



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:15 AM UTC

PDB ID : 7NXQ / pdb_00007nxq
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 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
Mogul : 2022.3.0, CSD as543be (2022)
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

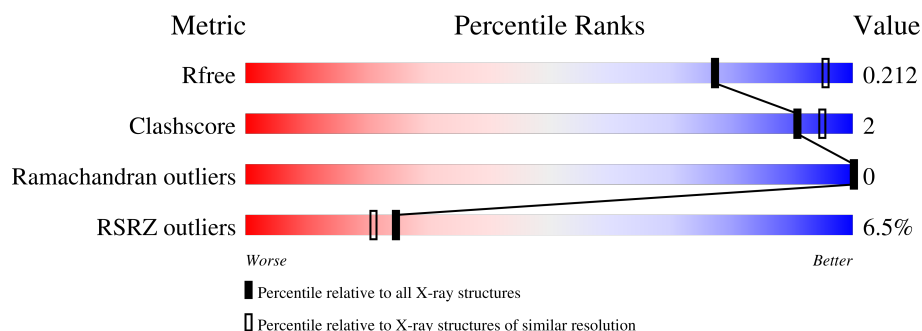
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
RSRZ outliers	180081	6066 (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 $\leq 5\%$. 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	443	7% 89% 7%
1	B	443	4% 87% 5% 9%
1	C	443	5% 88% 5% 7%
1	D	443	6% 87% 9%
1	E	443	7% 87% 5% 8%
1	F	443	6% 86% 5% 9%

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Mol	Chain	Length	Quality of chain
1	G	443	8% 87% 5% 9%
1	H	443	5% 87% • 9%
1	I	443	6% 86% 5% 9%
1	J	443	6% 87% • 9%

2 Entry composition

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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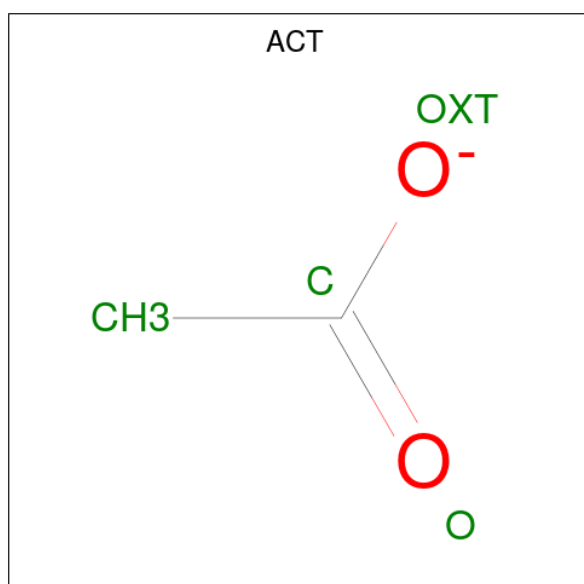
Chain	Residue	Modelled	Actual	Comment	Reference
F	562	HIS	-	expression tag	UNP Q76RI7
F	563	HIS	-	expression tag	UNP Q76RI7
F	564	HIS	-	expression tag	UNP Q76RI7
G	122	MET	-	initiating methionine	UNP Q76RI7
G	550	PRO	-	expression tag	UNP Q76RI7
G	551	ALA	-	expression tag	UNP Q76RI7
G	552	ALA	-	expression 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 (CCD ID: 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

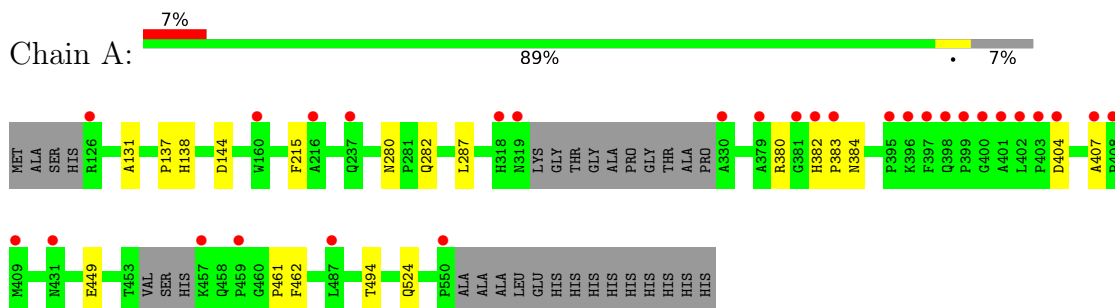
- Molecule 3 is water.

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

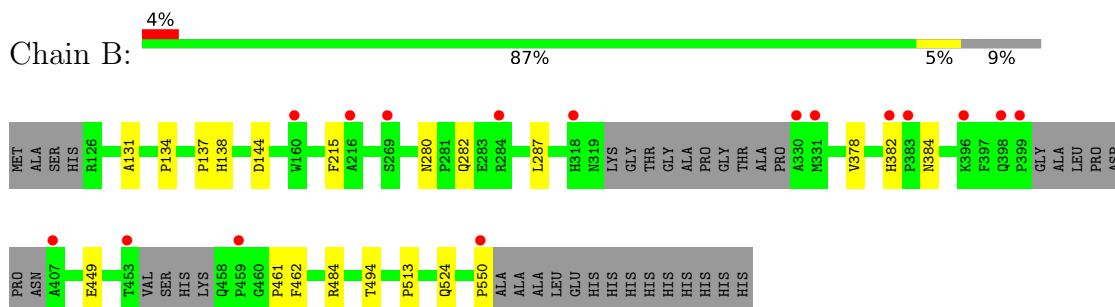
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

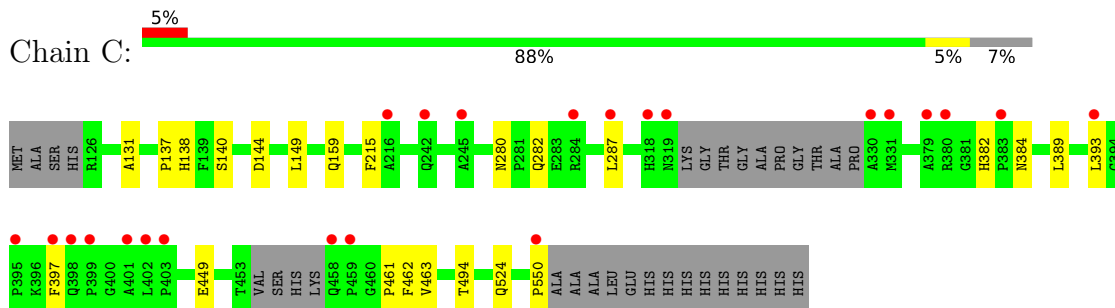
- Molecule 1: Capsid vertex component 2



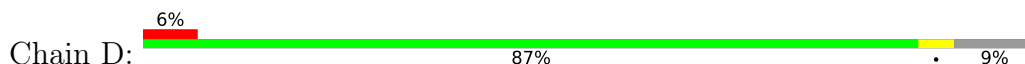
- Molecule 1: Capsid vertex component 2

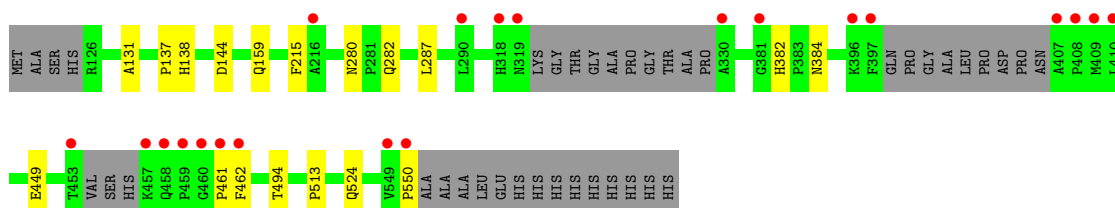


- Molecule 1: Capsid vertex component 2

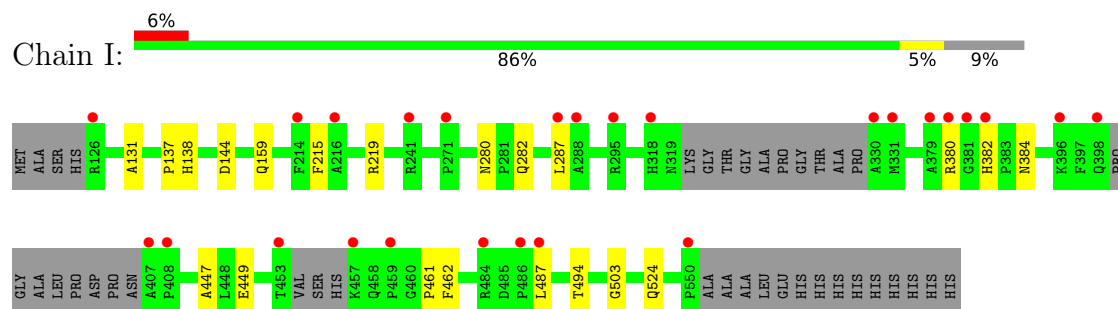


- Molecule 1: Capsid vertex component 2

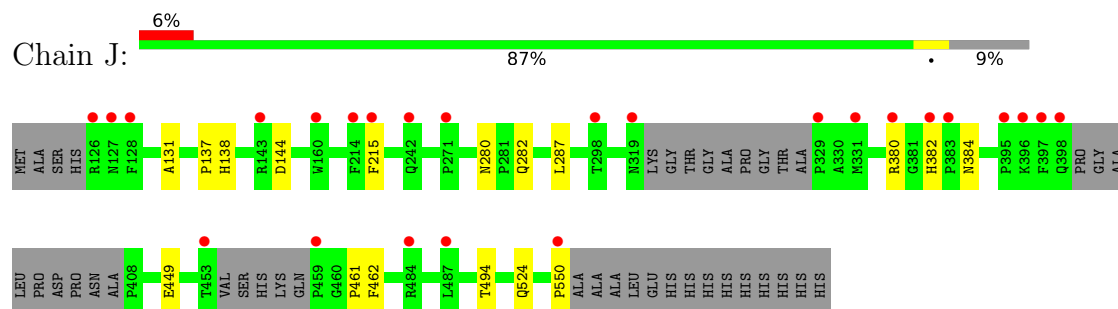




● Molecule 1: Capsid vertex component 2



● Molecule 1: Capsid vertex component 2



4 Data and refinement statistics

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) 75.7 (48.36-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.207 , 0.235 (Not available) , 0.212	Depositor DCC
R_{free} test set	8712 reflections (3.76%)	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)	0.31 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.61	0/3315	1.00	3/4514 (0.1%)
1	B	0.61	0/3256	0.99	4/4431 (0.1%)
1	C	0.61	0/3306	0.99	3/4503 (0.1%)
1	D	0.59	0/3256	0.98	3/4429 (0.1%)
1	E	0.59	0/3272	0.98	4/4453 (0.1%)
1	F	0.59	0/3271	1.00	3/4449 (0.1%)
1	G	0.59	0/3264	0.99	4/4442 (0.1%)
1	H	0.58	0/3248	0.99	4/4418 (0.1%)
1	I	0.59	0/3257	0.99	3/4430 (0.1%)
1	J	0.60	0/3242	0.99	3/4409 (0.1%)
All	All	0.60	0/32687	0.99	34/44478 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	462	PHE	CA-CB-CG	8.41	122.21	113.80
1	J	462	PHE	CA-CB-CG	7.77	121.57	113.80
1	E	462	PHE	CA-CB-CG	7.57	121.37	113.80
1	C	462	PHE	CA-CB-CG	7.54	121.33	113.80
1	D	462	PHE	CA-CB-CG	7.30	121.10	113.80
1	H	462	PHE	CA-CB-CG	7.27	121.07	113.80
1	F	462	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	462	PHE	CA-CB-CG	7.03	120.83	113.80
1	I	462	PHE	CA-CB-CG	7.03	120.83	113.80
1	B	462	PHE	CA-CB-CG	6.83	120.63	113.80
1	H	215	PHE	CA-CB-CG	6.34	120.14	113.80
1	E	215	PHE	CA-CB-CG	6.32	120.12	113.80
1	C	215	PHE	CA-CB-CG	6.31	120.11	113.80
1	J	215	PHE	CA-CB-CG	6.13	119.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	PHE	CA-CB-CG	6.13	119.93	113.80
1	F	215	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	215	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	215	PHE	CA-CB-CG	6.00	119.80	113.80
1	G	215	PHE	CA-CB-CG	5.97	119.77	113.80
1	C	144	ASP	CA-CB-CG	5.84	118.44	112.60
1	I	215	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	144	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	144	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	144	ASP	CA-CB-CG	5.47	118.07	112.60
1	J	144	ASP	CA-CB-CG	5.35	117.95	112.60
1	H	144	ASP	CA-CB-CG	5.32	117.92	112.60
1	E	144	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	397	PHE	CA-CB-CG	5.24	119.04	113.80
1	E	345	ASP	CA-CB-CG	5.21	117.81	112.60
1	I	144	ASP	CA-CB-CG	5.20	117.80	112.60
1	G	144	ASP	CA-CB-CG	5.17	117.77	112.60
1	H	513	PRO	N-CA-C	5.11	116.93	110.70
1	B	513	PRO	N-CA-C	5.10	116.92	110.70
1	F	144	ASP	CA-CB-CG	5.07	117.67	112.60

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	362/443 (82%)	356 (98%)	6 (2%)	0	100	100
1	C	405/443 (91%)	400 (99%)	5 (1%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	3946/4430 (89%)	3884 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	H	601	-	3,3,3	1.10	0	3,3,3	0.98	0
2	ACT	H	602	-	3,3,3	1.08	0	3,3,3	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	601	-	3,3,3	1.10	0	3,3,3	0.82	0
2	ACT	G	602	-	3,3,3	1.15	0	3,3,3	0.85	0
2	ACT	G	601	-	3,3,3	1.17	0	3,3,3	0.85	0
2	ACT	I	602	-	3,3,3	1.10	0	3,3,3	0.86	0
2	ACT	J	601	-	3,3,3	1.04	0	3,3,3	0.97	0
2	ACT	I	601	-	3,3,3	1.09	0	3,3,3	0.84	0
2	ACT	E	602	-	3,3,3	1.07	0	3,3,3	0.97	0
2	ACT	C	601	-	3,3,3	1.09	0	3,3,3	0.88	0
2	ACT	A	602	-	3,3,3	1.17	0	3,3,3	0.83	0
2	ACT	C	602	-	3,3,3	1.13	0	3,3,3	1.04	0
2	ACT	F	602	-	3,3,3	1.15	0	3,3,3	1.04	0
2	ACT	D	601	-	3,3,3	1.07	0	3,3,3	0.84	0
2	ACT	B	602	-	3,3,3	1.14	0	3,3,3	0.86	0
2	ACT	E	601	-	3,3,3	1.08	0	3,3,3	1.02	0
2	ACT	A	601	-	3,3,3	1.17	0	3,3,3	0.86	0
2	ACT	D	602	-	3,3,3	1.13	0	3,3,3	0.86	0
2	ACT	F	601	-	3,3,3	1.04	0	3,3,3	0.88	0
2	ACT	J	602	-	3,3,3	1.15	0	3,3,3	0.98	0

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 [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	412/443 (93%)	0.12	29 (7%)	22	19	29, 47, 87, 114	0
1	B	404/443 (91%)	0.22	16 (3%)	42	38	34, 57, 88, 109	0
1	C	411/443 (92%)	0.23	23 (5%)	30	26	30, 54, 96, 112	0
1	D	404/443 (91%)	0.25	28 (6%)	23	19	33, 56, 90, 106	0
1	E	406/443 (91%)	0.39	33 (8%)	18	14	34, 60, 100, 120	0
1	F	405/443 (91%)	0.27	26 (6%)	25	22	28, 57, 108, 127	0
1	G	405/443 (91%)	0.41	37 (9%)	15	12	34, 60, 102, 117	0
1	H	403/443 (90%)	0.31	21 (5%)	33	29	38, 61, 97, 122	0
1	I	404/443 (91%)	0.25	26 (6%)	25	22	31, 54, 94, 112	0
1	J	402/443 (90%)	0.38	25 (6%)	26	23	38, 61, 97, 110	0
All	All	4056/4430 (91%)	0.28	264 (6%)	25	21	28, 57, 98, 127	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	512	SER	5.8
1	E	379	ALA	5.5
1	C	330	ALA	5.3
1	G	453	THR	5.3
1	I	216	ALA	5.2
1	D	381	GLY	5.1
1	G	399	PRO	4.8
1	A	400	GLY	4.5
1	J	459	PRO	4.5
1	C	395	PRO	4.5
1	J	453	THR	4.3
1	A	382	HIS	4.3
1	H	550	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	457	LYS	4.3
1	B	330	ALA	4.2
1	E	405	PRO	4.2
1	E	216	ALA	4.1
1	I	407	ALA	4.0
1	G	319	ASN	4.0
1	D	407	ALA	3.9
1	A	398	GLN	3.9
1	E	380	ARG	3.9
1	G	380	ARG	3.9
1	E	378	VAL	3.9
1	G	398	GLN	3.8
1	D	395	PRO	3.8
1	E	550	PRO	3.8
1	H	407	ALA	3.8
1	F	456	HIS	3.8
1	B	550	PRO	3.8
1	D	240	SER	3.7
1	A	402	LEU	3.7
1	B	453	THR	3.7
1	D	397	PHE	3.7
1	E	381	GLY	3.7
1	C	459	PRO	3.7
1	E	215	PHE	3.7
1	G	331	MET	3.6
1	B	383	PRO	3.6
1	G	329	PRO	3.6
1	I	457	LYS	3.5
1	I	381	GLY	3.5
1	C	397	PHE	3.5
1	I	550	PRO	3.5
1	G	381	GLY	3.5
1	B	399	PRO	3.5
1	E	399	PRO	3.4
1	J	396	LYS	3.4
1	E	330	ALA	3.4
1	D	396	LYS	3.4
1	E	459	PRO	3.4
1	G	461	PRO	3.3
1	G	550	PRO	3.3
1	H	318	HIS	3.3
1	H	459	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	379	ALA	3.3
1	F	550	PRO	3.2
1	E	453	THR	3.2
1	G	269	SER	3.2
1	C	319	ASN	3.2
1	F	408	PRO	3.2
1	D	380	ARG	3.2
1	E	344	SER	3.2
1	D	319	ASN	3.2
1	G	330	ALA	3.1
1	J	380	ARG	3.1
1	C	550	PRO	3.1
1	A	409	MET	3.1
1	F	399	PRO	3.1
1	B	407	ALA	3.0
1	H	330	ALA	3.0
1	I	453	THR	3.0
1	B	331	MET	3.0
1	A	401	ALA	3.0
1	A	550	PRO	3.0
1	G	160	TRP	3.0
1	A	399	PRO	3.0
1	J	398	GLN	3.0
1	A	459	PRO	2.9
1	D	329	PRO	2.9
1	H	396	LYS	2.9
1	G	215	PHE	2.9
1	B	269	SER	2.9
1	H	319	ASN	2.9
1	A	381	GLY	2.9
1	F	240	SER	2.9
1	J	329	PRO	2.9
1	G	287	LEU	2.9
1	E	214	PHE	2.9
1	E	398	GLN	2.9
1	A	319	ASN	2.9
1	H	460	GLY	2.9
1	H	216	ALA	2.9
1	I	330	ALA	2.9
1	H	458	GLN	2.9
1	G	452	SER	2.8
1	J	382	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	398	GLN	2.8
1	A	431	ASN	2.8
1	D	484	ARG	2.8
1	D	550	PRO	2.8
1	F	288	ALA	2.8
1	F	398	GLN	2.8
1	F	319	ASN	2.8
1	I	486	PRO	2.8
1	B	382	HIS	2.8
1	A	403	PRO	2.7
1	J	127	ASN	2.7
1	J	271	PRO	2.7
1	D	330	ALA	2.7
1	F	216	ALA	2.7
1	H	453	THR	2.7
1	I	380	ARG	2.7
1	G	382	HIS	2.7
1	C	383	PRO	2.7
1	D	453	THR	2.7
1	D	457	LYS	2.7
1	C	458	GLN	2.7
1	G	316	PHE	2.7
1	G	407	ALA	2.7
1	G	460	GLY	2.7
1	H	408	PRO	2.7
1	J	143	ARG	2.7
1	A	216	ALA	2.6
1	G	458	GLN	2.6
1	J	160	TRP	2.6
1	H	381	GLY	2.6
1	C	331	MET	2.6
1	E	331	MET	2.6
1	C	401	ALA	2.6
1	G	318	HIS	2.6
1	E	383	PRO	2.5
1	D	215	PHE	2.5
1	I	487	LEU	2.5
1	C	242	GLN	2.5
1	B	216	ALA	2.5
1	E	407	ALA	2.5
1	G	240	SER	2.5
1	I	241	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	550	PRO	2.5
1	A	487	LEU	2.5
1	D	243	LEU	2.5
1	A	237	GLN	2.5
1	A	379	ALA	2.5
1	F	453	THR	2.5
1	A	160	TRP	2.5
1	A	397	PHE	2.5
1	I	214	PHE	2.5
1	J	487	LEU	2.5
1	B	398	GLN	2.5
1	D	242	GLN	2.5
1	C	379	ALA	2.5
1	I	287	LEU	2.5
1	I	396	LYS	2.5
1	C	398	GLN	2.5
1	E	397	PHE	2.5
1	F	397	PHE	2.5
1	J	397	PHE	2.5
1	A	330	ALA	2.5
1	G	379	ALA	2.5
1	D	459	PRO	2.4
1	A	396	LYS	2.4
1	F	458	GLN	2.4
1	A	126	ARG	2.4
1	B	160	TRP	2.4
1	F	459	PRO	2.4
1	B	396	LYS	2.4
1	D	462	PHE	2.4
1	G	214	PHE	2.4
1	J	126	ARG	2.4
1	B	459	PRO	2.4
1	H	461	PRO	2.4
1	D	378	VAL	2.4
1	C	393	LEU	2.4
1	D	458	GLN	2.4
1	E	318	HIS	2.4
1	G	315	LEU	2.4
1	I	318	HIS	2.4
1	H	397	PHE	2.4
1	A	407	ALA	2.4
1	A	408	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	160	TRP	2.4
1	J	484	ARG	2.3
1	A	318	HIS	2.3
1	E	458	GLN	2.3
1	F	330	ALA	2.3
1	A	395	PRO	2.3
1	A	383	PRO	2.3
1	E	461	PRO	2.3
1	G	216	ALA	2.3
1	I	459	PRO	2.3
1	I	126	ARG	2.3
1	B	318	HIS	2.3
1	E	483	PHE	2.3
1	C	403	PRO	2.3
1	G	408	PRO	2.3
1	I	379	ALA	2.3
1	F	409	MET	2.3
1	F	342	PHE	2.3
1	B	284	ARG	2.3
1	E	395	PRO	2.3
1	F	395	PRO	2.3
1	F	484	ARG	2.3
1	G	351	ALA	2.2
1	F	215	PHE	2.2
1	E	394	GLY	2.2
1	C	287	LEU	2.2
1	H	409	MET	2.2
1	J	214	PHE	2.2
1	E	319	ASN	2.2
1	E	382	HIS	2.2
1	G	490	LEU	2.2
1	H	410	LEU	2.2
1	D	344	SER	2.2
1	I	295	ARG	2.2
1	D	408	PRO	2.2
1	A	457	LYS	2.2
1	C	245	ALA	2.2
1	F	457	LYS	2.2
1	J	331	MET	2.2
1	C	284	ARG	2.2
1	G	271	PRO	2.2
1	E	245	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	331	MET	2.1
1	C	402	LEU	2.1
1	J	298	THR	2.1
1	G	344	SER	2.1
1	C	399	PRO	2.1
1	H	462	PHE	2.1
1	J	215	PHE	2.1
1	H	549	VAL	2.1
1	J	242	GLN	2.1
1	G	487	LEU	2.1
1	C	380	ARG	2.1
1	I	408	PRO	2.1
1	D	318	HIS	2.1
1	I	382	HIS	2.1
1	F	126	ARG	2.1
1	I	484	ARG	2.1
1	I	271	PRO	2.1
1	J	383	PRO	2.1
1	J	128	PHE	2.1
1	F	485	ASP	2.1
1	E	452	SER	2.1
1	G	409	MET	2.1
1	E	342	PHE	2.0
1	G	462	PHE	2.0
1	C	216	ALA	2.0
1	F	380	ARG	2.0
1	J	319	ASN	2.0
1	G	270	GLY	2.0
1	F	396	LYS	2.0
1	A	404	ASP	2.0
1	C	318	HIS	2.0
1	E	316	PHE	2.0
1	D	393	LEU	2.0
1	E	285	ALA	2.0
1	H	290	LEU	2.0
1	I	288	ALA	2.0
1	E	127	ASN	2.0
1	F	127	ASN	2.0
1	D	485	ASP	2.0
1	J	395	PRO	2.0
1	F	318	HIS	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	ACT	F	602	4/4	0.85	0.20	81,81,81,82	0
2	ACT	H	602	4/4	0.85	0.19	87,87,87,88	0
2	ACT	J	602	4/4	0.85	0.22	90,91,91,91	0
2	ACT	C	602	4/4	0.86	0.19	84,84,84,84	0
2	ACT	D	602	4/4	0.87	0.16	76,76,77,77	0
2	ACT	A	602	4/4	0.88	0.15	76,76,76,76	0
2	ACT	E	602	4/4	0.89	0.16	88,88,88,88	0
2	ACT	G	602	4/4	0.89	0.17	79,79,79,79	0
2	ACT	J	601	4/4	0.90	0.14	53,53,53,53	0
2	ACT	B	602	4/4	0.91	0.17	89,89,89,90	0
2	ACT	I	602	4/4	0.91	0.13	70,70,70,70	0
2	ACT	D	601	4/4	0.92	0.13	54,54,55,55	0
2	ACT	H	601	4/4	0.92	0.15	65,65,66,66	0
2	ACT	G	601	4/4	0.92	0.14	52,52,53,54	0
2	ACT	E	601	4/4	0.94	0.10	58,58,58,58	0
2	ACT	F	601	4/4	0.94	0.10	47,48,48,48	0
2	ACT	I	601	4/4	0.96	0.09	54,54,54,55	0
2	ACT	B	601	4/4	0.97	0.07	52,52,52,52	0
2	ACT	A	601	4/4	0.97	0.07	53,53,53,53	0
2	ACT	C	601	4/4	0.97	0.06	42,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.