wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 02:53 PM EDT

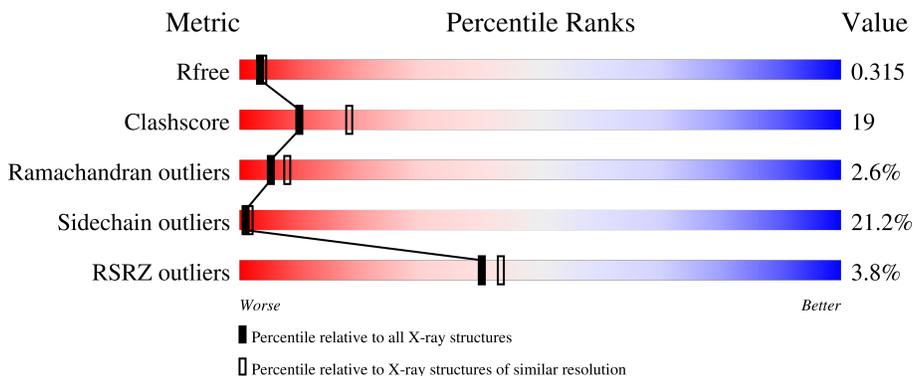|		
PDB ID	:	1V7M
Title	:	Human Thrombopoietin Functional Domain Complexed To Neutralizing Antibody TN1 Fab
Authors	:	Feese, M.D.; Tamada, T.; Kato, Y.; Maeda, Y.; Hirose, M.; Matsukura, Y.; Shigematsu, H.; Kato, T.; Miyazaki, H.; Kuroki, R.
Deposited on	:	2003-12-18
Resolution	:	2.51 Å(reported)

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 2.51 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		0.315
Clashscore		19
Ramachandran outliers		2.6%
Sidechain outliers		21.2%
RSRZ outliers		3.8%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	L	213	70% 23% 6%
1	M	213	62% 32% 5%
2	H	217	% 55% 35% 9% ·
2	I	217	% 61% 29% 9%
3	V	163	15% 45% 30% 12% · 11%

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Mol	Chain	Length	Quality of chain
3	X	163	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8902 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 Monoclonal TN1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total 1632	C 1015	N 277	O 332	S 8	0	0	0
1	M	212	Total 1632	C 1015	N 277	O 332	S 8	0	0	0

- Molecule 2 is a protein called Monoclonal TN1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total 1643	C 1038	N 273	O 324	S 8	0	0	0
2	I	217	Total 1643	C 1038	N 273	O 324	S 8	0	0	0

- Molecule 3 is a protein called Thrombopoietin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	145	Total 1098	C 699	N 196	O 196	S 7	0	0	0
3	X	145	Total 1098	C 699	N 196	O 196	S 7	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	27	Total 27	O 27	0	0
4	H	35	Total 35	O 35	0	0
4	V	12	Total 12	O 12	0	0
4	M	36	Total 36	O 36	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	33	Total 33	O 33	0	0
4	X	13	Total 13	O 13	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.
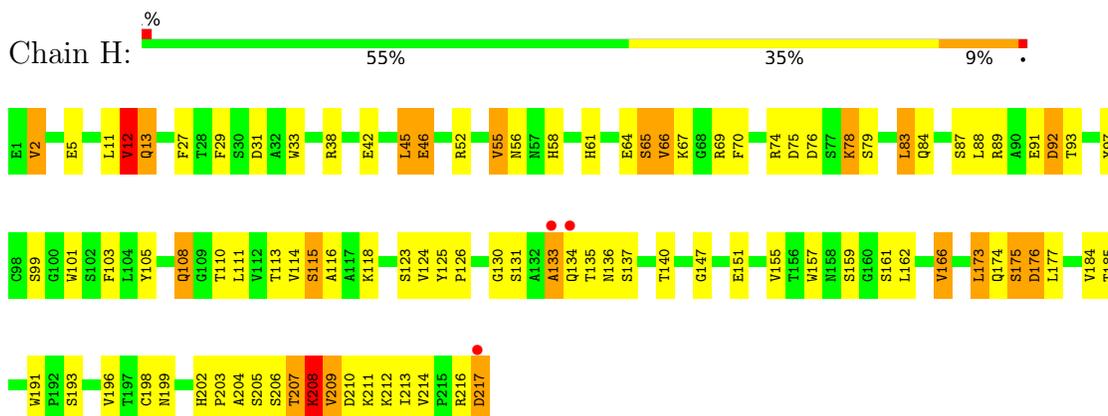
• Molecule 1: Monoclonal TN1 Fab Light Chain
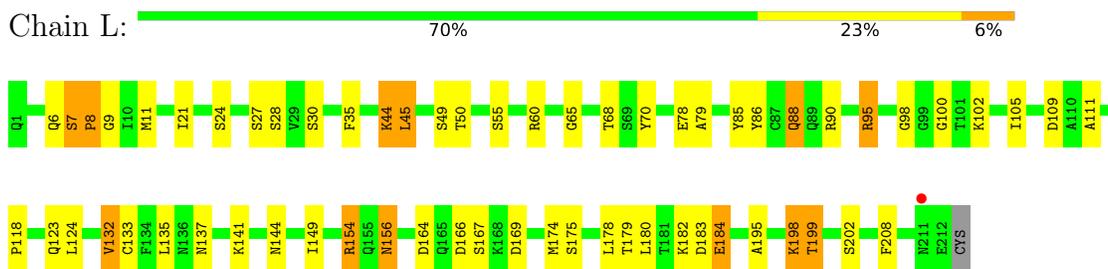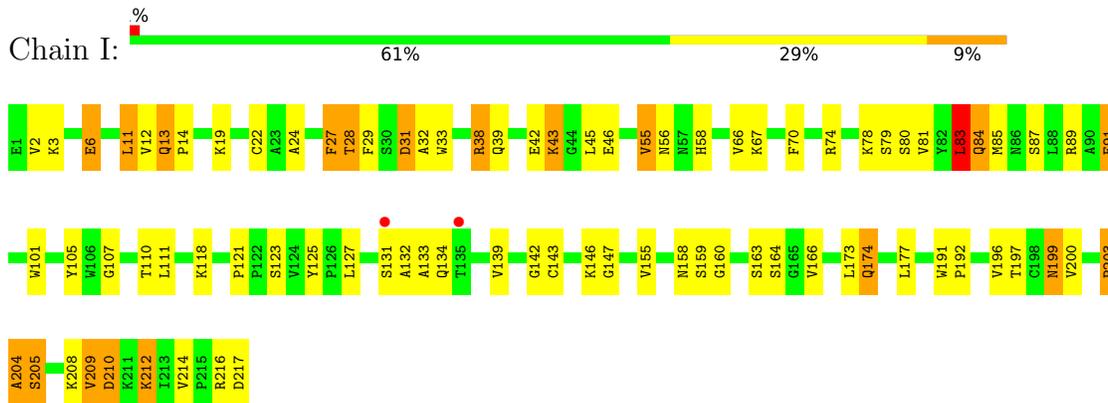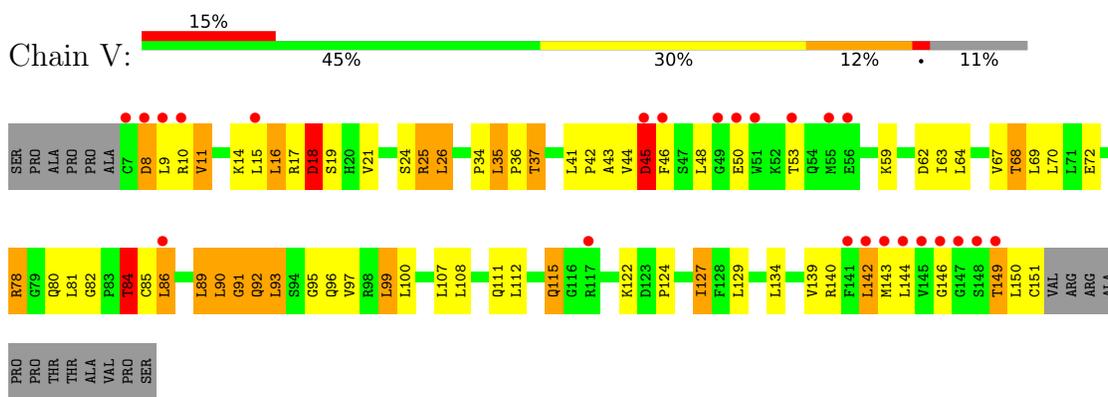

• Molecule 1: Monoclonal TN1 Fab Light Chain
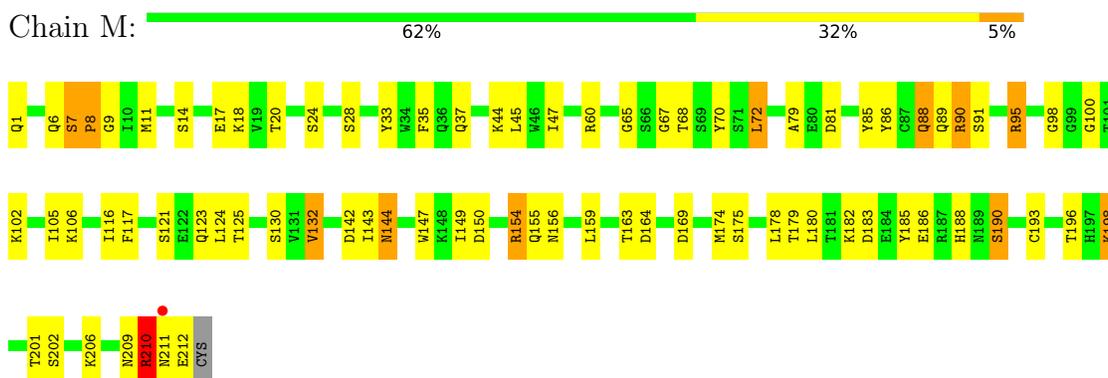
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

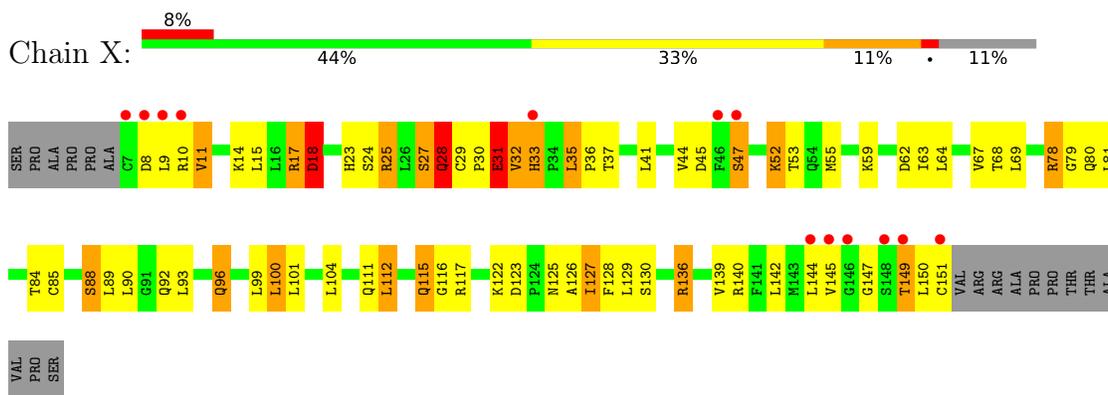• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain I:

• Molecule 3: Thrombopoietin

Chain V:

• Molecule 3: Thrombopoietin

Chain X:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.10Å 46.77Å 185.15Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	45.28 – 2.51 45.28 – 2.51	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.28-2.51) 92.8 (45.28-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.228 , 0.316 0.230 , 0.315	Depositor DCC
R_{free} test set	1852 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.9	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8902	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2117e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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	L	0.91	1/1670 (0.1%)	1.07	9/2266 (0.4%)
1	M	0.98	1/1670 (0.1%)	1.11	10/2266 (0.4%)
2	H	0.98	1/1687 (0.1%)	1.13	14/2302 (0.6%)
2	I	0.96	2/1687 (0.1%)	1.05	4/2302 (0.2%)
3	V	0.79	0/1117	1.05	4/1515 (0.3%)
3	X	0.81	0/1117	1.01	3/1515 (0.2%)
All	All	0.92	5/8948 (0.1%)	1.08	44/12166 (0.4%)

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
2	H	0	1
3	X	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	184	GLU	CD-OE2	6.08	1.32	1.25
1	M	147	TRP	CB-CG	-5.46	1.40	1.50
2	H	208	LYS	CD-CE	5.18	1.64	1.51
2	I	55	VAL	CB-CG2	5.14	1.63	1.52
2	I	43	LYS	CD-CE	5.12	1.64	1.51

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	62	ASP	CB-CG-OD2	8.94	126.34	118.30
3	X	62	ASP	CB-CG-OD2	8.79	126.21	118.30
2	H	31	ASP	CB-CG-OD2	8.54	125.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	109	ASP	CB-CG-OD2	8.18	125.67	118.30
1	M	60	ARG	NE-CZ-NH2	-7.89	116.36	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	203	PRO	Peptide
3	X	33	HIS	Peptide

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	L	1632	0	1568	44	0
1	M	1632	0	1568	52	0
2	H	1643	0	1594	61	0
2	I	1643	0	1594	93	0
3	V	1098	0	1152	45	0
3	X	1098	0	1152	54	0
4	H	35	0	0	10	0
4	I	33	0	0	22	0
4	L	27	0	0	8	0
4	M	36	0	0	12	0
4	V	12	0	0	7	0
4	X	13	0	0	7	0
All	All	8902	0	8628	332	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 19.

The worst 5 of 332 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)
2:I:11:LEU:HG	4:I:227:HOH:O	1.20	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:85:CYS:HA	4:X:173:HOH:O	1.17	1.30
1:M:8:PRO:HD2	4:M:241:HOH:O	1.17	1.27
2:I:209:VAL:HG12	4:I:231:HOH:O	1.19	1.27
2:H:209:VAL:HG23	4:H:228:HOH:O	1.18	1.26

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	L	210/213 (99%)	201 (96%)	7 (3%)	2 (1%)	15	28
1	M	210/213 (99%)	197 (94%)	9 (4%)	4 (2%)	8	13
2	H	215/217 (99%)	197 (92%)	13 (6%)	5 (2%)	6	10
2	I	215/217 (99%)	202 (94%)	9 (4%)	4 (2%)	8	13
3	V	143/163 (88%)	116 (81%)	20 (14%)	7 (5%)	2	2
3	X	143/163 (88%)	113 (79%)	22 (15%)	8 (6%)	2	1
All	All	1136/1186 (96%)	1026 (90%)	80 (7%)	30 (3%)	5	8

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	SER
2	H	65	SER
2	H	134	GLN
2	H	137	SER
2	H	204	ALA

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	L	185/186 (100%)	156 (84%)	29 (16%)	2	4
1	M	185/186 (100%)	153 (83%)	32 (17%)	2	3
2	H	185/185 (100%)	148 (80%)	37 (20%)	1	2
2	I	185/185 (100%)	146 (79%)	39 (21%)	1	2
3	V	124/138 (90%)	86 (69%)	38 (31%)	0	0
3	X	124/138 (90%)	90 (73%)	34 (27%)	0	0
All	All	988/1018 (97%)	779 (79%)	209 (21%)	1	2

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	105	ILE
2	I	28	THR
3	X	100	LEU
1	M	144	ASN
1	M	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	158	ASN
3	X	132	GLN
2	I	199	ASN
3	X	105	GLN
3	V	92	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	L	212/213 (99%)	-0.45	1 (0%)	91	91	26, 39, 57, 75	0
1	M	212/213 (99%)	-0.40	1 (0%)	91	91	26, 39, 60, 77	0
2	H	217/217 (100%)	-0.33	3 (1%)	75	77	26, 41, 62, 86	0
2	I	217/217 (100%)	-0.30	2 (0%)	84	86	29, 42, 62, 79	0
3	V	145/163 (88%)	0.83	24 (16%)	1	1	30, 75, 112, 118	0
3	X	145/163 (88%)	0.55	13 (8%)	9	9	32, 66, 101, 116	0
All	All	1148/1186 (96%)	-0.10	44 (3%)	40	43	26, 44, 93, 118	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	144	LEU	14.8
3	X	7	CYS	9.8
3	V	7	CYS	7.9
3	V	145	VAL	6.7
3	V	46	PHE	6.2

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.