wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 02:38 AM EDT

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PDB ID	:	7SFX
Title	:	10A1 Fab in complex with CD99 peptide
Authors	:	Romero, L.A.; Hattori, T.; Koide, S.
Deposited on	:	2021-10-04
Resolution	:	3.10 Å(reported)

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 3.10 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.
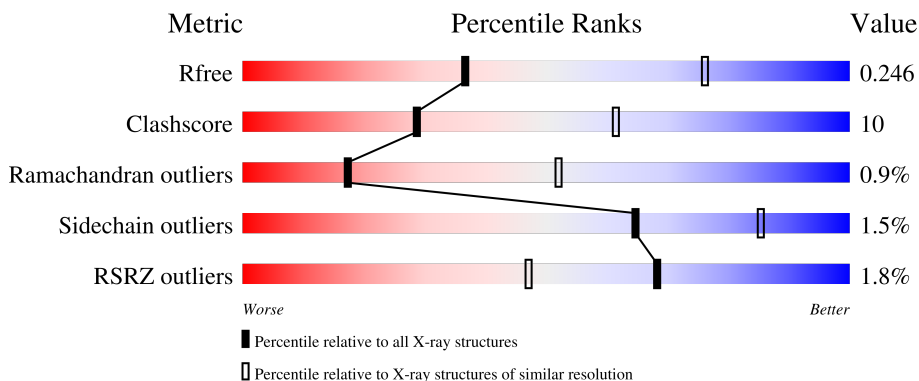
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 >=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	247	·% 72% 17% 11%
1	C	247	71% 19% 11%
1	G	247	69% 19% 11%
1	J	247	4% 68% 17% 14%
2	B	215	2% 82% 17%

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Mol	Chain	Length	Quality of chain
2	D	215	86% ▬▬▬▬▬▬▬▬▬▬▬▬▬ 14%
2	H	215	73% ▬▬▬▬▬▬▬▬▬▬ 24% •
2	K	215	4% 70% ▬▬▬▬▬▬▬ 23% • 6%
3	E	14	14% 21% 29% 50%
3	F	14	29% 21% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25893 atoms, of which 12755 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 10A1 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	221	Total 3286	C 1046	H 1626	N 280	O 329	S 5	0	0	0
1	A	221	Total 3286	C 1046	H 1626	N 280	O 329	S 5	0	0	0
1	G	219	Total 3262	C 1039	H 1615	N 278	O 325	S 5	0	0	0
1	J	213	Total 3206	C 1023	H 1590	N 270	O 319	S 4	0	0	0

- Molecule 2 is a protein called 10A1 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	214	Total 3185	C 1015	H 1560	N 271	O 335	S 4	0	0	0
2	B	214	Total 3185	C 1015	H 1560	N 271	O 335	S 4	0	0	0
2	H	214	Total 3185	C 1015	H 1560	N 271	O 335	S 4	0	0	0
2	K	203	Total 3070	C 983	H 1506	N 260	O 317	S 4	0	0	0

- Molecule 3 is a protein called CD99 antigen peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	7	Total 109	C 35	H 56	N 9	O 8	S 1	0	0	0
3	E	7	Total 109	C 35	H 56	N 9	O 8	S 1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	O 2	0	0
4	F	1	Total 1	O 1	0	0
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0
4	E	1	Total 1	O 1	0	0
4	H	3	Total 3	O 3	0	0
4	J	1	Total 1	O 1	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.
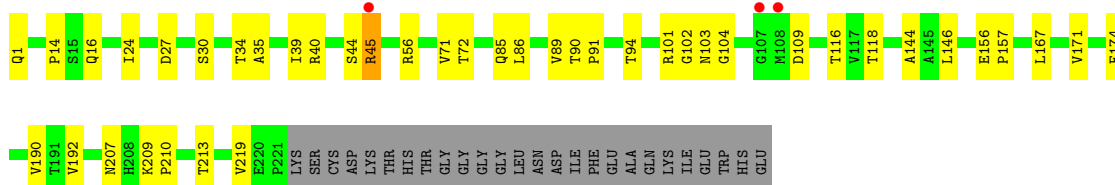
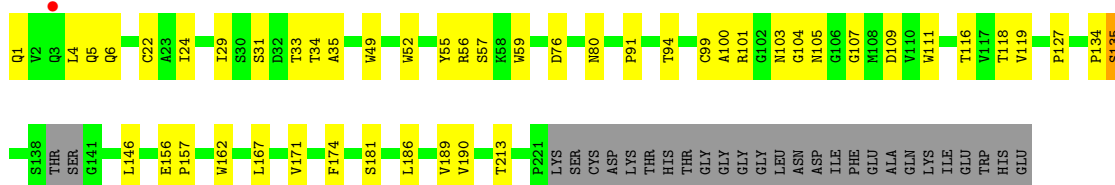- Molecule 1: 10A1 Fab heavy chain

Chain C: 71% 19% 11%

Q1 V2 L11 T17 L18 S25 I29 D32 T33 T34 A35 W36 S37 W38 I39 S42 P43 S44 R45 W49 L50 G51 W52 Y55 R56 S57 K58 W59 F60 V71 L86 G102 N105 D109 V117 A122 P127 S140 V150 K151 D152

E156 P157 V158 V171 Q179 V189 V190 S196 T199 H208 P221 LYS SER CYS ASP LYS THR HIS THR GLY GLY GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU

- Molecule 1: 10A1 Fab heavy chain

Chain A: % 72% 17% 11%

Q1 P14 S15 Q16 I24 D27 S30 T34 A35 I39 R40 S44 R45 R56 V71 T72 Q85 L86 V89 T90 P91 T94 R101 G102 N103 G104 G107 M108 D109 T116 V117 T118 A144 A145 L146 E156 P157 L167 V171 F174

V190 T191 V192 N207 H208 K209 P210 T213 V219 E220 P221 LYS SER CYS ASP LYS THR HIS THR GLY GLY GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU

- Molecule 1: 10A1 Fab heavy chain

Chain G: 69% 19% 11%

Q1 V2 Q3 L4 Q5 Q6 C22 A23 I24 I29 S30 S31 D32 T33 T34 A35 W49 W52 Y55 R56 S57 K58 W59 D76 N80 P91 T94 C99 A100 R101 G102 N103 G104 N105 G106 G107 M108 D109 V110 W111 T116 V117 T118 V119 P127 P134 S135

S138 THR SER G141 L146 E156 P157 W162 L167 V171 F174 S181 L186 V189 V190 T213 P221 LYS SER CYS ASP LYS THR HIS THR GLY GLY GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU
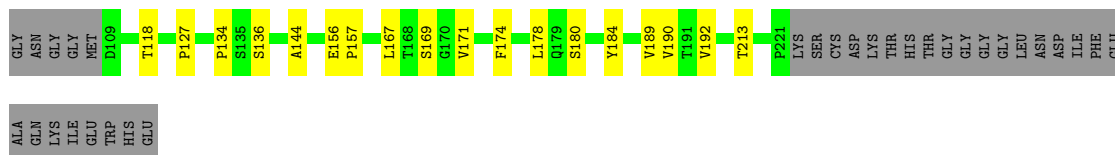
- Molecule 1: 10A1 Fab heavy chain

Chain J: 4% 68% 17% 14%

Q1 V2 Q3 L4 Q5 P14 L20 T21 C22 A23 I24 S25 GLY D27 S28 I29 T34 A35 W36 S37 R41 W52 T53 Y54 Y55 R56 S57 K58 W59 F60 V65 S66 N74 P75 D76 T77 S78 K79 N80 L84 V89 T94 A95 Y98 C99 A100 R101 GLY ASN

GLY ASN GLY MET D109 T118 P127 P134 S135 S136 A144 E156 P157 L167 T168 S169 G170 V171 F174 L178 Q179 S180 Y184 V189 V190 T191 V192 T213 P221 LYS SER CYS ASP LYS THR HIS THR GLY GLY GLY LEU ASN ASP ILE PHE GLU

ALA GLN LYS ILE GLU TRP HIS GLU

- Molecule 2: 10A1 Fab light chain

Chain D:

86%   14%

S1 Y2 Y31 Y35 A79 Q88 S89 V90 S93 G94 L105 T106 V107 L108 R109 T110 V111 F119 V134 C135 L136 Y141 P142 V151 D152 E162 S163 V164 T165 E166 S172 T173 Y174 S175 L176 Y187 V192 Y193 E214 CYS

- Molecule 2: 10A1 Fab light chain

Chain B:

2%   82%   17%

S1 Y2 V3 I20 L27 P28 W34 Y35 Q36 Q37 K38 P39 G40 Q41 L45 V46 I47 F48 K49 E52 R60 S64 V70 T71 C87 D91 G94 F95 R109 Q125 Y141 P142 V151 D152 Q156 S163 V164 T165 L176 S177 A185

D186 Y187 E188 K189 H190 M191 C195 E214 CYS
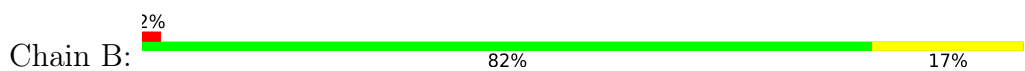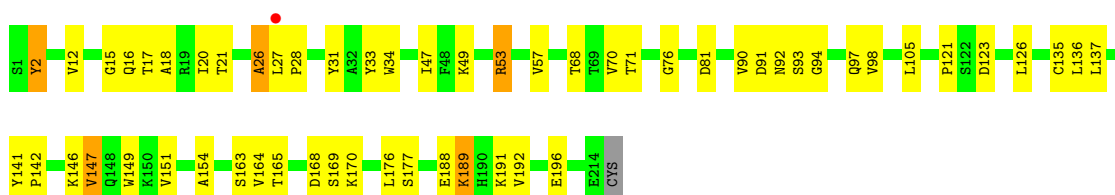
- Molecule 2: 10A1 Fab light chain

Chain H:

73%   24%   •

S1 Y2 V12 G15 Q16 T17 A18 R19 I20 T21 A26 L27 P28 Y31 A32 Y33 W34 I47 F48 K49 R53 V57 T68 T69 V70 T71 G76 D81 V90 D91 N92 S93 G94 Q97 V98 L105 P121 S122 D123 L126 C135 L136 L137

Y141 P142 K146 V147 Q148 W149 K150 V151 A154 S163 V164 T165 D168 S169 K170 L176 S177 E188 K189 H190 K191 V192 E196 E214 CYS

- Molecule 2: 10A1 Fab light chain

Chain K:

4%   70%   23%   •   6%

SER Y2 V3 A8 S11 V12 SER PRO GLY Q16 T17 A18 R19 I20 T21 C22 SER GLY D25 A26 L27 P28 K29 Q30 Y31 A32 Y33 W34 Y35 A42 V46 P54 F61 SER GLY SER S66 G67 T68 T71 L72 T73 A79 E80 D81 Y85 Q88 SER V90

D91 Y96 Q97 G102 T106 V107 L108 R109 T110 V111 V116 L136 L137 Y141 P142 R143 V147 Q148 V151 T165 E166 Q167 K170 D171 S172 L182 D186 H190 K191 V192 E196 V206 R212 G213 E214 CYS

- Molecule 3: CD99 antigen peptide

Chain F:

29%   21%   50%

GLU ASN ASP ASP PRO ARG PRO P5 N6 P7 P8 K9 P10 M11

• Molecule 3: CD99 antigen peptide

Chain E:

14%

21% 29% 50%

GLU ASN ASP ASP PRO ARG PRO P5 N6 P7 P8 K9 P10 M11

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.41Å 131.55Å 119.81Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	46.38 – 3.10 46.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.38-3.10) 97.4 (46.38-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.248 0.226 , 0.246	Depositor DCC
R_{free} test set	1847 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 8.1	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	25893	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 ⓘ

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	0/1703	0.60	0/2330
1	C	0.32	0/1703	0.61	0/2330
1	G	0.31	0/1689	0.59	0/2309
1	J	0.41	0/1657	0.66	0/2267
2	B	0.30	0/1661	0.61	0/2261
2	D	0.35	0/1661	0.62	0/2261
2	H	0.37	0/1661	0.63	0/2261
2	K	0.33	0/1595	0.61	0/2166
3	E	0.32	0/56	0.54	0/76
3	F	0.35	0/56	0.46	0/76
All	All	0.34	0/13442	0.62	0/18337

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	1660	1626	1626	31	0
1	C	1660	1626	1626	28	0
1	G	1647	1615	1613	45	0
1	J	1616	1590	1588	28	0
2	B	1625	1560	1560	28	0
2	D	1625	1560	1560	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1625	1560	1560	45	0
2	K	1564	1506	1502	37	0
3	E	53	56	56	7	0
3	F	53	56	56	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	3	0	0	0	0
4	J	1	0	0	0	0
All	All	13138	12755	12747	251	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 10.

The worst 5 of 251 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:ASN:HB2	3:E:7:PRO:HD2	1.36	1.06
2:D:93:SER:O	3:F:7:PRO:HG3	1.76	0.86
1:J:24:ILE:HD12	1:J:24:ILE:O	1.79	0.82
1:G:4:LEU:HD21	1:G:99:CYS:SG	2.19	0.82
1:G:107:GLY:HA2	2:H:33:TYR:HE2	1.45	0.81

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	219/247 (89%)	202 (92%)	16 (7%)	1 (0%)	29	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	219/247 (89%)	198 (90%)	21 (10%)	0	100	100
1	G	215/247 (87%)	195 (91%)	19 (9%)	1 (0%)	29	64
1	J	207/247 (84%)	180 (87%)	26 (13%)	1 (0%)	29	64
2	B	212/215 (99%)	193 (91%)	17 (8%)	2 (1%)	17	52
2	D	212/215 (99%)	191 (90%)	20 (9%)	1 (0%)	29	64
2	H	212/215 (99%)	184 (87%)	23 (11%)	5 (2%)	6	27
2	K	193/215 (90%)	167 (86%)	22 (11%)	4 (2%)	7	30
3	E	5/14 (36%)	1 (20%)	4 (80%)	0	100	100
3	F	5/14 (36%)	4 (80%)	1 (20%)	0	100	100
All	All	1699/1876 (91%)	1515 (89%)	169 (10%)	15 (1%)	17	52

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
2	B	191	LYS
2	H	147	VAL
2	H	189	LYS
2	K	3	VAL

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	191/212 (90%)	190 (100%)	1 (0%)	88	94
1	C	191/212 (90%)	187 (98%)	4 (2%)	53	79
1	G	189/212 (89%)	187 (99%)	2 (1%)	73	89
1	J	188/212 (89%)	184 (98%)	4 (2%)	53	79
2	B	183/184 (100%)	180 (98%)	3 (2%)	62	84
2	D	183/184 (100%)	180 (98%)	3 (2%)	62	84
2	H	183/184 (100%)	179 (98%)	4 (2%)	52	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	175/184 (95%)	173 (99%)	2 (1%)	73	89
3	E	7/14 (50%)	7 (100%)	0	100	100
3	F	7/14 (50%)	7 (100%)	0	100	100
All	All	1497/1612 (93%)	1474 (98%)	23 (2%)	65	85

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	53	ARG
1	J	22	CYS
2	H	123	ASP
1	J	52	TRP
2	D	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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(Å²)	Q<0.9
1	A	221/247 (89%)	0.02	3 (1%)	75	56	34, 55, 101, 141	0
1	C	221/247 (89%)	-0.07	0	100	100	32, 44, 82, 113	0
1	G	219/247 (88%)	0.13	1 (0%)	91	81	33, 63, 108, 135	0
1	J	213/247 (86%)	0.30	11 (5%)	27	12	34, 73, 131, 153	0
2	B	214/215 (99%)	0.20	5 (2%)	60	39	41, 73, 114, 159	0
2	D	214/215 (99%)	0.10	0	100	100	34, 61, 85, 126	0
2	H	214/215 (99%)	0.12	1 (0%)	91	81	35, 80, 113, 138	0
2	K	203/215 (94%)	0.33	9 (4%)	34	17	40, 82, 136, 181	0
3	E	7/14 (50%)	1.60	2 (28%)	0	0	55, 67, 110, 122	0
3	F	7/14 (50%)	0.37	0	100	100	60, 61, 72, 72	0
All	All	1733/1876 (92%)	0.15	32 (1%)	68	47	32, 66, 117, 181	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	36	TRP	4.5
3	E	6	ASN	4.4
2	K	32	ALA	4.2
1	J	2	VAL	3.8
3	E	5	PRO	3.6

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.