Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 04:11 PM EDT

PDB ID	:	8DTR
Title	:	Crystal structure of SARS-CoV-2 spike stem helix peptide in complex with neutralizing antibody COV30-14
Authors	:	Lee, C.C.D.; Lin, T.H.; Wilson, I.A.
Deposited on	:	2022-07-26
Resolution	:	1.50 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:

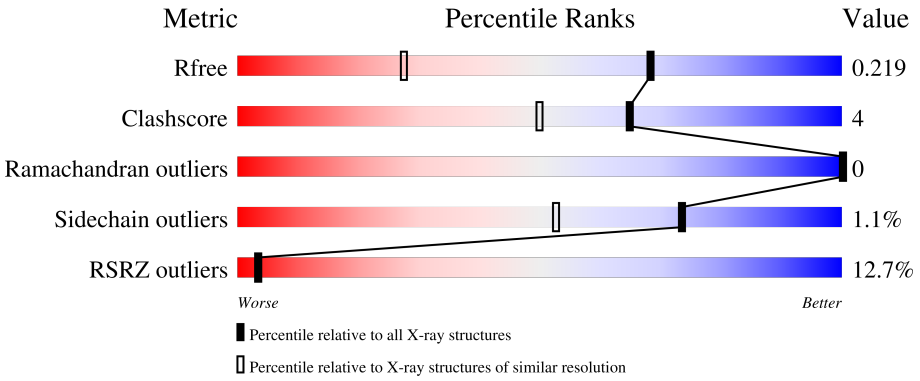
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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.



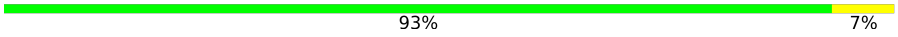
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	221	5% 85% 9% 6%
1	E	221	10% 87% 8%
2	B	217	3% 95%
2	F	217	34% 86% 13%
3	G	15	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	15	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7812 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 COV30-14 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1546	975	257	305	9			
1	E	213	Total	C	N	O	S	0	0	0
			1594	1005	263	317	9			

- Molecule 2 is a protein called COV30-14 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1667	1043	285	334	5			
2	F	216	Total	C	N	O	S	0	0	0
			1667	1043	285	334	5			

- Molecule 3 is a protein called Spike protein S2' stem helix peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	15	Total	C	N	O	0	0	0
			135	88	21	26			
3	J	15	Total	C	N	O	0	0	0
			135	88	21	26			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total	O	0	0
			299	299		
4	B	330	Total	O	0	0
			330	330		
4	G	19	Total	O	0	0
			19	19		
4	E	234	Total	O	0	0
			234	234		

Continued on next page...

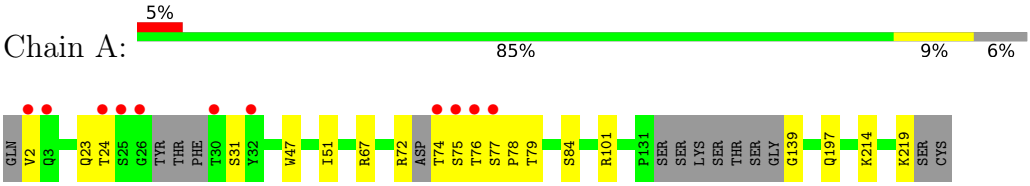
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	170	Total O 170 170	0	0
4	J	16	Total O 16 16	0	0

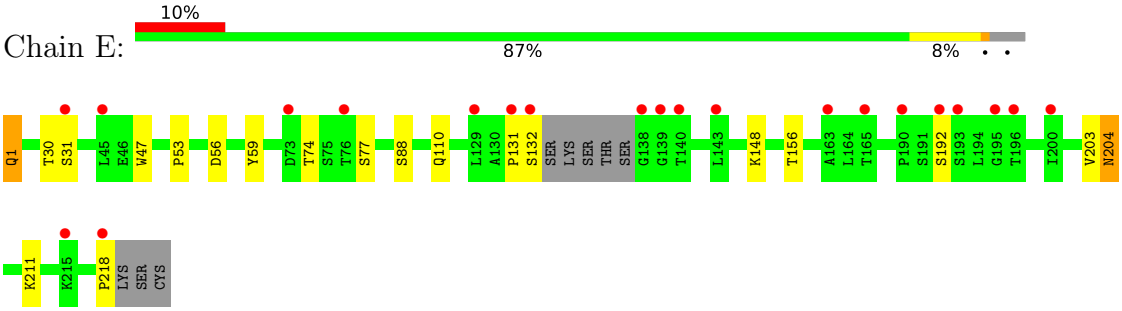
3 Residue-property plots (i)

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.

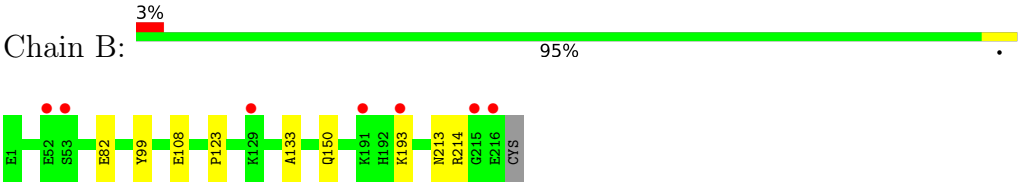
• Molecule 1: COV30-14 heavy chain



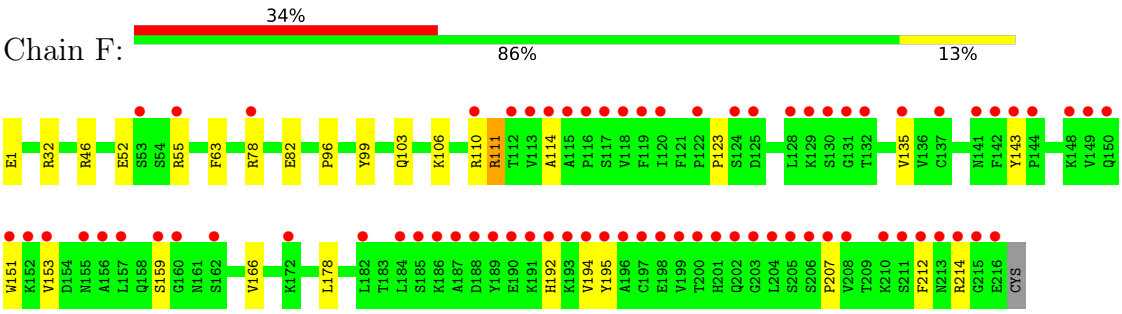
• Molecule 1: COV30-14 heavy chain



• Molecule 2: COV30-14 light chain



• Molecule 2: COV30-14 light chain



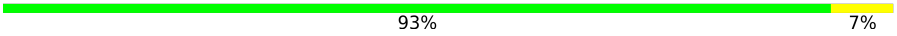
• Molecule 3: Spike protein S2' stem helix peptide

Chain G:

There are no outlier residues recorded for this chain.

• Molecule 3: Spike protein S2' stem helix peptide

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.36Å 83.21Å 170.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 1.50 46.91 – 1.50	Depositor EDS
% Data completeness (in resolution range)	80.5 (46.91-1.50) 80.5 (46.91-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.198 , 0.222 0.196 , 0.219	Depositor DCC
R_{free} test set	6790 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7812	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 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.35	0/1581	0.58	0/2152
1	E	0.36	0/1633	0.58	0/2227
2	B	0.40	0/1705	0.65	0/2315
2	F	0.34	0/1705	0.59	0/2315
3	G	0.35	0/138	0.57	0/182
3	J	0.33	0/138	0.47	0/182
All	All	0.36	0/6900	0.60	0/9373

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	A	1546	0	1515	14	0
1	E	1594	0	1552	14	1
2	B	1667	0	1617	6	0
2	F	1667	0	1617	22	0
3	G	135	0	125	0	0
3	J	135	0	125	1	0
4	A	299	0	0	7	0
4	B	330	0	0	2	3
4	E	234	0	0	5	0
4	F	170	0	0	11	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	19	0	0	0	1
4	J	16	0	0	1	0
All	All	7812	0	6551	54	4

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 (54) 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:E:1:GLN:N	4:E:301:HOH:O	1.86	1.05
2:F:207:PRO:O	4:F:302:HOH:O	2.03	0.74
2:B:82:GLU:OE2	4:B:301:HOH:O	2.08	0.71
1:A:75:SER:O	4:A:901:HOH:O	2.10	0.70
1:E:56:ASP:OD2	4:E:302:HOH:O	2.09	0.70
2:F:212:PHE:O	4:F:303:HOH:O	2.08	0.69
2:F:82:GLU:OE2	4:F:304:HOH:O	2.11	0.68
2:B:150:GLN:NE2	4:B:304:HOH:O	2.29	0.66
2:F:103:GLN:HG2	4:F:365:HOH:O	1.98	0.64
1:A:197:GLN:OE1	4:A:902:HOH:O	2.15	0.64
1:E:132:SER:O	4:E:303:HOH:O	2.15	0.62
2:F:195:TYR:O	4:F:303:HOH:O	2.16	0.61
2:F:46:ARG:NH1	4:F:301:HOH:O	1.97	0.60
1:E:31:SER:HB3	1:E:53:PRO:HB3	1.83	0.59
1:E:148:LYS:HE3	4:F:307:HOH:O	2.01	0.59
2:B:193:LYS:NZ	2:B:214:ARG:O	2.28	0.58
1:A:139:GLY:N	4:A:909:HOH:O	2.38	0.57
1:E:74:THR:H	1:E:77:SER:HB2	1.70	0.55
2:F:106:LYS:NZ	4:F:308:HOH:O	2.40	0.54
1:E:192:SER:O	4:E:304:HOH:O	2.19	0.54
2:F:123:PRO:HD3	2:F:135:VAL:HG22	1.88	0.54
2:F:111:ARG:NH2	2:F:114:ALA:HB2	2.22	0.54
1:A:31:SER:HB3	4:A:908:HOH:O	2.08	0.53
1:A:214:LYS:HD2	4:A:1081:HOH:O	2.10	0.52
1:A:2:VAL:HG13	1:A:24:THR:HG23	1.92	0.52
2:F:135:VAL:HG12	2:F:151:TRP:CH2	2.45	0.52
2:F:195:TYR:N	4:F:306:HOH:O	2.20	0.51
1:E:110:GLN:NE2	4:E:308:HOH:O	2.45	0.50
1:E:47:TRP:CD2	2:F:99:TYR:HB2	2.49	0.48
2:B:193:LYS:HE3	2:B:213:ASN:HB3	1.95	0.48
2:F:1:GLU:OE1	4:F:305:HOH:O	2.19	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:THR:HG23	1:E:31:SER:O	2.15	0.47
1:A:219:LYS:N	4:A:904:HOH:O	2.31	0.47
3:J:1157:LYS:NZ	4:J:1201:HOH:O	2.37	0.46
1:A:23:GLN:CG	1:A:78:PRO:HB3	2.46	0.45
2:F:166:VAL:HG22	2:F:178:LEU:HD12	1.98	0.45
1:A:47:TRP:CD2	2:B:99:TYR:HB2	2.52	0.44
2:F:123:PRO:HD3	2:F:135:VAL:CG2	2.48	0.43
2:F:153:VAL:HA	2:F:194:VAL:O	2.18	0.43
1:E:203:VAL:O	1:E:211:LYS:HD2	2.18	0.43
1:A:67:ARG:HD2	1:A:84:SER:O	2.18	0.43
1:A:51:ILE:HD13	1:A:72:ARG:HG3	2.00	0.42
1:E:131:PRO:HG2	1:E:218:PRO:HG3	2.01	0.42
2:B:123:PRO:HG3	2:B:133:ALA:HB1	2.02	0.42
1:A:72:ARG:HG2	1:A:79:THR:HB	2.00	0.42
1:E:59:TYR:CZ	2:F:96:PRO:HB2	2.55	0.42
2:F:110:ARG:HA	2:F:143:TYR:OH	2.20	0.42
2:F:55:ARG:NE	2:F:63:PHE:O	2.48	0.41
1:A:76:THR:HA	4:A:901:HOH:O	2.21	0.41
1:E:156:THR:OG1	1:E:204:ASN:HB3	2.20	0.41
2:F:192:HIS:O	2:F:214:ARG:NE	2.46	0.40
1:A:74:THR:OG1	1:A:75:SER:N	2.55	0.40
2:F:32:ARG:N	2:F:52:GLU:HG3	2.37	0.40
2:F:212:PHE:O	4:F:306:HOH:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:606:HOH:O	4:F:451:HOH:O[3_454]	1.84	0.36
1:E:1:GLN:OE1	1:E:88:SER:N[3_454]	1.89	0.31
4:B:359:HOH:O	4:G:1214:HOH:O[4_455]	2.15	0.05
4:B:402:HOH:O	4:F:416:HOH:O[3_454]	2.19	0.01

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	199/221 (90%)	197 (99%)	2 (1%)	0	100	100
1	E	209/221 (95%)	208 (100%)	1 (0%)	0	100	100
2	B	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
2	F	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
3	G	13/15 (87%)	13 (100%)	0	0	100	100
3	J	13/15 (87%)	13 (100%)	0	0	100	100
All	All	862/906 (95%)	848 (98%)	14 (2%)	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	175/188 (93%)	173 (99%)	2 (1%)	73	53
1	E	180/188 (96%)	178 (99%)	2 (1%)	73	53
2	B	187/188 (100%)	186 (100%)	1 (0%)	88	78
2	F	187/188 (100%)	184 (98%)	3 (2%)	62	36
3	G	15/15 (100%)	15 (100%)	0	100	100
3	J	15/15 (100%)	15 (100%)	0	100	100
All	All	759/782 (97%)	751 (99%)	8 (1%)	73	53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	101	ARG
2	B	108	GLU
1	E	1	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	204	ASN
2	F	78	ARG
2	F	111	ARG
2	F	159	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1	GLN
1	E	62	GLN
1	E	204	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 monosaccharides 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

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^{th} 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	207/221 (93%)	0.25	11 (5%) 26 29	14, 24, 48, 76	0
1	E	213/221 (96%)	0.64	21 (9%) 7 7	14, 30, 53, 75	0
2	B	216/217 (99%)	0.14	7 (3%) 47 52	13, 20, 39, 66	0
2	F	216/217 (99%)	1.78	73 (33%) 0 0	13, 41, 65, 77	0
3	G	15/15 (100%)	-0.28	0 100 100	18, 23, 37, 39	0
3	J	15/15 (100%)	0.05	0 100 100	20, 30, 42, 47	0
All	All	882/906 (97%)	0.68	112 (12%) 3 3	13, 26, 59, 77	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	208	VAL	11.5
2	F	155	ASN	9.8
2	F	194	VAL	9.8
2	F	128	LEU	9.5
1	A	75	SER	8.7
2	F	184	LEU	8.3
1	E	138	GLY	8.2
2	F	204	LEU	7.2
2	F	205	SER	7.1
2	F	157	LEU	6.3
2	F	196	ALA	6.2
2	F	142	PHE	6.1
2	F	197	CYS	6.1
2	F	189	TYR	6.0
2	F	113	VAL	6.0
1	E	195	GLY	6.0
2	F	144	PRO	5.8
2	F	188	ASP	5.7
2	F	156	ALA	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	195	TYR	5.4
1	A	74	THR	5.3
2	F	216	GLU	5.3
1	E	196	THR	5.2
2	F	151	TRP	5.1
2	F	182	LEU	5.0
2	B	215	GLY	4.9
2	F	213	ASN	4.9
2	F	203	GLY	4.8
2	F	131	GLY	4.4
2	F	191	LYS	4.4
2	F	153	VAL	4.4
1	E	139	GLY	4.3
2	F	212	PHE	4.3
2	F	202	GLN	4.3
2	F	200	THR	4.2
2	F	199	VAL	4.2
2	F	143	TYR	4.2
2	F	207	PRO	4.2
2	F	160	GLY	4.1
2	F	210	LYS	4.0
2	F	187	ALA	4.0
2	F	206	SER	4.0
2	F	119	PHE	3.9
2	F	185	SER	3.9
1	E	163	ALA	3.9
1	A	30	THR	3.8
1	E	31	SER	3.7
1	A	26	GLY	3.7
2	F	186	LYS	3.7
1	E	76	THR	3.6
2	F	112	THR	3.6
1	A	76	THR	3.5
2	F	198	GLU	3.5
1	E	132	SER	3.5
2	F	148	LYS	3.5
2	F	192	HIS	3.5
2	F	150	GLN	3.5
2	F	122	PRO	3.5
1	A	77	SER	3.4
2	F	117	SER	3.4
2	F	132	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	215	GLY	3.4
1	E	193	SER	3.4
1	E	131	PRO	3.3
2	F	149	VAL	3.2
2	F	116	PRO	3.2
2	F	115	ALA	3.2
2	F	214	ARG	3.2
2	B	53	SER	3.1
2	F	114	ALA	3.1
2	F	152	LYS	3.1
2	F	135	VAL	3.0
2	F	159	SER	3.0
1	E	215	LYS	2.9
1	E	165	THR	2.8
2	F	172	LYS	2.8
2	F	110	ARG	2.8
1	A	24	THR	2.7
1	E	190	PRO	2.7
1	A	25	SER	2.7
2	F	193	LYS	2.6
2	F	130	SER	2.6
2	F	55	ARG	2.5
1	E	192	SER	2.5
1	E	218	PRO	2.5
2	F	201	HIS	2.5
1	E	143	LEU	2.4
2	F	129	LYS	2.4
1	E	129	LEU	2.4
2	F	190	GLU	2.4
2	F	118	VAL	2.4
1	E	73	ASP	2.4
1	E	45	LEU	2.3
1	A	2	VAL	2.3
2	B	216	GLU	2.3
2	B	191	LYS	2.3
2	F	137	CYS	2.3
2	F	124	SER	2.2
1	E	140	THR	2.2
2	B	52	GLU	2.2
2	F	211	SER	2.2
2	F	78	ARG	2.2
1	E	200	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	53	SER	2.2
2	F	125	ASP	2.1
2	B	129	LYS	2.1
1	A	3	GLN	2.1
2	F	141	ASN	2.1
2	F	162	SER	2.1
1	A	32	TYR	2.1
2	F	120	ILE	2.0
2	B	193	LYS	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 monosaccharides 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.