



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2018 – 11:05 AM EST

PDB ID : 3SKB
Title : Structural characterization of a GII.4 2004 norovirus variant (TCH05)
Authors : Shanker, S.; Choi, J.-M.; Sankaran, B.; Atmar, R.L.; Estes, M.K.; Prasad, B.V.V.
Deposited on : 2011-06-22
Resolution : 3.22 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

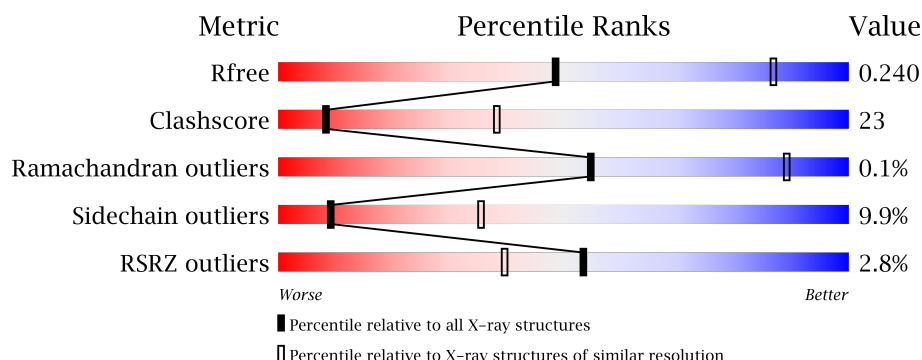
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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. 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	311	<div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
1	B	311	<div> <div>61%</div> <div>34%</div> <div>5%</div> </div>
1	C	311	<div> <div>63%</div> <div>31%</div> <div>5%</div> </div>
1	D	311	<div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
1	E	311	<div> <div>61%</div> <div>33%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain	
1	F	311		• •
1	G	311		•
1	H	311		•
1	I	311		• • • 6%
1	J	311		• 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23592 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 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2389	1510	411	458	10			
1	B	309	Total	C	N	O	S	0	0	0
			2394	1513	412	459	10			
1	C	308	Total	C	N	O	S	0	0	0
			2389	1510	411	458	10			
1	D	308	Total	C	N	O	S	0	0	0
			2387	1509	411	457	10			
1	E	309	Total	C	N	O	S	0	0	0
			2400	1516	415	459	10			
1	F	309	Total	C	N	O	S	0	0	0
			2394	1513	412	459	10			
1	G	308	Total	C	N	O	S	0	0	0
			2389	1510	411	458	10			
1	H	308	Total	C	N	O	S	0	0	0
			2389	1510	411	458	10			
1	I	291	Total	C	N	O	S	0	0	0
			2257	1435	389	425	8			
1	J	283	Total	C	N	O	S	0	0	0
			2204	1406	378	413	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
A	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
A	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
B	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
B	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
B	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
C	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
C	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
C	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

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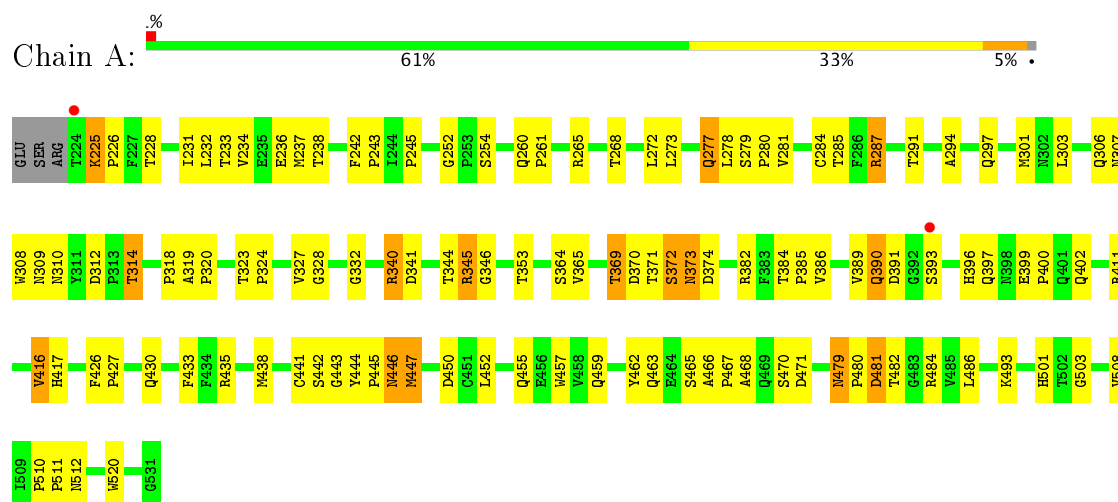
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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
D	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
D	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
E	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
E	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
E	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
F	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
F	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
F	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
G	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
G	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
G	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
H	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
H	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
H	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
I	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
I	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
I	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8
J	228	THR	SER	SEE REMARK 999	UNP Q5EGK8
J	271	ALA	VAL	SEE REMARK 999	UNP Q5EGK8
J	282	ASP	ASN	SEE REMARK 999	UNP Q5EGK8

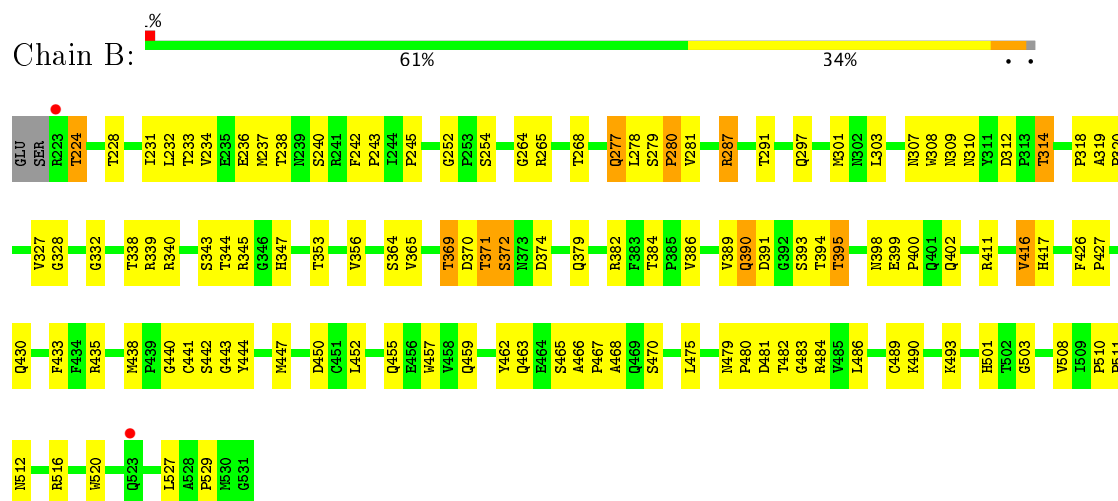
3 Residue-property plots

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: Capsid

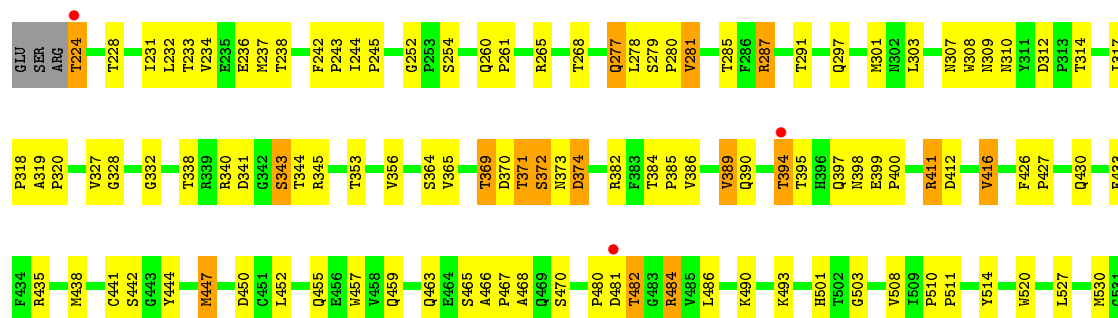


• Molecule 1: Capsid

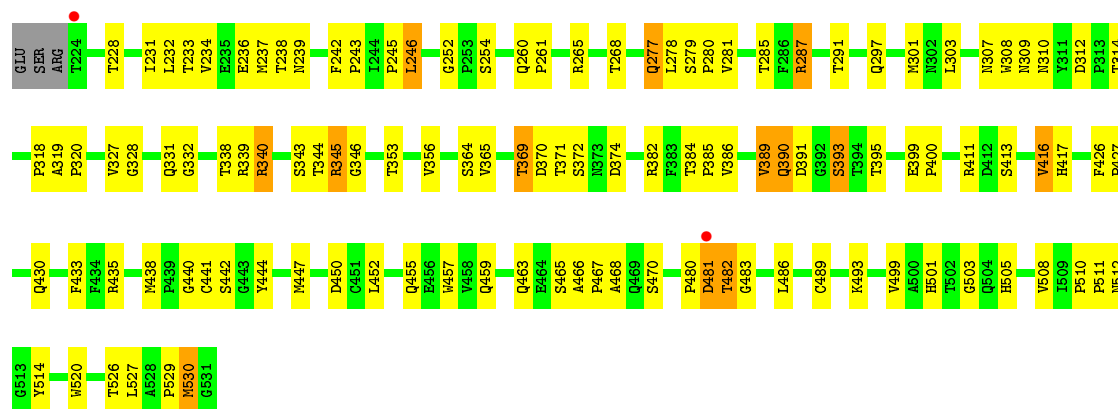


• Molecule 1: Capsid

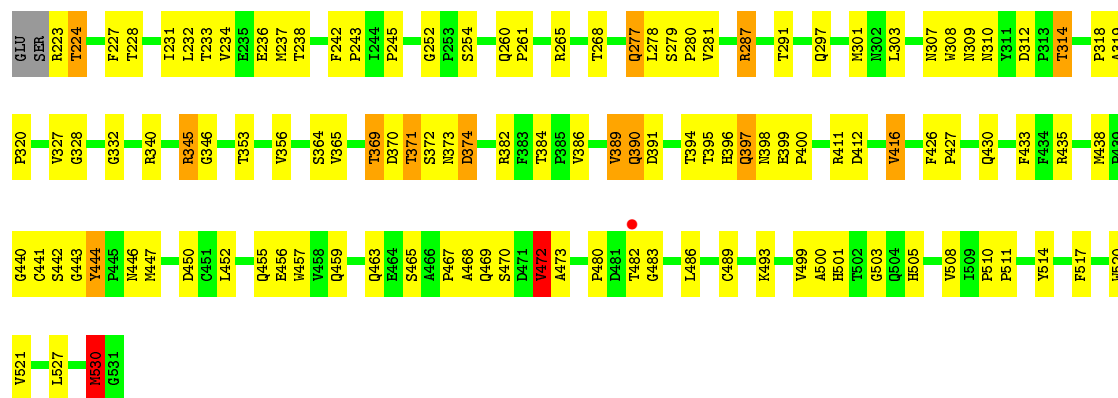




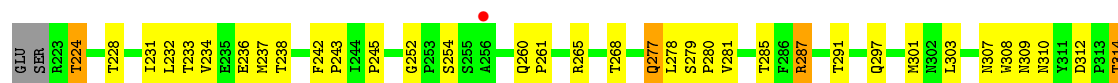
• Molecule 1: Capsid

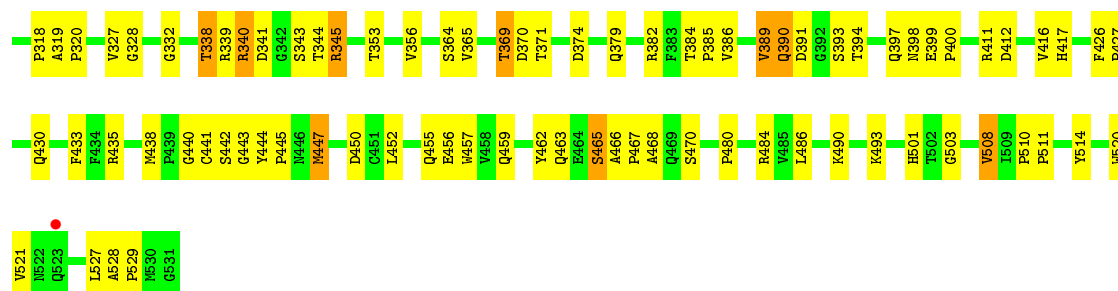


• Molecule 1: Capsid

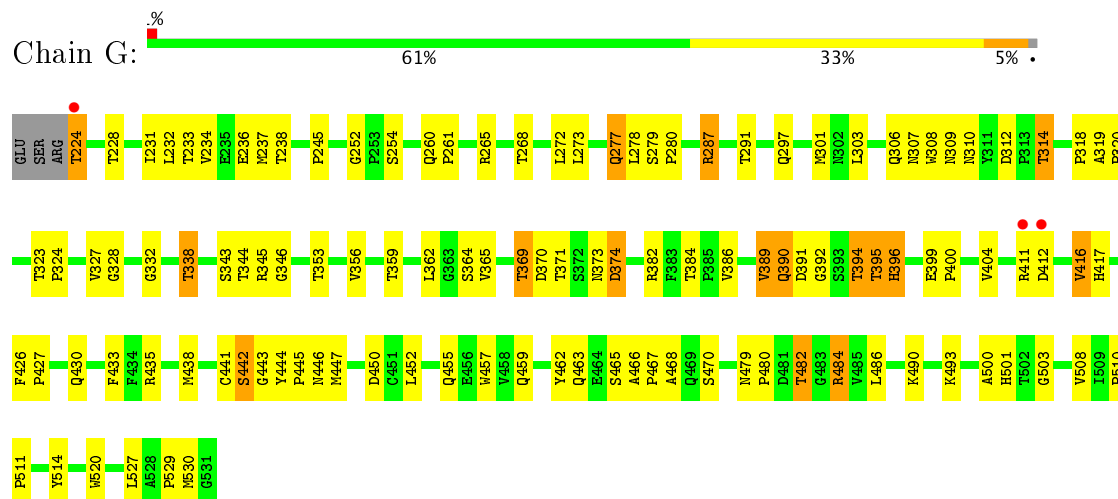


• Molecule 1: Capsid

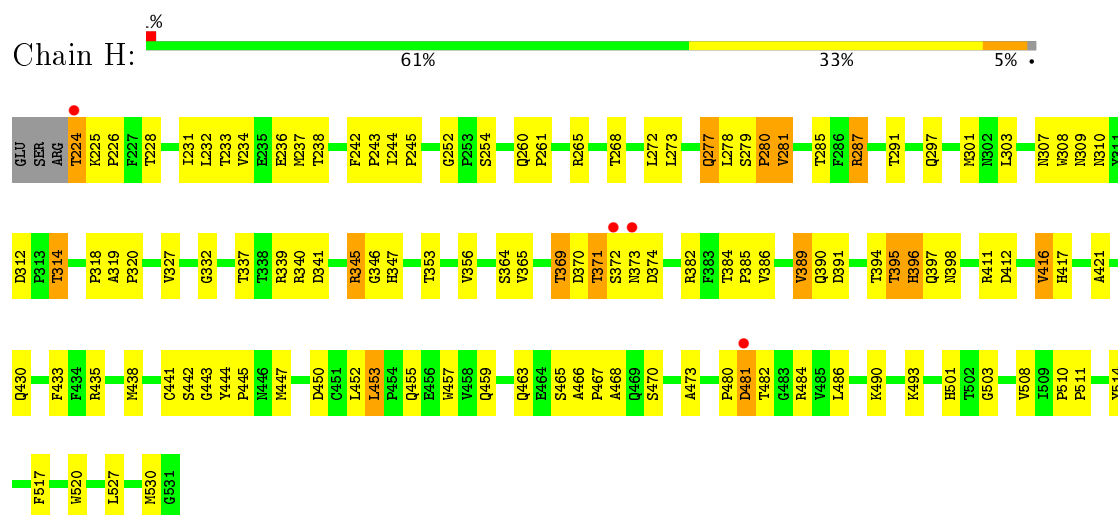




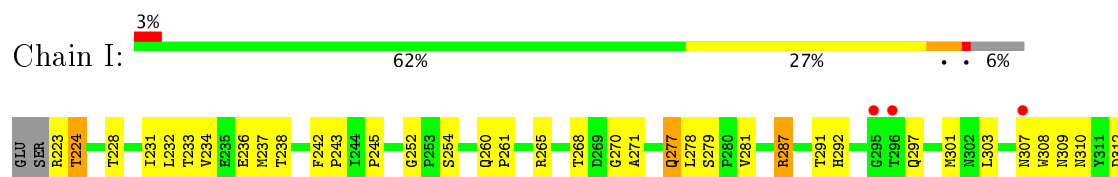
• Molecule 1: Capsid

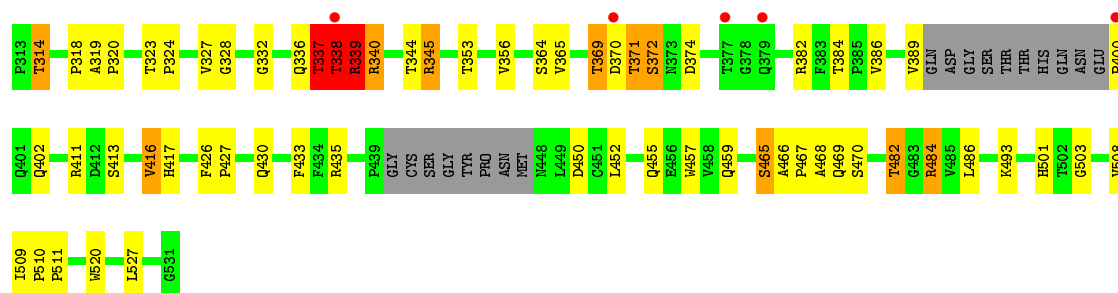


• Molecule 1: Capsid

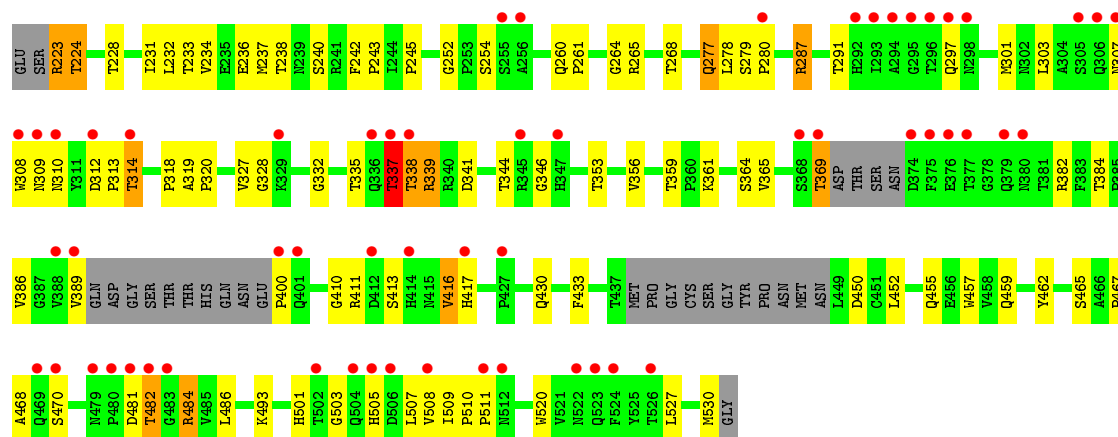


• Molecule 1: Capsid





• Molecule 1: Capsid



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	243.91Å 339.12Å 125.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.57 – 3.22 27.57 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.3 (27.57-3.22) 94.3 (27.57-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.201 , 0.245 0.196 , 0.240	Depositor DCC
R_{free} test set	3950 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23592	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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	0.62	1/2459 (0.0%)	0.68	1/3366 (0.0%)
1	B	0.58	0/2464	0.69	0/3373
1	C	0.57	0/2459	0.67	1/3366 (0.0%)
1	D	0.55	0/2457	0.68	0/3363
1	E	0.60	1/2470 (0.0%)	0.69	2/3380 (0.1%)
1	F	0.59	1/2464 (0.0%)	0.68	0/3373
1	G	0.51	0/2459	0.69	1/3366 (0.0%)
1	H	0.52	0/2459	0.69	2/3366 (0.1%)
1	I	0.63	2/2322 (0.1%)	0.76	5/3177 (0.2%)
1	J	0.57	0/2267	0.66	3/3099 (0.1%)
All	All	0.57	5/24280 (0.0%)	0.69	15/33229 (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	2
1	J	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	338	THR	N-CA	8.49	1.63	1.46
1	I	338	THR	CB-CG2	5.55	1.70	1.52
1	E	444	TYR	CD1-CE1	-5.54	1.31	1.39
1	A	284	CYS	CB-SG	-5.33	1.73	1.81
1	F	441	CYS	CB-SG	-5.02	1.73	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	338	THR	N-CA-C	9.02	135.34	111.00
1	I	337	THR	CA-C-N	-8.06	99.46	117.20
1	I	337	THR	O-C-N	7.86	135.27	122.70
1	I	338	THR	CB-CA-C	-7.10	92.44	111.60
1	I	339	ARG	N-CA-C	6.21	127.77	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	337	THR	Mainchain,Peptide
1	J	337	THR	Mainchain,Peptide
1	J	339	ARG	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	A	2389	0	2277	135	0
1	B	2394	0	2279	135	0
1	C	2389	0	2277	107	0
1	D	2387	0	2272	105	0
1	E	2400	0	2290	120	0
1	F	2394	0	2279	134	0
1	G	2389	0	2277	119	0
1	H	2389	0	2277	114	0
1	I	2257	0	2162	114	0
1	J	2204	0	2117	78	0
All	All	23592	0	22507	1067	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 23.

The worst 5 of 1067 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)
1:A:480:PRO:HG2	1:A:512:ASN:ND2	1.49	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:O	1:E:442:SER:HA	1.39	1.22
1:E:390:GLN:NE2	1:E:391:ASP:O	1.82	1.12
1:B:480:PRO:HG2	1:B:512:ASN:ND2	1.64	1.11
1:A:480:PRO:HD2	1:A:481:ASP:H	1.17	1.06

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	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	B	307/311 (99%)	294 (96%)	12 (4%)	1 (0%)	44	81
1	C	306/311 (98%)	292 (95%)	14 (5%)	0	100	100
1	D	306/311 (98%)	295 (96%)	11 (4%)	0	100	100
1	E	307/311 (99%)	293 (95%)	13 (4%)	1 (0%)	44	81
1	F	307/311 (99%)	292 (95%)	15 (5%)	0	100	100
1	G	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	H	306/311 (98%)	293 (96%)	13 (4%)	0	100	100
1	I	285/311 (92%)	272 (95%)	13 (5%)	0	100	100
1	J	275/311 (88%)	260 (94%)	15 (6%)	0	100	100
All	All	3011/3110 (97%)	2877 (96%)	132 (4%)	2 (0%)	55	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	483	GLY
1	E	397	GLN

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	267/272 (98%)	239 (90%)	28 (10%)	8	32
1	B	267/272 (98%)	243 (91%)	24 (9%)	11	40
1	C	267/272 (98%)	236 (88%)	31 (12%)	6	28
1	D	266/272 (98%)	239 (90%)	27 (10%)	8	34
1	E	268/272 (98%)	242 (90%)	26 (10%)	9	36
1	F	267/272 (98%)	245 (92%)	22 (8%)	13	47
1	G	267/272 (98%)	242 (91%)	25 (9%)	10	38
1	H	267/272 (98%)	238 (89%)	29 (11%)	7	31
1	I	250/272 (92%)	224 (90%)	26 (10%)	8	33
1	J	244/272 (90%)	221 (91%)	23 (9%)	10	38
All	All	2630/2720 (97%)	2369 (90%)	261 (10%)	9	35

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	314	THR
1	F	340	ARG
1	J	254	SER
1	E	364	SER
1	E	465	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	505	HIS
1	E	505	HIS
1	I	505	HIS
1	E	277	GLN
1	E	396	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	308/311 (99%)	-0.45	2 (0%) 89 83	22, 43, 81, 112	0
1	B	309/311 (99%)	-0.45	2 (0%) 89 83	21, 43, 81, 110	0
1	C	308/311 (99%)	-0.41	3 (0%) 82 73	20, 44, 81, 112	0
1	D	308/311 (99%)	-0.44	2 (0%) 89 83	22, 45, 82, 111	0
1	E	309/311 (99%)	-0.46	1 (0%) 93 92	22, 44, 81, 109	0
1	F	309/311 (99%)	-0.41	2 (0%) 89 83	23, 44, 83, 110	0
1	G	308/311 (99%)	-0.38	3 (0%) 82 73	27, 46, 82, 169	0
1	H	308/311 (99%)	-0.39	4 (1%) 77 65	24, 47, 82, 111	0
1	I	291/311 (93%)	-0.21	8 (2%) 55 41	26, 47, 86, 134	0
1	J	283/311 (90%)	1.04	58 (20%) 1 1	37, 71, 113, 218	0
All	All	3041/3110 (97%)	-0.27	85 (2%) 53 40	20, 46, 87, 218	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	338	THR	6.6
1	J	523	GLN	6.2
1	C	224	THR	5.9
1	J	377	THR	5.4
1	J	307	ASN	4.7

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.