14	12	13	0	0
5	H	24	0	0	0	0
5	K	22	0	0	0	0
5	R	19	0	0	0	0
All	All	4717	4297	4270	33	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 (33) 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:H:57:ILE:O	1:H:57:ILE:HD12	1.86	0.73
1:H:178:LEU:HD12	1:H:179:SER:N	2.14	0.62
3:R:336:CYS:HB2	3:R:363:ALA:HB2	1.82	0.61
3:R:440:ASN:N	3:R:440:ASN:OD1	2.35	0.58
1:H:57:ILE:HD13	1:H:59:TYR:CE2	2.39	0.58
1:H:29:PHE:O	1:H:71:ARG:NH2	2.37	0.57
2:K:33:LEU:HD22	2:K:71:PHE:CG	2.40	0.56
1:H:94:LYS:HB3	1:H:102:ASN:HB2	1.89	0.55
2:K:21:ILE:HG12	2:K:102:THR:HG21	1.90	0.53
1:H:48:VAL:HG13	1:H:63:VAL:HG21	1.91	0.52
3:R:368:LEU:HD12	3:R:371:SER:OG	2.11	0.51
1:H:67:PHE:HB3	1:H:80:LEU:HD11	1.94	0.49
1:H:57:ILE:HD13	1:H:59:TYR:HE2	1.75	0.49
1:H:20:LEU:HG	1:H:82:MET:HE2	1.95	0.49
3:R:364:ASP:HA	3:R:388:ASN:OD1	2.13	0.48
1:H:100:GLY:HA3	2:K:91:TYR:CD1	2.48	0.48
3:R:395:VAL:HG22	3:R:515:PHE:HD1	1.78	0.48
2:K:113:PRO:HB3	2:K:139:PHE:HB3	1.98	0.46
3:R:366:SER:H	3:R:388:ASN:HD21	1.63	0.45
2:K:140:TYR:CG	2:K:141:PRO:HA	2.51	0.45
3:R:431:GLY:HA2	3:R:515:PHE:CE2	2.51	0.45
1:H:34:MET:HB3	1:H:78:LEU:HD22	2.00	0.44
3:R:461:LEU:HD22	3:R:465:GLU:HB3	1.99	0.43
1:H:192:GLN:OE1	1:H:193:THR:N	2.52	0.43
1:H:131:THR:HB	1:H:186:SER:OG	2.19	0.42
2:K:142:ARG:CZ	2:K:163:VAL:HG11	2.51	0.41
1:H:139:GLY:HA2	1:H:154:TRP:CZ2	2.56	0.41
1:H:34:MET:O	1:H:51:ILE:HG22	2.21	0.40
1:H:39:GLN:O	1:H:88:ALA:HB1	2.21	0.40
1:H:201:LYS:N	1:H:202:PRO:CD	2.84	0.40
2:K:158:ASN:OD1	2:K:158:ASN:N	2.53	0.40
1:H:195:ILE:HG23	1:H:209:LYS:O	2.21	0.40
2:K:145:LYS:HB3	2:K:197:THR:HB	2.04	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	H	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
2	K	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
3	R	187/249 (75%)	179 (96%)	8 (4%)	0	100	100
All	All	619/693 (89%)	598 (97%)	21 (3%)	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	H	168/192 (88%)	166 (99%)	2 (1%)	63	84
2	K	182/188 (97%)	181 (100%)	1 (0%)	81	92
3	R	140/216 (65%)	139 (99%)	1 (1%)	76	90
All	All	490/596 (82%)	486 (99%)	4 (1%)	73	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	130	SER
1	H	179	SER
2	K	11	LEU
3	R	514	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	76	ASN
1	H	164	HIS
2	K	79	GLN
2	K	138	ASN
2	K	147	GLN
2	K	199	GLN
2	K	210	ASN
3	R	394	ASN
3	R	498	GLN

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](#)

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	R	601	3	14,14,15	1.01	1 (7%)	17,19,21	0.84	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	R	601	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	601	NAG	C1-C2	2.99	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	601	NAG	O5-C5-C6-O6
4	R	601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	H	221/230 (96%)	0.43	3 (1%) 73 72	42, 53, 65, 74	0
2	K	214/214 (100%)	0.35	5 (2%) 61 58	38, 50, 61, 72	0
3	R	191/249 (76%)	0.91	24 (12%) 8 7	44, 60, 85, 93	0
All	All	626/693 (90%)	0.55	32 (5%) 33 29	38, 53, 77, 93	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	517	LEU	5.5
3	R	372	ALA	4.6
2	K	7	SER	4.4
3	R	385	THR	4.2
3	R	335	LEU	4.0
3	R	389	ASP	3.4
3	R	524	VAL	3.3
3	R	367	VAL	3.2
3	R	364	ASP	3.2
1	H	207	VAL	3.1
3	R	521	PRO	3.0
3	R	382	VAL	3.0
3	R	369	TYR	2.9
3	R	384	PRO	2.8
1	H	214	LYS	2.8
3	R	368	LEU	2.7
2	K	95	SER	2.6
3	R	366	SER	2.5
3	R	383	SER	2.5
2	K	3	GLN	2.4
3	R	522	ALA	2.4
3	R	486	PHE	2.3
3	R	338	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	21	ILE	2.3
2	K	214	CYS	2.2
3	R	500	THR	2.2
3	R	386	LYS	2.1
1	H	26	GLY	2.1
3	R	520	ALA	2.1
3	R	393	THR	2.0
3	R	394	ASN	2.0
3	R	527	PRO	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(\AA^2)	Q<0.9
4	NAG	R	601	14/15	0.46	0.21	44,73,83,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.