



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2025 – 02:13 PM JST

PDB ID : 8YDK / pdb\_00008ydk  
Title : Crystal structure of a novel design for RSV F protein in pre-fusion state  
Authors : Qi, J.X.; Li, J.  
Deposited on : 2024-02-20  
Resolution : 2.10 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

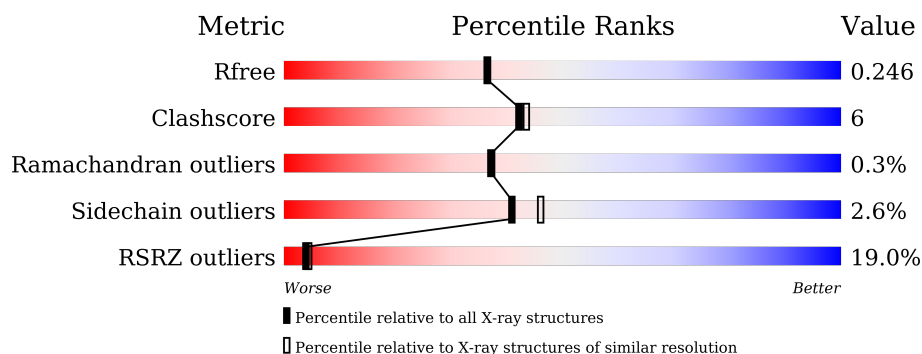
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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  $\geq 3$ , 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	249	<div> <div>19%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>.</div> <div>.</div> </div> </div>
1	B	249	<div> <div>15%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	249	<div> <div>21%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5831 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 Fusion glycoprotein F2, F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	2	0
			1867	1183	308	365	11			
1	B	240	Total	C	N	O	S	0	1	0
			1867	1183	308	367	9			
1	C	240	Total	C	N	O	S	0	3	0
			1872	1186	309	366	11			

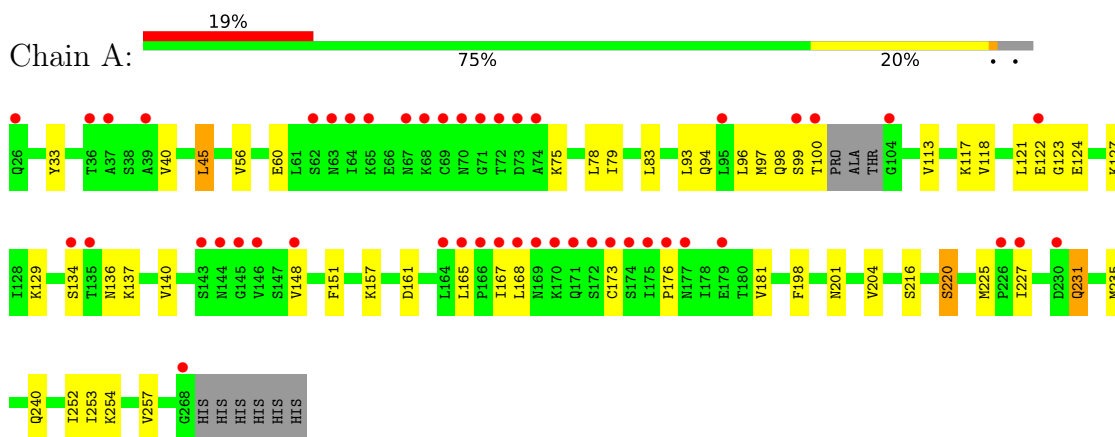
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total	O	0	0
			47	47		
2	B	99	Total	O	0	0
			99	99		
2	C	79	Total	O	0	0
			79	79		

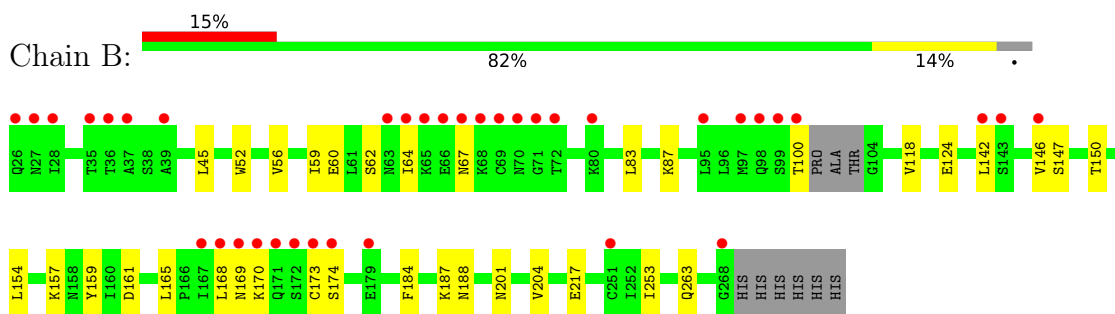
### 3 Residue-property plots [i](#)

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.

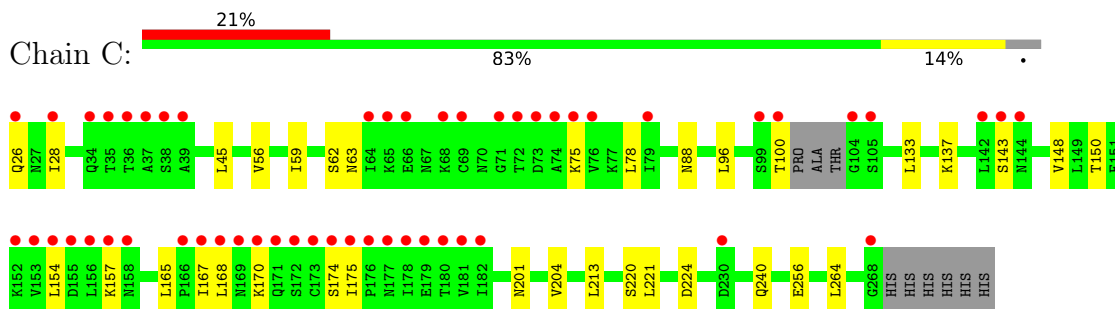
- Molecule 1: Fusion glycoprotein F2, F1



- Molecule 1: Fusion glycoprotein F2, F1



- Molecule 1: Fusion glycoprotein F2, F1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.24Å 64.91Å 109.94Å 90.00° 130.28° 90.00°	Depositor
Resolution (Å)	32.76 – 2.10 32.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (32.76-2.10) 92.6 (32.76-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.220 , 0.246 0.220 , 0.246	Depositor DCC
$R_{free}$ test set	2248 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.15	0/1892	0.37	0/2560
1	B	0.15	0/1889	0.35	0/2556
1	C	0.21	1/1900 (0.1%)	0.39	0/2571
All	All	0.17	1/5681 (0.0%)	0.37	0/7687

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	ASN	C-O	-5.40	1.17	1.24

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	1867	0	1943	35	0
1	B	1867	0	1941	17	0
1	C	1872	0	1949	22	0
2	A	47	0	0	1	0
2	B	99	0	0	1	0
2	C	79	0	0	2	0
All	All	5831	0	5833	71	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 6.

All (71) 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:134:SER:OG	1:B:67:ASN:ND2	2.09	0.85
1:C:26:GLN:N	2:C:301:HOH:O	2.22	0.72
1:A:122:GLU:OE1	1:A:254:LYS:NZ	2.23	0.71
1:A:167:ILE:HG22	1:A:168:LEU:HG	1.74	0.70
1:A:93:LEU:HB2	1:A:253:ILE:HD11	1.78	0.65
1:A:60:GLU:HG3	1:A:157:LYS:HB3	1.79	0.64
1:C:137:LYS:HE3	1:C:224:ASP:OD2	1.97	0.64
1:C:221:LEU:HD23	1:C:264:LEU:HD11	1.80	0.64
1:A:161:ASP:HA	1:A:165:LEU:HG	1.80	0.63
1:C:137:LYS:NZ	1:C:220:SER:OG	2.30	0.63
1:A:75:LYS:HA	1:A:78:LEU:HD12	1.82	0.61
1:C:174:SER:OG	1:C:175:ILE:N	2.34	0.61
1:C:240:GLN:H	1:C:240:GLN:CD	2.08	0.60
1:A:40:VAL:HG11	1:A:45:LEU:HG	1.85	0.59
1:C:170:LYS:NZ	1:C:174:SER:HB2	2.19	0.56
1:C:213:LEU:HD21	1:C:221:LEU:HD22	1.87	0.56
1:A:127:LYS:HE3	1:A:140:VAL:HG13	1.88	0.55
1:A:94:GLN:O	1:A:98:GLN:NE2	2.39	0.55
1:A:56:VAL:HG23	1:A:148:VAL:HG11	1.88	0.55
1:C:63:ASN:HB2	1:C:256:GLU:HG2	1.89	0.55
1:A:225:MET:HE1	1:A:235:MET:HE1	1.89	0.54
1:A:79:ILE:HG12	1:A:181:VAL:HG22	1.89	0.53
1:A:93:LEU:CB	1:A:253:ILE:HD11	2.38	0.53
1:C:56:VAL:HG23	1:C:148:VAL:HG11	1.90	0.53
1:A:118:VAL:O	1:A:124:GLU:HG3	2.09	0.53
1:C:75:LYS:HA	1:C:78:LEU:HD12	1.91	0.52
1:C:62:SER:OG	1:C:157:LYS:HA	2.09	0.52
1:B:64:ILE:HD11	1:B:168:LEU:HD11	1.92	0.51
1:A:113:VAL:O	1:A:117:LYS:HG2	2.11	0.51
1:A:136:ASN:OD1	1:A:137:LYS:HE3	2.12	0.50
1:B:161:ASP:HA	1:B:165:LEU:HD12	1.94	0.50
1:B:56:VAL:HB	1:B:150:THR:HG22	1.95	0.49
1:B:159:TYR:OH	1:B:184:PHE:HB2	2.13	0.49
1:C:59:ILE:HG23	1:C:154:LEU:HB3	1.94	0.49
1:C:143:SER:HB2	2:C:336:HOH:O	2.13	0.48
1:B:62:SER:HB2	1:B:157:LYS:HA	1.95	0.48
1:B:64:ILE:O	1:B:87:LYS:HD3	2.14	0.47
1:C:167:ILE:HG22	1:C:168:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLN:NE2	2:A:303:HOH:O	2.37	0.46
1:C:167:ILE:O	1:C:174:SER:HB3	2.16	0.46
1:B:187:LYS:HE2	2:B:311:HOH:O	2.16	0.45
1:A:96:LEU:CD2	1:A:198:PHE:HB3	2.46	0.45
1:A:75:LYS:HD2	1:A:176:PRO:O	2.16	0.44
1:A:227:ILE:HD12	1:A:231:GLN:HB3	1.98	0.44
1:B:184:PHE:O	1:B:188:ASN:HB2	2.18	0.44
1:C:170:LYS:HZ2	1:C:174:SER:HB2	1.81	0.44
1:C:201:ASN:HB3	1:C:204:VAL:O	2.18	0.44
1:B:59:ILE:HG23	1:B:154:LEU:HB3	1.99	0.43
1:B:217:GLU:HA	1:C:133:LEU:HD21	1.99	0.43
1:C:137:LYS:HA	1:C:150:THR:O	2.18	0.43
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.86	0.43
1:A:33:TYR:N	1:A:40:VAL:O	2.49	0.43
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.88	0.43
1:B:52:TRP:CE3	1:B:263:GLN:HG2	2.54	0.42
1:C:28:ILE:O	1:C:28:ILE:HG12	2.18	0.42
1:A:127:LYS:HA	1:A:127:LYS:HD2	1.92	0.42
1:B:118:VAL:O	1:B:124:GLU:HG3	2.19	0.42
1:A:99:SER:O	1:A:100:THR:OG1	2.28	0.42
1:A:122:GLU:OE2	1:A:123:GLY:N	2.52	0.42
1:A:97:MET:CE	1:A:252:ILE:HG13	2.50	0.42
1:A:201:ASN:HB3	1:A:204:VAL:O	2.19	0.42
1:A:216:SER:O	1:A:220:SER:OG	2.38	0.41
1:A:121:LEU:O	1:A:124:GLU:HG2	2.20	0.41
1:C:170:LYS:HZ3	1:C:174:SER:HB2	1.84	0.41
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.86	0.41
1:A:134:SER:HG	1:B:67:ASN:ND2	2.16	0.41
1:A:129:LYS:HE2	1:A:257:VAL:HG23	2.02	0.41
1:A:129:LYS:HE2	1:A:257:VAL:CG2	2.51	0.41
1:B:201:ASN:HB3	1:B:204:VAL:O	2.20	0.41
1:A:137:LYS:HG2	1:A:151:PHE:CZ	2.57	0.40
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.98	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	238/249 (96%)	234 (98%)	4 (2%)	0	100	100
1	B	237/249 (95%)	227 (96%)	8 (3%)	2 (1%)	16	13
1	C	239/249 (96%)	227 (95%)	12 (5%)	0	100	100
All	All	714/747 (96%)	688 (96%)	24 (3%)	2 (0%)	37	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	ASN
1	B	170	LYS

### 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	220/226 (97%)	216 (98%)	4 (2%)	54	61
1	B	219/226 (97%)	209 (95%)	10 (5%)	23	23
1	C	221/226 (98%)	217 (98%)	4 (2%)	54	61
All	All	660/678 (97%)	642 (97%)	18 (3%)	41	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	173	CYS
1	A	220	SER
1	A	231	GLN
1	B	60[A]	GLU
1	B	60[B]	GLU
1	B	83	LEU
1	B	100	THR
1	B	142	LEU
1	B	146	VAL
1	B	147	SER
1	B	173	CYS
1	B	174	SER
1	B	253	ILE
1	C	45	LEU
1	C	96	LEU
1	C	100	THR
1	C	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	223	ASN
1	B	67	ASN
1	B	126	ASN
1	B	158	ASN
1	B	177	ASN
1	B	229	ASN
1	B	245	GLN
1	C	27	ASN
1	C	67	ASN
1	C	186	GLN
1	C	223	ASN
1	C	245	GLN

### 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 oligosaccharides 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	240/249 (96%)	0.78	47 (19%) 4 4	15, 38, 112, 159	2 (0%)
1	B	240/249 (96%)	0.63	37 (15%) 6 7	14, 28, 100, 173	1 (0%)
1	C	240/249 (96%)	0.97	53 (22%) 3 3	12, 29, 134, 217	3 (1%)
All	All	720/747 (96%)	0.80	137 (19%) 4 4	12, 31, 118, 217	6 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	THR	10.4
1	C	37	ALA	8.1
1	C	38	SER	7.9
1	C	64	ILE	6.9
1	C	36	THR	6.6
1	C	99	SER	6.5
1	C	268	GLY	6.3
1	C	176	PRO	6.0
1	C	104	GLY	5.7
1	C	175	ILE	5.7
1	A	146	VAL	5.6
1	B	68	LYS	5.5
1	B	65	LYS	5.4
1	C	177	ASN	5.4
1	B	170	LYS	5.0
1	C	143	SER	5.0
1	A	100	THR	5.0
1	C	178	ILE	4.8
1	C	144	ASN	4.8
1	A	72	THR	4.7
1	C	100	THR	4.6
1	C	73	ASP	4.5
1	B	173	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	37	ALA	4.4
1	A	70	ASN	4.4
1	C	173	CYS	4.3
1	A	69	CYS	4.2
1	B	69	CYS	4.1
1	A	99	SER	4.1
1	B	70	ASN	4.1
1	B	171	GLN	4.1
1	A	166	PRO	4.0
1	A	268	GLY	4.0
1	A	173	CYS	3.9
1	C	34	GLN	3.8
1	B	100	THR	3.8
1	C	171	GLN	3.8
1	B	268	GLY	3.7
1	C	72	THR	3.6
1	C	76	VAL	3.6
1	C	167	ILE	3.6
1	B	168	LEU	3.6
1	A	143	SER	3.6
1	C	68	LYS	3.5
1	C	75	LYS	3.5
1	A	64	ILE	3.5
1	B	36	THR	3.5
1	C	180	THR	3.5
1	B	143	SER	3.5
1	C	169	ASN	3.5
1	B	169	ASN	3.4
1	A	39	ALA	3.4
1	C	105	SER	3.4
1	A	172	SER	3.4
1	B	27	ASN	3.4
1	B	28	ILE	3.4
1	B	67	ASN	3.3
1	A	174	SER	3.3
1	B	174	SER	3.3
1	C	179	GLU	3.3
1	C	182	ILE	3.3
1	C	174	SER	3.3
1	A	68	LYS	3.2
1	B	26	GLN	3.2
1	A	144	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	VAL	3.1
1	A	104	GLY	3.1
1	C	65	LYS	3.1
1	C	66	GLU	3.1
1	C	170	LYS	3.1
1	C	166	PRO	3.1
1	B	71	GLY	3.1
1	A	175	ILE	3.1
1	C	152	LYS	3.1
1	C	69	CYS	3.0
1	C	155	ASP	3.0
1	B	179	GLU	3.0
1	A	169	ASN	2.9
1	A	145	GLY	2.9
1	C	168	LEU	2.9
1	B	39	ALA	2.9
1	B	64	ILE	2.8
1	A	65	LYS	2.8
1	B	142	LEU	2.8
1	C	172	SER	2.8
1	B	66	GLU	2.8
1	C	157	LYS	2.7
1	B	72	THR	2.7
1	A	73	ASP	2.7
1	B	63	ASN	2.6
1	A	37	ALA	2.6
1	B	99	SER	2.6
1	B	146	VAL	2.6
1	B	98	GLN	2.6
1	C	28	ILE	2.6
1	C	79	ILE	2.6
1	B	167	ILE	2.5
1	A	71	GLY	2.5
1	A	135	THR	2.5
1	C	74	ALA	2.5
1	A	26	GLN	2.5
1	C	26	GLN	2.5
1	A	164	LEU	2.4
1	C	230	ASP	2.4
1	B	35	THR	2.4
1	A	148	VAL	2.4
1	C	142	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	63	ASN	2.4
1	A	170	LYS	2.4
1	A	227	ILE	2.4
1	C	158	ASN	2.3
1	A	36	THR	2.3
1	B	172	SER	2.3
1	A	165	LEU	2.3
1	A	176	PRO	2.3
1	A	230	ASP	2.3
1	A	167	ILE	2.2
1	A	177	ASN	2.2
1	B	97	MET	2.2
1	A	171	GLN	2.2
1	C	39	ALA	2.2
1	A	67	ASN	2.2
1	A	179	GLU	2.1
1	A	95	LEU	2.1
1	A	168	LEU	2.1
1	A	134	SER	2.1
1	C	181	VAL	2.1
1	C	71	GLY	2.1
1	A	62	SER	2.1
1	C	154	LEU	2.1
1	C	156	LEU	2.1
1	A	74	ALA	2.0
1	A	122	GLU	2.0
1	B	80	LYS	2.0
1	B	95	LEU	2.0
1	A	226	PRO	2.0
1	B	251	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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.