wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 06:47 pm BST

PDB ID	:	5XOV
Title	:	Crystal structure of peptide-HLA-A24 bound to S19-2 V-delta/V-beta TCR
Authors	:	Shi, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2017-05-31
Resolution	:	2.68 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.68 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.
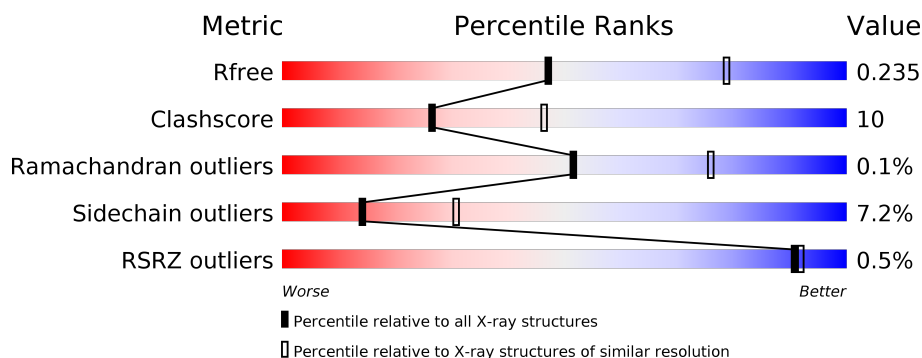
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 on 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	274	75% 25%
1	D	274	% 73% 25% •
2	B	100	2% 77% 19% •
2	E	100	2% 79% 17% •
3	C	10	40% 60%
3	F	10	50% 50%

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Mol	Chain	Length	Quality of chain
4	G	207	73% 23%
4	I	207	76% 18% 5%
5	H	245	79% 19%
5	J	245	% 80% 16%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13812 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 HLA class I histocompatibility antigen, A-24 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2221	C 1382	N 403	O 426	S 10	0	0	0
1	D	274	Total 2221	C 1382	N 403	O 426	S 10	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total 836	C 533	N 141	O 158	S 4	0	0	0
2	E	100	Total 836	C 533	N 141	O 158	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called HIV-1 Nef138-10 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total 91	C 64	N 14	O 12	S 1	0	0	0
3	F	10	Total 91	C 64	N 14	O 12	S 1	0	0	0

- Molecule 4 is a protein called V-delta chain of T cell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	207	Total 1631	C 1033	N 270	O 319	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	207	Total 1631	C 1033	N 270	O 319	S 9	0	0	0

- Molecule 5 is a protein called V-beta chain of T cell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	245	Total 1929	C 1229	N 330	O 365	S 5	0	0	0
5	H	245	Total 1929	C 1229	N 330	O 365	S 5	0	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total 47	O 47	0	0
6	B	24	Total 24	O 24	0	0
6	C	5	Total 5	O 5	0	0
6	D	49	Total 49	O 49	0	0
6	E	23	Total 23	O 23	0	0
6	F	2	Total 2	O 2	0	0
6	I	58	Total 58	O 58	0	0
6	J	57	Total 57	O 57	0	0
6	G	68	Total 68	O 68	0	0
6	H	63	Total 63	O 63	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
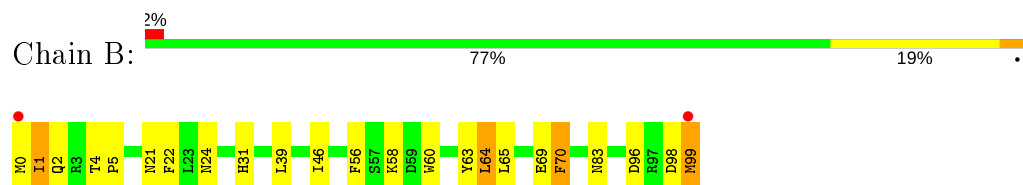
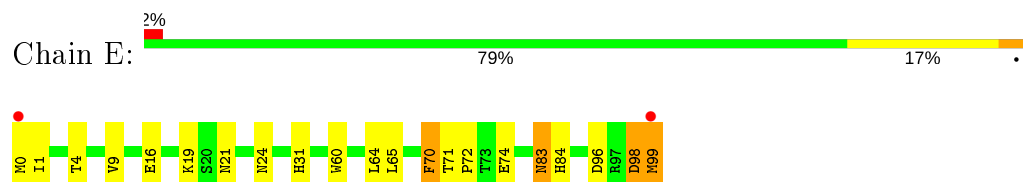- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain
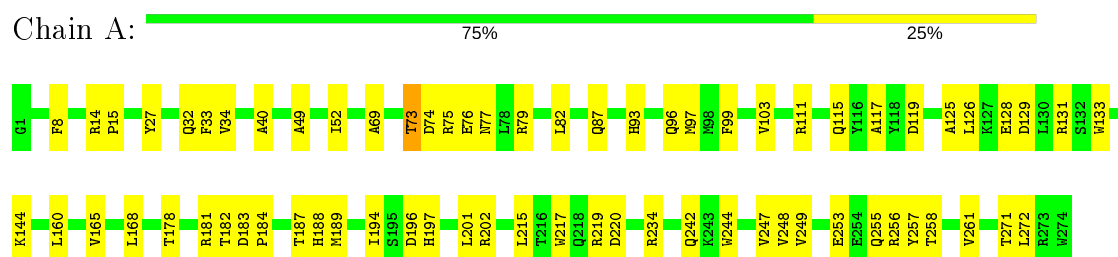
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain
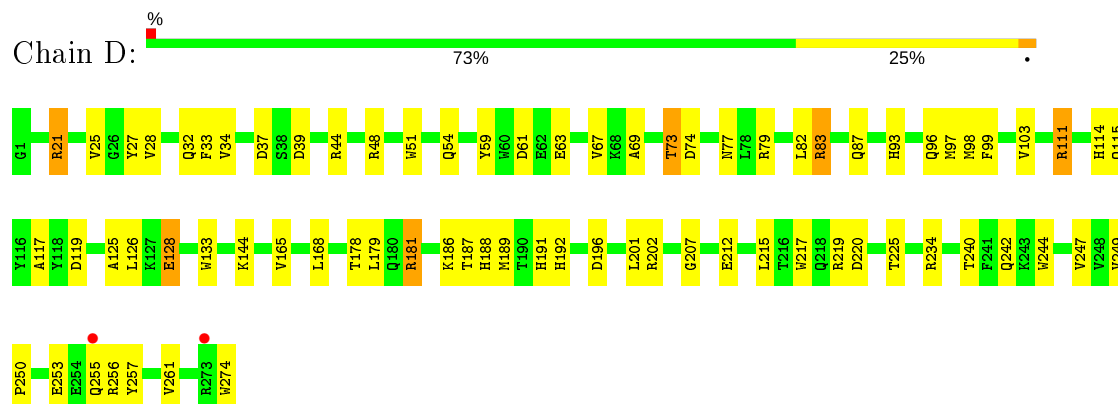
- Molecule 2: Beta-2-microglobulin

- Molecule 2: Beta-2-microglobulin

• Molecule 3: HIV-1 Nef138-10 peptide

Chain C:
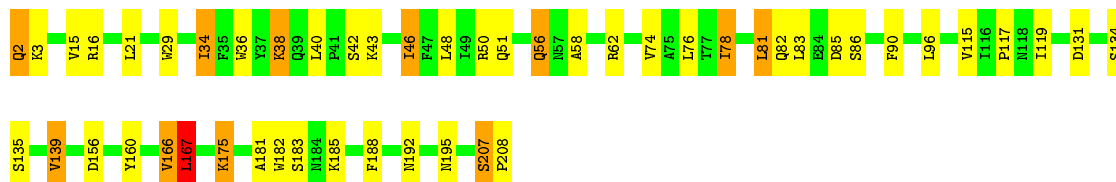

• Molecule 3: HIV-1 Nef138-10 peptide

Chain F:

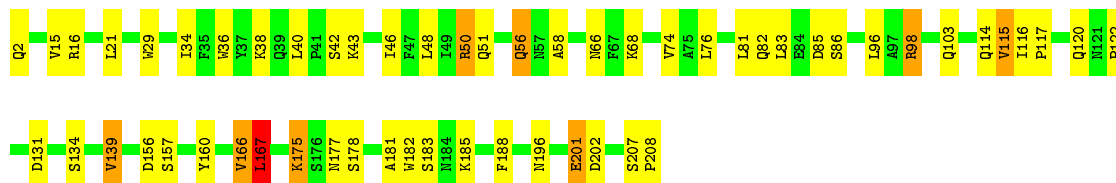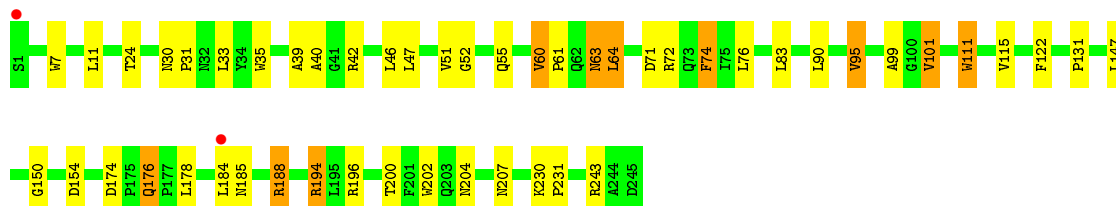• Molecule 4: V-delta chain of T cell receptor

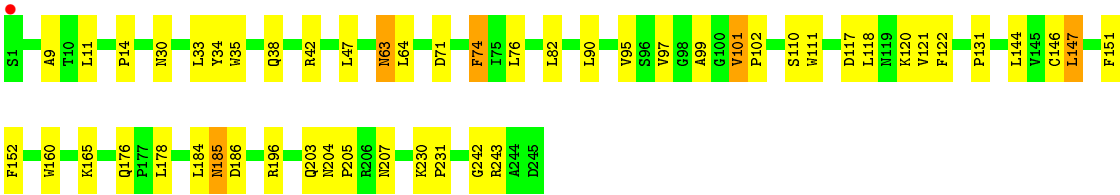Chain I:

• Molecule 4: V-delta chain of T cell receptor

Chain G:

• Molecule 5: V-beta chain of T cell receptor

Chain J:

• Molecule 5: V-beta chain of T cell receptor

Chain H:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.99Å 73.79Å 163.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.68 40.31 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.00-2.68) 99.7 (40.31-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.203 , 0.245 0.195 , 0.235	Depositor DCC
R_{free} test set	3462 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.9	EDS
L-test for twinning[2]	$<|L|>$ = 0.51, $<L^2>$ = 0.34	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13812	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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	0.28	0/2281	0.45	0/3092
1	D	0.29	0/2281	0.48	0/3092
2	B	0.30	0/859	0.47	0/1162
2	E	0.29	0/859	0.46	0/1162
3	C	0.31	0/96	0.42	0/130
3	F	0.34	0/96	0.45	0/130
4	G	0.31	0/1667	0.50	1/2256 (0.0%)
4	I	0.31	0/1667	0.49	1/2256 (0.0%)
5	H	0.30	0/1985	0.47	0/2713
5	J	0.29	0/1985	0.47	0/2713
All	All	0.30	0/13776	0.47	2/18706 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	167	LEU	CA-CB-CG	6.05	129.22	115.30
4	G	167	LEU	CA-CB-CG	5.13	127.11	115.30

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	2221	0	2082	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2221	0	2082	62	0
2	B	836	0	803	15	0
2	E	836	0	803	15	0
3	C	91	0	85	5	0
3	F	91	0	85	7	0
4	G	1631	0	1587	38	0
4	I	1631	0	1587	42	0
5	H	1929	0	1853	40	0
5	J	1929	0	1853	33	0
6	A	47	0	0	3	0
6	B	24	0	0	0	0
6	C	5	0	0	2	0
6	D	49	0	0	2	0
6	E	23	0	0	0	0
6	F	2	0	0	1	0
6	G	68	0	0	4	0
6	H	63	0	0	1	0
6	I	58	0	0	3	0
6	J	57	0	0	2	0
All	All	13812	0	12820	271	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 271 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)
5:H:117:ASP:HB3	5:H:120:LYS:HD3	1.32	1.10
1:D:83:ARG:HH11	1:D:83:ARG:HG2	1.26	0.97
1:A:76:GLU:HG2	6:A:343:HOH:O	1.68	0.92
4:G:50:ARG:HH22	5:H:101:VAL:HG21	1.32	0.91
6:A:343:HOH:O	3:C:9:CYS:SG	2.29	0.90

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	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	E	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	F	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	G	205/207 (99%)	197 (96%)	8 (4%)	0	100	100
4	I	205/207 (99%)	193 (94%)	10 (5%)	2 (1%)	15	34
5	H	243/245 (99%)	233 (96%)	10 (4%)	0	100	100
5	J	243/245 (99%)	233 (96%)	10 (4%)	0	100	100
All	All	1652/1672 (99%)	1588 (96%)	62 (4%)	2 (0%)	51	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	207	SER
4	I	81	LEU

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	230/230 (100%)	220 (96%)	10 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	230/230 (100%)	218 (95%)	12 (5%)	23	46
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	29
2	E	95/95 (100%)	87 (92%)	8 (8%)	11	22
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
4	G	184/184 (100%)	165 (90%)	19 (10%)	7	15
4	I	184/184 (100%)	167 (91%)	17 (9%)	9	19
5	H	212/212 (100%)	201 (95%)	11 (5%)	23	46
5	J	212/212 (100%)	191 (90%)	21 (10%)	8	16
All	All	1460/1460 (100%)	1355 (93%)	105 (7%)	14	31

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	83	LEU
5	J	60	VAL
5	H	63	ASN
4	I	96	LEU
4	I	175	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	2	GLN
4	I	196	ASN
5	H	63	ASN
4	I	51	GLN
4	I	150	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 (i)

There are no carbohydrates 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	274/274 (100%)	-0.02	0 100	100	34, 51, 78, 101	0
1	D	274/274 (100%)	-0.00	2 (0%) 87	88	35, 50, 78, 104	0
2	B	100/100 (100%)	-0.08	2 (2%) 65	65	37, 53, 75, 88	0
2	E	100/100 (100%)	-0.05	2 (2%) 65	65	36, 53, 76, 83	0
3	C	10/10 (100%)	-0.03	0 100	100	37, 39, 44, 44	0
3	F	10/10 (100%)	0.04	0 100	100	37, 39, 44, 45	0
4	G	207/207 (100%)	-0.01	0 100	100	37, 49, 79, 92	0
4	I	207/207 (100%)	-0.01	0 100	100	37, 49, 78, 91	0
5	H	245/245 (100%)	-0.05	1 (0%) 92	93	37, 48, 71, 89	0
5	J	245/245 (100%)	-0.06	2 (0%) 86	86	35, 48, 71, 83	0
All	All	1672/1672 (100%)	-0.03	9 (0%) 91	92	34, 50, 76, 104	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	MET	4.3
2	E	0	MET	4.1
5	J	1	SER	3.6
2	E	99	MET	3.1
2	B	99	MET	2.5

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 (i)

There are no carbohydrates 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.