



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:16 am GMT

PDB ID : 6GSI
EMDB ID : EMD-0056
Title : Feline Calicivirus Strain F9 bound to a soluble ectodomain fragment of feline junctional adhesion molecule A - leading to assembly of a portal structure at a unique three-fold axis.
Authors : Conley, M.J.; Bhella, D.
Deposited on : 2018-06-14
Resolution : 3.75 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

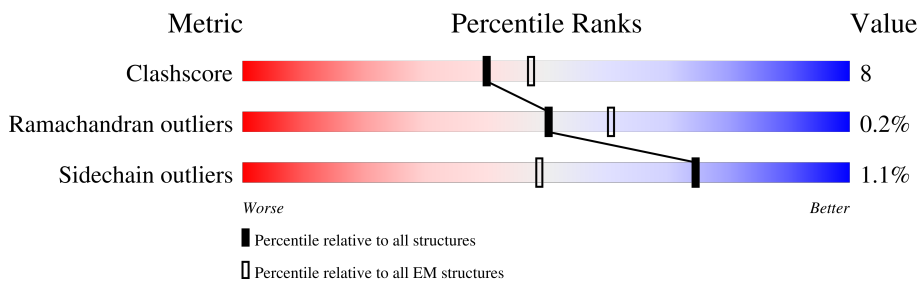
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.75 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.



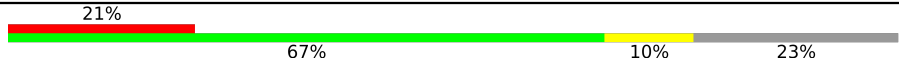
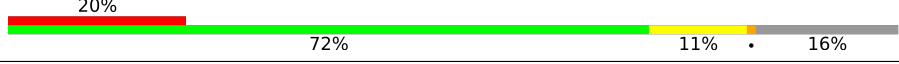
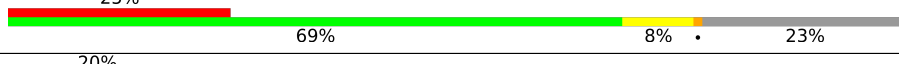

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	669	
1	B	669	
1	C	669	
1	D	669	
2	E	202	
2	F	202	
2	G	202	
2	H	202	

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Mol	Chain	Length	Quality of chain
3	I	106	
3	J	106	
3	K	106	
3	L	106	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 50126 atoms, of which 24749 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	534	8123	2612	4026	684	790	11	0	0
1	B	530	8061	2596	3990	680	784	11	0	0
1	C	534	8121	2612	4024	684	790	11	0	0
1	D	534	8123	2612	4026	684	790	11	0	0

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	ASP	conflict	UNP P27406
A	19	ARG	LYS	conflict	UNP P27406
A	23	ASP	ASN	conflict	UNP P27406
A	26	LYS	ASN	conflict	UNP P27406
A	34	ASP	SER	conflict	UNP P27406
A	56	GLN	ARG	conflict	UNP P27406
A	60	GLN	GLU	conflict	UNP P27406
A	76	TYR	PHE	conflict	UNP P27406
A	77	GLU	ASP	conflict	UNP P27406
A	79	ILE	VAL	conflict	UNP P27406
A	82	ALA	VAL	conflict	UNP P27406
A	89	ASP	GLY	conflict	UNP P27406
A	109	GLU	LYS	conflict	UNP P27406
A	112	LYS	ALA	conflict	UNP P27406
A	113	ALA	GLY	conflict	UNP P27406
A	117	ASN	ASP	conflict	UNP P27406
A	120	MET	LEU	conflict	UNP P27406
A	121	PHE	ILE	conflict	UNP P27406
A	127	GLY	-	insertion	UNP P27406
A	139	PRO	MET	conflict	UNP P27406
A	153	ALA	THR	conflict	UNP P27406
A	217	ASP	GLU	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
A	268	SER	CYS	conflict	UNP P27406
A	269	ILE	LEU	conflict	UNP P27406
A	304	SER	ALA	conflict	UNP P27406
A	319	ALA	PRO	conflict	UNP P27406
A	338	VAL	ILE	conflict	UNP P27406
A	346	SER	THR	conflict	UNP P27406
A	355	HIS	TYR	conflict	UNP P27406
A	357	THR	SER	conflict	UNP P27406
A	389	TYR	PHE	conflict	UNP P27406
A	393	THR	SER	conflict	UNP P27406
A	394	ILE	VAL	conflict	UNP P27406
A	397	SER	THR	conflict	UNP P27406
A	399	LYS	GLN	conflict	UNP P27406
A	428	GLU	GLY	conflict	UNP P27406
A	429	LYS	GLU	conflict	UNP P27406
A	431	THR	ILE	conflict	UNP P27406
A	441	LYS	GLY	conflict	UNP P27406
A	442	SER	THR	conflict	UNP P27406
A	450	ALA	THR	conflict	UNP P27406
A	454	GLY	THR	conflict	UNP P27406
A	457	VAL	ILE	conflict	UNP P27406
A	459	VAL	LYS	conflict	UNP P27406
A	465	LYS	ARG	conflict	UNP P27406
A	493	LYS	-	insertion	UNP P27406
A	494	VAL	LEU	conflict	UNP P27406
A	?	-	GLY	deletion	UNP P27406
A	?	-	ASP	deletion	UNP P27406
A	?	-	ASN	deletion	UNP P27406
A	?	-	ASN	deletion	UNP P27406
A	497	ALA	LYS	conflict	UNP P27406
A	499	GLU	ASN	conflict	UNP P27406
A	501	SER	CYS	conflict	UNP P27406
A	503	VAL	THR	conflict	UNP P27406
A	506	MET	GLN	conflict	UNP P27406
A	507	THR	SER	conflict	UNP P27406
A	510	ALA	VAL	conflict	UNP P27406
A	512	TYR	PHE	conflict	UNP P27406
A	515	THR	ASN	conflict	UNP P27406
A	520	GLU	LYS	conflict	UNP P27406
A	521	VAL	ALA	conflict	UNP P27406
A	529	SER	ALA	conflict	UNP P27406
A	553	VAL	THR	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
A	636	SER	GLY	conflict	UNP P27406
A	637	ILE	PHE	conflict	UNP P27406
A	645	THR	SER	conflict	UNP P27406
A	665	SER	PRO	conflict	UNP P27406
B	13	ASN	ASP	conflict	UNP P27406
B	19	ARG	LYS	conflict	UNP P27406
B	23	ASP	ASN	conflict	UNP P27406
B	26	LYS	ASN	conflict	UNP P27406
B	34	ASP	SER	conflict	UNP P27406
B	56	GLN	ARG	conflict	UNP P27406
B	60	GLN	GLU	conflict	UNP P27406
B	76	TYR	PHE	conflict	UNP P27406
B	77	GLU	ASP	conflict	UNP P27406
B	79	ILE	VAL	conflict	UNP P27406
B	82	ALA	VAL	conflict	UNP P27406
B	89	ASP	GLY	conflict	UNP P27406
B	109	GLU	LYS	conflict	UNP P27406
B	112	LYS	ALA	conflict	UNP P27406
B	113	ALA	GLY	conflict	UNP P27406
B	117	ASN	ASP	conflict	UNP P27406
B	120	MET	LEU	conflict	UNP P27406
B	121	PHE	ILE	conflict	UNP P27406
B	127	GLY	-	insertion	UNP P27406
B	139	PRO	MET	conflict	UNP P27406
B	153	ALA	THR	conflict	UNP P27406
B	217	ASP	GLU	conflict	UNP P27406
B	268	SER	CYS	conflict	UNP P27406
B	269	ILE	LEU	conflict	UNP P27406
B	304	SER	ALA	conflict	UNP P27406
B	319	ALA	PRO	conflict	UNP P27406
B	338	VAL	ILE	conflict	UNP P27406
B	346	SER	THR	conflict	UNP P27406
B	355	HIS	TYR	conflict	UNP P27406
B	357	THR	SER	conflict	UNP P27406
B	389	TYR	PHE	conflict	UNP P27406
B	393	THR	SER	conflict	UNP P27406
B	394	ILE	VAL	conflict	UNP P27406
B	397	SER	THR	conflict	UNP P27406
B	399	LYS	GLN	conflict	UNP P27406
B	428	GLU	GLY	conflict	UNP P27406
B	429	LYS	GLU	conflict	UNP P27406
B	431	THR	ILE	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
B	441	LYS	GLY	conflict	UNP P27406
B	442	SER	THR	conflict	UNP P27406
B	450	ALA	THR	conflict	UNP P27406
B	454	GLY	THR	conflict	UNP P27406
B	457	VAL	ILE	conflict	UNP P27406
B	459	VAL	LYS	conflict	UNP P27406
B	465	LYS	ARG	conflict	UNP P27406
B	493	LYS	-	insertion	UNP P27406
B	494	VAL	LEU	conflict	UNP P27406
B	?	-	GLY	deletion	UNP P27406
B	?	-	ASP	deletion	UNP P27406
B	?	-	ASN	deletion	UNP P27406
B	?	-	ASN	deletion	UNP P27406
B	497	ALA	LYS	conflict	UNP P27406
B	499	GLU	ASN	conflict	UNP P27406
B	501	SER	CYS	conflict	UNP P27406
B	503	VAL	THR	conflict	UNP P27406
B	506	MET	GLN	conflict	UNP P27406
B	507	THR	SER	conflict	UNP P27406
B	510	ALA	VAL	conflict	UNP P27406
B	512	TYR	PHE	conflict	UNP P27406
B	515	THR	ASN	conflict	UNP P27406
B	520	GLU	LYS	conflict	UNP P27406
B	521	VAL	ALA	conflict	UNP P27406
B	529	SER	ALA	conflict	UNP P27406
B	553	VAL	THR	conflict	UNP P27406
B	636	SER	GLY	conflict	UNP P27406
B	637	ILE	PHE	conflict	UNP P27406
B	645	THR	SER	conflict	UNP P27406
B	665	SER	PRO	conflict	UNP P27406
C	13	ASN	ASP	conflict	UNP P27406
C	19	ARG	LYS	conflict	UNP P27406
C	23	ASP	ASN	conflict	UNP P27406
C	26	LYS	ASN	conflict	UNP P27406
C	34	ASP	SER	conflict	UNP P27406
C	56	GLN	ARG	conflict	UNP P27406
C	60	GLN	GLU	conflict	UNP P27406
C	76	TYR	PHE	conflict	UNP P27406
C	77	GLU	ASP	conflict	UNP P27406
C	79	ILE	VAL	conflict	UNP P27406
C	82	ALA	VAL	conflict	UNP P27406
C	89	ASP	GLY	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
C	109	GLU	LYS	conflict	UNP P27406
C	112	LYS	ALA	conflict	UNP P27406
C	113	ALA	GLY	conflict	UNP P27406
C	117	ASN	ASP	conflict	UNP P27406
C	120	MET	LEU	conflict	UNP P27406
C	121	PHE	ILE	conflict	UNP P27406
C	127	GLY	-	insertion	UNP P27406
C	139	PRO	MET	conflict	UNP P27406
C	153	ALA	THR	conflict	UNP P27406
C	217	ASP	GLU	conflict	UNP P27406
C	268	SER	CYS	conflict	UNP P27406
C	269	ILE	LEU	conflict	UNP P27406
C	304	SER	ALA	conflict	UNP P27406
C	319	ALA	PRO	conflict	UNP P27406
C	338	VAL	ILE	conflict	UNP P27406
C	346	SER	THR	conflict	UNP P27406
C	355	HIS	TYR	conflict	UNP P27406
C	357	THR	SER	conflict	UNP P27406
C	389	TYR	PHE	conflict	UNP P27406
C	393	THR	SER	conflict	UNP P27406
C	394	ILE	VAL	conflict	UNP P27406
C	397	SER	THR	conflict	UNP P27406
C	399	LYS	GLN	conflict	UNP P27406
C	428	GLU	GLY	conflict	UNP P27406
C	429	LYS	GLU	conflict	UNP P27406
C	431	THR	ILE	conflict	UNP P27406
C	441	LYS	GLY	conflict	UNP P27406
C	442	SER	THR	conflict	UNP P27406
C	450	ALA	THR	conflict	UNP P27406
C	454	GLY	THR	conflict	UNP P27406
C	457	VAL	ILE	conflict	UNP P27406
C	459	VAL	LYS	conflict	UNP P27406
C	465	LYS	ARG	conflict	UNP P27406
C	493	LYS	-	insertion	UNP P27406
C	494	VAL	LEU	conflict	UNP P27406
C	?	-	GLY	deletion	UNP P27406
C	?	-	ASP	deletion	UNP P27406
C	?	-	ASN	deletion	UNP P27406
C	?	-	ASN	deletion	UNP P27406
C	497	ALA	LYS	conflict	UNP P27406
C	499	GLU	ASN	conflict	UNP P27406
C	501	SER	CYS	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	VAL	THR	conflict	UNP P27406
C	506	MET	GLN	conflict	UNP P27406
C	507	THR	SER	conflict	UNP P27406
C	510	ALA	VAL	conflict	UNP P27406
C	512	TYR	PHE	conflict	UNP P27406
C	515	THR	ASN	conflict	UNP P27406
C	520	GLU	LYS	conflict	UNP P27406
C	521	VAL	ALA	conflict	UNP P27406
C	529	SER	ALA	conflict	UNP P27406
C	553	VAL	THR	conflict	UNP P27406
C	636	SER	GLY	conflict	UNP P27406
C	637	ILE	PHE	conflict	UNP P27406
C	645	THR	SER	conflict	UNP P27406
C	665	SER	PRO	conflict	UNP P27406
D	13	ASN	ASP	conflict	UNP P27406
D	19	ARG	LYS	conflict	UNP P27406
D	23	ASP	ASN	conflict	UNP P27406
D	26	LYS	ASN	conflict	UNP P27406
D	34	ASP	SER	conflict	UNP P27406
D	56	GLN	ARG	conflict	UNP P27406
D	60	GLN	GLU	conflict	UNP P27406
D	76	TYR	PHE	conflict	UNP P27406
D	77	GLU	ASP	conflict	UNP P27406
D	79	ILE	VAL	conflict	UNP P27406
D	82	ALA	VAL	conflict	UNP P27406
D	89	ASP	GLY	conflict	UNP P27406
D	109	GLU	LYS	conflict	UNP P27406
D	112	LYS	ALA	conflict	UNP P27406
D	113	ALA	GLY	conflict	UNP P27406
D	117	ASN	ASP	conflict	UNP P27406
D	120	MET	LEU	conflict	UNP P27406
D	121	PHE	ILE	conflict	UNP P27406
D	127	GLY	-	insertion	UNP P27406
D	139	PRO	MET	conflict	UNP P27406
D	153	ALA	THR	conflict	UNP P27406
D	217	ASP	GLU	conflict	UNP P27406
D	268	SER	CYS	conflict	UNP P27406
D	269	ILE	LEU	conflict	UNP P27406
D	304	SER	ALA	conflict	UNP P27406
D	319	ALA	PRO	conflict	UNP P27406
D	338	VAL	ILE	conflict	UNP P27406
D	346	SER	THR	conflict	UNP P27406

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Chain	Residue	Modelled	Actual	Comment	Reference
D	355	HIS	TYR	conflict	UNP P27406
D	357	THR	SER	conflict	UNP P27406
D	389	TYR	PHE	conflict	UNP P27406
D	393	THR	SER	conflict	UNP P27406
D	394	ILE	VAL	conflict	UNP P27406
D	397	SER	THR	conflict	UNP P27406
D	399	LYS	GLN	conflict	UNP P27406
D	428	GLU	GLY	conflict	UNP P27406
D	429	LYS	GLU	conflict	UNP P27406
D	431	THR	ILE	conflict	UNP P27406
D	441	LYS	GLY	conflict	UNP P27406
D	442	SER	THR	conflict	UNP P27406
D	450	ALA	THR	conflict	UNP P27406
D	454	GLY	THR	conflict	UNP P27406
D	457	VAL	ILE	conflict	UNP P27406
D	459	VAL	LYS	conflict	UNP P27406
D	465	LYS	ARG	conflict	UNP P27406
D	493	LYS	-	insertion	UNP P27406
D	494	VAL	LEU	conflict	UNP P27406
D	?	-	GLY	deletion	UNP P27406
D	?	-	ASP	deletion	UNP P27406
D	?	-	ASN	deletion	UNP P27406
D	?	-	ASN	deletion	UNP P27406
D	497	ALA	LYS	conflict	UNP P27406
D	499	GLU	ASN	conflict	UNP P27406
D	501	SER	CYS	conflict	UNP P27406
D	503	VAL	THR	conflict	UNP P27406
D	506	MET	GLN	conflict	UNP P27406
D	507	THR	SER	conflict	UNP P27406
D	510	ALA	VAL	conflict	UNP P27406
D	512	TYR	PHE	conflict	UNP P27406
D	515	THR	ASN	conflict	UNP P27406
D	520	GLU	LYS	conflict	UNP P27406
D	521	VAL	ALA	conflict	UNP P27406
D	529	SER	ALA	conflict	UNP P27406
D	553	VAL	THR	conflict	UNP P27406
D	636	SER	GLY	conflict	UNP P27406
D	637	ILE	PHE	conflict	UNP P27406
D	645	THR	SER	conflict	UNP P27406
D	665	SER	PRO	conflict	UNP P27406

- Molecule 2 is a protein called Junctional adhesion molecule A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	201	Total	C	H	N	O	S	0	0
			3023	970	1473	259	311	10		
2	F	202	Total	C	H	N	O	S	0	0
			3033	973	1478	260	312	10		
2	G	200	Total	C	H	N	O	S	0	0
			3013	967	1468	258	310	10		
2	H	200	Total	C	H	N	O	S	0	0
			3008	965	1467	258	308	10		

- Molecule 3 is a protein called VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	82	Total	C	H	N	O	S	0	0
			1341	421	666	126	127	1		
3	J	89	Total	C	H	N	O	S	0	0
			1467	459	732	139	136	1		
3	K	82	Total	C	H	N	O	S	0	0
			1341	421	666	126	127	1		
3	L	89	Total	C	H	N	O	S	0	0
			1468	459	733	139	136	1		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	37	LYS	GLN	conflict	UNP P28711
I	39	MET	ILE	conflict	UNP P28711
I	40	LYS	GLY	conflict	UNP P28711
I	43	HIS	ARG	conflict	UNP P28711
I	85	ASP	ASN	conflict	UNP P28711
I	101	ARG	LYS	conflict	UNP P28711
I	106	ASN	ILE	conflict	UNP P28711
J	37	LYS	GLN	conflict	UNP P28711
J	39	MET	ILE	conflict	UNP P28711
J	40	LYS	GLY	conflict	UNP P28711
J	43	HIS	ARG	conflict	UNP P28711
J	85	ASP	ASN	conflict	UNP P28711
J	101	ARG	LYS	conflict	UNP P28711
J	106	ASN	ILE	conflict	UNP P28711
K	37	LYS	GLN	conflict	UNP P28711
K	39	MET	ILE	conflict	UNP P28711
K	40	LYS	GLY	conflict	UNP P28711
K	43	HIS	ARG	conflict	UNP P28711
K	85	ASP	ASN	conflict	UNP P28711

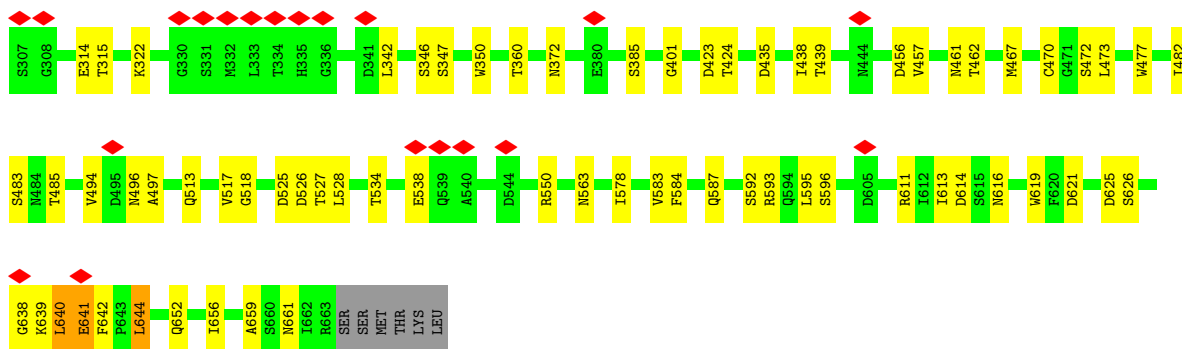
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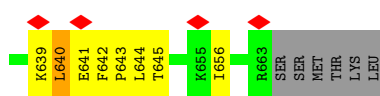
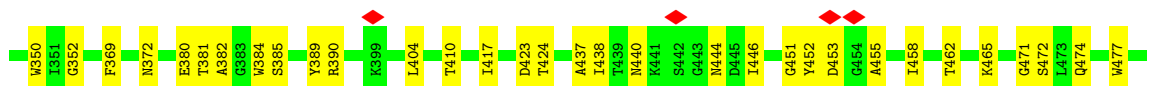
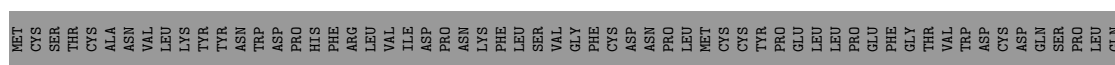
Chain	Residue	Modelled	Actual	Comment	Reference
K	101	ARG	LYS	conflict	UNP P28711
K	106	ASN	ILE	conflict	UNP P28711
L	37	LYS	GLN	conflict	UNP P28711
L	39	MET	ILE	conflict	UNP P28711
L	40	LYS	GLY	conflict	UNP P28711
L	43	HIS	ARG	conflict	UNP P28711
L	85	ASP	ASN	conflict	UNP P28711
L	101	ARG	LYS	conflict	UNP P28711
L	106	ASN	ILE	conflict	UNP P28711

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

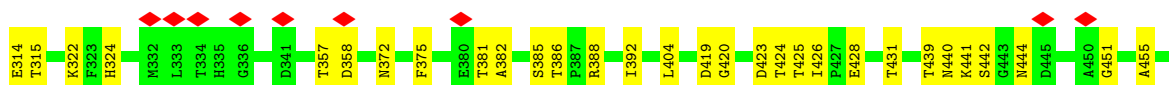
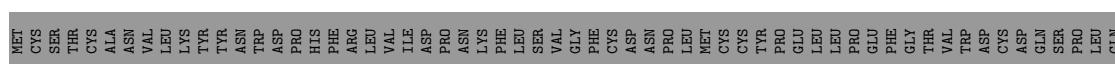
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total K 1 1	0
4	B	1	Total K 1 1	0
4	C	1	Total K 1 1	0
4	D	1	Total K 1 1	0

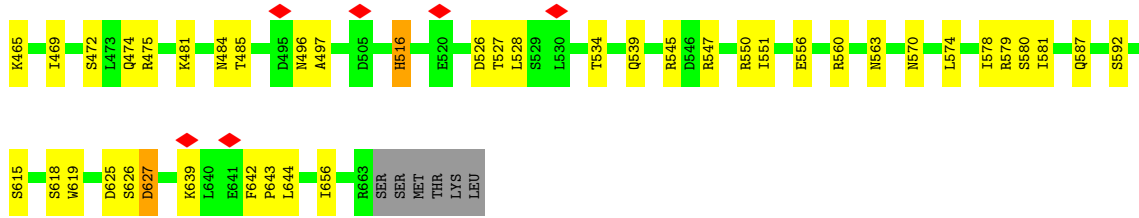


• Molecule 1: Capsid protein

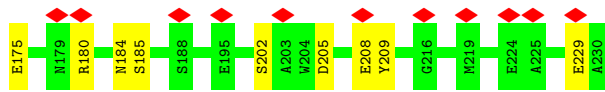
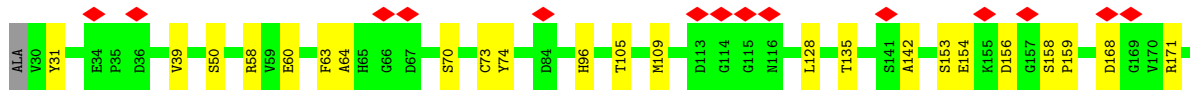
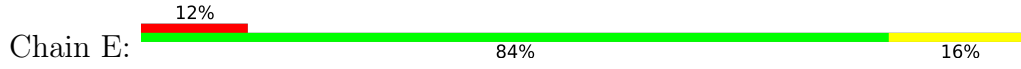


• Molecule 1: Capsid protein

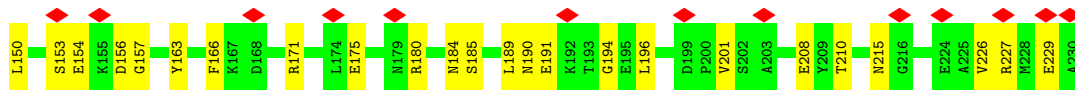
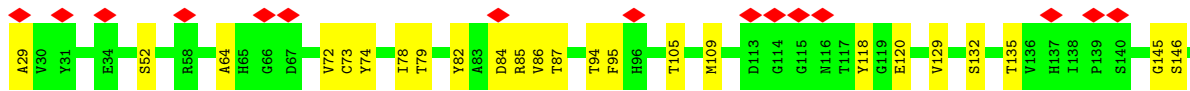
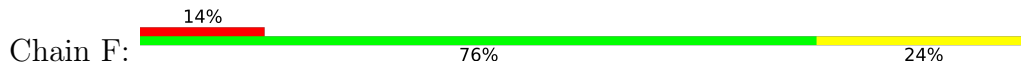




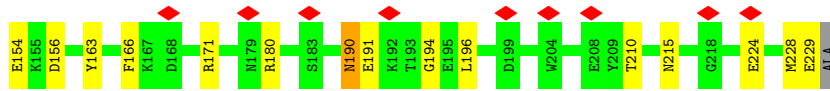
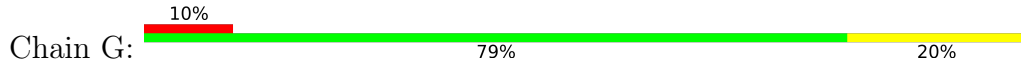
• Molecule 2: Junctional adhesion molecule A



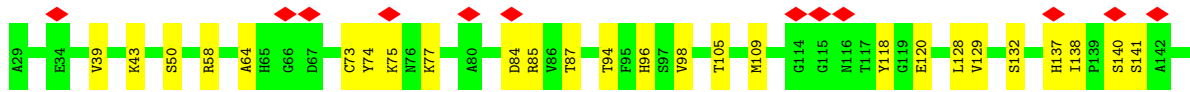
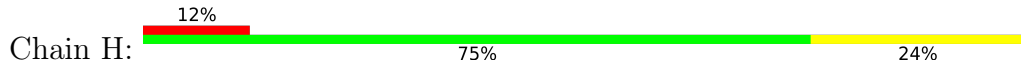
• Molecule 2: Junctional adhesion molecule A

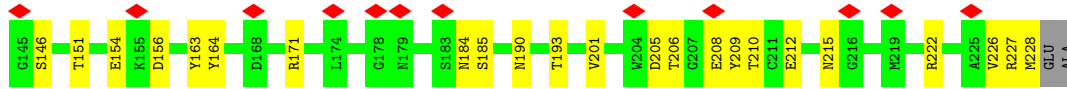


• Molecule 2: Junctional adhesion molecule A

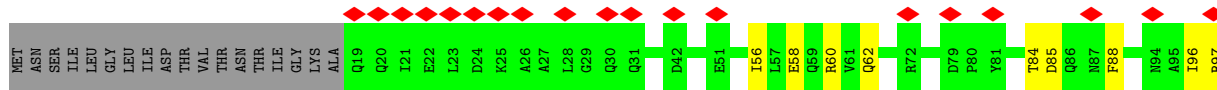


• Molecule 2: Junctional adhesion molecule A

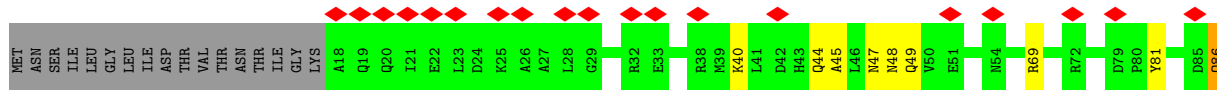
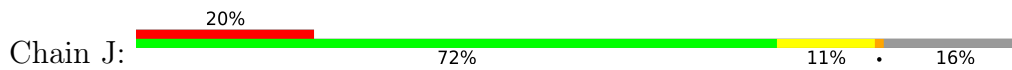




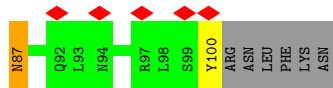
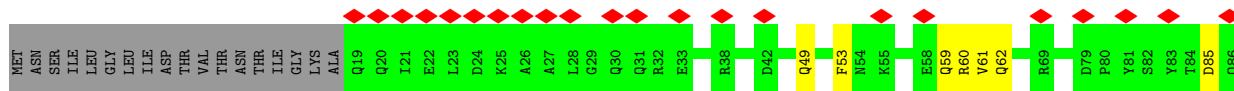
• Molecule 3: VP2



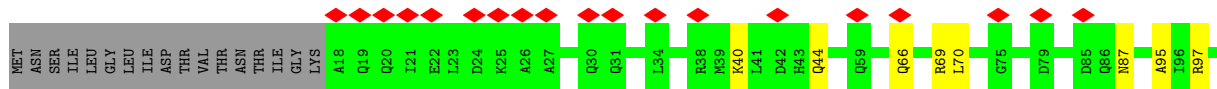
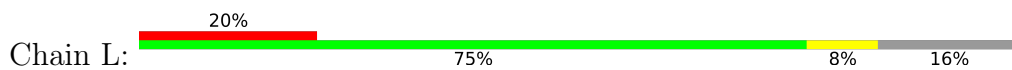
• Molecule 3: VP2



• Molecule 3: VP2



• Molecule 3: VP2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was implemented through Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	639.00006, 639.00006, 639.00006	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.53	0/4199	0.61	0/5725
1	B	0.55	0/4173	0.64	0/5688
1	C	0.54	0/4199	0.63	0/5725
1	D	0.54	0/4199	0.61	0/5725
2	E	0.40	0/1591	0.60	0/2164
2	F	0.40	0/1596	0.59	0/2171
2	G	0.42	0/1586	0.59	0/2157
2	H	0.41	0/1582	0.60	0/2152
3	I	0.37	0/684	0.61	0/920
3	J	0.43	0/745	0.62	0/1001
3	K	0.38	0/684	0.65	0/920
3	L	0.41	0/745	0.58	0/1001
All	All	0.50	0/25983	0.61	0/35349

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	2
3	I	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	ASN	Peptide
1	A	446	ILE	Peptide
3	I	96	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4097	4026	4029	86	0
1	B	4071	3990	4002	66	0
1	C	4097	4024	4030	57	0
1	D	4097	4026	4030	76	0
2	E	1550	1473	1472	18	0
2	F	1555	1478	1477	28	0
2	G	1545	1468	1467	23	0
2	H	1541	1467	1466	30	0
3	I	675	666	670	6	0
3	J	735	732	733	10	0
3	K	675	666	670	6	0
3	L	735	733	733	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	25377	24749	24779	379	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 8.

All (379) 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:642:PHE:O	1:A:644:LEU:CD2	1.72	1.37
1:D:481:LYS:O	1:D:516:HIS:CE1	1.82	1.33
1:D:481:LYS:O	1:D:516:HIS:HE1	1.04	1.26
1:A:642:PHE:C	1:A:644:LEU:HD23	1.53	1.26
1:A:642:PHE:O	1:A:644:LEU:HD23	1.03	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:PHE:HA	1:A:644:LEU:CD2	1.88	1.03
1:B:616:ASN:HB2	1:B:641:GLU:HG2	1.44	0.98
1:A:642:PHE:C	1:A:644:LEU:CD2	2.23	0.97
1:C:642:PHE:O	1:C:644:LEU:N	1.98	0.96
1:A:642:PHE:CA	1:A:644:LEU:CD2	2.47	0.92
1:B:616:ASN:HB2	1:B:641:GLU:CG	2.03	0.89
1:A:642:PHE:HA	1:A:644:LEU:HD21	1.51	0.89
1:A:502:ASN:OD1	1:A:550:ARG:NH2	2.08	0.85
1:B:614:ASP:HA	1:B:644:LEU:HB3	1.60	0.84
1:B:642:PHE:O	1:B:644:LEU:HG	1.78	0.83
1:D:215:SER:O	1:D:216:ILE:HG12	1.80	0.81
1:A:548:VAL:O	1:A:550:ARG:NH2	2.15	0.80
1:C:465:LYS:O	1:C:534:THR:OG1	2.00	0.80
1:B:496:ASN:ND2	2:G:96:HIS:O	2.16	0.79
3:K:85:ASP:O	3:K:87:ASN:OD1	2.01	0.79
1:A:642:PHE:CA	1:A:644:LEU:HD21	2.14	0.77
1:A:642:PHE:O	1:A:644:LEU:N	2.18	0.76
1:D:472:SER:OG	1:D:484:ASN:O	2.03	0.76
1:A:642:PHE:O	1:A:644:LEU:HD21	1.85	0.76
1:D:639:LYS:NZ	3:L:87:ASN:OD1	2.17	0.76
1:B:613:ILE:O	1:B:644:LEU:HB2	1.85	0.76
1:B:470:CYS:O	1:B:485:THR:OG1	2.04	0.75
1:B:472:SER:OG	1:B:513:GLN:NE2	2.20	0.74
1:A:644:LEU:HD23	1:A:644:LEU:N	2.02	0.74
2:H:205:ASP:O	2:H:209:TYR:OH	2.05	0.74
1:C:372:ASN:O	1:C:385:SER:OG	2.05	0.73
1:C:440:ASN:ND2	1:C:444:ASN:O	2.22	0.73
1:C:640:LEU:HD12	1:C:640:LEU:N	2.01	0.73
3:K:59:GLN:O	3:K:61:VAL:N	2.21	0.73
1:C:483:SER:O	1:D:485:THR:OG1	2.06	0.73
1:D:587:GLN:OE1	1:D:592:SER:OG	2.04	0.73
1:A:640:LEU:HD12	1:A:640:LEU:N	2.02	0.73
1:C:328:PRO:O	1:C:331:SER:OG	2.05	0.72
2:H:87:THR:OG1	2:H:94:THR:OG1	2.08	0.72
1:B:640:LEU:HD12	1:B:640:LEU:H	1.54	0.71
1:D:440:ASN:ND2	1:D:451:GLY:O	2.24	0.71
1:A:640:LEU:HD12	1:A:640:LEU:H	1.55	0.70
1:B:640:LEU:HD12	1:B:640:LEU:N	2.05	0.70
3:K:59:GLN:O	3:K:62:GLN:N	2.24	0.70
1:C:587:GLN:OE1	1:C:592:SER:OG	2.10	0.69
1:A:587:GLN:OE1	1:A:592:SER:OG	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ARG:NE	1:B:621:ASP:OD1	2.22	0.69
1:B:372:ASN:OD1	1:B:385:SER:OG	2.05	0.69
3:L:40:LYS:O	3:L:44:GLN:N	2.26	0.68
1:D:481:LYS:HB2	1:D:516:HIS:ND1	2.07	0.68
1:C:410:THR:O	3:L:97:ARG:NH1	2.28	0.67
1:D:539:GLN:O	3:J:81:TYR:OH	2.10	0.67
1:C:572:ILE:O	1:C:580:SER:OG	2.07	0.67
2:G:163:TYR:N	2:G:191:GLU:O	2.27	0.67
1:B:563:ASN:ND2	1:B:656:ILE:O	2.28	0.67
1:D:299:PRO:HG2	1:D:300:TYR:CE1	2.29	0.67
1:C:640:LEU:HD12	1:C:640:LEU:H	1.60	0.66
1:D:218:VAL:HG13	1:D:315:THR:HG22	1.77	0.66
1:A:485:THR:OG1	1:B:483:SER:O	2.13	0.66
3:K:87:ASN:OD1	3:K:87:ASN:N	2.27	0.66
2:G:132:SER:OG	2:G:156:ASP:OD2	2.12	0.66
1:A:533:TYR:OH	1:A:538:GLU:OE1	2.13	0.66
2:F:190:ASN:O	2:F:194:GLY:N	2.29	0.66
2:H:118:TYR:OH	2:H:120:GLU:OE2	2.13	0.65
1:A:452:TYR:CD1	1:A:453:ASP:N	2.65	0.65
1:A:545:ARG:NH2	1:A:556:GLU:OE2	2.29	0.65
1:D:563:ASN:ND2	1:D:656:ILE:O	2.29	0.64
1:C:156:ASP:OD2	1:D:322:LYS:NZ	2.30	0.64
1:C:644:LEU:O	1:C:644:LEU:HD12	1.97	0.64
1:D:545:ARG:NH1	1:D:556:GLU:OE2	2.30	0.64
1:D:455:ALA:O	3:J:69:ARG:NH2	2.30	0.64
1:B:587:GLN:OE1	1:B:592:SER:OG	2.09	0.64
2:E:39:VAL:O	2:E:128:LEU:N	2.31	0.63
1:C:352:GLY:O	1:C:389:TYR:OH	2.15	0.63
2:H:208:GLU:OE2	2:H:226:VAL:N	2.32	0.63
1:B:613:ILE:O	1:B:644:LEU:CB	2.47	0.63
1:D:439:THR:OG1	1:D:444:ASN:O	2.10	0.63
2:E:109:MET:SD	2:F:180:ARG:NH2	2.72	0.62
1:B:593:ARG:O	1:B:596:SER:OG	2.11	0.62
1:B:614:ASP:HB2	1:B:641:GLU:O	2.00	0.62
1:A:642:PHE:HA	1:A:644:LEU:HD22	1.80	0.62
1:C:563:ASN:ND2	1:C:656:ILE:O	2.33	0.62
2:H:129:VAL:O	2:H:215:ASN:ND2	2.32	0.62
2:G:118:TYR:OH	2:G:120:GLU:OE2	2.18	0.61
2:E:180:ARG:NH2	2:F:109:MET:SD	2.73	0.61
1:D:615:SER:OG	1:D:643:PRO:O	2.18	0.61
1:B:435:ASP:O	1:B:462:THR:OG1	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:N	1:C:314:GLU:O	2.34	0.61
1:D:392:ILE:N	1:D:528:LEU:O	2.33	0.61
1:B:423:ASP:O	1:B:424:THR:OG1	2.17	0.60
1:D:560:ARG:NH1	1:D:625:ASP:OD2	2.34	0.60
1:C:390:ARG:NH2	1:D:358:ASP:OD1	2.35	0.59
1:D:465:LYS:O	1:D:534:THR:OG1	2.04	0.59
1:A:433:ALA:O	1:A:512:TYR:OH	2.20	0.59
2:H:206:THR:HG23	2:H:228:MET:O	2.03	0.59
1:C:343:ILE:HD12	1:C:610:TYR:HD2	1.68	0.59
1:B:438:ILE:O	1:B:439:THR:HG22	2.02	0.59
1:C:644:LEU:HD12	1:C:644:LEU:C	2.22	0.59
2:G:133:LYS:NZ	2:G:224:GLU:OE2	2.35	0.59
2:H:190:ASN:ND2	2:H:193:THR:OG1	2.35	0.59
2:G:87:THR:OG1	2:G:94:THR:OG1	2.21	0.59
2:H:164:TYR:O	2:H:212:GLU:N	2.36	0.59
1:A:615:SER:HB2	1:A:641:GLU:HB3	1.85	0.58
2:E:31:TYR:N	2:E:50:SER:O	2.37	0.58
1:B:347:SER:OG	1:B:644:LEU:HD12	2.04	0.58
1:B:219:ARG:N	1:B:314:GLU:O	2.36	0.58
2:F:129:VAL:O	2:F:215:ASN:ND2	2.36	0.58
2:F:154:GLU:N	2:F:163:TYR:OH	2.35	0.58
2:G:180:ARG:NH2	2:H:109:MET:SD	2.76	0.58
1:B:298:ASN:ND2	1:B:301:ALA:HB3	2.19	0.58
2:E:64:ALA:O	2:E:105:THR:N	2.36	0.57
2:F:135:THR:N	2:F:153:SER:O	2.37	0.57
1:B:494:VAL:N	1:B:497:ALA:O	2.37	0.57
1:A:392:ILE:O	1:A:528:LEU:N	2.37	0.57
1:D:299:PRO:HD2	1:D:300:TYR:CE1	2.39	0.57
2:G:154:GLU:N	2:G:163:TYR:OH	2.38	0.57
1:A:452:TYR:HD1	1:A:453:ASP:N	2.03	0.57
1:B:642:PHE:O	1:B:644:LEU:N	2.37	0.57
1:B:538:GLU:N	1:B:538:GLU:OE1	2.38	0.56
1:C:258:ASP:OD1	1:C:259:ALA:N	2.38	0.56
2:F:29:ALA:N	2:F:52:SER:O	2.38	0.56
1:B:616:ASN:CB	1:B:641:GLU:HG2	2.29	0.56
1:D:643:PRO:HG3	3:L:95:ALA:HB1	1.88	0.56
1:C:570:ASN:ND2	1:C:585:ASN:OD1	2.39	0.56
1:D:516:HIS:N	1:D:516:HIS:CD2	2.73	0.56
2:H:138:ILE:HB	2:H:226:VAL:HG11	1.87	0.55
2:E:184:ASN:OD1	2:E:185:SER:N	2.38	0.55
2:G:39:VAL:O	2:G:128:LEU:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:PHE:C	1:C:644:LEU:N	2.59	0.55
1:D:627:ASP:OD1	1:D:627:ASP:N	2.39	0.55
2:G:85:ARG:NH2	2:G:102:ASP:OD1	2.40	0.55
1:A:156:ASP:OD2	1:B:322:LYS:NZ	2.39	0.55
1:A:496:ASN:ND2	2:H:96:HIS:O	2.39	0.55
1:D:560:ARG:O	1:D:563:ASN:N	2.40	0.55
2:F:118:TYR:OH	2:F:120:GLU:OE2	2.24	0.55
1:D:300:TYR:CD1	1:D:300:TYR:N	2.75	0.54
2:F:163:TYR:N	2:F:191:GLU:O	2.40	0.54
2:G:190:ASN:O	2:G:194:GLY:N	2.41	0.54
1:D:526:ASP:OD1	1:D:527:THR:N	2.40	0.54
2:F:64:ALA:HB3	2:F:105:THR:O	2.06	0.54
3:I:97:ARG:NH1	3:K:100:TYR:OH	2.41	0.54
1:A:217:ASP:HB2	1:A:316:LYS:O	2.07	0.54
1:C:625:ASP:OD1	1:C:626:SER:N	2.40	0.54
1:A:355:HIS:CD2	1:A:357:THR:HG23	2.43	0.53
2:F:87:THR:OG1	2:F:94:THR:OG1	2.26	0.53
2:F:132:SER:OG	2:F:156:ASP:OD2	2.26	0.53
1:C:437:ALA:O	1:C:462:THR:OG1	2.26	0.53
2:F:208:GLU:OE2	2:F:226:VAL:N	2.41	0.53
1:C:642:PHE:O	1:C:644:LEU:HG	2.08	0.53
1:D:299:PRO:HD2	1:D:300:TYR:CD1	2.42	0.53
1:D:375:PHE:CE1	1:D:381:THR:HG21	2.44	0.53
2:E:135:THR:N	2:E:153:SER:O	2.41	0.53
2:E:205:ASP:O	2:E:209:TYR:OH	2.23	0.53
1:D:218:VAL:O	1:D:266:ILE:O	2.26	0.53
2:H:132:SER:OG	2:H:156:ASP:OD2	2.25	0.53
1:A:641:GLU:OE2	1:A:641:GLU:N	2.41	0.53
1:D:130:SER:OG	1:D:131:ILE:N	2.42	0.53
1:D:618:SER:OG	1:D:619:TRP:N	2.42	0.53
1:D:474:GLN:CD	1:D:474:GLN:O	2.48	0.53
2:H:73:CYS:SG	2:H:74:TYR:N	2.82	0.53
3:L:66:GLN:OE1	3:L:69:ARG:NH2	2.42	0.53
1:A:275:THR:OG1	1:A:277:TYR:O	2.20	0.52
2:E:202:SER:N	2:E:205:ASP:OD2	2.42	0.52
1:A:627:ASP:OD1	1:A:627:ASP:N	2.42	0.52
1:A:614:ASP:HB2	1:A:641:GLU:O	2.10	0.52
1:B:439:THR:HG21	1:B:461:ASN:ND2	2.24	0.52
1:B:616:ASN:ND2	1:B:641:GLU:OE2	2.42	0.52
1:D:469:ILE:HG22	1:D:469:ILE:O	2.10	0.52
2:H:84:ASP:OD1	2:H:85:ARG:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:NH2	1:A:314:GLU:OE1	2.42	0.52
2:E:73:CYS:SG	2:E:74:TYR:N	2.82	0.52
1:C:560:ARG:NH1	1:C:625:ASP:OD2	2.42	0.52
1:A:328:PRO:O	1:A:331:SER:OG	2.21	0.52
3:J:47:ASN:OD1	3:J:48:ASN:N	2.43	0.51
3:L:66:GLN:O	3:L:70:LEU:N	2.42	0.51
1:B:467:MET:O	1:B:534:THR:HG22	2.11	0.51
1:D:357:THR:OG1	1:D:570:ASN:OD1	2.07	0.51
2:F:227:ARG:NH2	2:F:229:GLU:OE2	2.43	0.51
1:D:642:PHE:O	1:D:644:LEU:N	2.43	0.51
1:A:303:ASP:OD1	1:A:304:SER:N	2.44	0.51
1:B:198:LEU:O	1:B:315:THR:OG1	2.17	0.50
1:B:456:ASP:OD1	1:B:457:VAL:N	2.45	0.50
1:C:211:ALA:HB3	1:C:324:HIS:HB2	1.92	0.50
3:I:85:ASP:OD2	3:I:88:PHE:N	2.45	0.50
1:D:219:ARG:N	1:D:314:GLU:O	2.44	0.50
1:C:452:TYR:CE1	1:C:458:ILE:HD13	2.47	0.50
1:C:477:TRP:NE1	1:D:578:ILE:HD12	2.26	0.50
1:A:475:ARG:NH2	1:B:578:ILE:O	2.44	0.50
1:D:215:SER:O	1:D:216:ILE:CG1	2.55	0.50
2:H:137:HIS:N	2:H:151:THR:OG1	2.45	0.50
3:J:40:LYS:O	3:J:44:GLN:N	2.45	0.50
1:A:347:SER:HB2	1:A:642:PHE:CE2	2.47	0.50
1:A:441:LYS:N	1:A:444:ASN:OD1	2.43	0.50
2:G:103:THR:HG23	2:G:126:THR:HA	1.93	0.50
1:C:474:GLN:CD	1:C:474:GLN:O	2.49	0.49
1:A:423:ASP:O	1:A:424:THR:OG1	2.29	0.49
3:I:56:ILE:O	3:I:60:ARG:N	2.40	0.49
1:B:240:GLY:N	1:B:284:ASP:OD1	2.44	0.49
1:D:258:ASP:OD1	1:D:259:ALA:N	2.44	0.49
1:A:142:GLY:N	1:B:268:SER:OG	2.45	0.49
1:A:400:ASN:N	1:A:518:GLY:O	2.46	0.49
1:C:526:ASP:OD1	1:C:527:THR:N	2.45	0.49
1:B:526:ASP:OD1	1:B:527:THR:N	2.45	0.49
2:F:84:ASP:OD1	2:F:85:ARG:N	2.46	0.49
1:B:401:GLY:N	1:B:518:GLY:O	2.44	0.48
1:C:451:GLY:O	1:C:455:ALA:N	2.46	0.48
2:G:135:THR:N	2:G:153:SER:O	2.43	0.48
3:K:49:GLN:O	3:K:53:PHE:N	2.43	0.48
1:A:242:ASP:OD2	1:A:655:LYS:NZ	2.25	0.48
2:F:150:LEU:O	2:F:196:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:SER:O	1:B:350:TRP:NE1	2.47	0.48
1:D:178:ASN:OD1	1:D:179:TRP:N	2.46	0.48
1:D:211:ALA:O	1:D:324:HIS:N	2.47	0.48
2:H:39:VAL:O	2:H:128:LEU:N	2.40	0.48
1:A:505:ASP:OD1	1:A:506:MET:N	2.46	0.48
1:C:325:LEU:HD21	1:D:159:THR:HG22	1.95	0.48
2:E:154:GLU:OE2	2:E:156:ASP:N	2.46	0.48
1:C:143:VAL:HG23	1:C:144:ILE:HG23	1.95	0.48
1:C:423:ASP:O	1:C:424:THR:OG1	2.27	0.48
2:G:154:GLU:OE2	2:G:156:ASP:N	2.46	0.48
1:A:452:TYR:CD1	1:A:452:TYR:C	2.85	0.47
1:D:426:ILE:HD12	1:D:428:GLU:O	2.13	0.47
2:G:150:LEU:HD12	2:G:196:LEU:HD23	1.96	0.47
1:D:423:ASP:O	1:D:424:THR:OG1	2.29	0.47
1:A:258:ASP:OD1	1:A:259:ALA:N	2.47	0.47
1:A:411:ASP:OD1	1:A:412:TYR:N	2.47	0.47
1:A:447:THR:HG21	1:A:452:TYR:HB2	1.97	0.47
1:A:615:SER:HB2	1:A:641:GLU:CB	2.44	0.47
1:D:469:ILE:HD11	1:D:534:THR:CG2	2.45	0.47
1:B:644:LEU:HD12	1:B:644:LEU:H	1.79	0.47
1:A:404:LEU:HD13	1:A:404:LEU:O	2.15	0.47
1:B:219:ARG:NH2	1:B:314:GLU:OE1	2.43	0.47
1:B:625:ASP:OD1	1:B:626:SER:N	2.46	0.47
2:F:184:ASN:OD1	2:F:185:SER:N	2.48	0.47
1:D:133:ALA:HB1	1:D:134:PRO:CD	2.45	0.47
2:F:154:GLU:OE1	2:F:157:GLY:N	2.48	0.47
2:F:166:PHE:N	2:F:210:THR:O	2.44	0.47
1:C:161:LYS:NZ	1:C:166:GLU:OE2	2.37	0.47
2:E:63:PHE:N	2:E:70:SER:O	2.47	0.47
1:C:347:SER:OG	1:C:644:LEU:HD12	2.14	0.46
1:D:299:PRO:CG	1:D:300:TYR:CE1	2.98	0.46
1:D:372:ASN:O	1:D:385:SER:OG	2.33	0.46
1:C:578:ILE:O	1:D:475:ARG:NH2	2.48	0.46
2:G:31:TYR:N	2:G:50:SER:O	2.48	0.46
1:A:644:LEU:HD23	1:A:644:LEU:H	1.76	0.46
1:B:201:TYR:OH	1:D:251:GLN:O	2.13	0.46
1:B:525:ASP:OD1	1:B:526:ASP:N	2.46	0.46
1:D:299:PRO:HG2	1:D:300:TYR:CD1	2.51	0.46
2:F:175:GLU:OE1	2:F:175:GLU:N	2.49	0.46
1:D:496:ASN:ND2	2:E:96:HIS:O	2.48	0.46
2:H:154:GLU:N	2:H:163:TYR:OH	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ILE:HD13	2:H:50:SER:OG	2.16	0.46
1:A:361:ASP:OD1	1:A:362:PHE:N	2.46	0.46
1:B:513:GLN:NE2	1:B:526:ASP:OD2	2.47	0.46
1:D:419:ASP:OD1	1:D:420:GLY:N	2.48	0.46
1:A:133:ALA:HB1	1:A:134:PRO:CD	2.45	0.46
1:A:352:GLY:O	1:A:389:TYR:OH	2.21	0.46
1:A:597:LEU:CD2	3:J:103:LEU:HD21	2.46	0.46
2:E:175:GLU:N	2:E:175:GLU:OE1	2.49	0.46
1:A:485:THR:HG22	1:A:486:ALA:H	1.80	0.45
1:B:401:GLY:HA2	1:B:517:VAL:HG23	1.98	0.45
1:B:641:GLU:HA	3:J:86:GLN:HE22	1.82	0.45
1:C:350:TRP:CZ3	1:C:644:LEU:HD11	2.52	0.45
1:C:472:SER:O	1:C:472:SER:OG	2.33	0.45
2:E:58:ARG:NH1	2:E:60:GLU:OE2	2.46	0.45
1:C:133:ALA:HB1	1:C:134:PRO:CD	2.47	0.45
1:D:381:THR:OG1	1:D:382:ALA:N	2.49	0.45
1:A:372:ASN:O	1:A:385:SER:OG	2.35	0.45
1:A:517:VAL:HG12	1:A:522:GLN:HB3	1.98	0.45
1:A:179:TRP:O	1:A:308:GLY:O	2.35	0.45
1:C:644:LEU:C	1:C:644:LEU:CD1	2.85	0.45
2:H:184:ASN:OD1	2:H:185:SER:N	2.50	0.45
1:A:388:ARG:NH2	1:A:419:ASP:OD2	2.50	0.45
2:F:154:GLU:OE2	2:F:156:ASP:N	2.49	0.45
1:C:615:SER:HB2	1:C:641:GLU:CB	2.47	0.45
1:D:625:ASP:OD1	1:D:626:SER:N	2.45	0.45
1:C:491:ALA:HB1	1:C:499:GLU:O	2.16	0.45
1:D:441:LYS:O	1:D:442:SER:OG	2.28	0.45
1:A:613:ILE:HG22	1:A:614:ASP:O	2.17	0.44
2:G:73:CYS:SG	2:G:77:LYS:N	2.90	0.44
1:B:583:VAL:HG12	1:B:584:PHE:N	2.32	0.44
1:C:345:LYS:O	1:C:645:THR:HA	2.17	0.44
2:H:146:SER:O	2:H:201:VAL:N	2.47	0.44
1:B:494:VAL:HG12	1:B:494:VAL:O	2.16	0.44
1:D:431:THR:HG22	1:D:497:ALA:HB2	1.99	0.44
1:B:178:ASN:ND2	1:B:659:ALA:HB2	2.33	0.44
1:A:424:THR:CB	1:A:468:TYR:HH	2.24	0.44
2:F:146:SER:O	2:F:201:VAL:N	2.48	0.44
1:A:479:ASP:O	1:A:481:LYS:N	2.50	0.44
1:D:180:SER:OG	1:D:181:THR:N	2.51	0.44
1:C:369:PHE:HE2	1:C:548:VAL:HG21	1.83	0.44
1:D:261:GLN:NE2	1:D:263:GLU:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:ALA:N	2:E:229:GLU:O	2.49	0.44
1:A:148:SER:OG	1:A:149:ALA:N	2.50	0.43
1:B:619:TRP:NE1	1:B:661:ASN:OD1	2.51	0.43
1:C:503:VAL:O	1:C:508:LYS:NZ	2.44	0.43
1:B:470:CYS:CB	1:B:528:LEU:HD12	2.48	0.43
1:D:222:ILE:HG22	1:D:223:SER:O	2.18	0.43
1:C:545:ARG:NH1	1:C:556:GLU:OE2	2.51	0.43
1:D:481:LYS:CB	1:D:516:HIS:ND1	2.80	0.43
1:B:360:THR:OG1	3:J:92:GLN:NE2	2.51	0.43
2:G:228:MET:SD	2:G:229:GLU:N	2.92	0.43
2:E:158:SER:N	2:E:159:PRO:O	2.52	0.43
2:F:86:VAL:HG22	2:F:95:PHE:CD1	2.53	0.43
1:A:163:VAL:HG13	1:A:163:VAL:O	2.19	0.43
1:A:471:GLY:N	1:A:529:SER:O	2.51	0.43
2:H:140:SER:O	2:H:141:SER:OG	2.28	0.43
2:G:86:VAL:HG22	2:G:95:PHE:CD1	2.54	0.43
1:A:550:ARG:HH11	1:A:554:LEU:HD22	1.83	0.42
3:I:58:GLU:O	3:I:62:GLN:N	2.48	0.42
2:F:189:LEU:HD21	2:F:196:LEU:HD13	2.01	0.42
2:G:129:VAL:O	2:G:215:ASN:ND2	2.45	0.42
1:A:409:ALA:HB2	1:A:416:GLY:O	2.20	0.42
1:A:489:THR:O	1:A:510:ALA:HB3	2.19	0.42
2:H:210:THR:HG21	2:H:222:ARG:CZ	2.49	0.42
1:A:452:TYR:HD1	1:A:453:ASP:H	1.67	0.42
1:C:477:TRP:HE1	1:D:578:ILE:HD12	1.85	0.42
1:D:404:LEU:HD23	1:D:404:LEU:H	1.84	0.42
2:F:145:GLY:N	2:F:201:VAL:O	2.50	0.42
1:D:386:THR:OG1	1:D:419:ASP:OD2	2.29	0.42
1:D:643:PRO:CG	3:L:95:ALA:HB1	2.49	0.42
1:D:425:THR:O	1:D:547:ARG:NH1	2.48	0.42
1:C:404:LEU:H	1:C:404:LEU:HD23	1.85	0.42
1:C:438:ILE:HD13	1:C:446:ILE:HG13	2.01	0.42
3:J:92:GLN:O	3:J:95:ALA:N	2.52	0.42
1:A:538:GLU:OE1	1:A:547:ARG:NH2	2.51	0.42
1:B:254:HIS:CD2	1:B:256:LEU:HD11	2.54	0.42
2:H:164:TYR:N	2:H:212:GLU:O	2.52	0.42
1:A:143:VAL:HG13	1:A:144:ILE:HG23	2.02	0.42
1:A:216:ILE:HG22	1:A:217:ASP:N	2.35	0.42
1:A:384:TRP:CG	1:A:417:ILE:HG21	2.55	0.42
1:B:640:LEU:N	1:B:640:LEU:CD1	2.75	0.41
1:A:250:LEU:HD13	1:A:293:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:OD1	1:A:526:ASP:N	2.53	0.41
2:G:146:SER:OG	2:G:147:ARG:N	2.53	0.41
1:A:469:ILE:HG21	1:B:473:LEU:HD12	2.01	0.41
1:A:568:TYR:N	1:A:585:ASN:O	2.48	0.41
1:A:642:PHE:O	1:A:644:LEU:CG	2.59	0.41
2:G:37:VAL:HG12	2:G:39:VAL:HG23	2.02	0.41
2:G:166:PHE:N	2:G:210:THR:O	2.43	0.41
2:H:64:ALA:O	2:H:105:THR:N	2.49	0.41
2:H:226:VAL:HG12	2:H:227:ARG:O	2.20	0.41
1:A:484:ASN:OD1	1:B:482:ILE:HD13	2.21	0.41
1:C:381:THR:OG1	1:C:382:ALA:N	2.54	0.41
1:D:469:ILE:HD11	1:D:534:THR:HG22	2.01	0.41
2:F:73:CYS:SG	2:F:74:TYR:N	2.93	0.41
1:A:477:TRP:CD1	1:B:578:ILE:HD12	2.56	0.41
1:B:342:LEU:HD11	1:B:595:LEU:HD21	2.02	0.41
1:C:380:GLU:OE1	3:L:106:ASN:ND2	2.49	0.41
1:D:183:GLU:OE1	1:D:183:GLU:N	2.53	0.41
2:H:43:LYS:O	2:H:98:VAL:HG22	2.21	0.41
1:A:484:ASN:OD1	1:A:485:THR:N	2.45	0.41
1:B:638:GLY:O	1:B:639:LYS:HG3	2.21	0.41
1:D:423:ASP:OD1	1:D:423:ASP:N	2.51	0.41
2:F:72:VAL:HG22	2:F:82:TYR:CD2	2.55	0.41
3:I:99:SER:OG	3:I:100:TYR:N	2.53	0.41
1:A:577:VAL:HG12	1:B:477:TRP:CZ3	2.56	0.41
2:H:58:ARG:HE	2:H:75:LYS:CD	2.34	0.41
1:A:337:SER:OG	1:A:338:VAL:N	2.53	0.41
2:H:185:SER:HG	2:H:205:ASP:CG	2.24	0.41
3:J:45:ALA:O	3:J:49:GLN:N	2.49	0.41
1:B:652:GLN:HE21	1:B:656:ILE:HG21	1.86	0.41
1:D:388:ARG:NH1	1:D:419:ASP:OD2	2.54	0.41
1:D:574:LEU:HD12	1:D:579:ARG:C	2.42	0.40
1:D:580:SER:OG	1:D:581:ILE:N	2.53	0.40
3:I:84:THR:O	3:I:84:THR:HG23	2.21	0.40
1:C:453:ASP:OD2	1:C:579:ARG:NH1	2.52	0.40
2:H:87:THR:OG1	2:H:94:THR:O	2.35	0.40
1:A:216:ILE:HG22	1:A:217:ASP:O	2.21	0.40
1:B:638:GLY:C	1:B:639:LYS:HG3	2.42	0.40
1:C:384:TRP:CG	1:C:417:ILE:HG21	2.56	0.40
2:E:168:ASP:N	2:E:208:GLU:O	2.48	0.40
1:B:144:ILE:HD12	1:B:145:ALA:HB2	2.04	0.40
1:B:641:GLU:OE1	3:J:86:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TRP:NE1	1:C:279:LEU:O	2.55	0.40
1:C:342:LEU:HD11	1:C:595:LEU:HD21	2.03	0.40
2:F:78:ILE:HG22	2:F:79:THR:O	2.20	0.40
1:D:382:ALA:O	1:D:551:ILE:HD12	2.21	0.40
2:H:74:TYR:N	2:H:77:LYS:O	2.47	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 PDB entries followed by that with respect to all EM entries.

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	532/669 (80%)	438 (82%)	92 (17%)	2 (0%)	34	69
1	B	528/669 (79%)	429 (81%)	99 (19%)	0	100	100
1	C	532/669 (80%)	433 (81%)	96 (18%)	3 (1%)	25	61
1	D	532/669 (80%)	445 (84%)	87 (16%)	0	100	100
2	E	199/202 (98%)	178 (89%)	21 (11%)	0	100	100
2	F	200/202 (99%)	185 (92%)	15 (8%)	0	100	100
2	G	198/202 (98%)	178 (90%)	20 (10%)	0	100	100
2	H	198/202 (98%)	180 (91%)	18 (9%)	0	100	100
3	I	80/106 (76%)	65 (81%)	15 (19%)	0	100	100
3	J	87/106 (82%)	80 (92%)	7 (8%)	0	100	100
3	K	80/106 (76%)	61 (76%)	18 (22%)	1 (1%)	12	48
3	L	87/106 (82%)	79 (91%)	8 (9%)	0	100	100
All	All	3253/3908 (83%)	2751 (85%)	496 (15%)	6 (0%)	50	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	60	ARG
1	A	447	THR
1	C	471	GLY
1	C	495	ASP
1	C	643	PRO
1	A	643	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	454/572 (79%)	447 (98%)	7 (2%)	65 81
1	B	451/572 (79%)	446 (99%)	5 (1%)	73 85
1	C	454/572 (79%)	450 (99%)	4 (1%)	78 88
1	D	454/572 (79%)	448 (99%)	6 (1%)	69 83
2	E	175/175 (100%)	174 (99%)	1 (1%)	86 93
2	F	175/175 (100%)	174 (99%)	1 (1%)	86 93
2	G	175/175 (100%)	173 (99%)	2 (1%)	73 85
2	H	174/175 (99%)	173 (99%)	1 (1%)	86 93
3	I	71/92 (77%)	71 (100%)	0	100 100
3	J	77/92 (84%)	75 (97%)	2 (3%)	46 70
3	K	71/92 (77%)	70 (99%)	1 (1%)	67 82
3	L	77/92 (84%)	77 (100%)	0	100 100
All	All	2808/3356 (84%)	2778 (99%)	30 (1%)	74 85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	TYR
1	A	550	ARG
1	A	627	ASP
1	A	639	LYS
1	A	640	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	641	GLU
1	A	644	LEU
1	B	300	TYR
1	B	550	ARG
1	B	640	LEU
1	B	641	GLU
1	B	644	LEU
1	C	489	THR
1	C	550	ARG
1	C	639	LYS
1	C	640	LEU
1	D	216	ILE
1	D	218	VAL
1	D	300	TYR
1	D	516	HIS
1	D	550	ARG
1	D	627	ASP
2	E	171	ARG
2	F	171	ARG
2	G	171	ARG
2	G	190	ASN
2	H	171	ARG
3	J	86	GLN
3	J	94	ASN
3	K	87	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	ASN
1	B	513	GLN
1	B	585	ASN
1	D	516	HIS
1	D	564	HIS
2	G	190	ASN
2	H	90	HIS
3	J	86	GLN
3	J	92	GLN
3	L	102	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

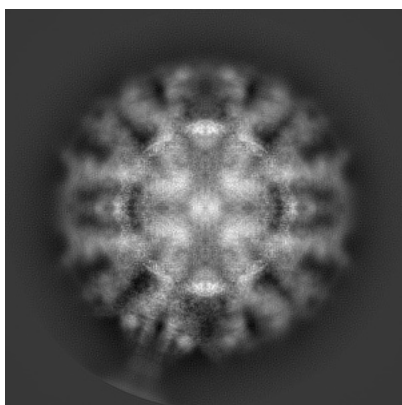
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0056. These allow visual inspection of the internal detail of the map and identification of artifacts.

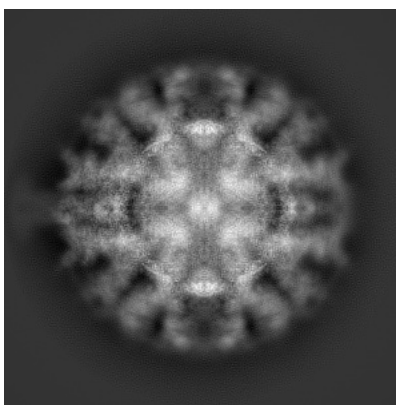
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

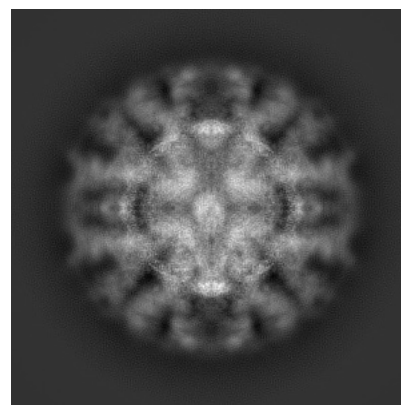
6.1.1 Primary map



X



Y

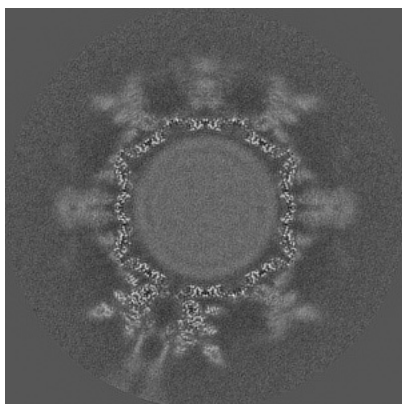


Z

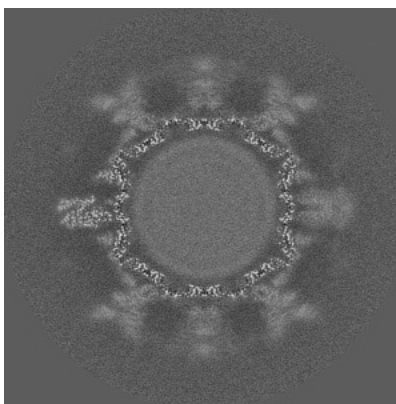
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

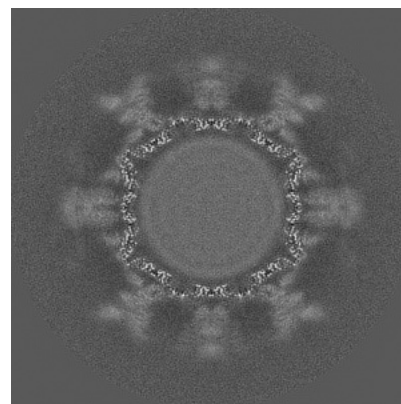
6.2.1 Primary map



X Index: 300



Y Index: 300

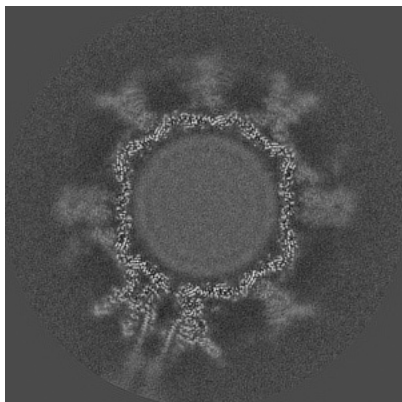


Z Index: 300

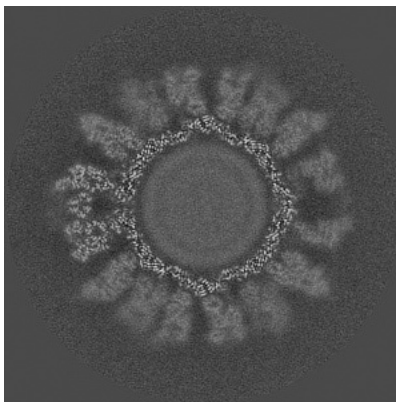
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

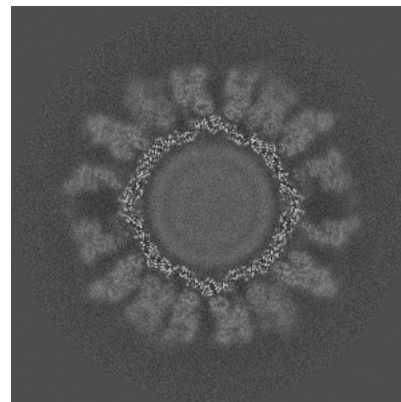
6.3.1 Primary map



X Index: 305



Y Index: 247

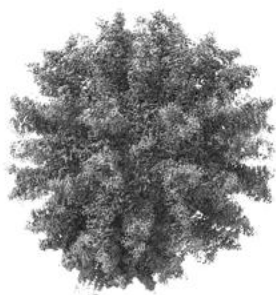


Z Index: 247

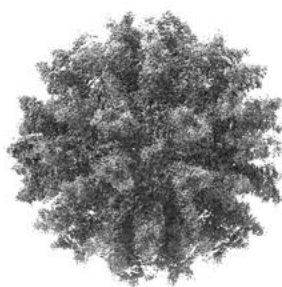
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

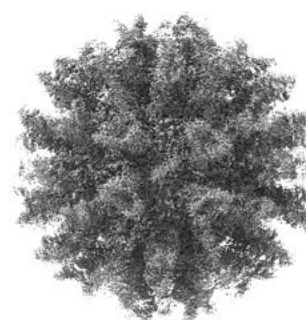
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

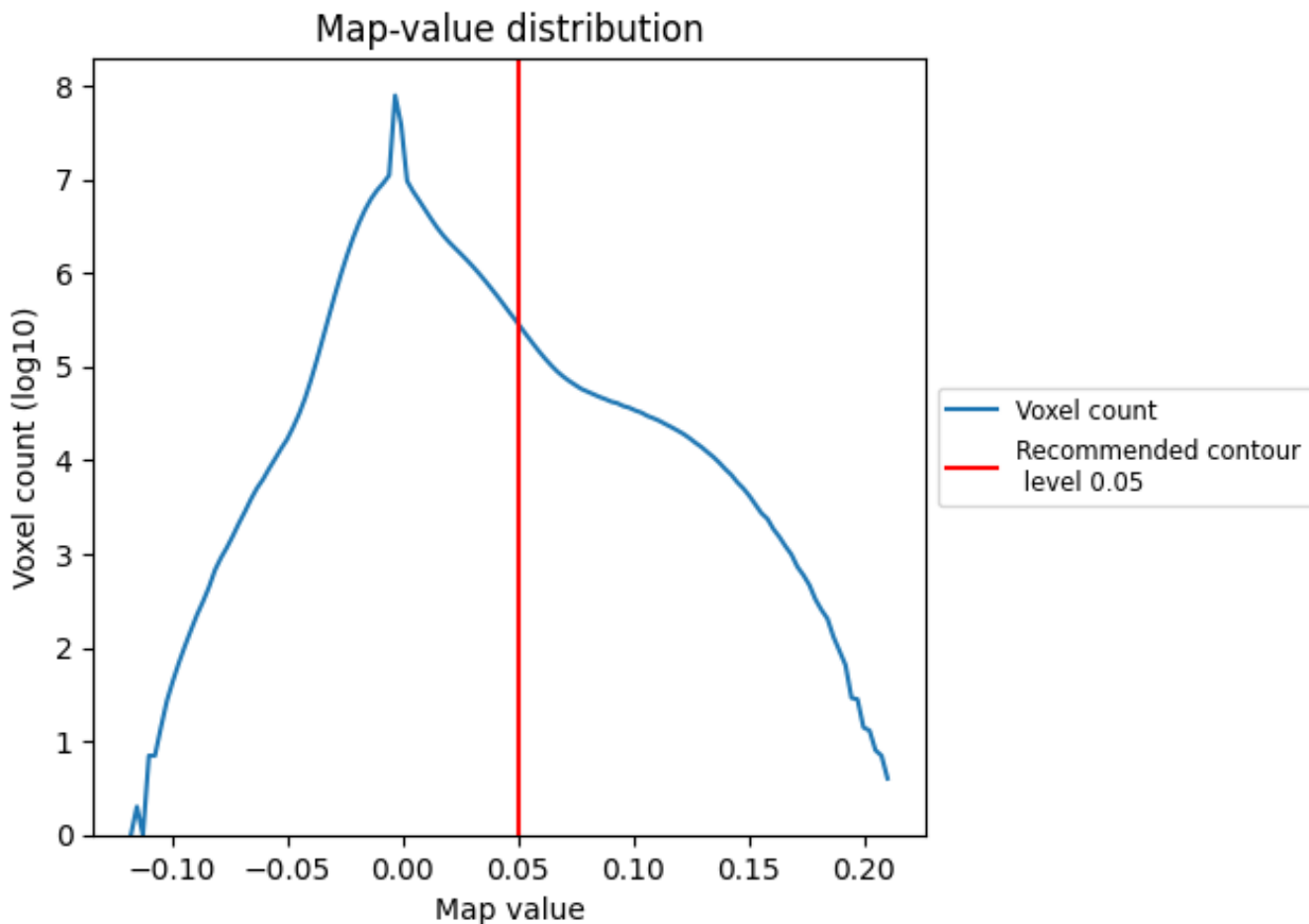
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

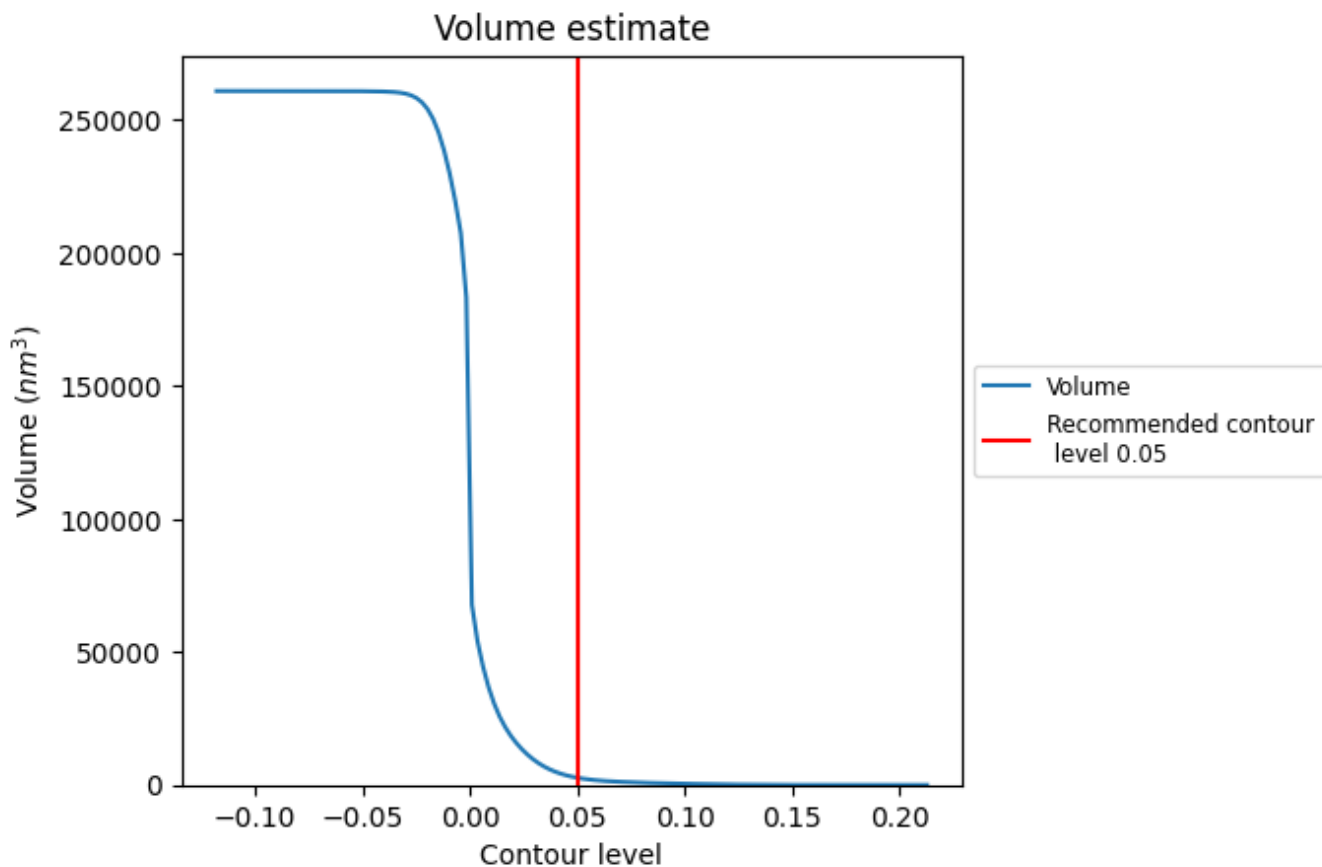
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

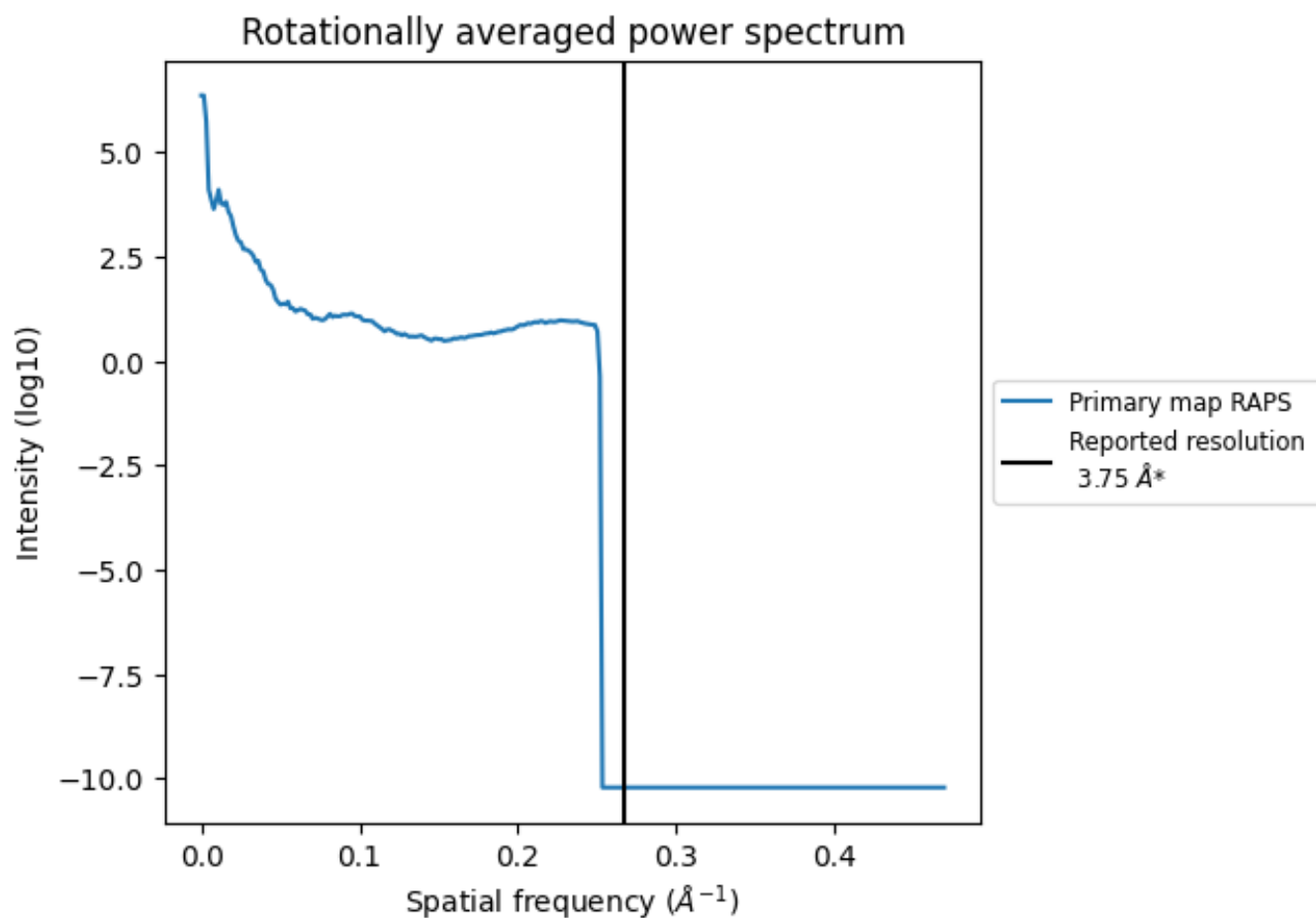
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2712 nm³; this corresponds to an approximate mass of 2450 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

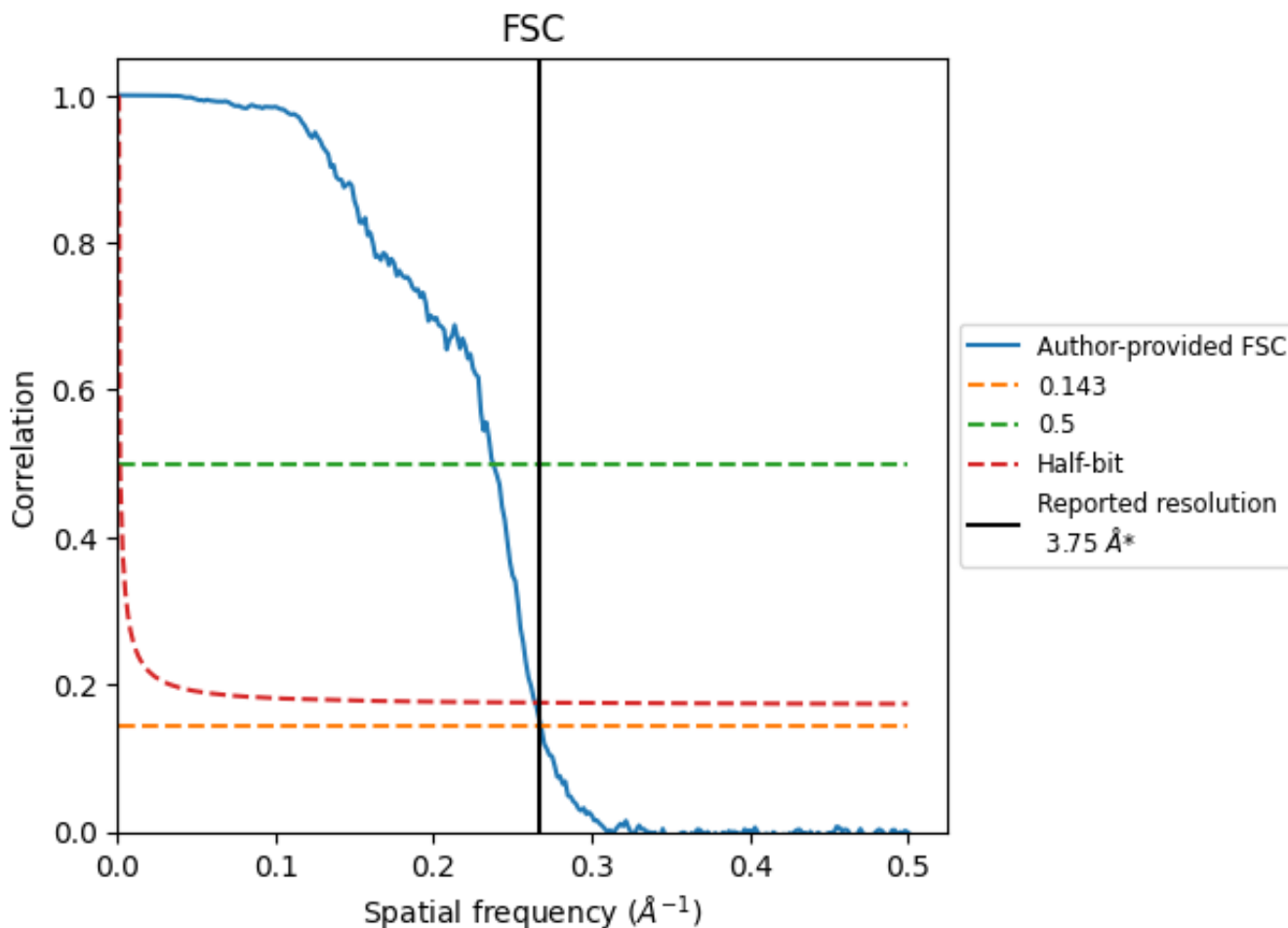


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.73	4.21	3.78
Unmasked-calculated*	-	-	-

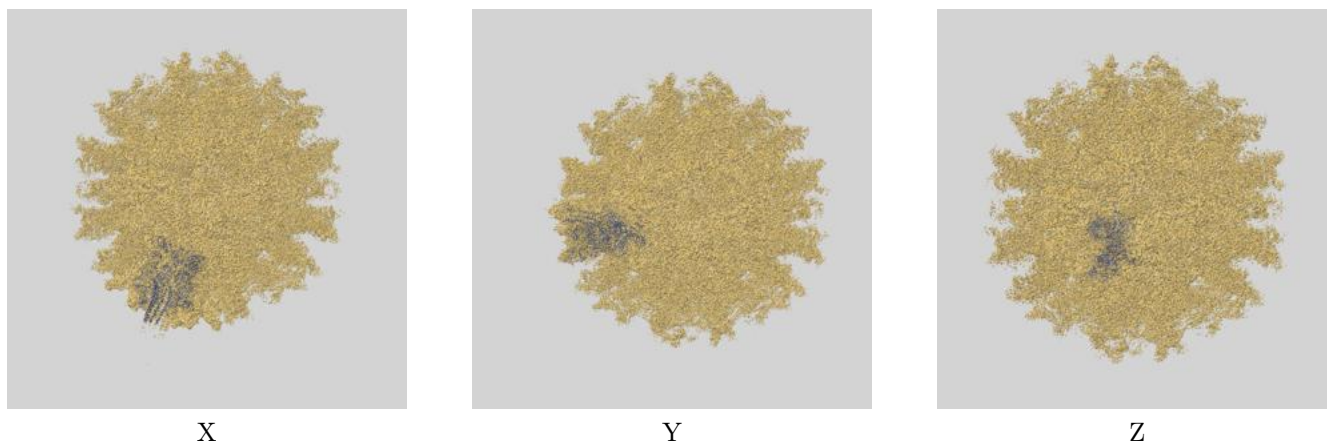
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

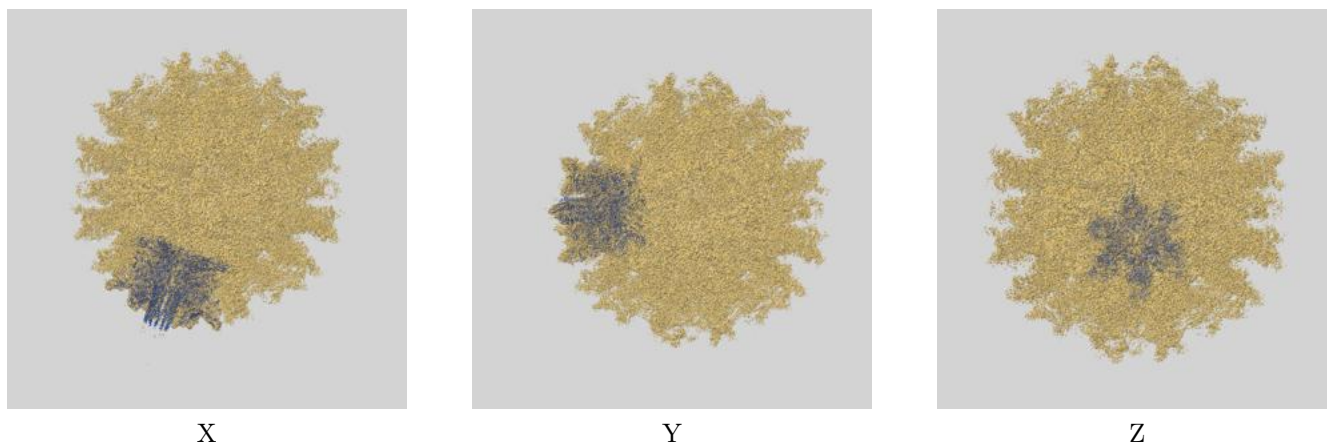
This section contains information regarding the fit between EMDB map EMD-0056 and PDB model 6GSI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

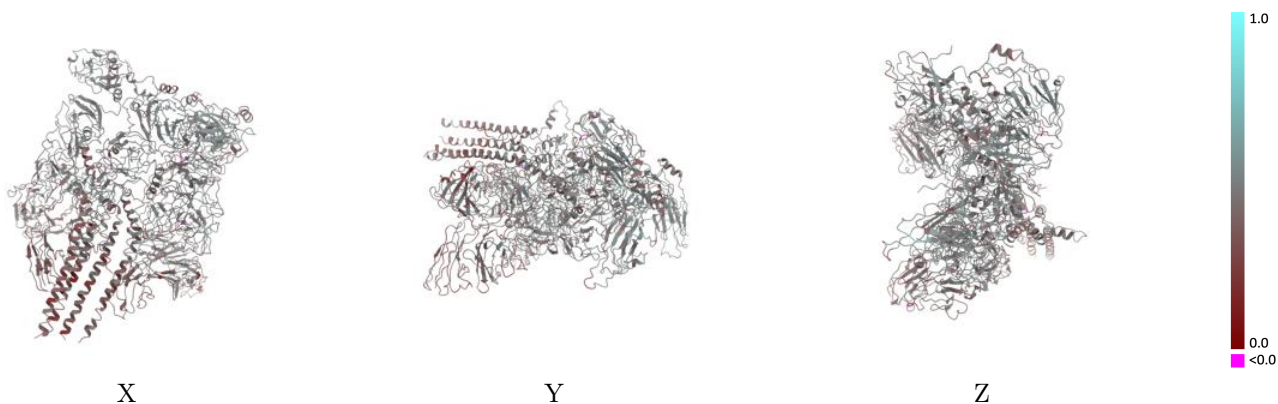


9.1.2 Map-model assembly overlay [i](#)



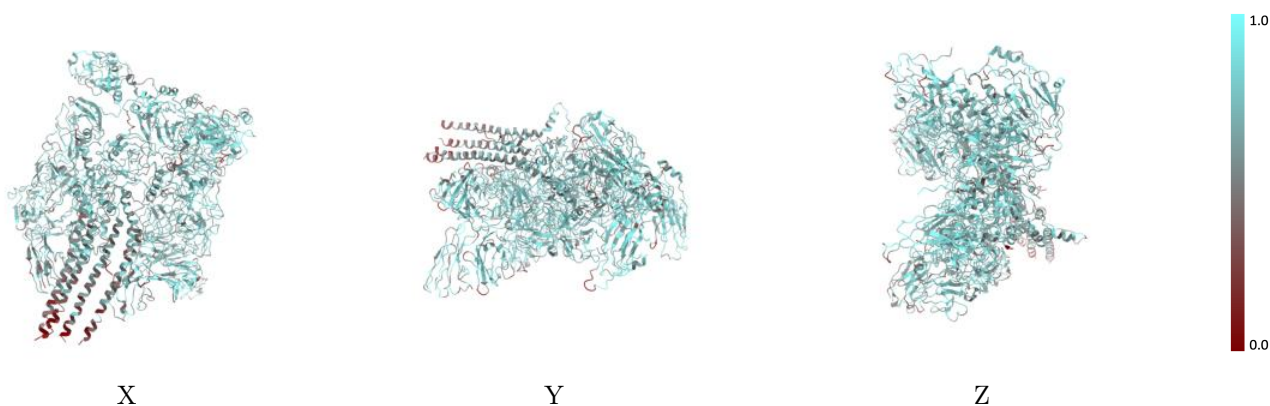
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



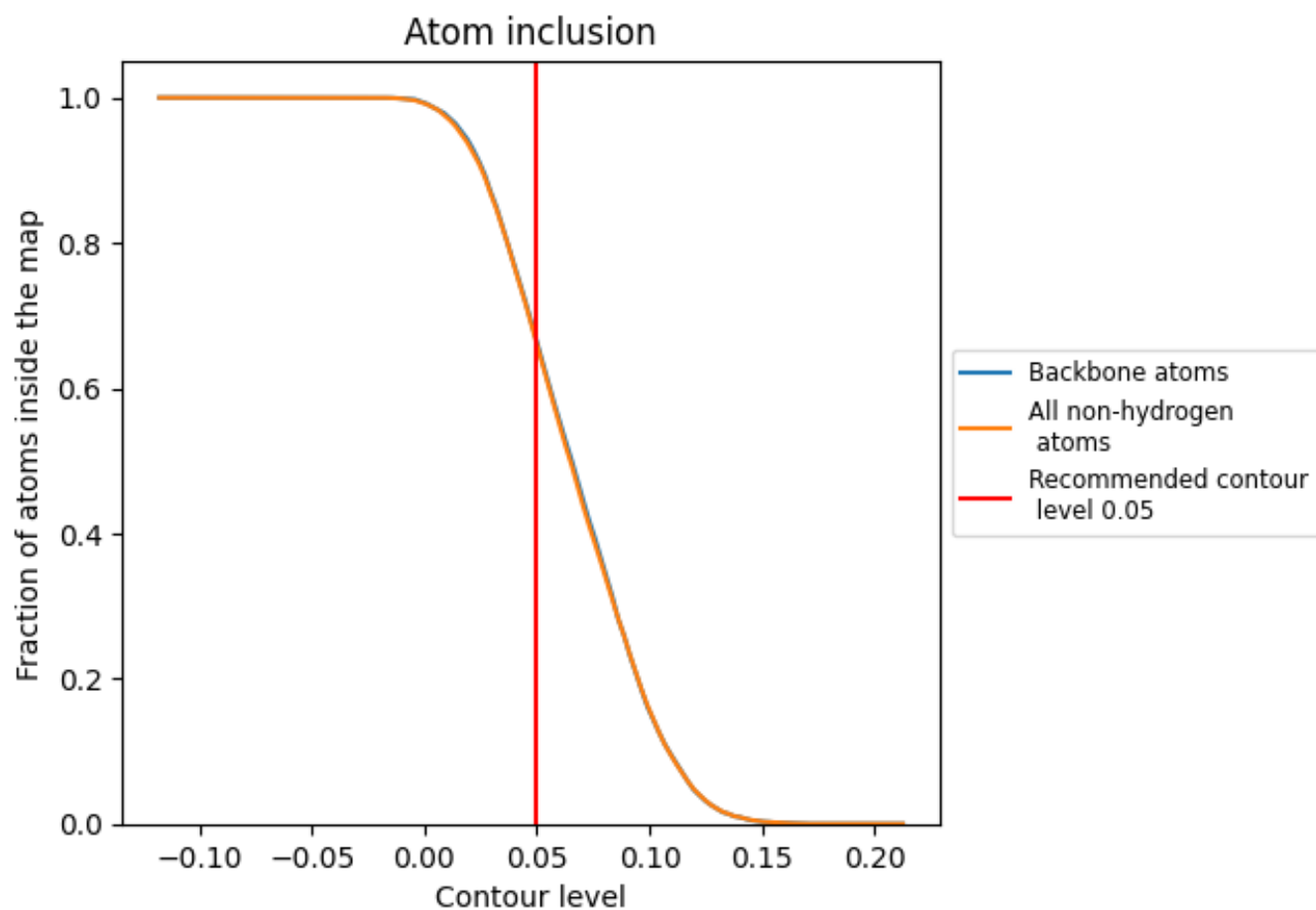
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6603	 0.4390
A	 0.7128	 0.4630
B	 0.6877	 0.4620
C	 0.6986	 0.4650
D	 0.6905	 0.4660
E	 0.6634	 0.3870
F	 0.6579	 0.3940
G	 0.6920	 0.3930
H	 0.6879	 0.4110
I	 0.5023	 0.3880
J	 0.5566	 0.4050
K	 0.4947	 0.3780
L	 0.5510	 0.3880

