Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 07:13 pm GMT

PDB ID	:	7NXQ
Title	:	Structure of the pentameric C-terminal domain of the capsid protein from Kaposi's sarcoma-associated herpesvirus (KSHV)
Authors	:	Naniima, P.; Legrand, P.; Krey, T.
Deposited on	:	2021-03-19
Resolution	:	2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references ⓘ) were used in the production of this report:

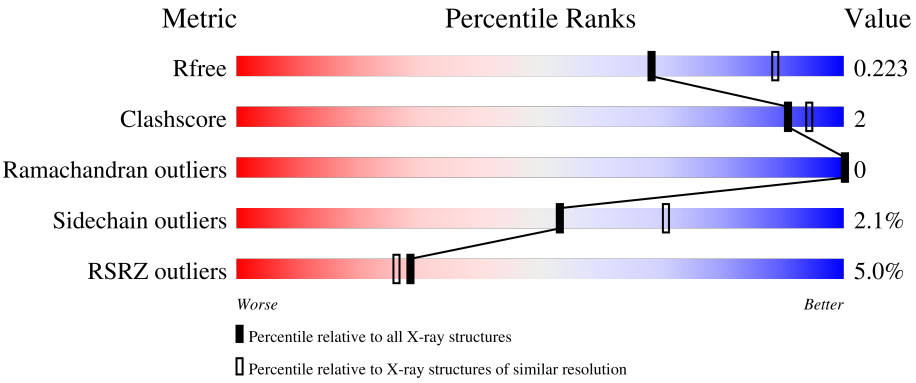
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	A	443	3% 88% 5% 7%
1	B	443	2% 86% 5% 9%
1	C	443	4% 87% 5% 7%
1	D	443	4% 86% 5% 9%
1	E	443	5% 87% 5% 8%

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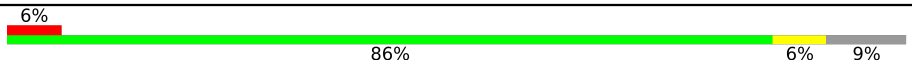
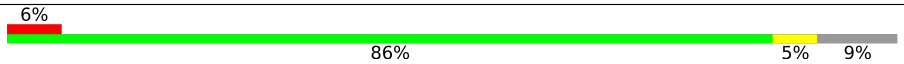
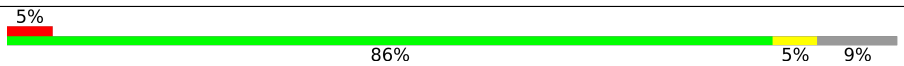
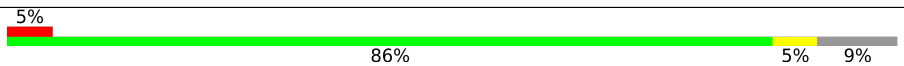
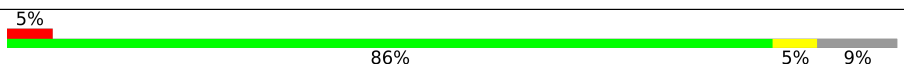
Mol	Chain	Length	Quality of chain
1	F	443	
1	G	443	
1	H	443	
1	I	443	
1	J	443	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33920 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 vertex component 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3230	2086	551	581	12			
1	B	404	Total	C	N	O	S	0	0	0
			3174	2051	541	570	12			
1	C	411	Total	C	N	O	S	0	0	0
			3221	2080	549	580	12			
1	D	404	Total	C	N	O	S	0	0	0
			3174	2052	541	569	12			
1	E	406	Total	C	N	O	S	0	0	0
			3189	2060	544	573	12			
1	F	405	Total	C	N	O	S	0	0	0
			3188	2060	545	571	12			
1	G	405	Total	C	N	O	S	0	0	0
			3181	2056	542	571	12			
1	H	403	Total	C	N	O	S	0	0	0
			3167	2047	540	568	12			
1	I	404	Total	C	N	O	S	0	0	0
			3176	2052	542	570	12			
1	J	402	Total	C	N	O	S	0	0	0
			3160	2043	538	567	12			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	-	initiating methionine	UNP Q76RI7
A	550	PRO	-	expression tag	UNP Q76RI7
A	551	ALA	-	expression tag	UNP Q76RI7
A	552	ALA	-	expression tag	UNP Q76RI7
A	553	ALA	-	expression tag	UNP Q76RI7
A	554	LEU	-	expression tag	UNP Q76RI7
A	555	GLU	-	expression tag	UNP Q76RI7
A	556	HIS	-	expression tag	UNP Q76RI7
A	557	HIS	-	expression tag	UNP Q76RI7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	558	HIS	-	expression tag	UNP Q76RI7
A	559	HIS	-	expression tag	UNP Q76RI7
A	560	HIS	-	expression tag	UNP Q76RI7
A	561	HIS	-	expression tag	UNP Q76RI7
A	562	HIS	-	expression tag	UNP Q76RI7
A	563	HIS	-	expression tag	UNP Q76RI7
A	564	HIS	-	expression tag	UNP Q76RI7
B	122	MET	-	initiating methionine	UNP Q76RI7
B	550	PRO	-	expression tag	UNP Q76RI7
B	551	ALA	-	expression tag	UNP Q76RI7
B	552	ALA	-	expression tag	UNP Q76RI7
B	553	ALA	-	expression tag	UNP Q76RI7
B	554	LEU	-	expression tag	UNP Q76RI7
B	555	GLU	-	expression tag	UNP Q76RI7
B	556	HIS	-	expression tag	UNP Q76RI7
B	557	HIS	-	expression tag	UNP Q76RI7
B	558	HIS	-	expression tag	UNP Q76RI7
B	559	HIS	-	expression tag	UNP Q76RI7
B	560	HIS	-	expression tag	UNP Q76RI7
B	561	HIS	-	expression tag	UNP Q76RI7
B	562	HIS	-	expression tag	UNP Q76RI7
B	563	HIS	-	expression tag	UNP Q76RI7
B	564	HIS	-	expression tag	UNP Q76RI7
C	122	MET	-	initiating methionine	UNP Q76RI7
C	550	PRO	-	expression tag	UNP Q76RI7
C	551	ALA	-	expression tag	UNP Q76RI7
C	552	ALA	-	expression tag	UNP Q76RI7
C	553	ALA	-	expression tag	UNP Q76RI7
C	554	LEU	-	expression tag	UNP Q76RI7
C	555	GLU	-	expression tag	UNP Q76RI7
C	556	HIS	-	expression tag	UNP Q76RI7
C	557	HIS	-	expression tag	UNP Q76RI7
C	558	HIS	-	expression tag	UNP Q76RI7
C	559	HIS	-	expression tag	UNP Q76RI7
C	560	HIS	-	expression tag	UNP Q76RI7
C	561	HIS	-	expression tag	UNP Q76RI7
C	562	HIS	-	expression tag	UNP Q76RI7
C	563	HIS	-	expression tag	UNP Q76RI7
C	564	HIS	-	expression tag	UNP Q76RI7
D	122	MET	-	initiating methionine	UNP Q76RI7
D	550	PRO	-	expression tag	UNP Q76RI7
D	551	ALA	-	expression tag	UNP Q76RI7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	552	ALA	-	expression tag	UNP Q76RI7
D	553	ALA	-	expression tag	UNP Q76RI7
D	554	LEU	-	expression tag	UNP Q76RI7
D	555	GLU	-	expression tag	UNP Q76RI7
D	556	HIS	-	expression tag	UNP Q76RI7
D	557	HIS	-	expression tag	UNP Q76RI7
D	558	HIS	-	expression tag	UNP Q76RI7
D	559	HIS	-	expression tag	UNP Q76RI7
D	560	HIS	-	expression tag	UNP Q76RI7
D	561	HIS	-	expression tag	UNP Q76RI7
D	562	HIS	-	expression tag	UNP Q76RI7
D	563	HIS	-	expression tag	UNP Q76RI7
D	564	HIS	-	expression tag	UNP Q76RI7
E	122	MET	-	initiating methionine	UNP Q76RI7
E	550	PRO	-	expression tag	UNP Q76RI7
E	551	ALA	-	expression tag	UNP Q76RI7
E	552	ALA	-	expression tag	UNP Q76RI7
E	553	ALA	-	expression tag	UNP Q76RI7
E	554	LEU	-	expression tag	UNP Q76RI7
E	555	GLU	-	expression tag	UNP Q76RI7
E	556	HIS	-	expression tag	UNP Q76RI7
E	557	HIS	-	expression tag	UNP Q76RI7
E	558	HIS	-	expression tag	UNP Q76RI7
E	559	HIS	-	expression tag	UNP Q76RI7
E	560	HIS	-	expression tag	UNP Q76RI7
E	561	HIS	-	expression tag	UNP Q76RI7
E	562	HIS	-	expression tag	UNP Q76RI7
E	563	HIS	-	expression tag	UNP Q76RI7
E	564	HIS	-	expression tag	UNP Q76RI7
F	122	MET	-	initiating methionine	UNP Q76RI7
F	550	PRO	-	expression tag	UNP Q76RI7
F	551	ALA	-	expression tag	UNP Q76RI7
F	552	ALA	-	expression tag	UNP Q76RI7
F	553	ALA	-	expression tag	UNP Q76RI7
F	554	LEU	-	expression tag	UNP Q76RI7
F	555	GLU	-	expression tag	UNP Q76RI7
F	556	HIS	-	expression tag	UNP Q76RI7
F	557	HIS	-	expression tag	UNP Q76RI7
F	558	HIS	-	expression tag	UNP Q76RI7
F	559	HIS	-	expression tag	UNP Q76RI7
F	560	HIS	-	expression tag	UNP Q76RI7
F	561	HIS	-	expression tag	UNP Q76RI7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	562	HIS	-	expression tag	UNP Q76RI7
F	563	HIS	-	expression tag	UNP Q76RI7
F	564	HIS	-	expression tag	UNP Q76RI7
G	122	MET	-	initiating methionine	UNP Q76RI7
G	550	PRO	-	expression tag	UNP Q76RI7
G	551	ALA	-	expression tag	UNP Q76RI7
G	552	ALA	-	expression tag	UNP Q76RI7
G	553	ALA	-	expression tag	UNP Q76RI7
G	554	LEU	-	expression tag	UNP Q76RI7
G	555	GLU	-	expression tag	UNP Q76RI7
G	556	HIS	-	expression tag	UNP Q76RI7
G	557	HIS	-	expression tag	UNP Q76RI7
G	558	HIS	-	expression tag	UNP Q76RI7
G	559	HIS	-	expression tag	UNP Q76RI7
G	560	HIS	-	expression tag	UNP Q76RI7
G	561	HIS	-	expression tag	UNP Q76RI7
G	562	HIS	-	expression tag	UNP Q76RI7
G	563	HIS	-	expression tag	UNP Q76RI7
G	564	HIS	-	expression tag	UNP Q76RI7
H	122	MET	-	initiating methionine	UNP Q76RI7
H	550	PRO	-	expression tag	UNP Q76RI7
H	551	ALA	-	expression tag	UNP Q76RI7
H	552	ALA	-	expression tag	UNP Q76RI7
H	553	ALA	-	expression tag	UNP Q76RI7
H	554	LEU	-	expression tag	UNP Q76RI7
H	555	GLU	-	expression tag	UNP Q76RI7
H	556	HIS	-	expression tag	UNP Q76RI7
H	557	HIS	-	expression tag	UNP Q76RI7
H	558	HIS	-	expression tag	UNP Q76RI7
H	559	HIS	-	expression tag	UNP Q76RI7
H	560	HIS	-	expression tag	UNP Q76RI7
H	561	HIS	-	expression tag	UNP Q76RI7
H	562	HIS	-	expression tag	UNP Q76RI7
H	563	HIS	-	expression tag	UNP Q76RI7
H	564	HIS	-	expression tag	UNP Q76RI7
I	122	MET	-	initiating methionine	UNP Q76RI7
I	550	PRO	-	expression tag	UNP Q76RI7
I	551	ALA	-	expression tag	UNP Q76RI7
I	552	ALA	-	expression tag	UNP Q76RI7
I	553	ALA	-	expression tag	UNP Q76RI7
I	554	LEU	-	expression tag	UNP Q76RI7
I	555	GLU	-	expression tag	UNP Q76RI7

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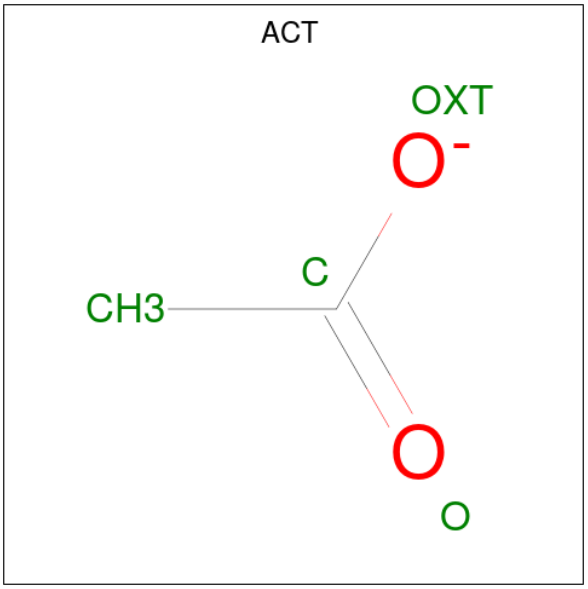
Chain	Residue	Modelled	Actual	Comment	Reference
I	556	HIS	-	expression tag	UNP Q76RI7
I	557	HIS	-	expression tag	UNP Q76RI7
I	558	HIS	-	expression tag	UNP Q76RI7
I	559	HIS	-	expression tag	UNP Q76RI7
I	560	HIS	-	expression tag	UNP Q76RI7
I	561	HIS	-	expression tag	UNP Q76RI7
I	562	HIS	-	expression tag	UNP Q76RI7
I	563	HIS	-	expression tag	UNP Q76RI7
I	564	HIS	-	expression tag	UNP Q76RI7
J	122	MET	-	initiating methionine	UNP Q76RI7
J	550	PRO	-	expression tag	UNP Q76RI7
J	551	ALA	-	expression tag	UNP Q76RI7
J	552	ALA	-	expression tag	UNP Q76RI7
J	553	ALA	-	expression tag	UNP Q76RI7
J	554	LEU	-	expression tag	UNP Q76RI7
J	555	GLU	-	expression tag	UNP Q76RI7
J	556	HIS	-	expression tag	UNP Q76RI7
J	557	HIS	-	expression tag	UNP Q76RI7
J	558	HIS	-	expression tag	UNP Q76RI7
J	559	HIS	-	expression tag	UNP Q76RI7
J	560	HIS	-	expression tag	UNP Q76RI7
J	561	HIS	-	expression tag	UNP Q76RI7
J	562	HIS	-	expression tag	UNP Q76RI7
J	563	HIS	-	expression tag	UNP Q76RI7
J	564	HIS	-	expression tag	UNP Q76RI7

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

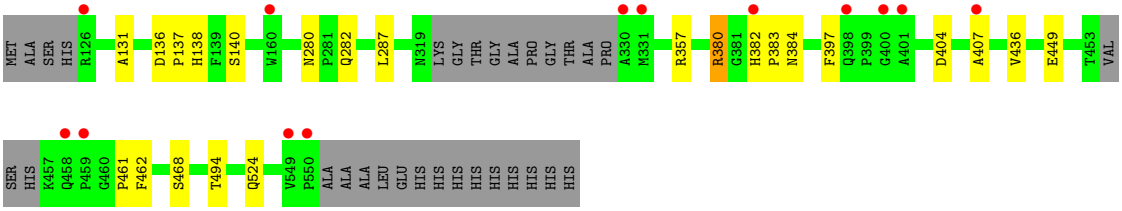
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	254	Total O 254 254	0	0
3	B	213	Total O 213 213	0	0
3	C	229	Total O 229 229	0	0
3	D	193	Total O 193 193	0	0
3	E	154	Total O 154 154	0	0
3	F	211	Total O 211 211	0	0
3	G	185	Total O 185 185	0	0
3	H	158	Total O 158 158	0	0
3	I	199	Total O 199 199	0	0
3	J	184	Total O 184 184	0	0

3 Residue-property plots (i)

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.

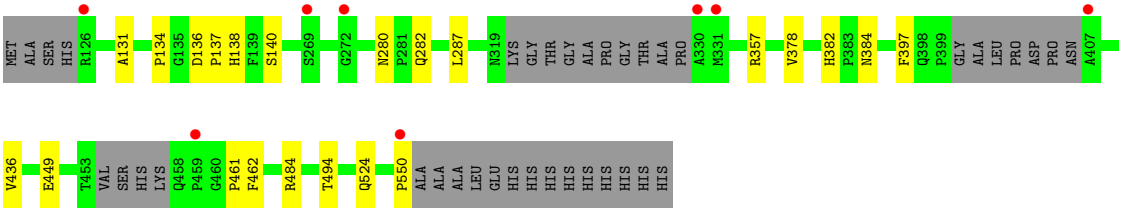
• Molecule 1: Capsid vertex component 2

Chain A:



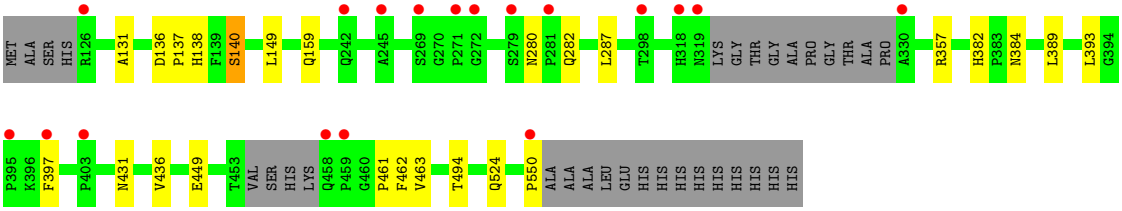
• Molecule 1: Capsid vertex component 2

Chain B:



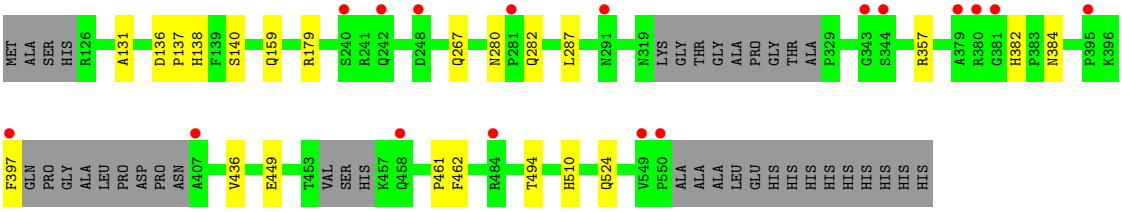
• Molecule 1: Capsid vertex component 2

Chain C:



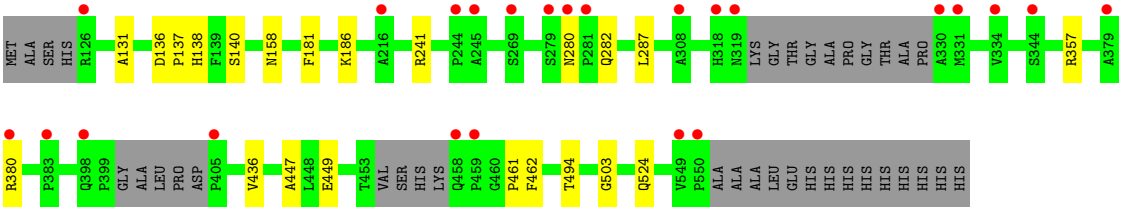
• Molecule 1: Capsid vertex component 2

Chain D:



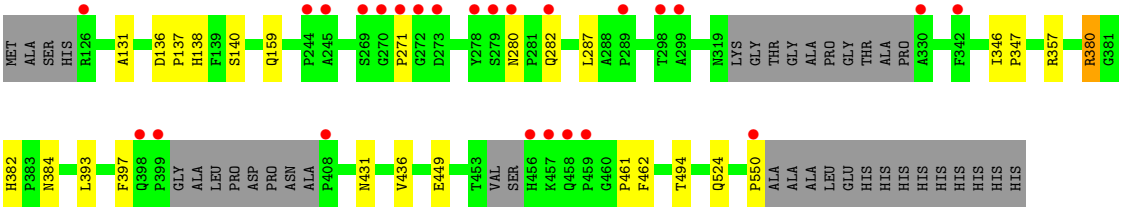
• Molecule 1: Capsid vertex component 2

Chain E:



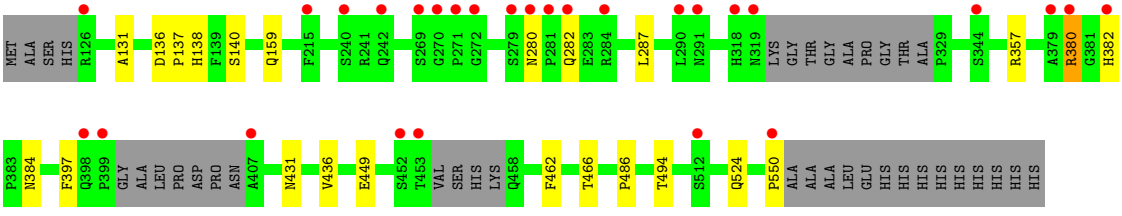
• Molecule 1: Capsid vertex component 2

Chain F:



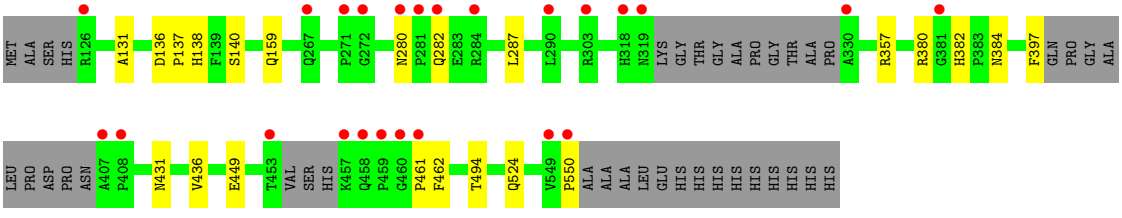
• Molecule 1: Capsid vertex component 2

Chain G:



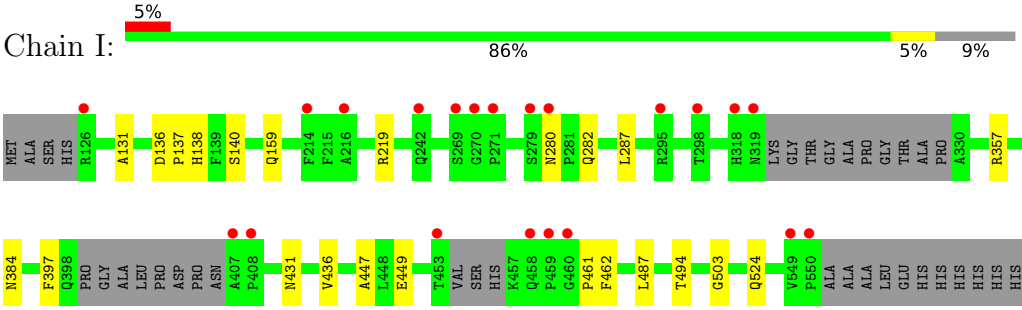
• Molecule 1: Capsid vertex component 2

Chain H:



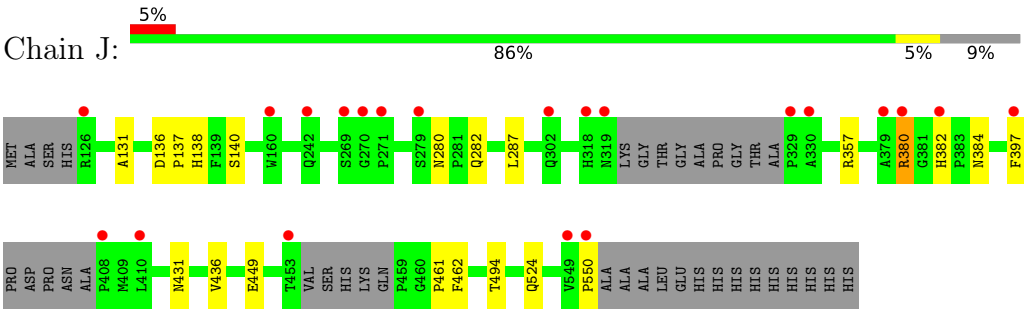
• Molecule 1: Capsid vertex component 2

Chain I:



• Molecule 1: Capsid vertex component 2

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.51Å 239.14Å 264.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.42 48.36 – 2.42	Depositor EDS
% Data completeness (in resolution range)	75.8 (48.36-2.42) 75.8 (48.36-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.207 , 0.235 0.197 , 0.223	Depositor DCC
R_{free} test set	8712 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33920	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.31	0/3315	0.50	0/4514
1	B	0.31	0/3256	0.49	0/4431
1	C	0.31	0/3306	0.50	0/4503
1	D	0.29	0/3256	0.49	0/4429
1	E	0.29	0/3272	0.49	0/4453
1	F	0.30	0/3271	0.49	0/4449
1	G	0.30	0/3264	0.49	0/4442
1	H	0.28	0/3248	0.48	0/4418
1	I	0.29	0/3257	0.49	0/4430
1	J	0.30	0/3242	0.49	0/4409
All	All	0.30	0/32687	0.49	0/44478

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3230	0	3232	18	0
1	B	3174	0	3175	16	0
1	C	3221	0	3219	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3174	0	3181	14	0
1	E	3189	0	3189	14	0
1	F	3188	0	3191	14	0
1	G	3181	0	3183	15	0
1	H	3167	0	3173	10	0
1	I	3176	0	3181	17	0
1	J	3160	0	3165	9	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
2	C	8	0	6	0	0
2	D	8	0	6	0	0
2	E	8	0	6	0	0
2	F	8	0	6	0	0
2	G	8	0	6	0	0
2	H	8	0	6	0	0
2	I	8	0	6	0	0
2	J	8	0	6	0	0
3	A	254	0	0	0	0
3	B	213	0	0	0	0
3	C	229	0	0	0	0
3	D	193	0	0	0	0
3	E	154	0	0	1	0
3	F	211	0	0	1	0
3	G	185	0	0	0	0
3	H	158	0	0	0	0
3	I	199	0	0	1	0
3	J	184	0	0	0	0
All	All	33920	0	31949	110	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 2.

All (110) 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:E:380:ARG:HA	1:G:486:PRO:HD2	1.38	1.02
1:E:380:ARG:HA	1:G:486:PRO:CD	2.01	0.91
1:A:380:ARG:HB3	1:B:484:ARG:HE	1.49	0.77
1:A:404:ASP:HB3	1:A:407:ALA:HB2	1.64	0.77
1:E:380:ARG:CA	1:G:486:PRO:HD2	2.17	0.71
1:A:461:PRO:HB2	1:E:137:PRO:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:HIS:CE1	1:I:487:LEU:HD21	2.29	0.67
1:A:382:HIS:HA	1:B:484:ARG:NH2	2.09	0.67
1:E:449:GLU:HG2	1:E:524:GLN:HG3	1.78	0.66
1:C:449:GLU:HG2	1:C:524:GLN:HG3	1.77	0.65
1:I:449:GLU:HG2	1:I:524:GLN:HG3	1.78	0.65
1:B:449:GLU:HG2	1:B:524:GLN:HG3	1.77	0.65
1:H:449:GLU:HG2	1:H:524:GLN:HG3	1.78	0.65
1:F:449:GLU:HG2	1:F:524:GLN:HG3	1.77	0.65
1:G:449:GLU:HG2	1:G:524:GLN:HG3	1.77	0.65
1:J:449:GLU:HG2	1:J:524:GLN:HG3	1.79	0.65
1:B:550:PRO:HG3	1:G:159:GLN:HG2	1.79	0.64
1:A:449:GLU:HG2	1:A:524:GLN:HG3	1.79	0.63
1:C:461:PRO:HB2	1:F:137:PRO:HB3	1.81	0.62
1:A:380:ARG:HG2	1:B:484:ARG:HH11	1.64	0.62
1:D:449:GLU:HG2	1:D:524:GLN:HG3	1.81	0.62
1:A:380:ARG:HB3	1:B:484:ARG:NE	2.15	0.61
1:D:510:HIS:HE1	1:I:487:LEU:HD21	1.68	0.57
1:F:461:PRO:HB2	1:I:137:PRO:HB3	1.87	0.57
1:B:137:PRO:HB3	1:I:461:PRO:HB2	1.87	0.56
1:F:382:HIS:CD2	1:F:384:ASN:HD22	2.25	0.55
1:F:271:PRO:HB3	3:F:888:HOH:O	2.08	0.54
1:A:280:ASN:HD21	1:A:282:GLN:HB3	1.72	0.53
1:D:267:GLN:HG2	1:I:219:ARG:NH1	2.24	0.52
1:A:382:HIS:CD2	1:A:384:ASN:HD22	2.27	0.52
1:I:280:ASN:HD21	1:I:282:GLN:HB2	1.75	0.51
1:C:280:ASN:HD21	1:C:282:GLN:HB2	1.76	0.51
1:H:280:ASN:HD21	1:H:282:GLN:HB2	1.75	0.51
1:J:280:ASN:HD21	1:J:282:GLN:HB2	1.75	0.51
1:D:280:ASN:HD21	1:D:282:GLN:HB2	1.76	0.51
1:B:280:ASN:HD21	1:B:282:GLN:HB2	1.76	0.51
1:G:280:ASN:HD21	1:G:282:GLN:HB2	1.76	0.50
1:E:280:ASN:HD21	1:E:282:GLN:HB2	1.76	0.50
1:F:280:ASN:HD21	1:F:282:GLN:HB2	1.76	0.50
1:D:137:PRO:HB3	1:H:461:PRO:HB2	1.92	0.50
1:D:287:LEU:HG	1:D:494:THR:HG23	1.94	0.50
1:E:287:LEU:HG	1:E:494:THR:HG23	1.94	0.50
1:E:380:ARG:HA	1:G:486:PRO:HD3	1.92	0.49
1:C:137:PRO:HG3	1:C:397:PHE:CD1	2.47	0.49
1:J:287:LEU:HG	1:J:494:THR:HG23	1.95	0.49
1:C:382:HIS:HD2	1:C:384:ASN:H	1.60	0.49
1:A:287:LEU:HG	1:A:494:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LEU:HG	1:F:494:THR:HG23	1.95	0.48
1:I:287:LEU:HG	1:I:494:THR:HG23	1.94	0.48
1:I:131:ALA:HB2	1:I:138:HIS:CD2	2.48	0.48
1:C:159:GLN:HG2	1:G:550:PRO:HG3	1.95	0.48
1:C:137:PRO:HG3	1:C:397:PHE:CE1	2.48	0.48
1:H:137:PRO:HB3	1:J:461:PRO:HB2	1.96	0.47
1:C:287:LEU:HG	1:C:494:THR:HG23	1.94	0.47
1:G:287:LEU:HG	1:G:494:THR:HG23	1.95	0.47
1:H:287:LEU:HG	1:H:494:THR:HG23	1.96	0.47
1:J:380:ARG:NH1	1:J:382:HIS:ND1	2.61	0.47
1:B:287:LEU:HG	1:B:494:THR:HG23	1.95	0.47
1:H:131:ALA:HB2	1:H:138:HIS:CD2	2.49	0.47
1:B:461:PRO:HB2	1:G:137:PRO:HB3	1.96	0.47
1:A:131:ALA:HB2	1:A:138:HIS:CD2	2.50	0.47
1:G:131:ALA:HB2	1:G:138:HIS:CD2	2.50	0.47
1:G:380:ARG:NH1	1:G:382:HIS:ND1	2.63	0.47
1:E:461:PRO:HB2	1:J:137:PRO:HB3	1.96	0.47
1:D:131:ALA:HB2	1:D:138:HIS:CD2	2.50	0.46
1:B:131:ALA:HB2	1:B:138:HIS:CD2	2.51	0.46
1:J:131:ALA:HB2	1:J:138:HIS:CD2	2.50	0.46
1:A:280:ASN:ND2	1:A:282:GLN:HB3	2.31	0.46
1:D:382:HIS:HD2	1:D:384:ASN:H	1.64	0.46
1:A:380:ARG:CB	1:B:484:ARG:HE	2.25	0.46
1:E:131:ALA:HB2	1:E:138:HIS:CD2	2.51	0.46
1:C:131:ALA:HB2	1:C:138:HIS:CD2	2.50	0.46
1:A:383:PRO:HD3	1:B:484:ARG:HH22	1.80	0.46
1:I:380:ARG:NH2	1:I:382:HIS:ND1	2.64	0.46
1:C:550:PRO:HG3	1:F:159:GLN:HG2	1.97	0.45
1:F:382:HIS:HD2	1:F:384:ASN:H	1.63	0.45
1:F:131:ALA:HB2	1:F:138:HIS:CD2	2.52	0.45
1:H:382:HIS:HD2	1:H:384:ASN:H	1.65	0.45
1:B:382:HIS:HE1	1:B:384:ASN:OD1	2.00	0.45
1:G:382:HIS:HD2	1:G:384:ASN:H	1.65	0.44
1:A:382:HIS:HD2	1:A:384:ASN:H	1.65	0.44
1:E:158:ASN:HB2	3:E:706:HOH:O	2.18	0.44
1:I:382:HIS:HD2	1:I:384:ASN:H	1.64	0.44
1:C:389:LEU:HD12	1:C:397:PHE:CE1	2.53	0.43
1:A:382:HIS:ND1	1:B:484:ARG:HD2	2.34	0.43
1:C:149:LEU:HD11	1:C:393:LEU:HD21	2.01	0.43
1:F:380:ARG:HD2	1:F:380:ARG:HA	1.77	0.43
1:J:382:HIS:HD2	1:J:384:ASN:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:380:ARG:HB2	3:I:852:HOH:O	2.19	0.43
1:A:137:PRO:HB3	1:D:461:PRO:HB2	2.01	0.42
1:D:510:HIS:HE1	1:I:487:LEU:CD2	2.32	0.42
1:D:159:GLN:HG2	1:H:550:PRO:HG3	2.02	0.42
1:F:550:PRO:HG3	1:I:159:GLN:HG2	2.02	0.41
1:I:280:ASN:ND2	1:I:282:GLN:HB2	2.35	0.41
1:F:346:ILE:HA	1:F:347:PRO:HD3	1.94	0.41
1:A:382:HIS:CD2	1:A:383:PRO:HD2	2.56	0.41
1:C:280:ASN:ND2	1:C:282:GLN:HB2	2.35	0.41
1:D:280:ASN:ND2	1:D:282:GLN:HB2	2.36	0.41
1:C:463:VAL:HG21	1:F:393:LEU:HD13	2.02	0.41
1:E:447:ALA:O	1:E:503:GLY:HA3	2.21	0.41
1:C:389:LEU:CD1	1:C:397:PHE:CE1	3.04	0.41
1:H:280:ASN:ND2	1:H:282:GLN:HB2	2.35	0.41
1:E:280:ASN:ND2	1:E:282:GLN:HB2	2.36	0.41
1:C:140:SER:HB3	1:G:466:THR:HG23	2.04	0.40
1:G:280:ASN:ND2	1:G:282:GLN:HB2	2.36	0.40
1:H:159:GLN:HG2	1:J:550:PRO:HG3	2.03	0.40
1:D:510:HIS:CE1	1:I:487:LEU:CD2	3.03	0.40
1:B:134:PRO:HD2	1:B:378:VAL:HG21	2.03	0.40
1:E:181:PHE:HB3	1:E:186:LYS:HE3	2.04	0.40
1:I:447:ALA:O	1:I:503:GLY:HA3	2.22	0.40

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	406/443 (92%)	399 (98%)	7 (2%)	0	100	100
1	B	396/443 (89%)	390 (98%)	6 (2%)	0	100	100
1	C	405/443 (91%)	400 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	396/443 (89%)	390 (98%)	6 (2%)	0	100	100
1	E	398/443 (90%)	390 (98%)	8 (2%)	0	100	100
1	F	397/443 (90%)	391 (98%)	6 (2%)	0	100	100
1	G	397/443 (90%)	391 (98%)	6 (2%)	0	100	100
1	H	395/443 (89%)	389 (98%)	6 (2%)	0	100	100
1	I	396/443 (89%)	390 (98%)	6 (2%)	0	100	100
1	J	394/443 (89%)	388 (98%)	6 (2%)	0	100	100
All	All	3980/4430 (90%)	3918 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	351/373 (94%)	343 (98%)	8 (2%)	50	68
1	B	345/373 (92%)	339 (98%)	6 (2%)	60	77
1	C	350/373 (94%)	344 (98%)	6 (2%)	60	77
1	D	345/373 (92%)	338 (98%)	7 (2%)	55	72
1	E	347/373 (93%)	341 (98%)	6 (2%)	60	77
1	F	347/373 (93%)	339 (98%)	8 (2%)	50	68
1	G	346/373 (93%)	338 (98%)	8 (2%)	50	68
1	H	344/373 (92%)	336 (98%)	8 (2%)	50	68
1	I	345/373 (92%)	337 (98%)	8 (2%)	50	68
1	J	344/373 (92%)	336 (98%)	8 (2%)	50	68
All	All	3464/3730 (93%)	3391 (98%)	73 (2%)	53	71

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	140	SER
1	A	357	ARG
1	A	380	ARG
1	A	397	PHE
1	A	436	VAL
1	A	462	PHE
1	A	468	SER
1	B	136	ASP
1	B	140	SER
1	B	357	ARG
1	B	397	PHE
1	B	436	VAL
1	B	462	PHE
1	C	136	ASP
1	C	140	SER
1	C	357	ARG
1	C	431	ASN
1	C	436	VAL
1	C	462	PHE
1	D	136	ASP
1	D	140	SER
1	D	179	ARG
1	D	357	ARG
1	D	397	PHE
1	D	436	VAL
1	D	462	PHE
1	E	136	ASP
1	E	140	SER
1	E	241	ARG
1	E	357	ARG
1	E	436	VAL
1	E	462	PHE
1	F	136	ASP
1	F	140	SER
1	F	357	ARG
1	F	380	ARG
1	F	397	PHE
1	F	431	ASN
1	F	436	VAL
1	F	462	PHE
1	G	136	ASP
1	G	140	SER

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Mol	Chain	Res	Type
1	G	357	ARG
1	G	380	ARG
1	G	397	PHE
1	G	431	ASN
1	G	436	VAL
1	G	462	PHE
1	H	136	ASP
1	H	140	SER
1	H	357	ARG
1	H	380	ARG
1	H	397	PHE
1	H	431	ASN
1	H	436	VAL
1	H	462	PHE
1	I	136	ASP
1	I	140	SER
1	I	357	ARG
1	I	380	ARG
1	I	397	PHE
1	I	431	ASN
1	I	436	VAL
1	I	462	PHE
1	J	136	ASP
1	J	140	SER
1	J	357	ARG
1	J	380	ARG
1	J	397	PHE
1	J	431	ASN
1	J	436	VAL
1	J	462	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	280	ASN
1	A	382	HIS
1	A	384	ASN
1	B	138	HIS
1	B	280	ASN
1	C	138	HIS
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	382	HIS
1	D	138	HIS
1	D	156	ASN
1	D	280	ASN
1	D	319	ASN
1	D	382	HIS
1	E	138	HIS
1	E	280	ASN
1	F	138	HIS
1	F	156	ASN
1	F	280	ASN
1	F	382	HIS
1	F	384	ASN
1	G	138	HIS
1	G	156	ASN
1	G	280	ASN
1	G	319	ASN
1	H	138	HIS
1	H	156	ASN
1	H	280	ASN
1	H	382	HIS
1	I	280	ASN
1	J	138	HIS
1	J	156	ASN
1	J	280	ASN
1	J	319	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 monosaccharides in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	412/443 (93%)	0.04	13 (3%) 47 45	29, 47, 87, 114	0
1	B	404/443 (91%)	-0.03	8 (1%) 65 62	34, 57, 88, 109	0
1	C	411/443 (92%)	0.17	18 (4%) 34 32	30, 54, 96, 112	0
1	D	404/443 (91%)	0.14	17 (4%) 36 34	33, 56, 90, 106	0
1	E	406/443 (91%)	0.27	24 (5%) 22 20	34, 60, 100, 120	0
1	F	405/443 (91%)	0.21	25 (6%) 20 19	28, 57, 108, 127	0
1	G	405/443 (91%)	0.27	28 (6%) 16 15	34, 60, 102, 117	0
1	H	403/443 (90%)	0.10	24 (5%) 21 20	38, 61, 97, 122	0
1	I	404/443 (91%)	0.10	23 (5%) 23 22	31, 54, 94, 112	0
1	J	402/443 (90%)	0.13	22 (5%) 25 23	38, 61, 97, 110	0
All	All	4056/4430 (91%)	0.14	202 (4%) 28 26	28, 57, 98, 127	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	GLY	10.7
1	A	398	GLN	5.8
1	F	330	ALA	5.7
1	G	319	ASN	5.5
1	E	550	PRO	5.4
1	G	453	THR	5.4
1	E	459	PRO	5.3
1	G	271	PRO	5.3
1	D	240	SER	4.9
1	G	512	SER	4.8
1	H	318	HIS	4.8
1	E	379	ALA	4.7
1	J	329	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	550	PRO	4.5
1	A	407	ALA	4.4
1	H	458	GLN	4.3
1	A	330	ALA	4.3
1	H	550	PRO	4.2
1	I	550	PRO	4.2
1	E	216	ALA	4.2
1	G	399	PRO	4.1
1	F	398	GLN	4.1
1	H	319	ASN	4.1
1	A	382	HIS	4.1
1	F	457	LYS	4.1
1	D	395	PRO	4.1
1	C	318	HIS	4.0
1	F	299	ALA	4.0
1	A	401	ALA	4.0
1	C	330	ALA	4.0
1	F	278	TYR	3.9
1	G	318	HIS	3.9
1	C	459	PRO	3.9
1	D	549	VAL	3.9
1	H	281	PRO	3.9
1	G	281	PRO	3.9
1	F	271	PRO	3.9
1	E	549	VAL	3.8
1	A	459	PRO	3.8
1	I	459	PRO	3.7
1	G	407	ALA	3.7
1	H	280	ASN	3.7
1	J	318	HIS	3.7
1	F	279	SER	3.6
1	F	456	HIS	3.6
1	A	550	PRO	3.6
1	J	379	ALA	3.6
1	I	380	ARG	3.6
1	H	549	VAL	3.6
1	F	272	GLY	3.5
1	J	550	PRO	3.5
1	I	269	SER	3.5
1	D	407	ALA	3.5
1	F	126	ARG	3.5
1	I	407	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	270	GLY	3.4
1	C	271	PRO	3.4
1	G	284	ARG	3.4
1	H	460	GLY	3.4
1	B	331	MET	3.4
1	A	458	GLN	3.4
1	C	126	ARG	3.4
1	B	407	ALA	3.4
1	B	550	PRO	3.3
1	C	458	GLN	3.3
1	I	458	GLN	3.3
1	I	270	GLY	3.3
1	I	319	ASN	3.2
1	D	242	GLN	3.2
1	G	126	ARG	3.2
1	E	331	MET	3.2
1	B	459	PRO	3.2
1	J	408	PRO	3.2
1	G	282	GLN	3.2
1	E	126	ARG	3.2
1	B	330	ALA	3.1
1	J	453	THR	3.1
1	D	484	ARG	3.1
1	H	407	ALA	3.1
1	H	457	LYS	3.1
1	B	269	SER	3.0
1	F	550	PRO	3.0
1	G	398	GLN	3.0
1	G	215	PHE	3.0
1	C	395	PRO	3.0
1	C	298	THR	3.0
1	H	303	ARG	3.0
1	J	382	HIS	2.9
1	G	452	SER	2.9
1	I	216	ALA	2.9
1	J	271	PRO	2.9
1	G	290	LEU	2.9
1	I	379	ALA	2.9
1	G	240	SER	2.9
1	E	344	SER	2.9
1	C	550	PRO	2.8
1	E	280	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	269	SER	2.8
1	H	284	ARG	2.8
1	F	458	GLN	2.8
1	H	272	GLY	2.8
1	H	459	PRO	2.8
1	J	549	VAL	2.7
1	D	397	PHE	2.7
1	B	272	GLY	2.7
1	E	279	SER	2.7
1	D	281	PRO	2.7
1	H	408	PRO	2.7
1	G	272	GLY	2.7
1	J	126	ARG	2.7
1	E	330	ALA	2.7
1	J	330	ALA	2.7
1	I	271	PRO	2.7
1	C	269	SER	2.7
1	D	343	GLY	2.7
1	G	280	ASN	2.7
1	H	267	GLN	2.7
1	J	398	GLN	2.7
1	C	279	SER	2.7
1	I	408	PRO	2.7
1	H	282	GLN	2.7
1	F	280	ASN	2.6
1	H	271	PRO	2.6
1	H	126	ARG	2.6
1	A	549	VAL	2.6
1	H	330	ALA	2.6
1	G	270	GLY	2.6
1	H	453	THR	2.6
1	I	318	HIS	2.6
1	J	279	SER	2.6
1	J	270	GLY	2.6
1	F	273	ASP	2.6
1	E	244	PRO	2.6
1	G	380	ARG	2.5
1	I	279	SER	2.5
1	H	381	GLY	2.5
1	G	242	GLN	2.5
1	F	269	SER	2.5
1	E	380	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	458	GLN	2.5
1	E	269	SER	2.5
1	J	319	ASN	2.5
1	E	308	ALA	2.4
1	C	242	GLN	2.4
1	G	344	SER	2.4
1	B	126	ARG	2.4
1	C	245	ALA	2.4
1	H	290	LEU	2.4
1	A	331	MET	2.4
1	G	550	PRO	2.4
1	G	279	SER	2.4
1	F	408	PRO	2.3
1	C	397	PHE	2.3
1	I	460	GLY	2.3
1	D	380	ARG	2.3
1	J	380	ARG	2.3
1	I	549	VAL	2.3
1	J	160	TRP	2.3
1	D	379	ALA	2.3
1	F	399	PRO	2.3
1	D	291	ASN	2.3
1	F	245	ALA	2.3
1	A	160	TRP	2.3
1	I	126	ARG	2.2
1	C	319	ASN	2.2
1	I	214	PHE	2.2
1	G	291	ASN	2.2
1	J	302	GLN	2.2
1	C	272	GLY	2.2
1	E	319	ASN	2.2
1	F	244	PRO	2.2
1	A	126	ARG	2.2
1	F	342	PHE	2.2
1	E	318	HIS	2.2
1	E	398	GLN	2.1
1	I	280	ASN	2.1
1	C	403	PRO	2.1
1	I	242	GLN	2.1
1	C	281	PRO	2.1
1	D	381	GLY	2.1
1	F	282	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	298	THR	2.1
1	I	298	THR	2.1
1	J	269	SER	2.1
1	E	245	ALA	2.1
1	E	334	VAL	2.1
1	J	410	LEU	2.1
1	E	458	GLN	2.1
1	F	459	PRO	2.0
1	G	379	ALA	2.0
1	G	382	HIS	2.0
1	J	397	PHE	2.0
1	I	295	ARG	2.0
1	E	281	PRO	2.0
1	E	383	PRO	2.0
1	F	289	PRO	2.0
1	H	461	PRO	2.0
1	I	453	THR	2.0
1	J	242	GLN	2.0
1	D	344	SER	2.0
1	D	248	ASP	2.0
1	E	405	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	C	602	4/4	0.80	0.43	84,84,84,84	0
2	ACT	F	602	4/4	0.80	0.23	81,81,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	G	602	4/4	0.81	0.23	79,79,79,79	0
2	ACT	B	602	4/4	0.85	0.17	89,89,89,90	0
2	ACT	J	602	4/4	0.86	0.49	90,91,91,91	0
2	ACT	H	602	4/4	0.89	0.15	87,87,87,88	0
2	ACT	A	602	4/4	0.89	0.19	76,76,76,76	0
2	ACT	D	602	4/4	0.90	0.17	76,76,77,77	0
2	ACT	I	602	4/4	0.92	0.24	70,70,70,70	0
2	ACT	E	602	4/4	0.92	0.39	88,88,88,88	0
2	ACT	J	601	4/4	0.93	0.16	53,53,53,53	0
2	ACT	H	601	4/4	0.93	0.21	65,65,66,66	0
2	ACT	G	601	4/4	0.95	0.22	52,52,53,54	0
2	ACT	D	601	4/4	0.97	0.15	54,54,55,55	0
2	ACT	A	601	4/4	0.97	0.13	53,53,53,53	0
2	ACT	E	601	4/4	0.97	0.18	58,58,58,58	0
2	ACT	F	601	4/4	0.98	0.20	47,48,48,48	0
2	ACT	B	601	4/4	0.98	0.14	52,52,52,52	0
2	ACT	I	601	4/4	0.98	0.14	54,54,54,55	0
2	ACT	C	601	4/4	0.99	0.15	42,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.