



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2025 – 06:11 PM JST

PDB ID : 9JPV / pdb_00009jpv
Title : A Fab Fragment of IgG
Authors : Makabe, K.
Deposited on : 2024-09-26
Resolution : 1.94 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

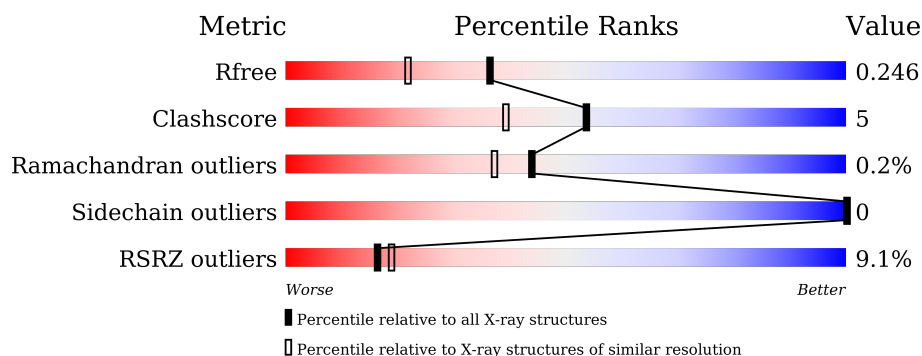
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	222	<div> <div>8%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	222	<div> <div>8%</div> <div>78%</div> <div>13%</div> <div>7%</div> <div>.</div> </div>
2	B	218	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>
2	D	218	<div> <div>17%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6951 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 Fab-VHCH1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1632	1034	268	325	5			
1	C	206	Total	C	N	O	S	0	0	0
			1544	974	256	309	5			

- Molecule 2 is a protein called Fab-CL-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1672	1044	285	337	6			
2	D	214	Total	C	N	O	S	0	1	0
			1653	1032	281	334	6			

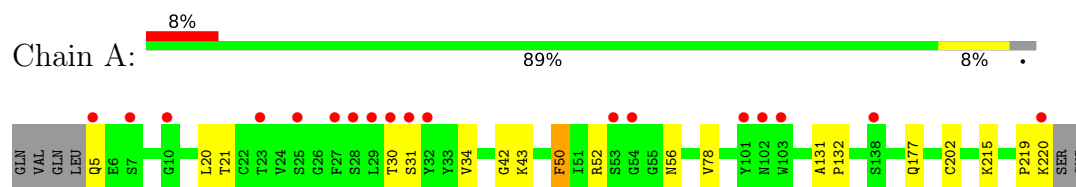
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	162	Total	O	0	0
			162	162		
3	C	84	Total	O	0	0
			84	84		
3	D	97	Total	O	0	0
			97	97		

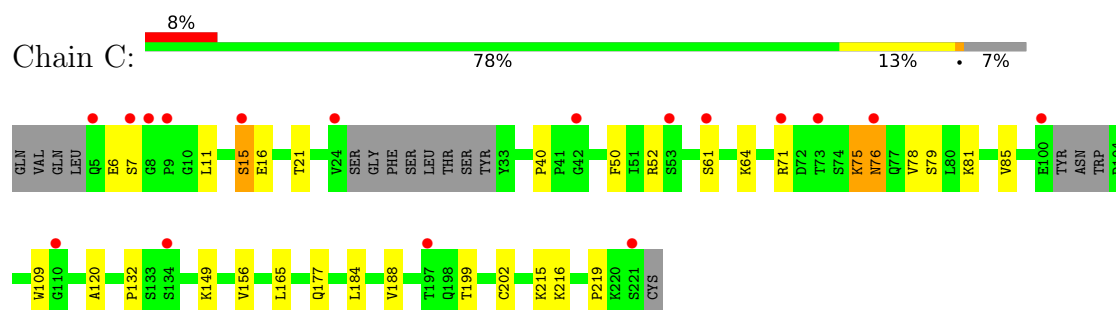
3 Residue-property plots [i](#)

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.

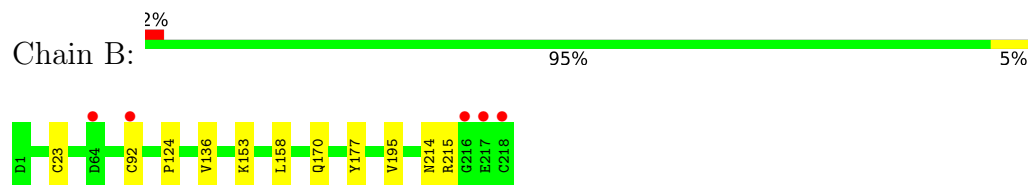
- Molecule 1: Fab-VHCH1-1



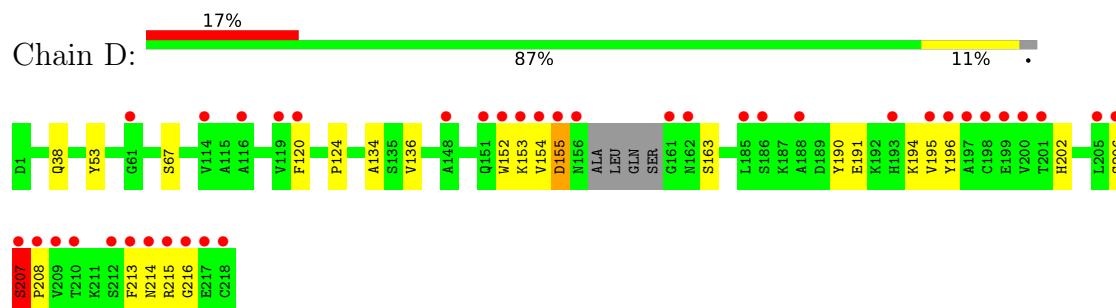
- Molecule 1: Fab-VHCH1-1



- Molecule 2: Fab-CL-1



- Molecule 2: Fab-CL-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.99Å 100.99Å 213.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.94 19.96 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.94) 99.9 (19.96-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.222 , 0.246 0.223 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6951	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.79% 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

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	0.97	0/1674	1.28	3/2283 (0.1%)
1	C	1.00	1/1579 (0.1%)	1.36	7/2149 (0.3%)
2	B	1.05	0/1706	1.26	2/2316 (0.1%)
2	D	1.01	0/1686	1.39	10/2287 (0.4%)
All	All	1.01	1/6645 (0.0%)	1.33	22/9035 (0.2%)

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	C	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	PRO	C-O	-5.30	1.20	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	SER	O-C-N	9.73	127.94	121.71
2	D	206	SER	CA-C-N	-8.70	107.53	123.11
2	D	206	SER	C-N-CA	-8.70	107.53	123.11
1	C	109	TRP	CA-C-N	-7.50	113.15	122.75
1	C	109	TRP	C-N-CA	-7.50	113.15	122.75
1	C	75	LYS	CA-C-N	-6.56	113.29	122.74
1	C	75	LYS	C-N-CA	-6.56	113.29	122.74
2	B	215	ARG	CA-C-N	-6.02	116.28	123.44
2	B	215	ARG	C-N-CA	-6.02	116.28	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	HIS	CA-C-N	5.97	128.56	120.38
2	D	202	HIS	C-N-CA	5.97	128.56	120.38
2	D	206	SER	O-C-N	5.96	129.41	122.20
1	A	50	PHE	CA-CB-CG	5.81	119.61	113.80
2	D	216	GLY	CA-C-N	-5.75	112.87	122.64
2	D	216	GLY	C-N-CA	-5.75	112.87	122.64
1	A	177	GLN	CA-C-N	5.66	128.13	120.38
1	A	177	GLN	C-N-CA	5.66	128.13	120.38
1	C	50	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	6	GLU	CA-C-N	5.19	131.45	121.54
1	C	6	GLU	C-N-CA	5.19	131.45	121.54
2	D	120	PHE	CA-CB-CG	5.11	118.91	113.80
2	D	155	ASP	N-CA-C	-5.02	105.82	112.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	76	ASN	Mainchain
2	D	207	SER	Mainchain

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	1632	0	1593	12	0
1	C	1544	0	1517	16	0
2	B	1672	0	1641	7	0
2	D	1653	0	1616	26	0
3	A	107	0	0	0	0
3	B	162	0	0	0	0
3	C	84	0	0	2	0
3	D	97	0	0	1	0
All	All	6951	0	6367	61	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 (61) 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)
2:D:155:ASP:OD1	2:D:195:VAL:HG22	1.69	0.93
2:D:153:LYS:HE3	2:D:153:LYS:HA	1.65	0.78
1:A:42:GLY:C	1:A:43:LYS:HD2	2.09	0.78
2:D:152:TRP:CD1	2:D:163:SER:HG	2.02	0.77
1:C:21:THR:HG22	1:C:79:SER:OG	1.85	0.77
2:D:155:ASP:H	2:D:195:VAL:HG23	1.52	0.75
2:B:153:LYS:HG2	2:B:158:LEU:HD12	1.71	0.72
2:B:153:LYS:HE2	2:B:158:LEU:HD11	1.71	0.72
2:D:153:LYS:HA	2:D:153:LYS:CE	2.18	0.70
2:B:23:CYS:SG	2:B:92:CYS:CB	2.81	0.68
2:D:154:VAL:HG21	2:D:196:TYR:CE2	2.30	0.67
1:C:149:LYS:HE3	3:C:308:HOH:O	1.94	0.67
2:D:207:SER:OG	2:D:208:PRO:HD2	1.96	0.66
2:D:155:ASP:HA	2:D:195:VAL:CG2	2.27	0.65
1:C:11:LEU:HD21	1:C:120:ALA:O	1.99	0.62
1:C:202:CYS:SG	1:C:215:LYS:HB3	2.39	0.62
2:D:153:LYS:HE3	2:D:153:LYS:CA	2.25	0.62
1:A:131:ALA:HB3	1:A:220:LYS:HE3	1.81	0.62
1:A:34:VAL:HG11	1:A:78:VAL:HG21	1.83	0.60
1:C:71:ARG:HG3	1:C:78:VAL:HG22	1.84	0.59
1:A:202:CYS:SG	1:A:215:LYS:HB3	2.45	0.57
1:C:199:THR:HG23	1:C:216:LYS:HE3	1.89	0.54
1:C:149:LYS:NZ	1:C:177:GLN:OE1	2.41	0.52
1:C:15:SER:OG	1:C:16:GLU:HG2	2.09	0.52
2:D:136:VAL:HG11	2:D:213:PHE:HE2	1.74	0.52
2:D:67:SER:HB3	3:D:349:HOH:O	2.09	0.52
2:D:155:ASP:HA	2:D:195:VAL:HG22	1.92	0.52
1:A:5:GLN:HB2	1:A:21:THR:H	1.74	0.52
2:D:38:GLN:HG3	2:D:53:TYR:HA	1.90	0.52
1:C:15:SER:O	1:C:85:VAL:HG22	2.10	0.50
1:A:52:ARG:CG	1:A:56:ASN:HB2	2.42	0.49
1:A:5:GLN:HB3	1:A:20:LEU:HD23	1.95	0.49
1:A:50:PHE:HE1	1:A:52:ARG:HD3	1.76	0.49
1:A:30:THR:O	1:A:31:SER:HB3	2.12	0.48
2:B:170:GLN:HG3	2:B:177:TYR:CZ	2.49	0.48
2:B:153:LYS:HG2	2:B:158:LEU:CD1	2.42	0.47
2:D:152:TRP:O	2:D:153:LYS:HD2	2.15	0.47
2:D:136:VAL:CG1	2:D:213:PHE:HE2	2.28	0.47
2:D:207:SER:OG	2:D:208:PRO:CD	2.62	0.47
1:C:52:ARG:O	1:C:71:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:O	1:C:76:ASN:HB2	2.15	0.46
1:A:42:GLY:O	1:A:43:LYS:HD2	2.15	0.46
2:D:124:PRO:HG2	2:D:134:ALA:HB1	1.96	0.46
1:C:61:SER:OG	1:C:64:LYS:NZ	2.50	0.45
2:D:191:GLU:O	2:D:215:ARG:NH2	2.50	0.45
2:B:124:PRO:HD3	2:B:136:VAL:HG22	1.98	0.45
2:D:190:TYR:HA	2:D:196:TYR:OH	2.16	0.45
2:D:155:ASP:N	2:D:195:VAL:HG23	2.25	0.44
1:C:81:LYS:HG3	3:C:331:HOH:O	2.16	0.44
2:D:155:ASP:CA	2:D:195:VAL:CG2	2.93	0.43
1:A:132:PRO:HG2	1:A:219:PRO:HA	2.02	0.42
1:C:156:VAL:CG2	1:C:184:LEU:HD21	2.49	0.42
2:D:155:ASP:H	2:D:195:VAL:CG2	2.27	0.42
1:C:132:PRO:HG2	1:C:219:PRO:HA	2.02	0.42
2:B:195:VAL:HG22	2:B:214:ASN:OD1	2.20	0.41
2:D:154:VAL:HG21	2:D:196:TYR:CZ	2.56	0.41
1:C:165:LEU:HD21	1:C:188:VAL:HG21	2.03	0.41
2:D:195:VAL:HG23	2:D:195:VAL:O	2.21	0.41
2:D:191:GLU:HA	2:D:215:ARG:NE	2.36	0.41
2:D:194:LYS:O	2:D:214:ASN:HA	2.21	0.41
1:A:52:ARG:HG2	1:A:56:ASN:HB2	2.02	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	214/222 (96%)	209 (98%)	5 (2%)	0	100	100
1	C	200/222 (90%)	193 (96%)	5 (2%)	2 (1%)	13	5
2	B	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
2	D	211/218 (97%)	205 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	841/880 (96%)	819 (97%)	20 (2%)	2 (0%)	44	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	SER
1	C	15	SER

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	187/193 (97%)	187 (100%)	0	100	100
1	C	178/193 (92%)	178 (100%)	0	100	100
2	B	191/191 (100%)	191 (100%)	0	100	100
2	D	189/191 (99%)	189 (100%)	0	100	100
All	All	745/768 (97%)	745 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	C	39	GLN
1	C	111	GLN
2	D	42	GLN
2	D	46	GLN
2	D	156	ASN
2	D	203	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](#)

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, 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	216/222 (97%)	0.56	18 (8%) 19 21	27, 40, 66, 84	0
1	C	206/222 (92%)	0.71	17 (8%) 19 21	31, 44, 68, 83	0
2	B	218/218 (100%)	0.19	5 (2%) 61 67	26, 36, 50, 77	0
2	D	214/218 (98%)	0.90	38 (17%) 4 5	22, 43, 70, 84	1 (0%)
All	All	854/880 (97%)	0.59	78 (9%) 16 19	22, 41, 67, 84	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	SER	5.1
2	D	218	CYS	5.1
1	A	30	THR	5.1
1	C	221	SER	4.9
2	D	196	TYR	4.8
1	A	29	LEU	4.2
2	D	197	ALA	4.1
1	C	8	GLY	4.0
2	B	218	CYS	4.0
1	A	5	GLN	4.0
1	A	31	SER	3.9
1	A	10	GLY	3.8
1	A	32	TYR	3.8
2	D	198	CYS	3.7
2	D	195	VAL	3.7
2	D	213	PHE	3.5
1	A	220	LYS	3.4
2	D	209	VAL	3.4
2	D	185	LEU	3.4
1	A	101	TYR	3.3
1	A	102	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	215	ARG	3.2
2	D	212	SER	3.2
1	C	100	GLU	3.1
1	C	53	SER	3.1
1	C	134	SER	3.0
1	A	54	GLY	2.9
2	D	120	PHE	2.9
1	C	73	THR	2.8
2	D	162	ASN	2.8
2	D	199	GLU	2.8
2	D	161	GLY	2.8
2	D	119	VAL	2.8
2	D	200	VAL	2.7
1	C	110	GLY	2.7
2	D	152	TRP	2.6
2	D	153	LYS	2.6
1	C	9	PRO	2.6
2	D	205	LEU	2.6
1	C	42	GLY	2.6
2	D	216	GLY	2.5
1	C	197	THR	2.5
1	A	103	TRP	2.5
2	D	155	ASP	2.5
2	D	210	THR	2.5
1	C	76	ASN	2.5
2	D	148	ALA	2.4
2	D	186	SER	2.4
2	B	92	CYS	2.4
2	D	116	ALA	2.4
2	D	188	ALA	2.4
2	D	207	SER	2.4
1	A	27	PHE	2.4
1	A	23	THR	2.4
1	A	7	SER	2.4
2	D	154	VAL	2.4
1	A	53	SER	2.3
1	C	5	GLN	2.3
2	D	151	GLN	2.3
2	D	61	GLY	2.3
1	C	24	VAL	2.3
2	D	201	THR	2.3
2	B	64	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	156	ASN	2.3
2	D	193	HIS	2.3
2	D	214	ASN	2.2
2	D	206	SER	2.2
2	D	114	VAL	2.2
2	B	216	GLY	2.2
2	D	208	PRO	2.2
1	C	71	ARG	2.1
1	A	138	SER	2.1
1	A	28	SER	2.1
1	C	7	SER	2.1
1	C	61	SER	2.1
2	B	217	GLU	2.1
2	D	217	GLU	2.0
1	A	25	SER	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.