



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:28 AM UTC

PDB ID : 2BTV / pdb_00002btv
Title : ATOMIC MODEL FOR BLUETONGUE VIRUS (BTV) CORE
Authors : Grimes, J.M.; Burroughs, J.N.; Gouet, P.; Diprose, J.M.; Malby, R.; Zientras, S.; Mertens, P.P.C.; Stuart, D.I.
Deposited on : 1998-09-05
Resolution : 3.50 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

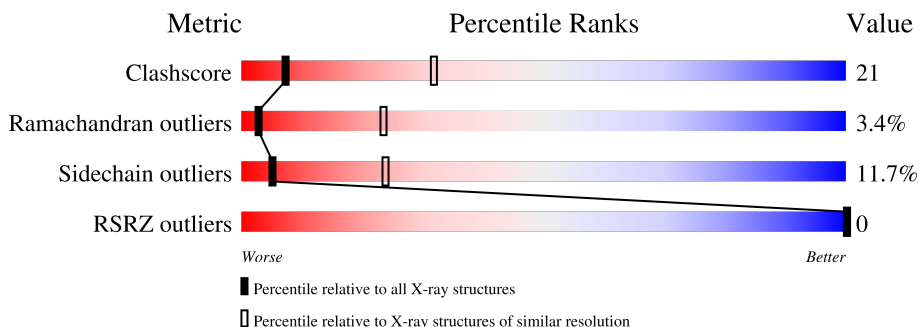
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	901	
1	B	901	
2	C	349	
2	D	349	
2	E	349	
2	F	349	
2	G	349	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	349	 64% 29% 6% •
2	I	349	 62% 31% 7% •
2	J	349	 64% 30% 6% •
2	P	349	 66% 30% •
2	Q	349	 61% 32% 6% •
2	R	349	 61% 30% 8% •
2	S	349	 58% 35% 5% •
2	T	349	 65% 30% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49061 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 PROTEIN (VP3 CORE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	0	0
			6824	4357	1181	1248	38			
1	B	885	Total	C	N	O	S	0	0	0
			7150	4561	1238	1311	40			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLU	ALA	conflict	UNP P56582
A	213	ILE	PHE	conflict	UNP P56582
A	220	LEU	PHE	conflict	UNP P56582
A	772	VAL	ILE	conflict	UNP P56582
A	773	ARG	GLY	conflict	UNP P56582
B	77	GLU	ALA	conflict	UNP P56582
B	213	ILE	PHE	conflict	UNP P56582
B	220	LEU	PHE	conflict	UNP P56582
B	772	VAL	ILE	conflict	UNP P56582
B	773	ARG	GLY	conflict	UNP P56582

- Molecule 2 is a protein called PROTEIN (VP7 CORE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	C	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	D	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	Q	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	E	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	R	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	G	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	H	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	S	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	I	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	J	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	T	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			

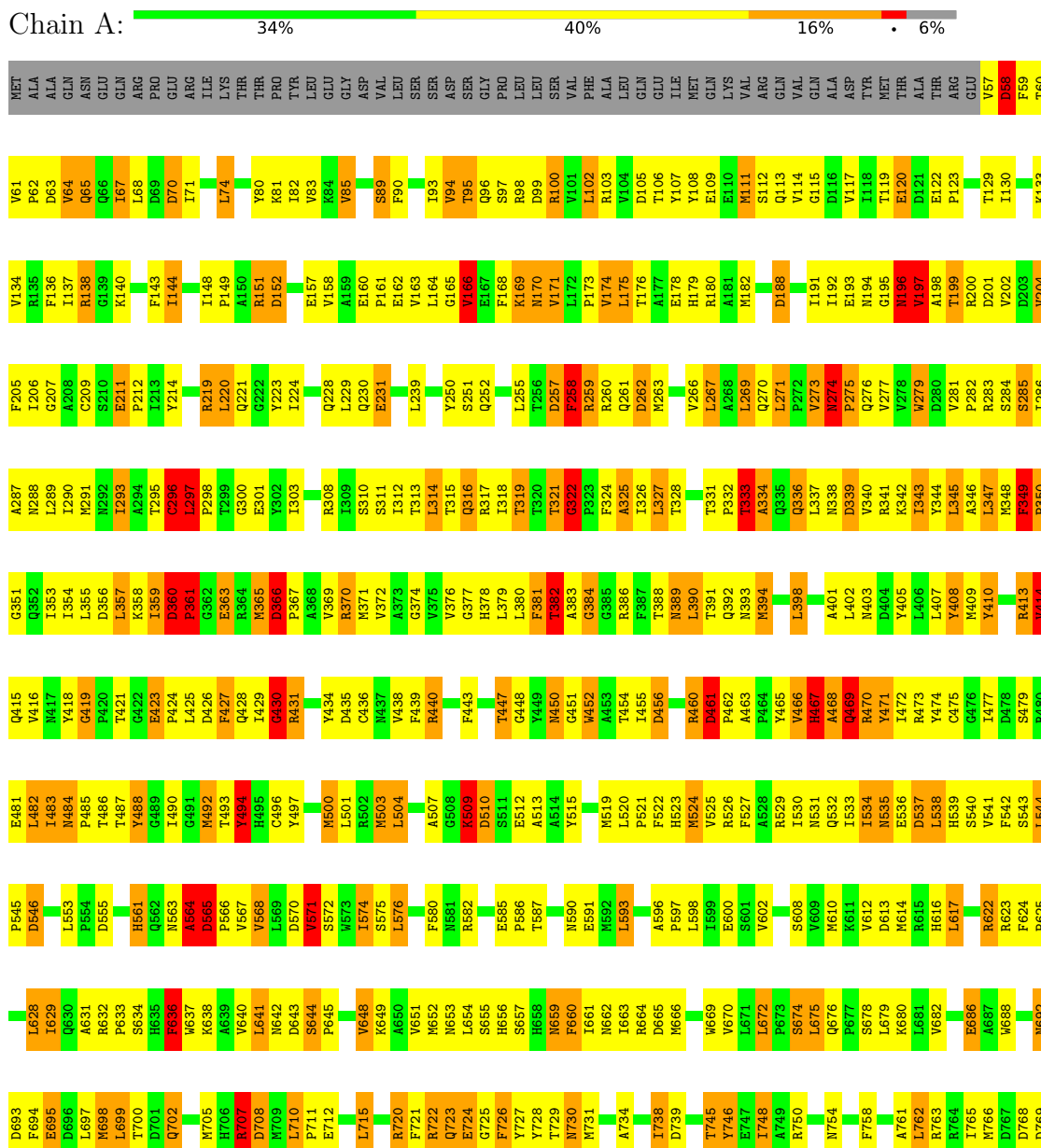
There are 13 discrepancies between the modelled and reference sequences:

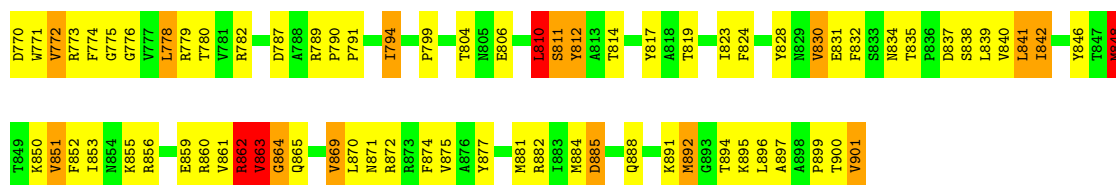
Chain	Residue	Modelled	Actual	Comment	Reference
P	278	TRP	GLY	conflict	UNP P18259
C	278	TRP	GLY	conflict	UNP P18259
D	278	TRP	GLY	conflict	UNP P18259
Q	278	TRP	GLY	conflict	UNP P18259
E	278	TRP	GLY	conflict	UNP P18259
F	278	TRP	GLY	conflict	UNP P18259
R	278	TRP	GLY	conflict	UNP P18259
G	278	TRP	GLY	conflict	UNP P18259
H	278	TRP	GLY	conflict	UNP P18259
S	278	TRP	GLY	conflict	UNP P18259
I	278	TRP	GLY	conflict	UNP P18259
J	278	TRP	GLY	conflict	UNP P18259
T	278	TRP	GLY	conflict	UNP P18259

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.

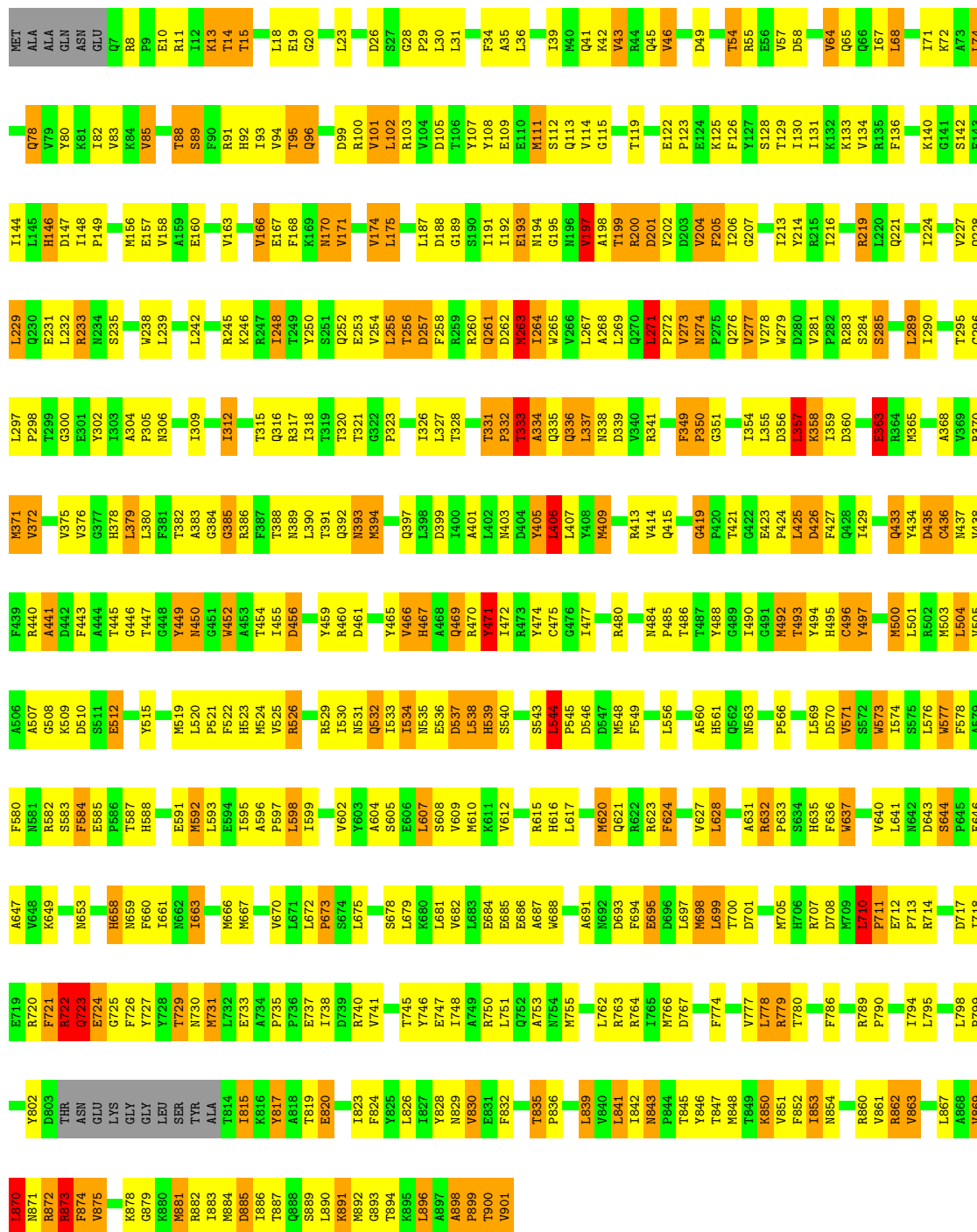
• Molecule 1: PROTEIN (VP3 CORE PROTEIN)





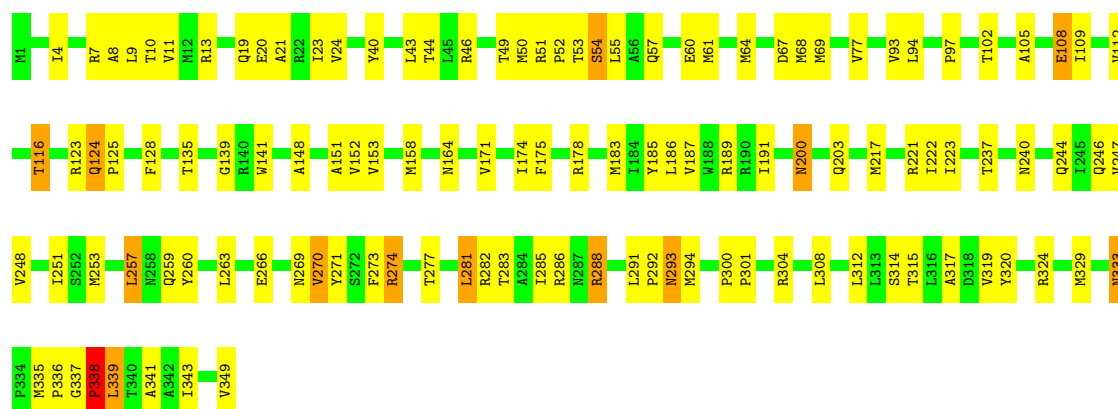
• Molecule 1: PROTEIN (VP3 CORE PROTEIN)

Chain B: 40% 41% 15% . .



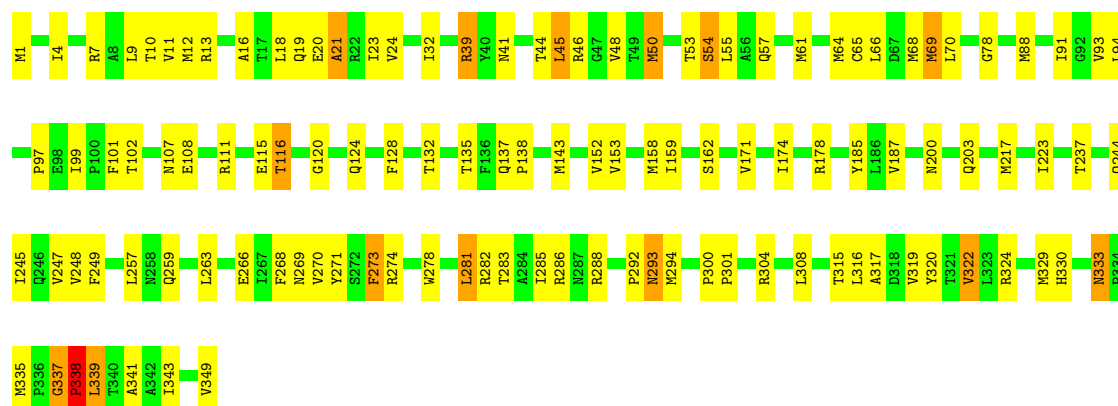
- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain P:  66% 30%



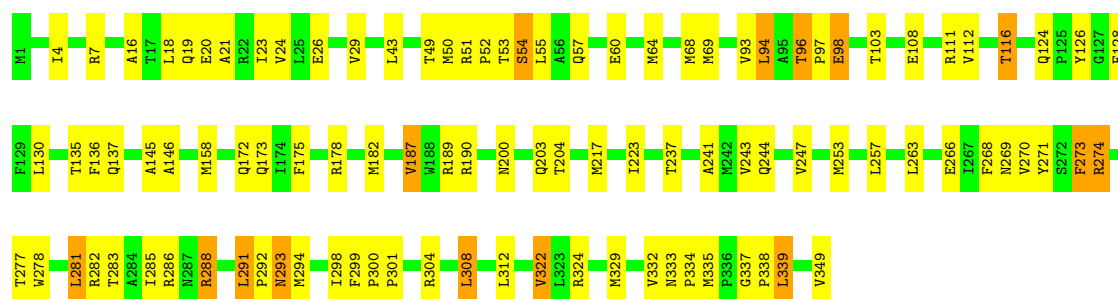
- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain C:  66% 29%



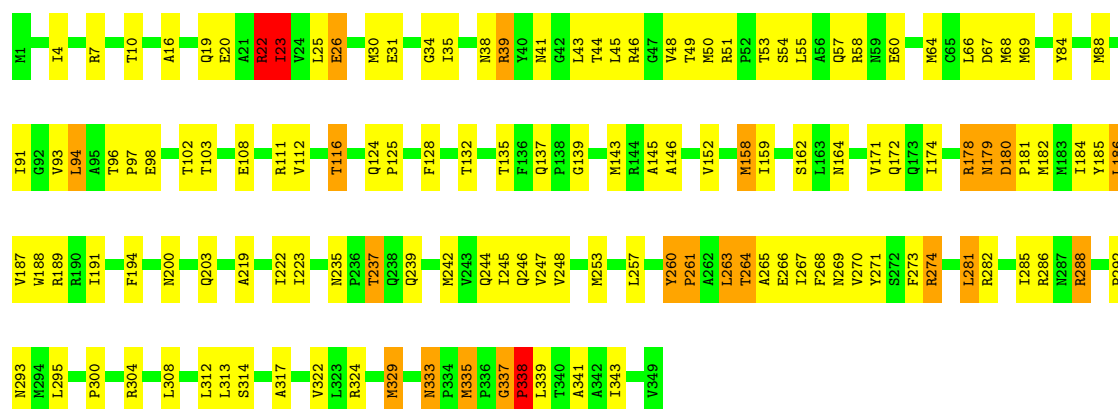
- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain D:  71% 25%

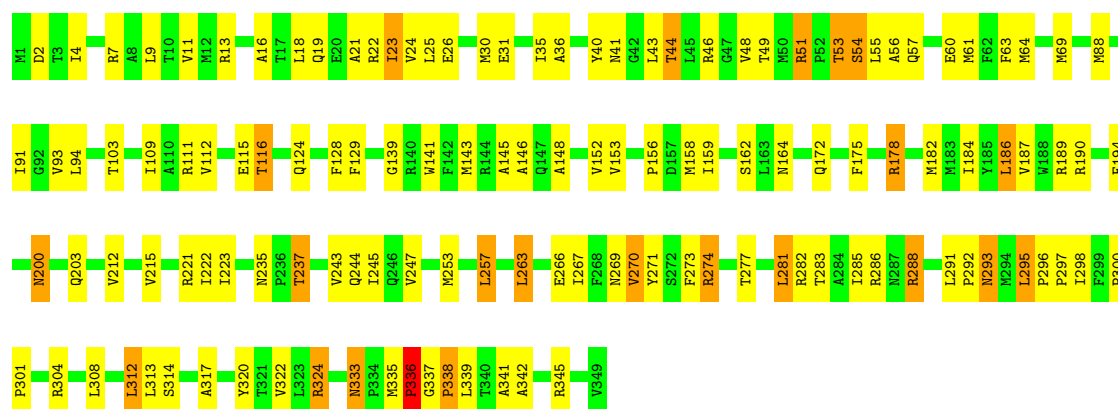


- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

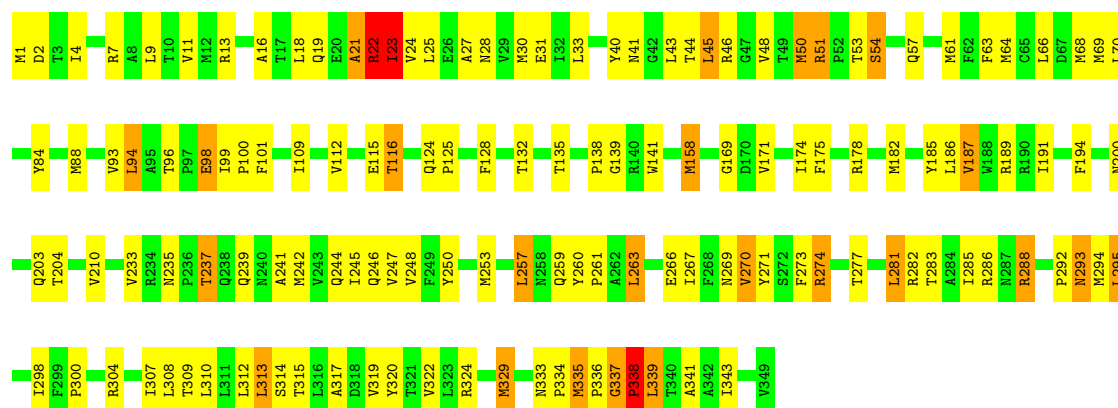
Chain Q:  61% 32% 6%



• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

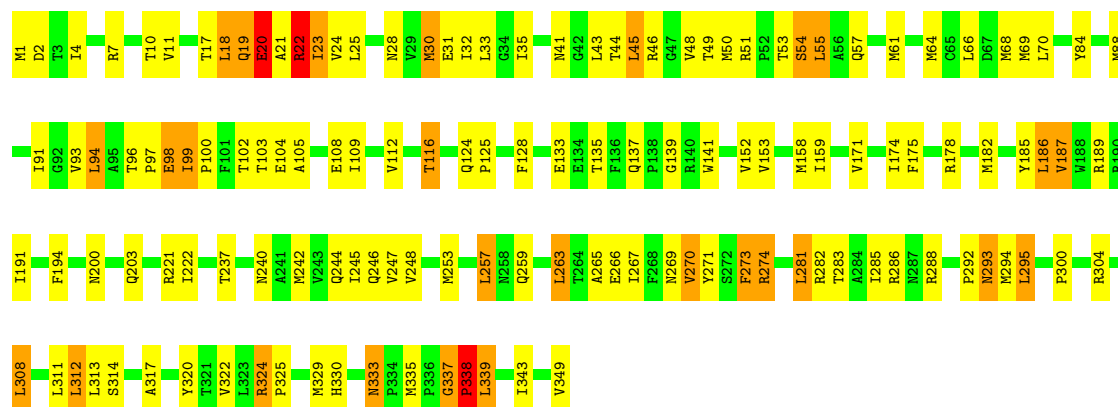


• Molecule 2: PROTEIN (VP7 CORE PROTEIN)



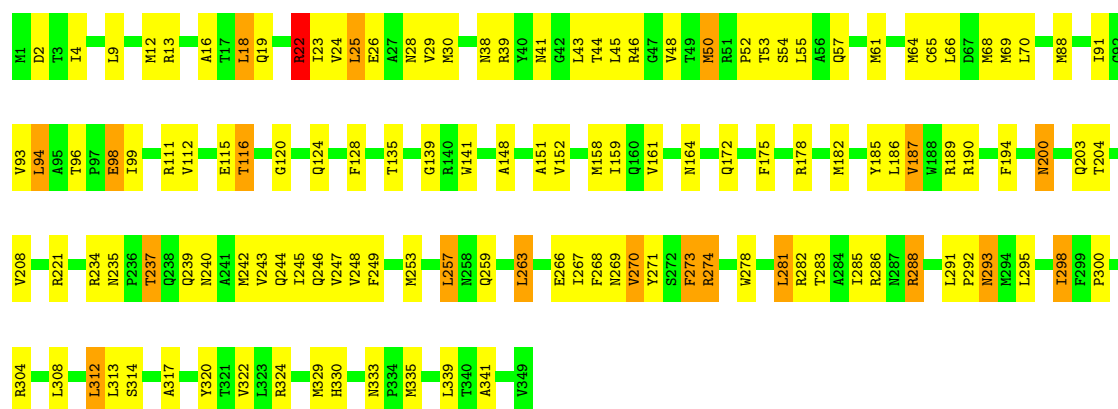
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)





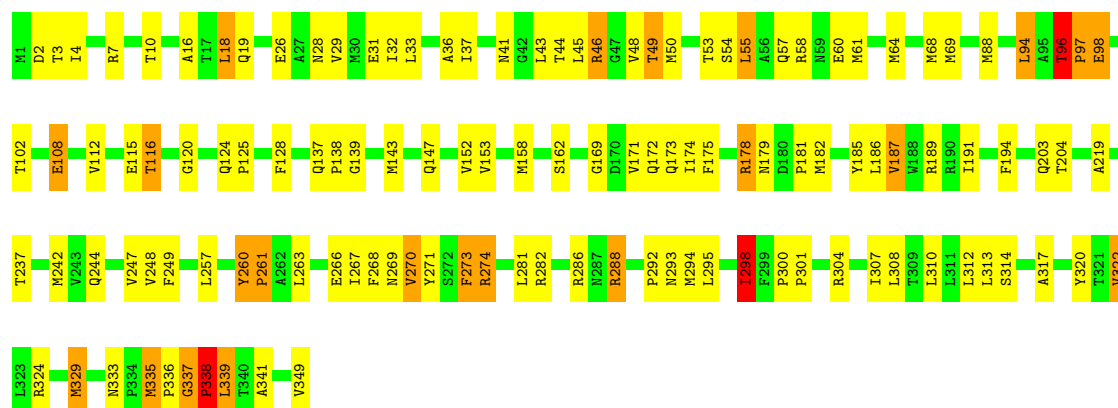
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain G: 63% 31% 5%



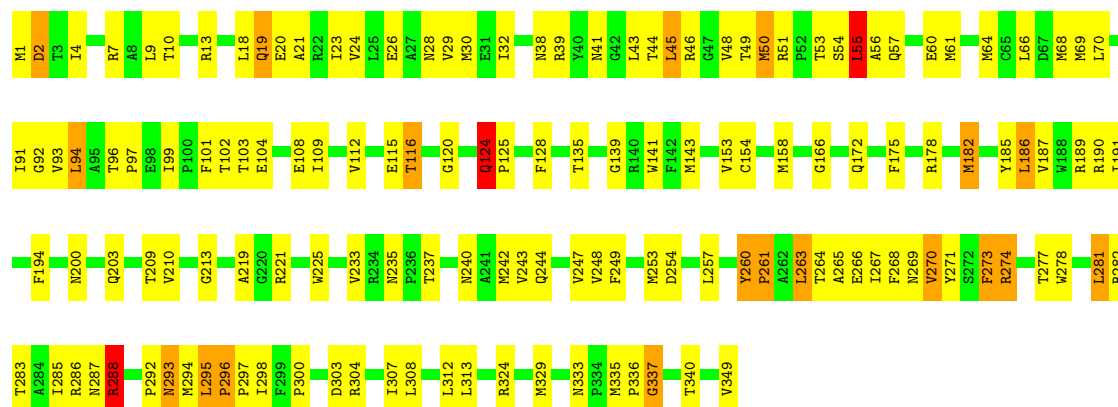
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain H: 64% 29% 6%



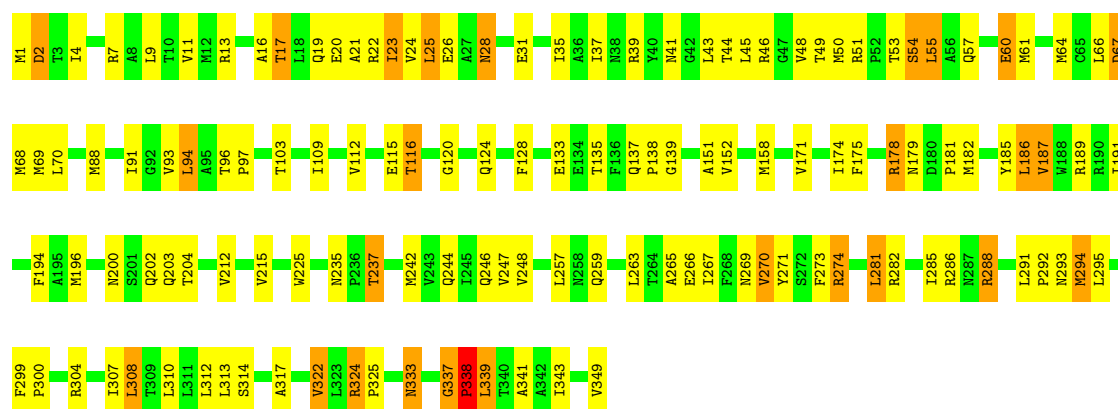
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain S: 58% 35% 5%



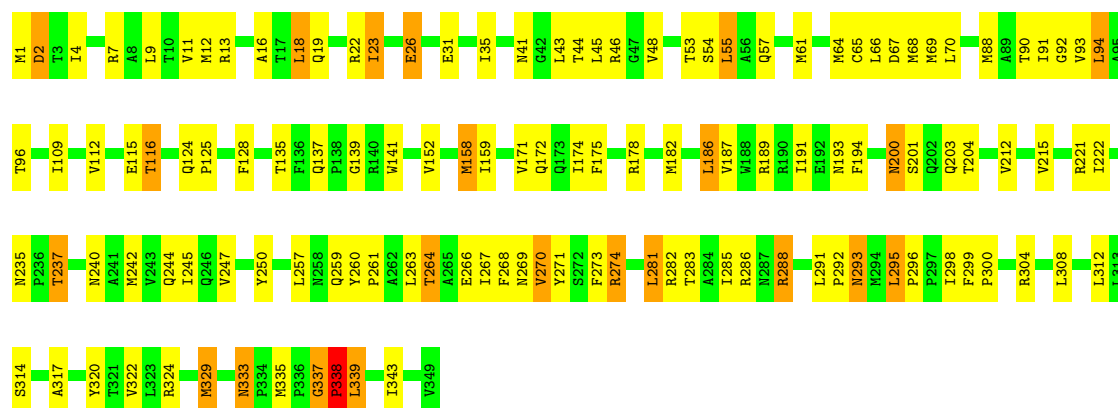
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain I: 62% 31% 7%



• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain J: 64% 30% 6%



• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain T: 65% 30% 5%

M1	D2	T3	I4	R7	A8	L9	T10	V11	M12	R13	A16	T17	L18	Q19	E20	A21	R22	I23	V24	L25	M30	R39	Y40	N41	G42	L43	T44	L45	R46	G47	V48	T53	S54	L55	A56	Q57	M61	M64	C65	L66	D67	M68	M69	L70	G78	P79	M88	I91	G92
V93	L94	A95	T96	P97	E98	T103	N107	E108	V112	E115	T116	G120	Q124	P125	F128	G139	R140	W141	V152	V153	M158	I159	G169	Q172	F175	R178	M182	Y185	L186	V187	W188	R189	R190	I191	F194	N200	Q203	V212											
V215	L231	N235	P236	T237	Q238	Q239	N240	A241	M242	W243	Q244	I245	Q246	V247	V248	L257	Y260	L263	T264	A265	E266	I267	F268	N269	V270	Y271	S272	F273	R274	L281	R282	I285	R286	N287	R288	L291	P292	N293	N294	L295	I298	F299	P300	R304	L308	T309	L312		
L313	S314	A317	Y320	T321	V322	L323	R324	P325	N333	P334	M335	P336	G337	P338	L339	T340	I343	V349																															

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	795.60Å 821.80Å 753.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.50 100.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	54.0 (100.00-3.50) 48.2 (100.00-3.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 3.49Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.266 , (Not available) 0.408 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	49061	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.12% 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	0.55	1/6978 (0.0%)	1.25	90/9479 (0.9%)
1	B	0.56	1/7308 (0.0%)	1.21	74/9925 (0.7%)
2	C	0.42	0/2757	1.03	15/3756 (0.4%)
2	D	0.41	0/2757	0.96	11/3756 (0.3%)
2	E	0.43	0/2757	1.04	17/3756 (0.5%)
2	F	0.44	0/2757	1.07	21/3756 (0.6%)
2	G	0.45	0/2757	1.04	14/3756 (0.4%)
2	H	0.46	0/2757	1.06	25/3756 (0.7%)
2	I	0.44	0/2757	1.06	21/3756 (0.6%)
2	J	0.43	0/2757	1.07	23/3756 (0.6%)
2	P	0.42	0/2757	1.03	13/3756 (0.3%)
2	Q	0.45	0/2757	1.08	22/3756 (0.6%)
2	R	0.46	0/2757	1.08	20/3756 (0.5%)
2	S	0.46	0/2757	1.03	17/3756 (0.5%)
2	T	0.45	0/2757	1.05	21/3756 (0.6%)
All	All	0.47	2/50127 (0.0%)	1.10	404/68232 (0.6%)

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	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	THR	CA-CB	5.26	1.61	1.53
1	A	95	THR	CA-CB	5.18	1.61	1.53

The worst 5 of 404 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	722	ARG	N-CA-C	-12.17	98.42	113.02
2	P	337	GLY	CA-C-N	11.39	134.08	119.84
2	P	337	GLY	C-N-CA	11.39	134.08	119.84
1	B	406	LEU	N-CA-C	-11.12	99.24	111.36
1	A	695	GLU	N-CA-C	-11.00	98.37	112.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	TYR	Sidechain
1	B	471	TYR	Sidechain

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	6824	0	6804	510	0
1	B	7150	0	7137	483	0
2	C	2699	0	2697	72	0
2	D	2699	0	2697	65	0
2	E	2699	0	2697	88	0
2	F	2699	0	2697	97	0
2	G	2699	0	2697	97	0
2	H	2699	0	2697	83	0
2	I	2699	0	2697	106	0
2	J	2699	0	2697	92	0
2	P	2699	0	2697	71	0
2	Q	2699	0	2697	103	0
2	R	2699	0	2697	101	0
2	S	2699	0	2697	108	0
2	T	2699	0	2697	73	0
All	All	49061	0	49002	2020	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 21.

The worst 5 of 2020 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:97:PRO:HD3	2:J:22:ARG:HH21	1.27	0.99
1:A:263:MET:HE2	1:A:882:ARG:HD2	1.46	0.97
2:E:158:MET:HE2	2:E:244:GLN:HB2	1.48	0.94
1:B:358:LYS:HB2	1:B:570:ASP:HB3	1.49	0.94
2:S:282:ARG:HD3	2:S:286:ARG:NH1	1.83	0.94

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	843/901 (94%)	674 (80%)	109 (13%)	60 (7%)	1	10
1	B	881/901 (98%)	715 (81%)	110 (12%)	56 (6%)	1	11
2	C	347/349 (99%)	313 (90%)	29 (8%)	5 (1%)	9	38
2	D	347/349 (99%)	316 (91%)	25 (7%)	6 (2%)	7	35
2	E	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	3	24
2	F	347/349 (99%)	305 (88%)	34 (10%)	8 (2%)	5	30
2	G	347/349 (99%)	303 (87%)	39 (11%)	5 (1%)	9	38
2	H	347/349 (99%)	302 (87%)	37 (11%)	8 (2%)	5	30
2	I	347/349 (99%)	300 (86%)	40 (12%)	7 (2%)	6	32
2	J	347/349 (99%)	296 (85%)	45 (13%)	6 (2%)	7	35
2	P	347/349 (99%)	312 (90%)	28 (8%)	7 (2%)	6	32
2	Q	347/349 (99%)	300 (86%)	39 (11%)	8 (2%)	5	30
2	R	347/349 (99%)	299 (86%)	39 (11%)	9 (3%)	4	27
2	S	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	3	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	347/349 (99%)	306 (88%)	35 (10%)	6 (2%)	7	35
All	All	6235/6339 (98%)	5333 (86%)	689 (11%)	213 (3%)	3	23

5 of 213 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	166	VAL
1	A	169	LYS
1	A	175	LEU
1	A	197	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	744/793 (94%)	597 (80%)	147 (20%)	1	7
1	B	782/793 (99%)	636 (81%)	146 (19%)	1	9
2	C	284/284 (100%)	263 (93%)	21 (7%)	13	37
2	D	284/284 (100%)	266 (94%)	18 (6%)	16	42
2	E	284/284 (100%)	258 (91%)	26 (9%)	8	32
2	F	284/284 (100%)	259 (91%)	25 (9%)	9	32
2	G	284/284 (100%)	257 (90%)	27 (10%)	8	31
2	H	284/284 (100%)	253 (89%)	31 (11%)	6	26
2	I	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	J	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	P	284/284 (100%)	262 (92%)	22 (8%)	12	37
2	Q	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	R	284/284 (100%)	257 (90%)	27 (10%)	8	31
2	S	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	T	284/284 (100%)	255 (90%)	29 (10%)	7	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5218/5278 (99%)	4607 (88%)	611 (12%)	5 24

5 of 611 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	115	GLU
2	J	270	VAL
2	G	291	LEU
2	G	111	ARG
2	S	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 182 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	200	ASN
2	H	244	GLN
2	G	19	GLN
2	G	269	ASN
2	S	269	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 ⓘ

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	845/901 (93%)	-1.26	0 100 100	0, 31, 86, 139	0
1	B	885/901 (98%)	-1.29	0 100 100	0, 24, 72, 141	0
2	C	349/349 (100%)	-0.95	0 100 100	18, 90, 152, 172	0
2	D	349/349 (100%)	-0.96	0 100 100	32, 102, 161, 182	0
2	E	349/349 (100%)	-1.08	0 100 100	1, 64, 122, 151	0
2	F	349/349 (100%)	-1.13	0 100 100	2, 61, 123, 151	0
2	G	349/349 (100%)	-1.15	0 100 100	0, 52, 107, 140	0
2	H	349/349 (100%)	-1.16	0 100 100	1, 51, 113, 148	0
2	I	349/349 (100%)	-1.16	0 100 100	0, 54, 120, 147	0
2	J	349/349 (100%)	-1.15	0 100 100	1, 56, 119, 142	0
2	P	349/349 (100%)	-0.86	0 100 100	35, 108, 162, 181	0
2	Q	349/349 (100%)	-1.11	0 100 100	1, 60, 125, 151	0
2	R	349/349 (100%)	-1.10	0 100 100	1, 57, 118, 146	0
2	S	349/349 (100%)	-1.19	0 100 100	0, 47, 116, 143	0
2	T	349/349 (100%)	-1.23	0 100 100	1, 48, 99, 134	0
All	All	6267/6339 (98%)	-1.14	0 100 100	0, 52, 135, 182	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.