Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 04:14 PM JST

PDB ID	:	8JEO
Title	:	Crystal structure of TIGIT in complexed with Tiragolumab
Authors	:	Sun, J.; Zhang, X.X.; Song, J.
Deposited on	:	2023-05-16
Resolution	:	2.06 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:

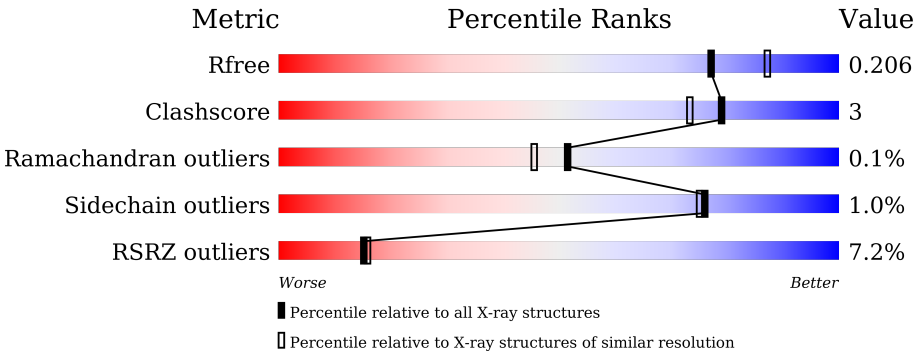
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	115	26% 79% 12% • 8%
1	D	115	4% 89% • 7%
2	B	235	% 92% • •
2	E	235	8% 91% • 6%
3	C	220	% 95% 5%
3	F	220	9% 88% 11% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9082 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 T-cell immunoreceptor with Ig and ITIM domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			811	511	133	163	4			
1	D	107	Total	C	N	O	S	0	0	0
			819	516	134	164	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	LEU	-	expression tag	UNP Q495A1
A	130	GLU	-	expression tag	UNP Q495A1
A	131	HIS	-	expression tag	UNP Q495A1
A	132	HIS	-	expression tag	UNP Q495A1
A	133	HIS	-	expression tag	UNP Q495A1
A	134	HIS	-	expression tag	UNP Q495A1
A	135	HIS	-	expression tag	UNP Q495A1
A	136	HIS	-	expression tag	UNP Q495A1
D	129	LEU	-	expression tag	UNP Q495A1
D	130	GLU	-	expression tag	UNP Q495A1
D	131	HIS	-	expression tag	UNP Q495A1
D	132	HIS	-	expression tag	UNP Q495A1
D	133	HIS	-	expression tag	UNP Q495A1
D	134	HIS	-	expression tag	UNP Q495A1
D	135	HIS	-	expression tag	UNP Q495A1
D	136	HIS	-	expression tag	UNP Q495A1

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1703	1079	281	338	5			
2	E	220	Total	C	N	O	S	0	0	0
			1672	1062	275	331	4			

- Molecule 3 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1705	1071	282	346	6			
3	F	218	Total	C	N	O	S	0	0	0
			1690	1063	280	342	5			

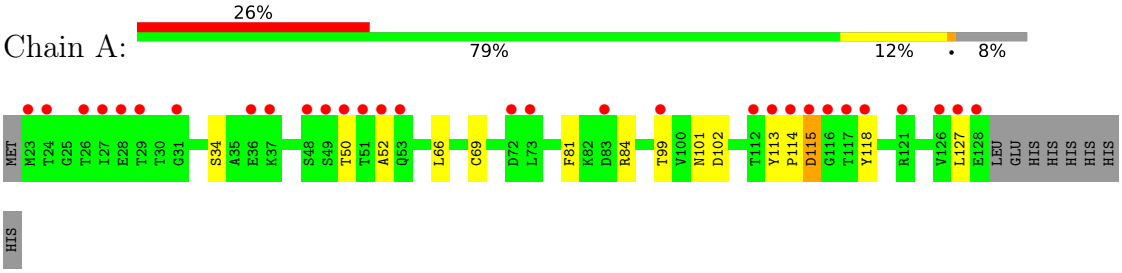
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	164	Total	O	0	0
			164	164		
4	C	162	Total	O	0	0
			162	162		
4	D	51	Total	O	0	0
			51	51		
4	E	172	Total	O	0	0
			172	172		
4	F	118	Total	O	0	0
			118	118		

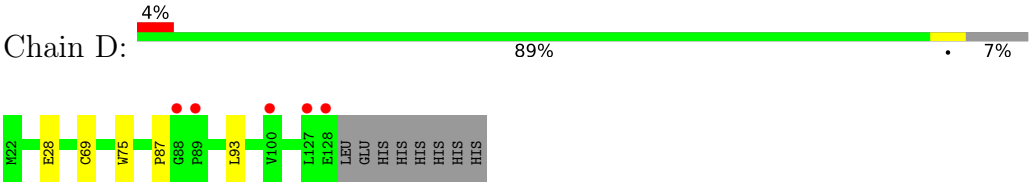
3 Residue-property plots (i)

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.

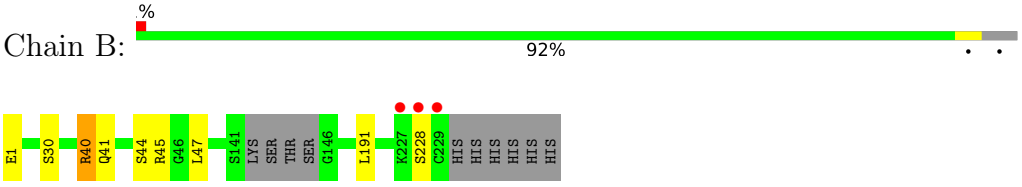
• Molecule 1: T-cell immunoreceptor with Ig and ITIM domains



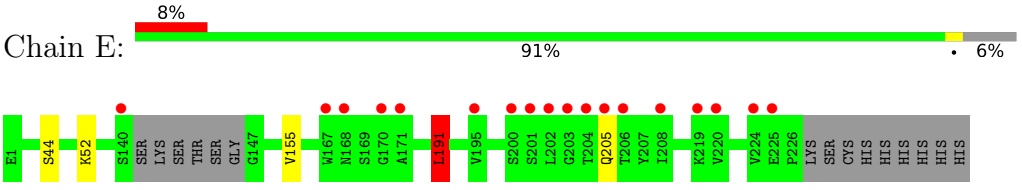
• Molecule 1: T-cell immunoreceptor with Ig and ITIM domains



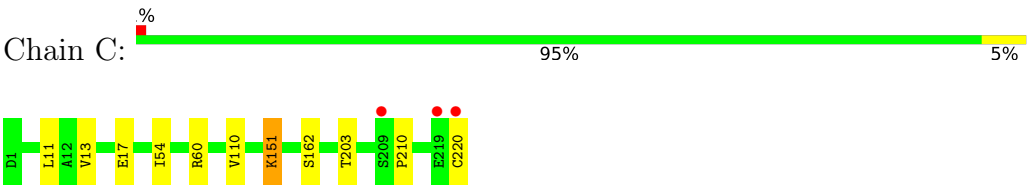
• Molecule 2: antibody heavy chain



• Molecule 2: antibody heavy chain

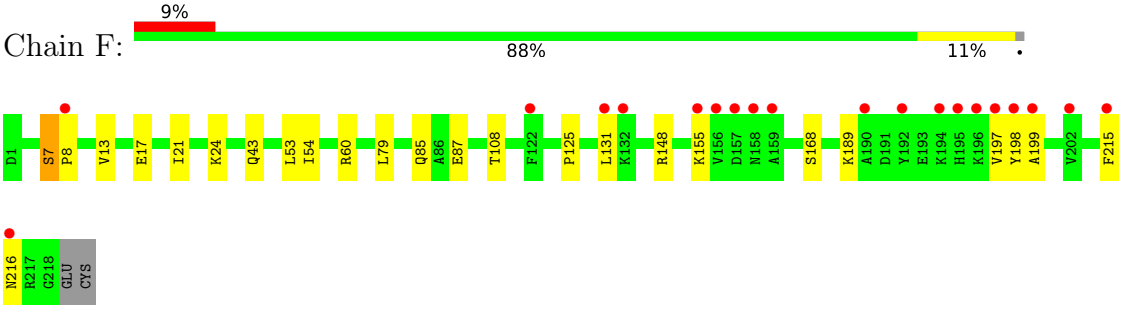


• Molecule 3: antibody light chain



• Molecule 3: antibody light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	214.16Å 214.16Å 66.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.06 48.81 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.81-2.06) 99.6 (48.81-2.06)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.172 , 0.205 0.172 , 0.206	Depositor DCC
R_{free} test set	4749 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9082	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.31	0/828	0.55	0/1130
1	D	0.36	0/836	0.57	0/1140
2	B	0.41	0/1747	0.60	1/2388 (0.0%)
2	E	0.42	0/1716	0.59	1/2348 (0.0%)
3	C	0.41	0/1744	0.56	0/2372
3	F	0.40	0/1729	0.57	1/2352 (0.0%)
All	All	0.40	0/8600	0.58	3/11730 (0.0%)

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
3	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	191	LEU	CA-CB-CG	6.16	129.48	115.30
2	E	191	LEU	CA-CB-CG	5.85	128.75	115.30
3	F	7	SER	C-N-CD	-5.70	108.05	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	7	SER	Peptide

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	811	0	779	11	0
1	D	819	0	788	3	0
2	B	1703	0	1662	4	0
2	E	1672	0	1632	4	0
3	C	1705	0	1648	7	0
3	F	1690	0	1638	18	0
4	A	15	0	0	2	0
4	B	164	0	0	1	0
4	C	162	0	0	0	0
4	D	51	0	0	1	0
4	E	172	0	0	1	0
4	F	118	0	0	3	0
All	All	9082	0	8147	46	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 3.

All (46) 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:D:69:CYS:SG	4:D:244:HOH:O	2.28	0.90
1:A:69:CYS:SG	4:A:214:HOH:O	2.38	0.81
3:C:203:THR:HG22	3:C:210:PRO:HG3	1.73	0.68
3:F:21:ILE:HD12	3:F:108:THR:HG21	1.74	0.68
3:F:13:VAL:HG13	3:F:17:GLU:HB2	1.80	0.64
1:A:50:THR:HG22	1:A:52:ALA:H	1.65	0.62
3:C:13:VAL:HG13	3:C:17:GLU:HB2	1.83	0.58
3:F:43:GLN:HB2	3:F:53:LEU:HD11	1.87	0.57
2:B:1:GLU:N	4:B:304:HOH:O	2.38	0.56
3:C:151:LYS:HE3	3:C:203:THR:OG1	2.06	0.56
3:F:155:LYS:HB2	3:F:199:ALA:HB3	1.88	0.56
3:F:198:TYR:HB2	3:F:215:PHE:CE1	2.42	0.55
3:C:11:LEU:HD21	3:C:110:VAL:HG22	1.89	0.54
1:A:34:SER:HB3	1:A:127:LEU:HD21	1.90	0.54
1:A:84:ARG:NH2	1:A:102:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:VAL:HB	2:E:191:LEU:HD12	1.92	0.52
3:F:54:ILE:HD13	3:F:79:LEU:HD13	1.92	0.52
3:F:85:GLN:HB3	3:F:87:GLU:OE1	2.10	0.51
3:F:125:PRO:HB3	3:F:215:PHE:CE2	2.46	0.50
3:F:60:ARG:NH1	4:F:302:HOH:O	2.39	0.49
3:F:87:GLU:OE2	4:F:301:HOH:O	2.20	0.48
1:A:115:ASP:HB3	1:A:118:TYR:OH	2.14	0.47
3:F:197:VAL:HG22	3:F:216:ASN:OD1	2.14	0.47
3:F:87:GLU:H	3:F:87:GLU:CD	2.17	0.47
3:F:148:ARG:HG2	3:F:148:ARG:HH11	1.80	0.47
2:B:40:ARG:NH2	2:B:45:ARG:HH22	2.13	0.45
1:A:34:SER:HB3	1:A:127:LEU:CD2	2.47	0.45
3:F:13:VAL:CG1	3:F:17:GLU:HB2	2.46	0.44
1:A:99:THR:HG23	1:A:101:ASN:N	2.33	0.44
3:C:151:LYS:HB3	3:C:203:THR:OG1	2.17	0.44
1:A:99:THR:HG23	1:A:101:ASN:H	1.82	0.44
3:F:148:ARG:HG2	3:F:148:ARG:NH1	2.32	0.43
1:A:84:ARG:HD3	4:A:206:HOH:O	2.18	0.43
3:C:151:LYS:HE3	3:C:151:LYS:HB3	1.73	0.42
2:B:44:SER:HB2	2:E:44:SER:HB2	2.02	0.42
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.90	0.42
1:A:66:LEU:HD23	1:A:81:PHE:CD2	2.55	0.42
2:E:52:LYS:NZ	4:E:310:HOH:O	2.53	0.41
3:F:53:LEU:HB2	3:F:54:ILE:HD12	2.02	0.41
2:E:205:GLN:HA	2:E:205:GLN:OE1	2.20	0.41
2:B:41:GLN:HB2	2:B:47:LEU:HD23	2.03	0.41
1:D:75:TRP:CE2	1:D:87:PRO:HB3	2.57	0.40
1:A:113:TYR:HA	1:A:114:PRO:HA	1.96	0.40
3:F:131:LEU:O	3:F:189:LYS:HE2	2.22	0.40
3:C:54:ILE:HD13	3:C:60:ARG:HA	2.03	0.40
3:F:24:LYS:NZ	4:F:304:HOH:O	2.54	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	104/115 (90%)	99 (95%)	5 (5%)	0	100	100
1	D	105/115 (91%)	101 (96%)	4 (4%)	0	100	100
2	B	221/235 (94%)	213 (96%)	8 (4%)	0	100	100
2	E	216/235 (92%)	209 (97%)	7 (3%)	0	100	100
3	C	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
3	F	216/220 (98%)	209 (97%)	6 (3%)	1 (0%)	29	19
All	All	1080/1140 (95%)	1044 (97%)	35 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	8	PRO

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	90/99 (91%)	89 (99%)	1 (1%)	73	72
1	D	91/99 (92%)	90 (99%)	1 (1%)	73	72
2	B	196/206 (95%)	193 (98%)	3 (2%)	65	62
2	E	192/206 (93%)	191 (100%)	1 (0%)	88	89
3	C	195/195 (100%)	192 (98%)	3 (2%)	65	62
3	F	193/195 (99%)	192 (100%)	1 (0%)	88	89
All	All	957/1000 (96%)	947 (99%)	10 (1%)	76	75

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

Mol	Chain	Res	Type
1	A	115	ASP

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Mol	Chain	Res	Type
2	B	30	SER
2	B	40	ARG
2	B	228	SER
3	C	151	LYS
3	C	162	SER
3	C	220	CYS
1	D	28	GLU
2	E	191	LEU
3	F	168	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	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 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	106/115 (92%)	1.35	30 (28%) 0 0	36, 73, 105, 119	0
1	D	107/115 (93%)	0.36	5 (4%) 31 32	34, 50, 80, 113	0
2	B	225/235 (95%)	0.23	3 (1%) 77 78	30, 40, 60, 116	0
2	E	220/235 (93%)	0.70	18 (8%) 11 12	30, 42, 86, 107	0
3	C	220/220 (100%)	0.10	3 (1%) 75 76	31, 42, 62, 119	0
3	F	218/220 (99%)	0.62	20 (9%) 9 9	31, 52, 92, 112	0
All	All	1096/1140 (96%)	0.50	79 (7%) 15 16	30, 45, 89, 119	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	9.1
3	C	220	CYS	6.9
2	E	202	LEU	6.6
1	A	24	THR	6.4
3	F	158	ASN	5.9
1	A	118	TYR	5.8
2	B	229	CYS	5.6
2	B	228	SER	5.4
1	A	113	TYR	5.3
1	A	26	THR	5.3
2	E	204	THR	5.3
3	F	132	LYS	4.6
1	A	48	SER	4.5
1	A	23	MET	4.1
3	F	159	ALA	4.0
1	A	36	GLU	3.9
2	E	205	GLN	3.7
2	E	224	VAL	3.7
1	D	127	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	203	GLY	3.6
1	A	50	THR	3.6
2	E	170	GLY	3.5
1	A	49	SER	3.5
3	F	131	LEU	3.4
1	D	89	PRO	3.4
3	F	202	VAL	3.4
2	E	171	ALA	3.4
3	F	196	LYS	3.4
2	E	167	TRP	3.3
3	F	157	ASP	3.3
1	A	116	GLY	3.3
1	A	51	THR	3.2
1	A	53	GLN	3.1
3	F	156	VAL	3.1
2	E	220	VAL	3.1
3	C	219	GLU	3.1
1	A	29	THR	3.1
3	F	197	VAL	3.1
2	E	201	SER	3.1
3	F	195	HIS	3.0
1	A	52	ALA	3.0
2	E	208	ILE	3.0
1	A	128	GLU	3.0
2	E	206	THR	2.9
3	F	194	LYS	2.8
3	C	209	SER	2.8
1	A	27	ILE	2.8
1	A	114	PRO	2.7
2	E	200	SER	2.7
1	D	100	VAL	2.7
2	E	219	LYS	2.7
3	F	8	PRO	2.6
1	A	117	THR	2.6
1	A	37	LYS	2.5
2	E	225	GLU	2.5
1	D	88	GLY	2.5
1	A	72	ASP	2.5
1	A	112	THR	2.5
2	E	140	SER	2.5
1	A	28	GLU	2.5
2	E	168	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	198	TYR	2.4
3	F	216	ASN	2.3
1	A	73	LEU	2.3
1	A	115	ASP	2.3
3	F	199	ALA	2.3
1	D	128	GLU	2.2
3	F	190	ALA	2.2
1	A	99	THR	2.2
1	A	31	GLY	2.2
1	A	126	VAL	2.2
3	F	215	PHE	2.1
3	F	122	PHE	2.1
2	B	227	LYS	2.1
1	A	83	ASP	2.1
1	A	121	ARG	2.1
3	F	155	LYS	2.1
3	F	192	TYR	2.1
2	E	195	VAL	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.