W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 11:39 AM EDT

PDB ID	:	5MHS
Title	:	T1L reovirus sigma1 complexed with 5C6 Fab fragments
Authors	:	Stehle, T.; Dietrich, M.H.
Deposited on	:	2016-11-25
Resolution	:	3.70 Å(reported)

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

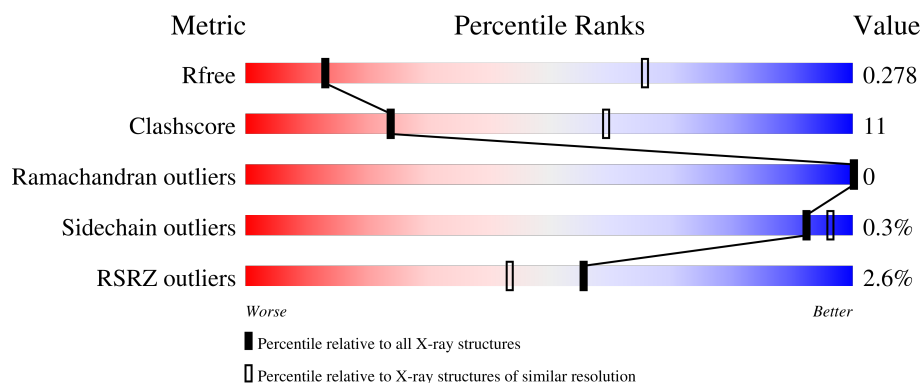|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.70 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		2.6%

Worse — *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	172	83% 12% 5%
1	B	172	74% 21% 5%
1	C	172	83% 12% 5%
2	D	217	2% 81% 18% •
2	F	217	6% 74% 23% •

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Mol	Chain	Length	Quality of chain
2	G	217	2% 75% 20% 6%
3	E	221	% 77% 17% 5%
3	H	221	7% 71% 20% 9%
3	N	221	3% 75% 18% 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11874 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1252	795	210	240	7			
1	B	163	Total	C	N	O	S	0	0	0
			1258	804	214	234	6			
1	C	163	Total	C	N	O	S	0	0	0
			1283	819	213	244	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLY	-	expression tag	UNP P04506
A	300	VAL	-	expression tag	UNP P04506
A	301	LEU	-	expression tag	UNP P04506
A	302	ASN	-	expression tag	UNP P04506
A	303	GLN	-	expression tag	UNP P04506
A	304	GLY	-	expression tag	UNP P04506
A	305	VAL	-	expression tag	UNP P04506
A	306	THR	-	expression tag	UNP P04506
A	307	SER	THR	conflict	UNP P04506
B	299	GLY	-	expression tag	UNP P04506
B	300	VAL	-	expression tag	UNP P04506
B	301	LEU	-	expression tag	UNP P04506
B	302	ASN	-	expression tag	UNP P04506
B	303	GLN	-	expression tag	UNP P04506
B	304	GLY	-	expression tag	UNP P04506
B	305	VAL	-	expression tag	UNP P04506
B	306	THR	-	expression tag	UNP P04506
B	307	SER	THR	conflict	UNP P04506
C	299	GLY	-	expression tag	UNP P04506
C	300	VAL	-	expression tag	UNP P04506
C	301	LEU	-	expression tag	UNP P04506
C	302	ASN	-	expression tag	UNP P04506
C	303	GLN	-	expression tag	UNP P04506

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Chain	Residue	Modelled	Actual	Comment	Reference
C	304	GLY	-	expression tag	UNP P04506
C	305	VAL	-	expression tag	UNP P04506
C	306	THR	-	expression tag	UNP P04506
C	307	SER	THR	conflict	UNP P04506

- Molecule 2 is a protein called 5C6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	214	Total 1392	C 870	N 244	O 272	S 6	0	0	0
2	F	212	Total 1375	C 852	N 241	O 276	S 6	0	0	0
2	G	205	Total 1352	C 843	N 240	O 264	S 5	0	0	0

- Molecule 3 is a protein called 5C6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	210	Total 1332	C 827	N 235	O 265	S 5	0	0	0
3	H	201	Total 1271	C 799	N 221	O 247	S 4	0	0	0
3	N	205	Total 1359	C 860	N 231	O 263	S 5	0	0	0

3 Residue-property plots ⓘ

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.
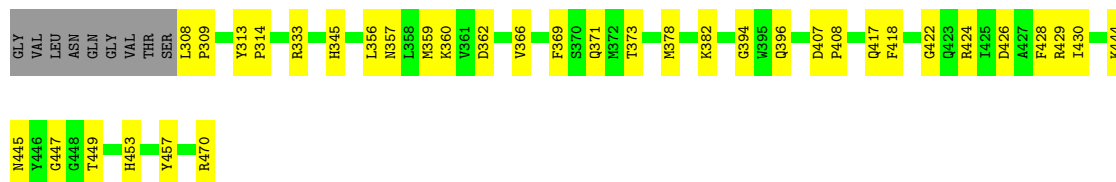
- Molecule 1: Outer capsid protein sigma-1

Chain A:

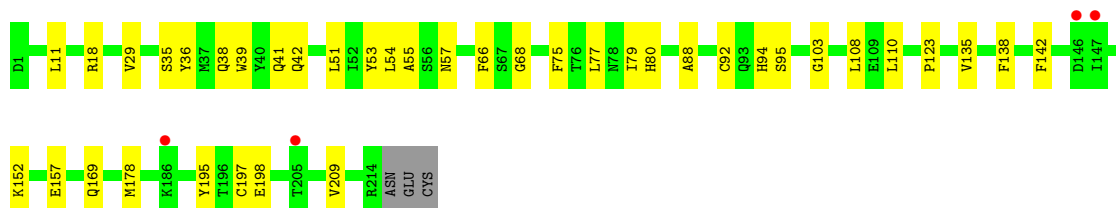- Molecule 1: Outer capsid protein sigma-1

Chain B:

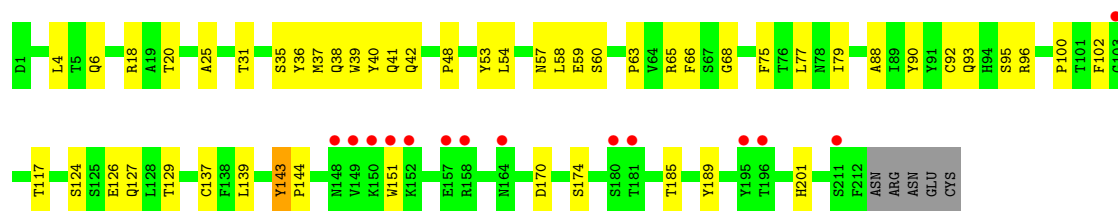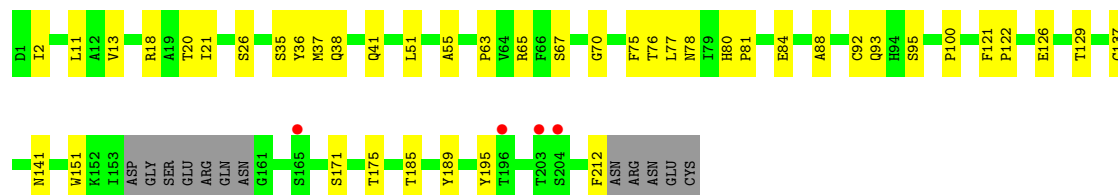- Molecule 1: Outer capsid protein sigma-1

Chain C:
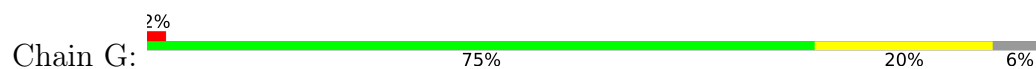

- Molecule 2: 5C6 Fab light chain

Chain D:

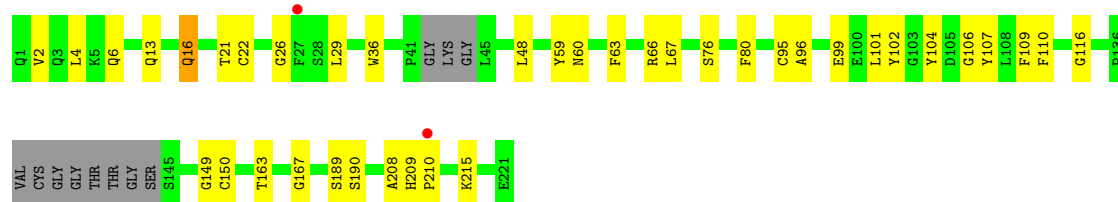- Molecule 2: 5C6 Fab light chain

Chain F:

D1 L4 T5 Q6 R18 A19 T20 A25 T31 S35 Y36 M37 Q38 W39 Y40 Q41 Q42 P48 Y53 L54 N57 L58 E59 S60 P63 V64 R65 F66 S67 G68 F75 T76 L77 N78 I79 A88 I89 Y90 C92 Q93 H94 S95 R96 P100 T101 F102 G103

T117 S124 S125 E126 Q127 L128 T129 C137 F138 L139 Y143 P144 N148 V149 K150 W151 K152 E157 R158 M164 D170 S174 S180 T181 T185 Y189 Y195 T196 H201 S211 F212 ASN ARG ASN GLU CYS

• Molecule 2: 5C6 Fab light chain

Chain G:

D1 I2 L11 A12 V13 R18 A19 T20 I21 S26 S35 Y36 M37 Q38 Q41 L51 A55 P63 V64 R65 F66 S67 G70 F75 T76 L77 N78 I79 H80 P81 E84 A88 C92 Q93 H94 S95 P100 F121 P122 E126 T129 C137

N141 W151 K152 I153 ASP GLY SER GLU ARG GLN ASN G161 S165 S171 T175 T185 Y189 Y195 T196 T203 S204 F212 ASN ARG ASN GLU CYS

• Molecule 3: 5C6 Fab heavy chain

Chain E:

Q1 V2 Q3 L4 K5 Q6 Q13 Q16 T21 C22 G26 F27 S28 L29 W36 P41 GLY LYS GLY L45 L48 Y59 N60 F63 R66 L67 S76 F80 C95 A96 E99 E100 L101 Y102 G103 Y104 D105 G106 Y107 L108 F109 F110 G116 P136

VAL CYS GLY GLY THR THR GLY SER S145 G149 C150 T163 G167 S189 S190 A208 H209 P210 K215 E221

• Molecule 3: 5C6 Fab heavy chain

Chain H:

GLN V2 Q3 L4 K5 Q6 P14 C22 G26 I34 H35 W36 V37 R38 Q39 S40 P41 GLY LYS G44 W47 L48 I51 W52 S56 N60 F63 R66 I69 F80 K81 M82 T90 A91 I92 C95 A96 R97 D105 G106 Y107 F110 D111 V112

W113 G114 A115 T118 V121 S122 S123 A124 T127 S130 V131 P136 VAL CYS GLY GLY THR THR GLY SER SER VAL THR LEU G149 K153 G154 Y155 F156 P157 E158 N165 SER GLY SER LEU SER S171 A178 L179 L180 L184 Y185 T186 N196 Q201 T202 I203

P210 E221

• Molecule 3: 5C6 Fab heavy chain

Chain N:

Q1 V2 Q3 L4 V12 L18 S19 C22 T23 V24 S25 I34 H35 W36 V37 R38 E46 W47 L48 G49 V50 I51 T57 D58 Y59 N60 F63 L67 F80 K81 L85 T90 C95 A96 Y107 F110 D111 G114 V121 T126 T127 A128 P129

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.61Å 129.08Å 87.86Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	48.99 – 3.70 48.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.99-3.70) 100.0 (48.99-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.49 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.261 , 0.278 0.261 , 0.278	Depositor DCC
R_{free} test set	1314 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	112.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 112.8	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.25	0/1288	0.50	0/1765
1	B	0.27	0/1294	0.53	0/1769
1	C	0.27	0/1319	0.50	0/1805
2	D	0.27	0/1427	0.52	0/1968
2	F	0.28	0/1407	0.51	0/1943
2	G	0.26	0/1384	0.50	0/1908
3	E	0.33	0/1365	0.56	0/1888
3	H	0.30	0/1303	0.54	0/1799
3	N	0.33	0/1394	0.59	0/1922
All	All	0.29	0/12181	0.53	0/16767

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 (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	1252	0	1128	14	1
1	B	1258	0	1156	26	0
1	C	1283	0	1206	16	1
2	D	1392	0	1072	33	0
2	F	1375	0	1060	40	0
2	G	1352	0	1065	27	0
3	E	1332	0	947	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1271	0	902	34	1
3	N	1359	0	1065	32	1
All	All	11874	0	9601	238	2

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 11.

The worst 5 of 238 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)
3:E:6:GLN:OE1	3:E:6:GLN:N	2.10	0.83
3:H:4:LEU:HB3	3:H:114:GLY:HA3	1.62	0.80
1:B:426:ASP:OD1	3:E:104:TYR:OH	2.03	0.77
3:H:4:LEU:HD21	3:H:22:CYS:HB3	1.67	0.77
2:G:36:TYR:HB3	2:G:95:SER:HB2	1.69	0.75

All (2) 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)
1:A:422:GLY:O	3:H:107:TYR:OH[2_756]	2.17	0.03
1:C:422:GLY:O	3:N:107:TYR:OH[4_756]	2.18	0.02

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	161/172 (94%)	160 (99%)	1 (1%)	0	100	100
1	B	161/172 (94%)	160 (99%)	1 (1%)	0	100	100
1	C	161/172 (94%)	160 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	212/217 (98%)	208 (98%)	4 (2%)	0	100	100
2	F	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
2	G	201/217 (93%)	195 (97%)	6 (3%)	0	100	100
3	E	204/221 (92%)	200 (98%)	4 (2%)	0	100	100
3	H	193/221 (87%)	190 (98%)	3 (2%)	0	100	100
3	N	201/221 (91%)	196 (98%)	5 (2%)	0	100	100
All	All	1704/1830 (93%)	1674 (98%)	30 (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	126/149 (85%)	126 (100%)	0	100	100
1	B	126/149 (85%)	126 (100%)	0	100	100
1	C	137/149 (92%)	137 (100%)	0	100	100
2	D	104/191 (54%)	104 (100%)	0	100	100
2	F	105/191 (55%)	104 (99%)	1 (1%)	76	86
2	G	105/191 (55%)	105 (100%)	0	100	100
3	E	90/190 (47%)	89 (99%)	1 (1%)	73	85
3	H	83/190 (44%)	83 (100%)	0	100	100
3	N	104/190 (55%)	103 (99%)	1 (1%)	76	86
All	All	980/1590 (62%)	977 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	16	GLN
2	F	143	TYR

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Mol	Chain	Res	Type
3	N	110	PHE

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

Mol	Chain	Res	Type
1	C	455	GLN
2	F	38	GLN
2	F	93	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, 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(Å²)	Q<0.9
1	A	163/172 (94%)	-0.20	0	100	100	67, 95, 152, 172	0
1	B	163/172 (94%)	-0.26	0	100	100	64, 92, 145, 172	0
1	C	163/172 (94%)	-0.23	0	100	100	57, 88, 150, 185	0
2	D	214/217 (98%)	-0.05	4 (1%)	66	55	86, 166, 239, 278	0
2	F	212/217 (97%)	0.24	14 (6%)	18	12	93, 167, 266, 283	0
2	G	205/217 (94%)	-0.16	4 (1%)	65	53	76, 142, 258, 328	0
3	E	210/221 (95%)	-0.28	2 (0%)	82	73	80, 158, 201, 217	0
3	H	201/221 (90%)	0.23	15 (7%)	14	10	90, 190, 255, 297	0
3	N	205/221 (92%)	-0.09	7 (3%)	45	34	77, 148, 241, 259	0
All	All	1736/1830 (94%)	-0.08	46 (2%)	56	43	57, 137, 247, 328	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	148	ASN	7.2
2	F	157	GLU	6.7
2	F	196	THR	6.4
2	F	152	LYS	5.7
3	H	203	ILE	5.2

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.