



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:52 AM UTC

PDB ID : 7SFX / pdb_00007sfx
Title : 10A1 Fab in complex with CD99 peptide
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Deposited on : 2021-10-04
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

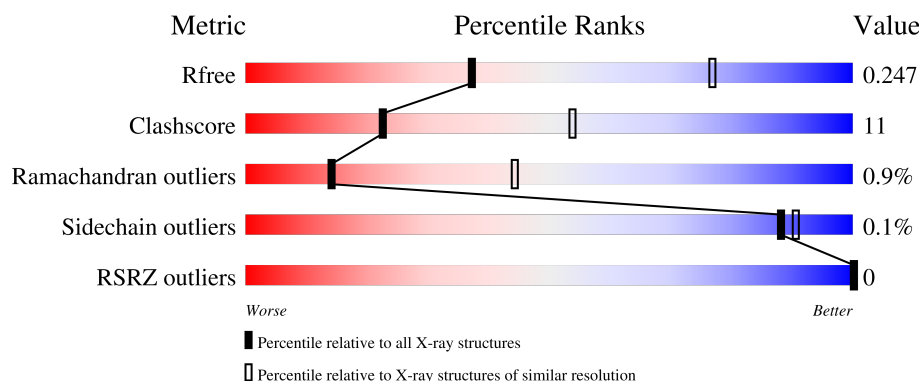
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	247	 71% 18% 11%
1	C	247	 72% 17% 11%
1	G	247	 70% 18% 11%
1	J	247	 67% 19% 14%
2	B	215	 81% 18% .

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Mol	Chain	Length	Quality of chain
2	D	215	 86% 13%
2	H	215	 72% 26%
2	K	215	 69% 24% 6%
3	E	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	C	H	N	O	S	0	0	0
			3286	1046	1626	280	329	5			
1	A	221	Total	C	H	N	O	S	0	0	0
			3286	1046	1626	280	329	5			
1	G	219	Total	C	H	N	O	S	0	0	0
			3262	1039	1615	278	325	5			
1	J	213	Total	C	H	N	O	S	0	0	0
			3206	1023	1590	270	319	4			

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

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

- Molecule 3 is a protein called CD99 antigen peptide.

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

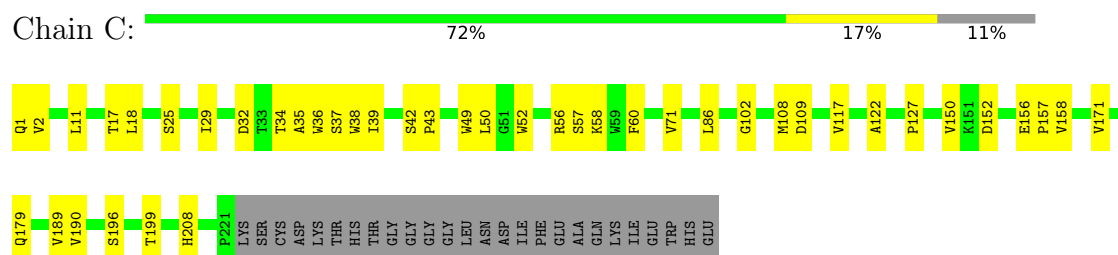
- Molecule 4 is water.

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

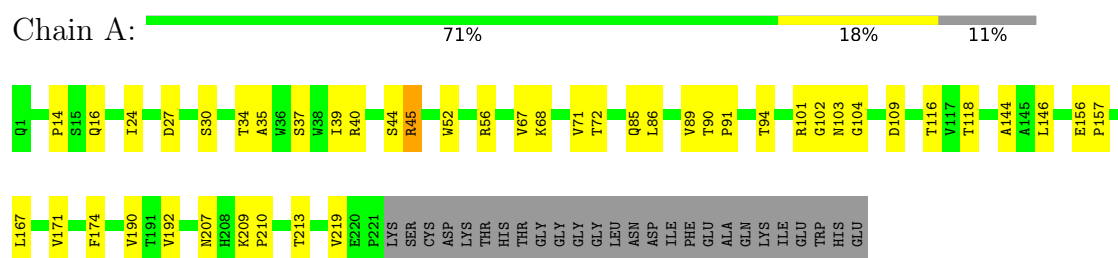
3 Residue-property plots [i](#)

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.

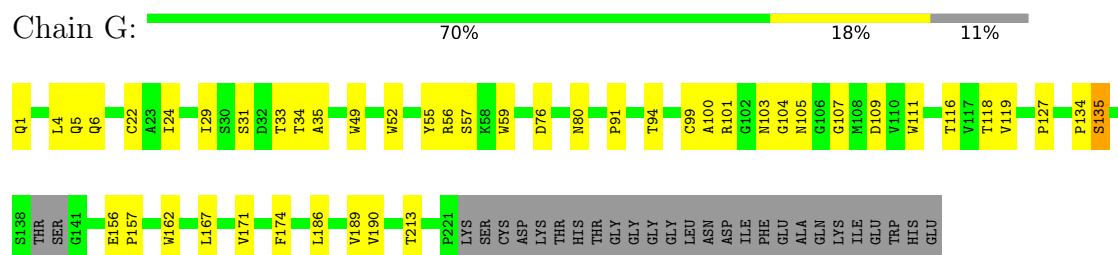
- Molecule 1: 10A1 Fab heavy chain



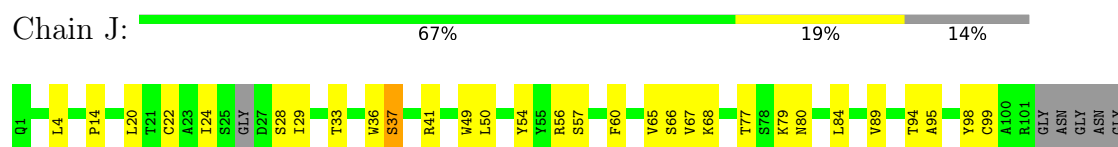
- Molecule 1: 10A1 Fab heavy chain

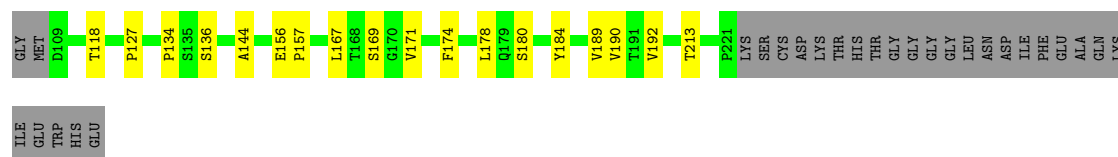


- Molecule 1: 10A1 Fab heavy chain



- Molecule 1: 10A1 Fab heavy chain





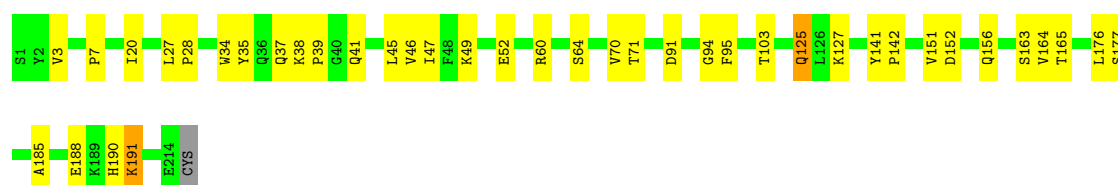
- Molecule 2: 10A1 Fab light chain

Chain D: 86% 13%



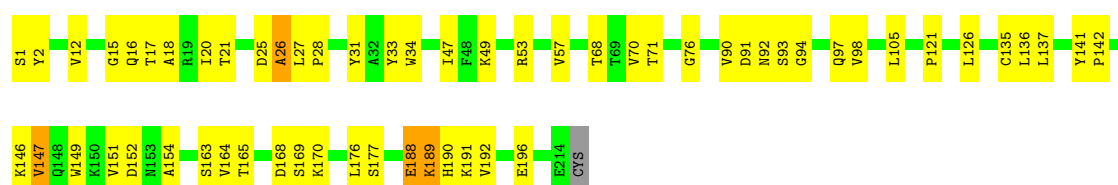
- Molecule 2: 10A1 Fab light chain

Chain B: 81% 18%



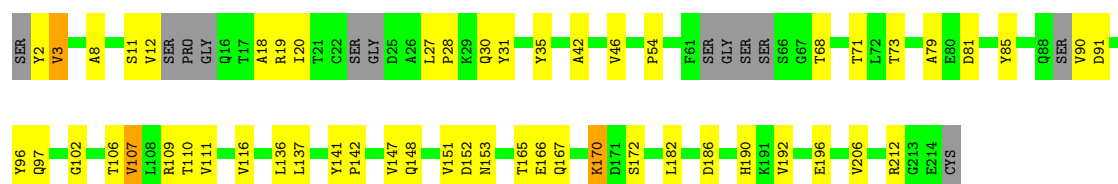
- Molecule 2: 10A1 Fab light chain

Chain H: 72% 26%



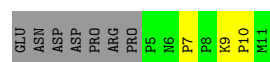
- Molecule 2: 10A1 Fab light chain

Chain K: 69% 24% 6%

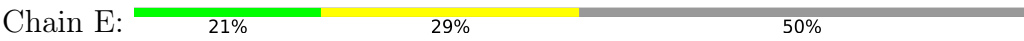


- Molecule 3: CD99 antigen peptide

Chain F: 29% 21% 50%



- Molecule 3: CD99 antigen peptide



GLU	ASN	ASP	ASP	PRO	ARG	PRO	P6	M6	P7	P8	K9	P10	R11
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4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.248 0.225 , 0.247	Depositor DCC
R_{free} test set	1847 reflections (5.00%)	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)	0.32 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	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.*

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	0.25	0/1703	0.54	0/2330
1	C	0.29	0/1703	0.57	0/2330
1	G	0.26	0/1689	0.55	0/2309
1	J	0.51	1/1657 (0.1%)	0.73	2/2267 (0.1%)
2	B	0.24	0/1661	0.58	0/2261
2	D	0.34	0/1661	0.64	0/2261
2	H	0.36	0/1661	0.66	2/2261 (0.1%)
2	K	0.32	0/1595	0.59	0/2166
3	E	0.29	0/56	0.57	0/76
3	F	0.36	0/56	0.62	0/76
All	All	0.33	1/13442 (0.0%)	0.61	4/18337 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	37	SER	N-CA	5.01	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	GLU	N-CA-C	-6.59	101.84	110.53
2	H	190	HIS	CA-C-O	-6.35	113.69	120.92
1	J	36	TRP	CA-C-O	-5.74	114.77	120.80
1	J	33	THR	N-CA-C	-5.62	104.55	111.75

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	33	0
1	C	1660	1626	1626	33	0
1	G	1647	1615	1613	46	0
1	J	1616	1590	1588	32	0
2	B	1625	1560	1560	31	0
2	D	1625	1560	1560	24	0
2	H	1625	1560	1560	49	0
2	K	1564	1506	1502	40	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	272	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 11.

The worst 5 of 272 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%)	24	57
1	C	219/247 (89%)	198 (90%)	21 (10%)	0	100	100
1	G	215/247 (87%)	195 (91%)	19 (9%)	1 (0%)	24	57
1	J	207/247 (84%)	180 (87%)	26 (13%)	1 (0%)	24	57
2	B	212/215 (99%)	193 (91%)	17 (8%)	2 (1%)	14	44
2	D	212/215 (99%)	191 (90%)	20 (9%)	1 (0%)	24	57
2	H	212/215 (99%)	184 (87%)	23 (11%)	5 (2%)	4	22
2	K	193/215 (90%)	167 (86%)	22 (11%)	4 (2%)	5	25
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%)	14	44

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%)	191 (100%)	0	100	100
1	C	191/212 (90%)	191 (100%)	0	100	100
1	G	189/212 (89%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	188/212 (89%)	187 (100%)	1 (0%)	81	85
2	B	183/184 (100%)	183 (100%)	0	100	100
2	D	183/184 (100%)	182 (100%)	1 (0%)	81	85
2	H	183/184 (100%)	183 (100%)	0	100	100
2	K	175/184 (95%)	175 (100%)	0	100	100
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%)	1495 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	31	TYR
1	J	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	16	GLN
2	K	97	GLN
2	K	156	GLN
2	K	148	GLN
1	G	212	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	221/247 (89%)	-1.14	0 100 100	35, 61, 110, 153	0
1	C	221/247 (89%)	-1.23	0 100 100	33, 48, 89, 127	0
1	G	219/247 (88%)	-1.13	0 100 100	34, 68, 119, 149	0
1	J	213/247 (86%)	-1.09	0 100 100	36, 80, 143, 169	0
2	B	214/215 (99%)	-1.05	0 100 100	45, 81, 126, 182	0
2	D	214/215 (99%)	-1.20	0 100 100	36, 67, 91, 139	0
2	H	214/215 (99%)	-1.03	0 100 100	37, 87, 125, 151	0
2	K	203/215 (94%)	-0.96	0 100 100	45, 91, 148, 196	0
3	E	7/14 (50%)	-0.84	0 100 100	53, 69, 109, 123	0
3	F	7/14 (50%)	-1.27	0 100 100	58, 60, 70, 71	0
All	All	1733/1876 (92%)	-1.10	0 100 100	33, 73, 128, 196	0

There are no RSRZ outliers to report.

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.