wwPDB X-ray Structure Validation Summary Report (i)

May 12, 2020 – 11:24 pm BST

PDB ID	:	3WOF
Title	:	Crystal structure of P23-45 gp39 (6-132) bound to Thermus thermophilus RNA polymerase beta-flap domain
Authors	:	Tagami, S.; Sekine, S.; Minakhin, L.; Esyunina, D.; Akasaka, R.; Shirouzu, M.; Kulbachinskiy, A.; Severinov, K.; Yokoyama, S.
Deposited on	:	2013-12-26
Resolution	:	3.30 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 (i) symbol.

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

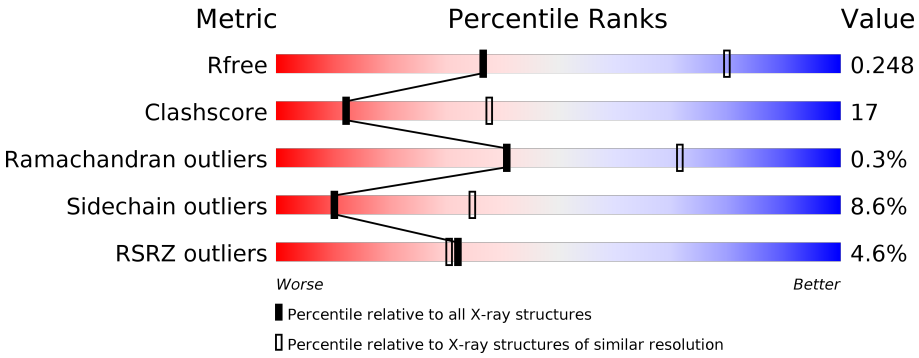
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	130	3% 60% 30% 9%
1	C	130	9% 76% 20%
1	E	130	3% 62% 28% 7%
1	G	130	2% 67% 27% 5%
1	I	130	7% 82% 13% 5%
1	K	130	8% 75% 18% 6%

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Mol	Chain	Length	Quality of chain
1	M	130	2% 66% 28% 5%
1	O	130	2% 74% 21% 5%
1	Q	130	9% 72% 22% 5%
1	S	130	5% 71% 25%
1	U	130	38% 72% 18% 7%
1	W	130	2% 70% 24% 5%
2	B	129	% 53% 23% 21%
2	D	129	% 57% 21% 20%
2	F	129	60% 17% 20%
2	H	129	57% 19% 21%
2	J	129	% 60% 16% 21%
2	L	129	60% 18% 21%
2	N	129	% 53% 24% 20%
2	P	129	58% 17% 21%
2	R	129	54% 20% 21%
2	T	129	61% 15% 21%
2	V	129	5% 60% 16% 21%
2	X	129	2% 57% 18% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22026 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 DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	0	0	0
			1009	627	191	191			
1	C	129	Total	C	N	O	0	0	0
			1009	627	191	191			
1	E	127	Total	C	N	O	0	0	0
			998	620	189	189			
1	G	129	Total	C	N	O	0	0	0
			1014	631	192	191			
1	I	129	Total	C	N	O	0	0	0
			1014	631	192	191			
1	K	128	Total	C	N	O	0	0	0
			1005	625	190	190			
1	M	128	Total	C	N	O	0	0	0
			1007	626	191	190			
1	O	129	Total	C	N	O	0	0	0
			1014	631	192	191			
1	Q	127	Total	C	N	O	0	0	0
			998	620	189	189			
1	S	129	Total	C	N	O	0	0	0
			1014	631	192	191			
1	U	121	Total	C	N	O	0	0	0
			949	589	180	180			
1	W	129	Total	C	N	O	0	0	0
			1014	631	192	191			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
A	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
C	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
C	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
E	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
G	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
G	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
I	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
I	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
K	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
K	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
M	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
M	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
O	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
O	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
Q	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
Q	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
S	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
S	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
U	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
U	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9
W	701	GLY	-	EXPRESSION TAG	UNP Q8RQE9
W	702	PRO	-	EXPRESSION TAG	UNP Q8RQE9

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	D	103	Total	C	N	O	S	0	0	0
			837	549	142	145	1			
2	F	103	Total	C	N	O	S	0	0	0
			837	549	142	145	1			
2	H	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	J	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	L	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	N	103	Total	C	N	O	S	0	0	0
			837	549	142	145	1			
2	P	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	R	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	T	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			
2	X	102	Total	C	N	O	S	0	0	0
			830	544	141	144	1			

There are 24 discrepancies between the modelled and reference sequences:

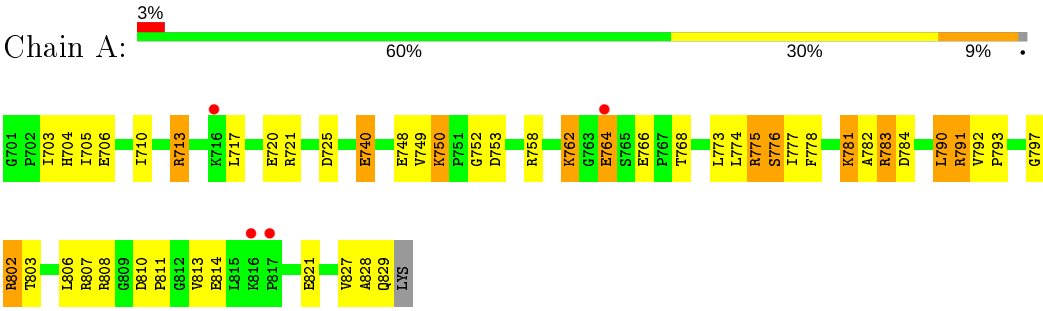
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLY	-	EXPRESSION TAG	UNP A7XX65
B	5	PRO	-	EXPRESSION TAG	UNP A7XX65
D	4	GLY	-	EXPRESSION TAG	UNP A7XX65
D	5	PRO	-	EXPRESSION TAG	UNP A7XX65
F	4	GLY	-	EXPRESSION TAG	UNP A7XX65
F	5	PRO	-	EXPRESSION TAG	UNP A7XX65
H	4	GLY	-	EXPRESSION TAG	UNP A7XX65
H	5	PRO	-	EXPRESSION TAG	UNP A7XX65
J	4	GLY	-	EXPRESSION TAG	UNP A7XX65
J	5	PRO	-	EXPRESSION TAG	UNP A7XX65
L	4	GLY	-	EXPRESSION TAG	UNP A7XX65
L	5	PRO	-	EXPRESSION TAG	UNP A7XX65
N	4	GLY	-	EXPRESSION TAG	UNP A7XX65
N	5	PRO	-	EXPRESSION TAG	UNP A7XX65
P	4	GLY	-	EXPRESSION TAG	UNP A7XX65
P	5	PRO	-	EXPRESSION TAG	UNP A7XX65
R	4	GLY	-	EXPRESSION TAG	UNP A7XX65
R	5	PRO	-	EXPRESSION TAG	UNP A7XX65
T	4	GLY	-	EXPRESSION TAG	UNP A7XX65
T	5	PRO	-	EXPRESSION TAG	UNP A7XX65
V	4	GLY	-	EXPRESSION TAG	UNP A7XX65
V	5	PRO	-	EXPRESSION TAG	UNP A7XX65
X	4	GLY	-	EXPRESSION TAG	UNP A7XX65
X	5	PRO	-	EXPRESSION TAG	UNP A7XX65

3 Residue-property plots (i)

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.

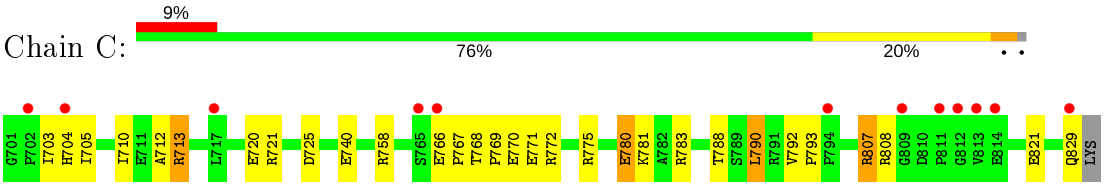
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain A:



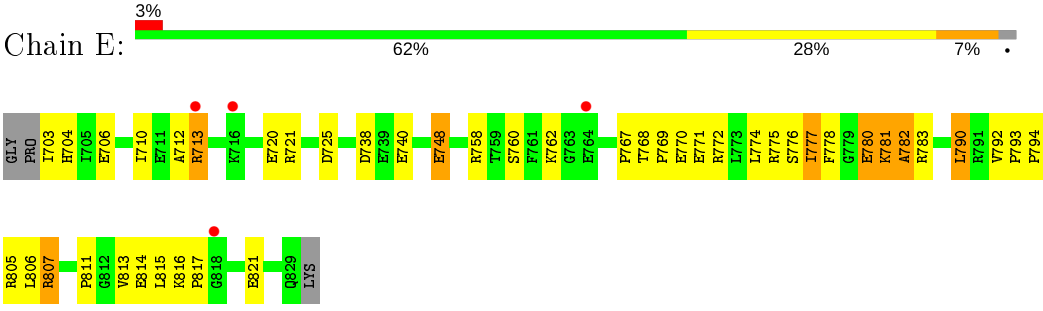
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain C:



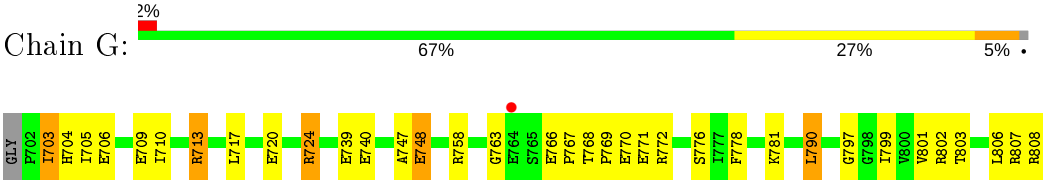
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain E:



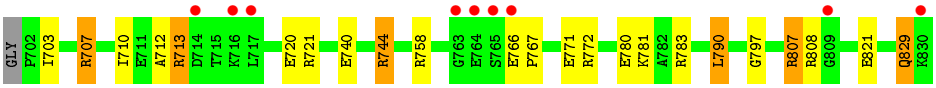
- Molecule 1: DNA-directed RNA polymerase subunit beta

Chain G:



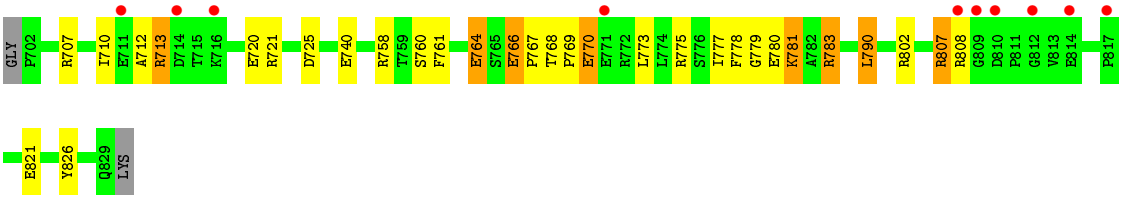
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain I:



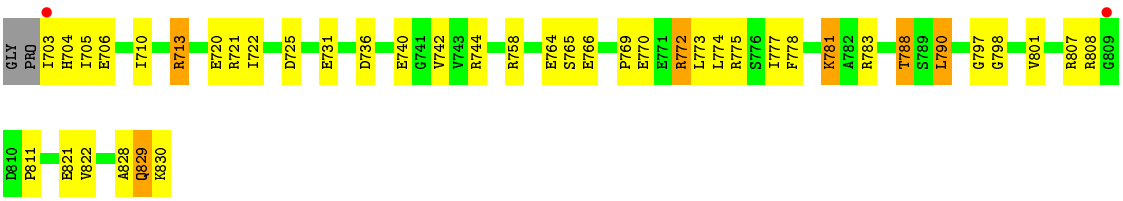
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain K:



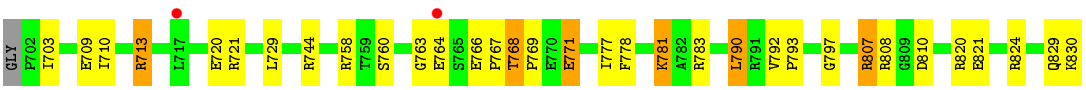
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain M:



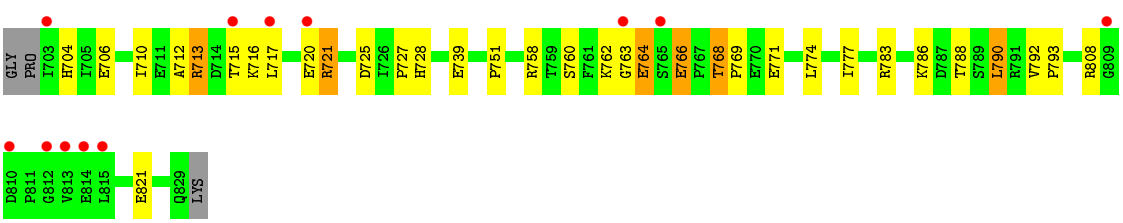
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain O:



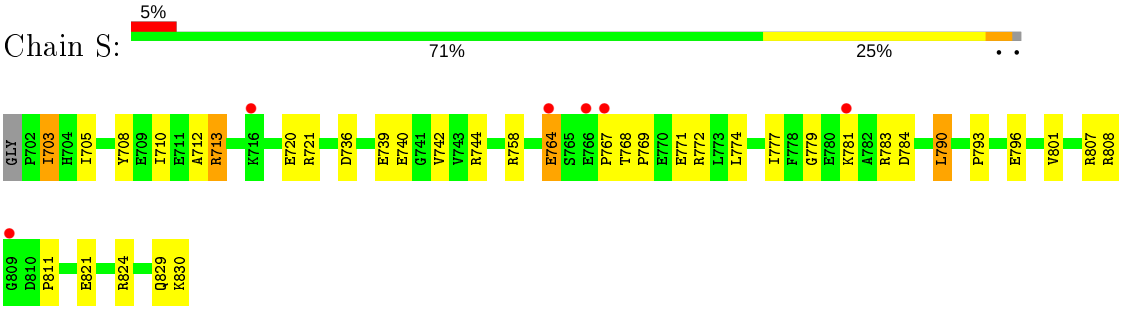
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain Q:



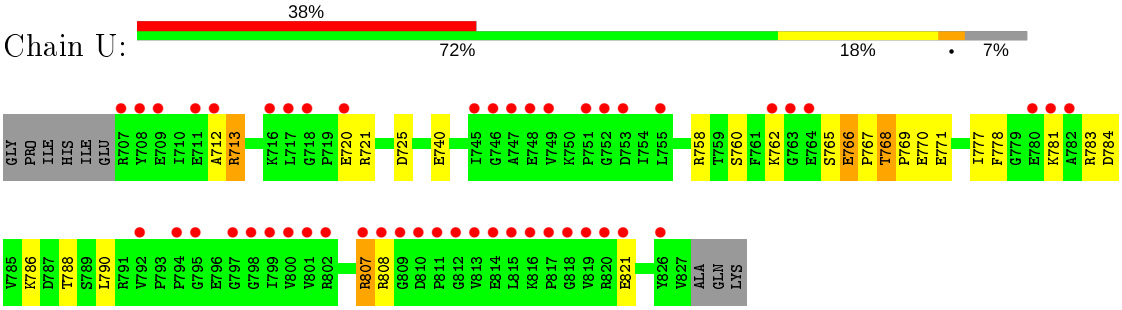
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain S:



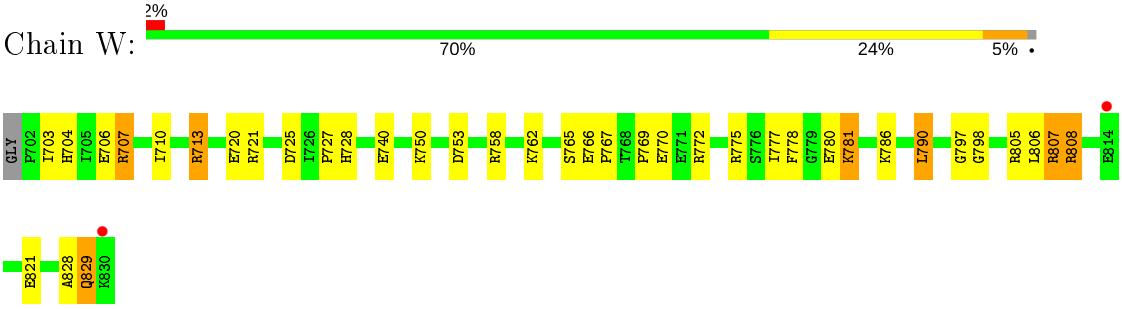
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain U:



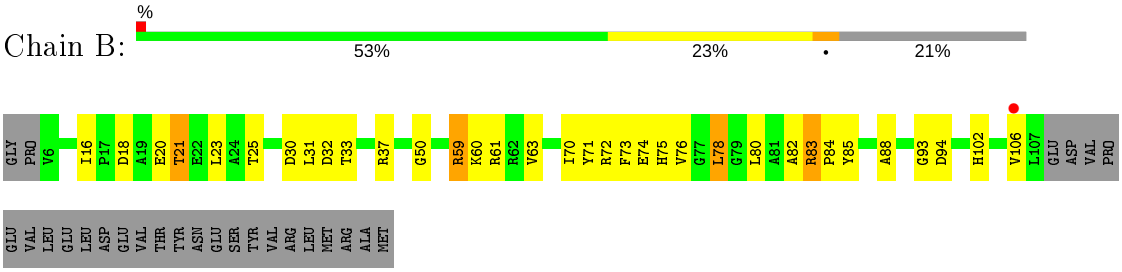
• Molecule 1: DNA-directed RNA polymerase subunit beta

Chain W:



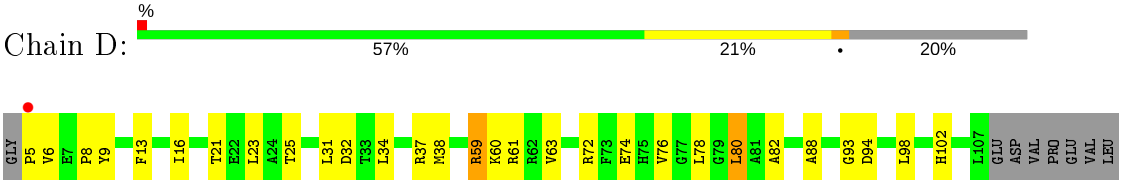
• Molecule 2: Putative uncharacterized protein

Chain B:



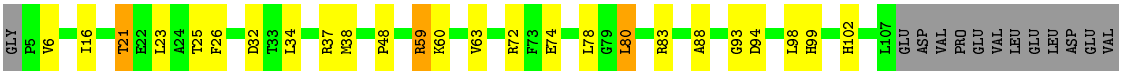
• Molecule 2: Putative uncharacterized protein

Chain D:



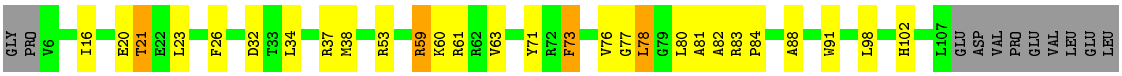
- Molecule 2: Putative uncharacterized protein

Chain F:



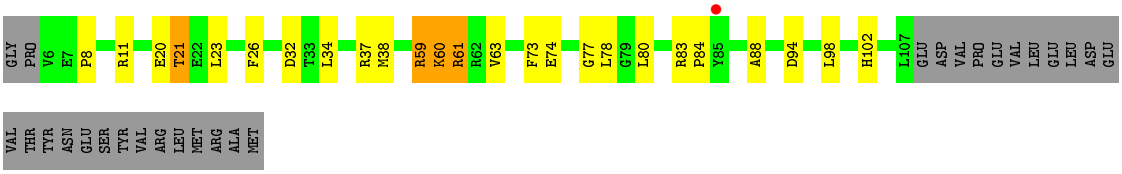
- Molecule 2: Putative uncharacterized protein

Chain H:



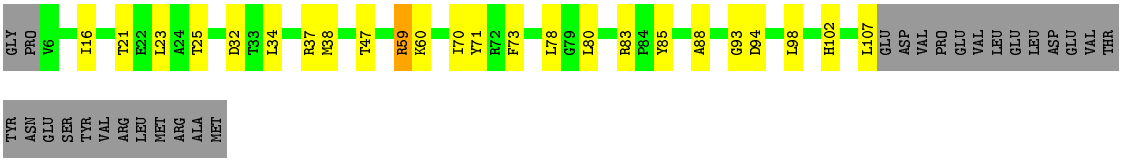
- Molecule 2: Putative uncharacterized protein

Chain J:



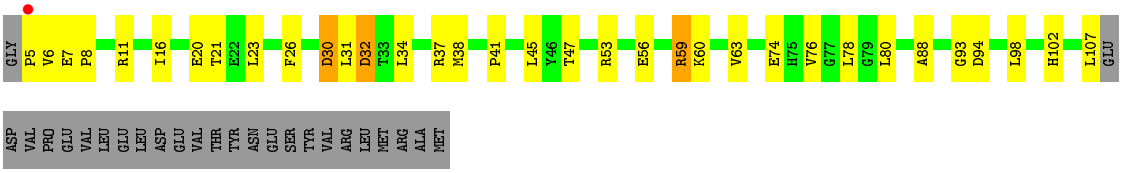
- Molecule 2: Putative uncharacterized protein

Chain L:



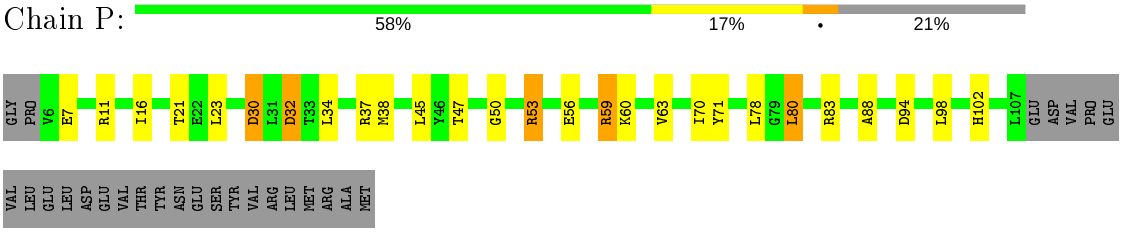
- Molecule 2: Putative uncharacterized protein

Chain N:



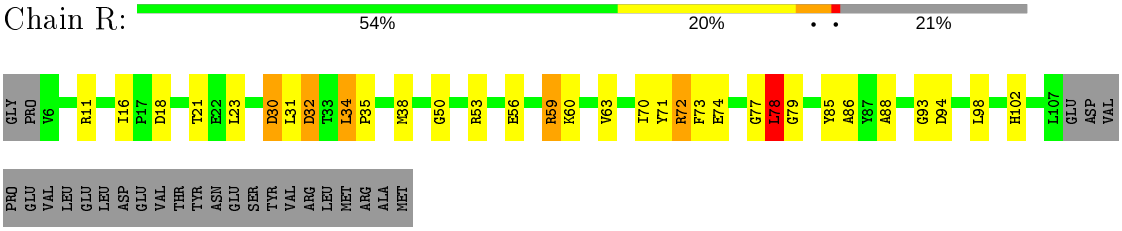
- Molecule 2: Putative uncharacterized protein

Chain P:



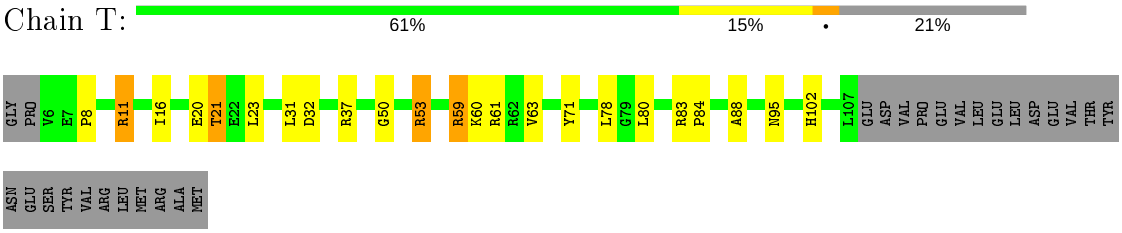
- Molecule 2: Putative uncharacterized protein

Chain R:



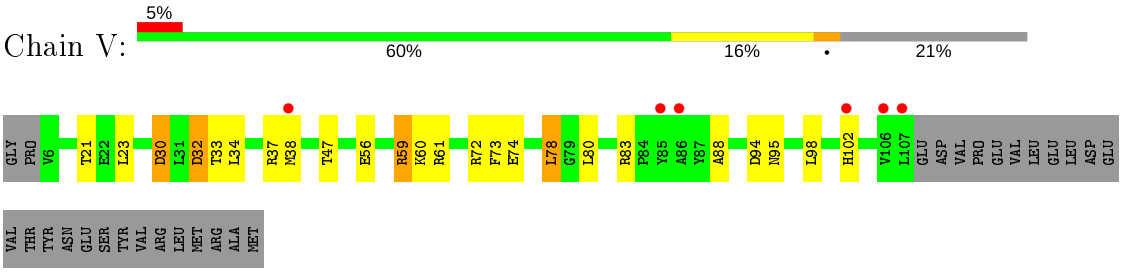
- Molecule 2: Putative uncharacterized protein

Chain T:



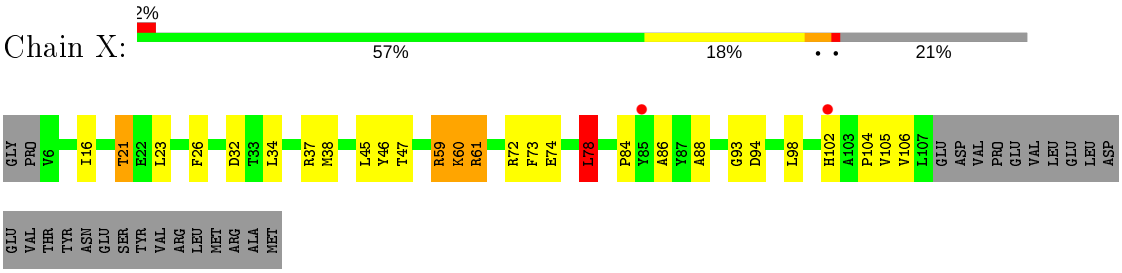
- Molecule 2: Putative uncharacterized protein

Chain V:



- Molecule 2: Putative uncharacterized protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	213.78Å 213.78Å 234.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 3.30 34.55 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.55-3.30) 99.9 (34.55-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	5.38 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.219 , 0.246 0.221 , 0.248	Depositor DCC
R_{free} test set	4107 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	68.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22026	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.46	0/1024	0.68	0/1382
1	C	0.44	0/1024	0.62	0/1382
1	E	0.48	0/1012	0.68	0/1365
1	G	0.41	0/1029	0.60	0/1387
1	I	0.40	0/1029	0.58	0/1387
1	K	0.40	0/1020	0.59	0/1376
1	M	0.42	0/1021	0.61	0/1376
1	O	0.41	0/1029	0.64	0/1387
1	Q	0.43	0/1012	0.60	0/1365
1	S	0.43	0/1029	0.65	1/1387 (0.1%)
1	U	0.40	0/962	0.62	0/1297
1	W	0.40	0/1029	0.58	0/1387
2	B	0.44	0/856	0.63	0/1169
2	D	0.42	0/864	0.60	0/1180
2	F	0.41	0/864	0.59	0/1180
2	H	0.41	0/856	0.59	0/1169
2	J	0.40	0/856	0.60	0/1169
2	L	0.39	0/856	0.61	0/1169
2	N	0.50	0/864	0.63	0/1180
2	P	0.44	0/856	0.63	0/1169
2	R	0.44	0/856	0.61	0/1169
2	T	0.43	0/856	0.60	0/1169
2	V	0.42	0/856	0.59	0/1169
2	X	0.41	0/856	0.63	1/1169 (0.1%)
All	All	0.42	0/22516	0.62	2/30539 (0.0%)

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
1	I	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	78	LEU	CA-CB-CG	6.61	130.49	115.30
1	S	779	GLY	N-CA-C	5.96	127.99	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	744	ARG	Sidechain

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	1009	0	1037	84	0
1	C	1009	0	1037	28	0
1	E	998	0	1027	47	2
1	G	1014	0	1048	66	0
1	I	1014	0	1048	17	5
1	K	1005	0	1035	32	0
1	M	1007	0	1040	47	0
1	O	1014	0	1048	23	6
1	Q	998	0	1027	33	2
1	S	1014	0	1048	56	0
1	U	949	0	979	23	0
1	W	1014	0	1048	38	0
2	B	830	0	829	56	0
2	D	837	0	837	37	0
2	F	837	0	837	32	0
2	H	830	0	829	39	0
2	J	830	0	829	38	2
2	L	830	0	829	32	0
2	N	837	0	837	69	0
2	P	830	0	829	36	0
2	R	830	0	829	45	1
2	T	830	0	829	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	830	0	829	34	0
2	X	830	0	829	55	0
All	All	22026	0	22394	751	9

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 17.

The worst 5 of 751 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:N:11:ARG:HB3	1:S:801:VAL:CG1	1.23	1.59
2:N:11:ARG:CB	1:S:801:VAL:HG11	1.38	1.51
2:R:34:LEU:CD2	2:R:35:PRO:HD2	1.53	1.39
2:H:20:GLU:HA	2:H:61:ARG:NH1	1.39	1.32
2:B:20:GLU:HA	2:B:61:ARG:NH1	1.43	1.32

The worst 5 of 9 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:Q:751:PRO:CD	2:R:11:ARG:NH2[7_555]	1.80	0.40
1:I:744:ARG:NH1	1:O:744:ARG:CZ[3_555]	1.83	0.37
1:I:744:ARG:NH2	1:O:744:ARG:NH2[3_555]	1.96	0.24
1:E:794:PRO:CB	1:Q:720:GLU:OE2[5_455]	2.00	0.20
1:I:744:ARG:NH1	1:O:744:ARG:NE[3_555]	2.00	0.20

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	127/130 (98%)	123 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
1	E	125/130 (96%)	119 (95%)	5 (4%)	1 (1%)	19	51
1	G	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
1	I	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
1	K	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
1	M	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
1	O	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	51
1	Q	125/130 (96%)	120 (96%)	4 (3%)	1 (1%)	19	51
1	S	127/130 (98%)	123 (97%)	3 (2%)	1 (1%)	19	51
1	U	119/130 (92%)	111 (93%)	8 (7%)	0	100	100
1	W	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	19	51
2	B	100/129 (78%)	99 (99%)	1 (1%)	0	100	100
2	D	101/129 (78%)	100 (99%)	1 (1%)	0	100	100
2	F	101/129 (78%)	100 (99%)	1 (1%)	0	100	100
2	H	100/129 (78%)	99 (99%)	1 (1%)	0	100	100
2	J	100/129 (78%)	100 (100%)	0	0	100	100
2	L	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
2	N	101/129 (78%)	98 (97%)	3 (3%)	0	100	100
2	P	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
2	R	100/129 (78%)	96 (96%)	3 (3%)	1 (1%)	15	46
2	T	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
2	V	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
2	X	100/129 (78%)	98 (98%)	1 (1%)	1 (1%)	15	46
All	All	2713/3108 (87%)	2636 (97%)	70 (3%)	7 (0%)	41	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	782	ALA
1	Q	763	GLY
1	S	764	GLU
2	R	78	LEU
2	X	84	PRO

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	109/110 (99%)	94 (86%)	15 (14%)	3 16
1	C	109/110 (99%)	104 (95%)	5 (5%)	27 58
1	E	108/110 (98%)	95 (88%)	13 (12%)	5 20
1	G	110/110 (100%)	101 (92%)	9 (8%)	11 36
1	I	110/110 (100%)	102 (93%)	8 (7%)	14 41
1	K	109/110 (99%)	99 (91%)	10 (9%)	9 31
1	M	109/110 (99%)	98 (90%)	11 (10%)	7 27
1	O	110/110 (100%)	100 (91%)	10 (9%)	9 31
1	Q	108/110 (98%)	100 (93%)	8 (7%)	13 40
1	S	110/110 (100%)	103 (94%)	7 (6%)	17 46
1	U	103/110 (94%)	96 (93%)	7 (7%)	16 44
1	W	110/110 (100%)	100 (91%)	10 (9%)	9 31
2	B	86/111 (78%)	78 (91%)	8 (9%)	9 30
2	D	87/111 (78%)	79 (91%)	8 (9%)	9 31
2	F	87/111 (78%)	79 (91%)	8 (9%)	9 31
2	H	86/111 (78%)	79 (92%)	7 (8%)	11 36
2	J	86/111 (78%)	78 (91%)	8 (9%)	9 30
2	L	86/111 (78%)	81 (94%)	5 (6%)	20 50
2	N	87/111 (78%)	79 (91%)	8 (9%)	9 31
2	P	86/111 (78%)	78 (91%)	8 (9%)	9 30
2	R	86/111 (78%)	78 (91%)	8 (9%)	9 30
2	T	86/111 (78%)	79 (92%)	7 (8%)	11 36
2	V	86/111 (78%)	79 (92%)	7 (8%)	11 36
2	X	86/111 (78%)	79 (92%)	7 (8%)	11 36
All	All	2340/2652 (88%)	2138 (91%)	202 (9%)	10 35

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	766	GLU
1	M	829	GLN
1	W	707	ARG
1	K	781	LYS
2	L	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	829	GLN
1	E	704	HIS
1	M	829	GLN
1	S	829	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 carbohydrates 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, 95^{th} 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	129/130 (99%)	0.11	4 (3%) 49 48	34, 63, 131, 166	0
1	C	129/130 (99%)	0.26	12 (9%) 8 9	45, 81, 147, 170	0
1	E	127/130 (97%)	0.21	4 (3%) 49 48	52, 81, 143, 162	0
1	G	129/130 (99%)	0.05	2 (1%) 72 70	30, 70, 143, 176	0
1	I	129/130 (99%)	0.53	9 (6%) 16 16	58, 101, 156, 182	0
1	K	128/130 (98%)	0.42	10 (7%) 13 12	60, 97, 145, 163	0
1	M	128/130 (98%)	0.09	2 (1%) 72 70	34, 67, 116, 142	0
1	O	129/130 (99%)	0.18	2 (1%) 72 70	51, 90, 134, 156	0
1	Q	127/130 (97%)	0.48	12 (9%) 8 9	61, 104, 155, 170	0
1	S	129/130 (99%)	0.12	6 (4%) 31 29	22, 62, 128, 183	0
1	U	121/130 (93%)	1.60	49 (40%) 0 0	84, 163, 197, 208	0
1	W	129/130 (99%)	-0.02	2 (1%) 72 70	41, 71, 121, 144	0
2	B	102/129 (79%)	-0.19	1 (0%) 82 82	26, 47, 81, 113	0
2	D	103/129 (79%)	-0.13	1 (0%) 82 82	36, 58, 93, 138	0
2	F	103/129 (79%)	-0.28	0 100 100	33, 56, 83, 123	0
2	H	102/129 (79%)	-0.16	0 100 100	35, 61, 93, 116	0
2	J	102/129 (79%)	-0.21	1 (0%) 82 82	47, 74, 98, 122	0
2	L	102/129 (79%)	-0.12	0 100 100	51, 78, 106, 128	0
2	N	103/129 (79%)	-0.23	1 (0%) 82 82	27, 44, 80, 117	0
2	P	102/129 (79%)	-0.35	0 100 100	38, 58, 82, 105	0
2	R	102/129 (79%)	-0.27	0 100 100	35, 58, 86, 115	0
2	T	102/129 (79%)	-0.29	0 100 100	31, 61, 97, 108	0
2	V	102/129 (79%)	0.26	6 (5%) 22 22	60, 101, 139, 180	0
2	X	102/129 (79%)	0.01	2 (1%) 65 64	51, 69, 106, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2761/3108 (88%)	0.11	126 (4%)	32	30	22, 73, 148, 208	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	717	LEU	6.0
1	I	764	GLU	5.8
1	U	709	GLU	5.0
1	U	815	LEU	4.9
1	I	765	SER	4.8

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 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.