Full wwPDB EM Validation Report ⓘ

Apr 16, 2023 – 03:13 am BST

PDB ID	:	8BP8
EMDB ID	:	EMD-16146
Title	:	SPA of Trypsin untreated Rotavirus TLP spike
Authors	:	Shah, P.N.M.; Stuart, D.I.
Deposited on	:	2022-11-16
Resolution	:	2.70 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:

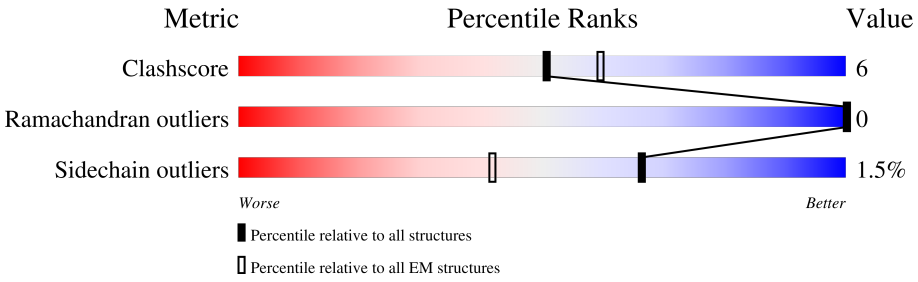
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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 <=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	776	56% 70% 23% • 6%
1	B	776	56% 68% 27% • •
1	C	776	33% 73% 15% • 11%
2	D	326	• 70% 10% • 20%
2	E	326	• 66% 8% 25%
2	F	326	• 70% 11% 18%
2	G	326	• 71% 11% 18%
2	H	326	64% 10% 26%

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Mol	Chain	Length	Quality of chain
2	I	326	71% 10% 19%
2	J	326	72% 8% 19%
2	K	326	68% 11% 21%
2	L	326	69% 12% 19%
2	M	326	72% 10% 18%
2	N	326	69% 12% 19%
2	O	326	73% 8% 19%
2	P	326	66% 9% 26%
3	d	397	99%
3	e	397	99%
3	f	397	99%
3	g	397	99%
3	h	397	99%
3	i	397	99%
3	j	397	99%
3	k	397	99%
3	l	397	100%
3	m	397	98%
3	n	397	99%
3	o	397	98%
3	p	397	99%
4	q	882	86% 13%
4	r	882	89% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 193677 atoms, of which 96046 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	726	Total	C	H	N	O	S	0	0
			11303	3616	5589	952	1127	19		
1	B	744	Total	C	H	N	O	S	0	0
			11596	3703	5737	977	1159	20		
1	C	692	Total	C	H	N	O	S	0	0
			10813	3466	5343	910	1074	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	THR	ARG	conflict	UNP A0A1Q2TSK9
A	323	MET	VAL	conflict	UNP A0A1Q2TSK9
A	737	SER	THR	conflict	UNP A0A1Q2TSK9
A	738	ARG	LYS	conflict	UNP A0A1Q2TSK9
B	185	THR	ARG	conflict	UNP A0A1Q2TSK9
B	323	MET	VAL	conflict	UNP A0A1Q2TSK9
B	737	SER	THR	conflict	UNP A0A1Q2TSK9
B	738	ARG	LYS	conflict	UNP A0A1Q2TSK9
C	185	THR	ARG	conflict	UNP A0A1Q2TSK9
C	323	MET	VAL	conflict	UNP A0A1Q2TSK9
C	737	SER	THR	conflict	UNP A0A1Q2TSK9
C	738	ARG	LYS	conflict	UNP A0A1Q2TSK9

- Molecule 2 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	262	Total	C	H	N	O	S	0	0
			4111	1324	2035	329	407	16		
2	E	244	Total	C	H	N	O	S	0	0
			3820	1227	1892	304	381	16		
2	F	267	Total	C	H	N	O	S	0	0
			4185	1348	2067	337	417	16		
2	G	268	Total	C	H	N	O	S	0	0
			4203	1354	2078	338	417	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	242	Total	C	H	N	O	S	0	0
			3787	1217	1874	302	378	16		
2	I	264	Total	C	H	N	O	S	0	0
			4144	1333	2048	334	413	16		
2	J	265	Total	C	H	N	O	S	0	0
			4153	1336	2053	335	413	16		
2	K	256	Total	C	H	N	O	S	0	0
			4021	1293	1991	323	398	16		
2	L	265	Total	C	H	N	O	S	0	0
			4154	1336	2053	335	414	16		
2	M	267	Total	C	H	N	O	S	0	0
			4185	1348	2067	337	417	16		
2	N	263	Total	C	H	N	O	S	0	0
			4131	1329	2044	333	409	16		
2	O	265	Total	C	H	N	O	S	0	0
			4154	1336	2053	335	414	16		
2	P	242	Total	C	H	N	O	S	0	0
			3787	1217	1874	302	378	16		

- Molecule 3 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	e	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	f	397	Total	C	H	N	O	S	0	0
			6277	2007	3114	550	592	14		
3	g	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	h	397	Total	C	H	N	O	S	0	0
			6277	2007	3114	550	592	14		
3	i	397	Total	C	H	N	O	S	0	0
			6277	2007	3114	550	592	14		
3	j	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	k	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	l	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	m	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	n	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	o	397	Total	C	H	N	O	S	0	0
			6276	2007	3113	550	592	14		
3	p	397	Total	C	H	N	O	S	0	0
			6277	2007	3114	550	592	14		

- Molecule 4 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	q	769	Total	C	H	N	O	S	0	0
			12520	3978	6273	1072	1161	36		
4	r	795	Total	C	H	N	O	S	0	0
			12974	4122	6502	1108	1206	36		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	118	ALA	LYS	conflict	UNP A2T3R1
q	129	ARG	LYS	conflict	UNP A2T3R1
q	131	LYS	LEU	conflict	UNP A2T3R1
q	135	ILE	ARG	conflict	UNP A2T3R1
q	140	LYS	ARG	conflict	UNP A2T3R1
q	142	ARG	LEU	conflict	UNP A2T3R1
q	146	ILE	TRP	conflict	UNP A2T3R1
q	152	LYS	ARG	conflict	UNP A2T3R1
q	175	THR	MET	conflict	UNP A2T3R1
q	206	SER	ALA	conflict	UNP A2T3R1
q	222	ALA	ARG	conflict	UNP A2T3R1
q	250	TYR	HIS	conflict	UNP A2T3R1
q	414	VAL	ILE	conflict	UNP A2T3R1
q	432	VAL	ILE	conflict	UNP A2T3R1
q	436	ILE	VAL	conflict	UNP A2T3R1
q	438	VAL	PRO	conflict	UNP A2T3R1
q	477	ASN	TYR	conflict	UNP A2T3R1
q	479	TYR	GLN	conflict	UNP A2T3R1
q	503	ILE	VAL	conflict	UNP A2T3R1
q	551	ALA	SER	conflict	UNP A2T3R1
q	553	SER	ASN	conflict	UNP A2T3R1
q	561	VAL	ILE	conflict	UNP A2T3R1
q	640	ALA	SER	conflict	UNP A2T3R1
q	650	HIS	GLN	conflict	UNP A2T3R1

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Chain	Residue	Modelled	Actual	Comment	Reference
q	656	VAL	ARG	conflict	UNP A2T3R1
q	657	ALA	VAL	conflict	UNP A2T3R1
q	676	VAL	ILE	conflict	UNP A2T3R1
q	686	LEU	ALA	conflict	UNP A2T3R1
q	688	ALA	ASN	conflict	UNP A2T3R1
q	690	ASP	GLU	conflict	UNP A2T3R1
q	741	THR	SER	conflict	UNP A2T3R1
q	743	SER	ASP	conflict	UNP A2T3R1
q	766	VAL	ILE	conflict	UNP A2T3R1
q	777	ILE	LYS	conflict	UNP A2T3R1
q	818	VAL	ILE	conflict	UNP A2T3R1
q	820	ILE	THR	conflict	UNP A2T3R1
q	831	VAL	GLN	conflict	UNP A2T3R1
q	837	ASN	ALA	conflict	UNP A2T3R1
r	118	ALA	LYS	conflict	UNP A2T3R1
r	129	ARG	LYS	conflict	UNP A2T3R1
r	131	LYS	LEU	conflict	UNP A2T3R1
r	135	ILE	ARG	conflict	UNP A2T3R1
r	140	LYS	ARG	conflict	UNP A2T3R1
r	142	ARG	LEU	conflict	UNP A2T3R1
r	146	ILE	TRP	conflict	UNP A2T3R1
r	152	LYS	ARG	conflict	UNP A2T3R1
r	175	THR	MET	conflict	UNP A2T3R1
r	206	SER	ALA	conflict	UNP A2T3R1
r	222	ALA	ARG	conflict	UNP A2T3R1
r	250	TYR	HIS	conflict	UNP A2T3R1
r	414	VAL	ILE	conflict	UNP A2T3R1
r	432	VAL	ILE	conflict	UNP A2T3R1
r	436	ILE	VAL	conflict	UNP A2T3R1
r	438	VAL	PRO	conflict	UNP A2T3R1
r	477	ASN	TYR	conflict	UNP A2T3R1
r	479	TYR	GLN	conflict	UNP A2T3R1
r	503	ILE	VAL	conflict	UNP A2T3R1
r	551	ALA	SER	conflict	UNP A2T3R1
r	553	SER	ASN	conflict	UNP A2T3R1
r	561	VAL	ILE	conflict	UNP A2T3R1
r	640	ALA	SER	conflict	UNP A2T3R1
r	650	HIS	GLN	conflict	UNP A2T3R1
r	656	VAL	ARG	conflict	UNP A2T3R1
r	657	ALA	VAL	conflict	UNP A2T3R1
r	676	VAL	ILE	conflict	UNP A2T3R1
r	686	LEU	ALA	conflict	UNP A2T3R1

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Chain	Residue	Modelled	Actual	Comment	Reference
r	688	ALA	ASN	conflict	UNP A2T3R1
r	690	ASP	GLU	conflict	UNP A2T3R1
r	741	THR	SER	conflict	UNP A2T3R1
r	743	SER	ASP	conflict	UNP A2T3R1
r	766	VAL	ILE	conflict	UNP A2T3R1
r	777	ILE	LYS	conflict	UNP A2T3R1
r	818	VAL	ILE	conflict	UNP A2T3R1
r	820	ILE	THR	conflict	UNP A2T3R1
r	831	VAL	GLN	conflict	UNP A2T3R1
r	837	ASN	ALA	conflict	UNP A2T3R1

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	D	3	Total Ca 3 3	0
5	E	3	Total Ca 3 3	0
5	F	3	Total Ca 3 3	0
5	G	3	Total Ca 3 3	0
5	H	3	Total Ca 3 3	0
5	I	3	Total Ca 3 3	0
5	J	3	Total Ca 3 3	0
5	K	3	Total Ca 3 3	0
5	L	3	Total Ca 3 3	0
5	M	3	Total Ca 3 3	0
5	N	3	Total Ca 3 3	0
5	O	3	Total Ca 3 3	0
5	P	3	Total Ca 3 3	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Inter-

est" by depositor).

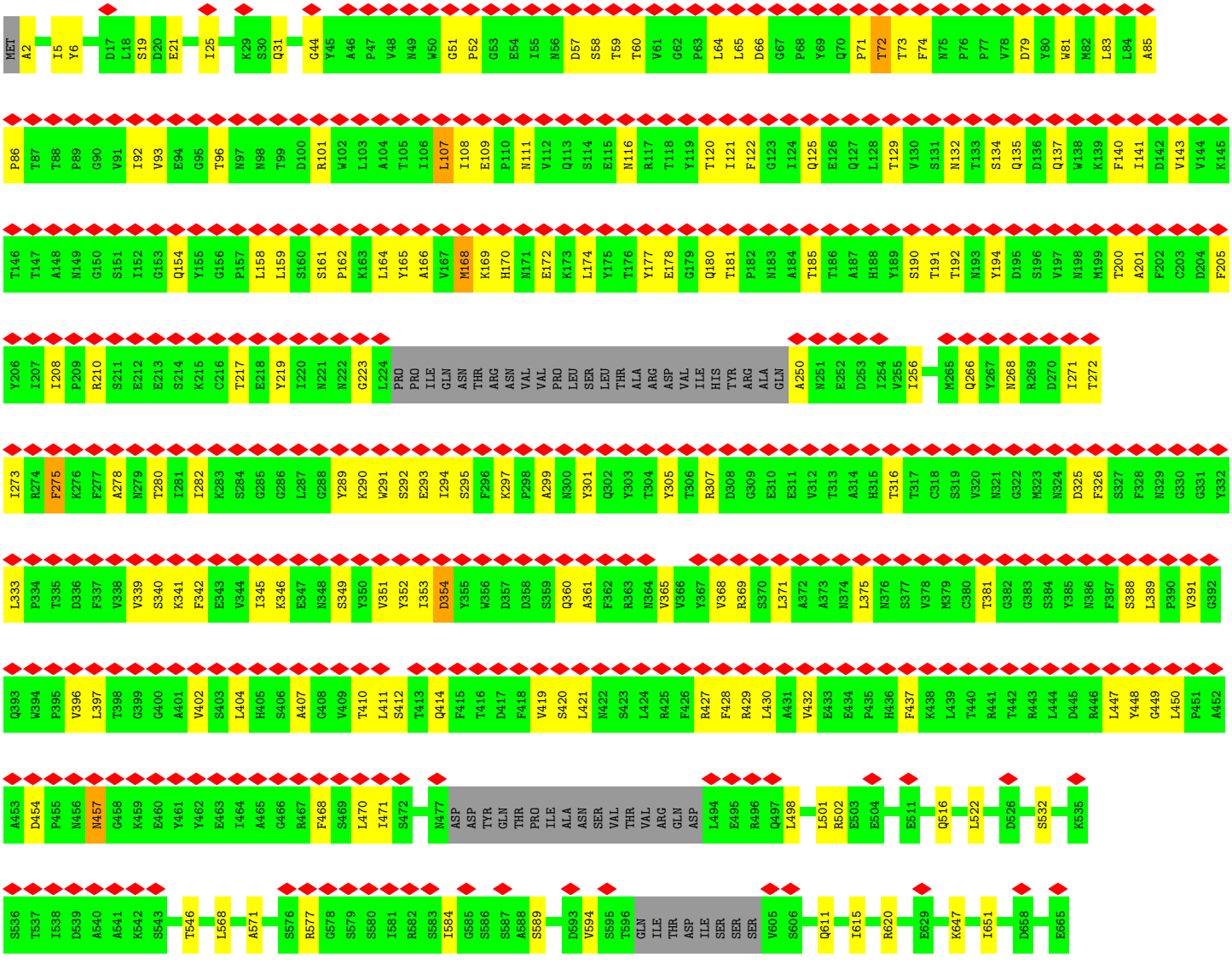
Mol	Chain	Residues	Atoms	AltConf
6	e	1	Total Zn 1 1	0
6	g	1	Total Zn 1 1	0
6	j	1	Total Zn 1 1	0
6	m	1	Total Zn 1 1	0
6	p	1	Total Zn 1 1	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

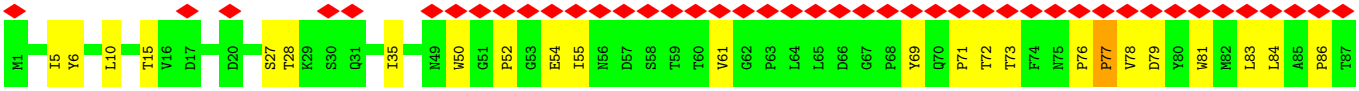
- Molecule 1: Outer capsid protein VP4

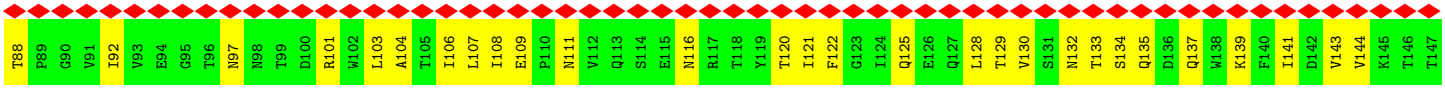
Chain A:

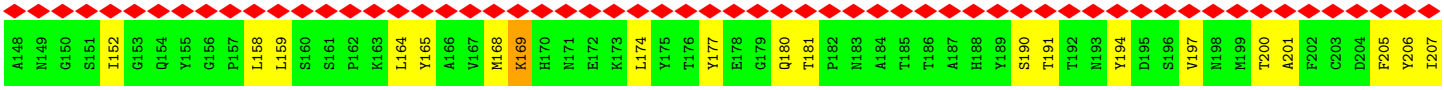


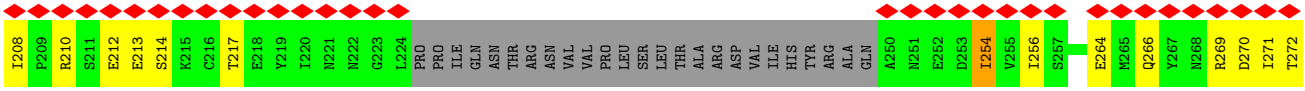
• Molecule 1: Outer capsid protein VP4

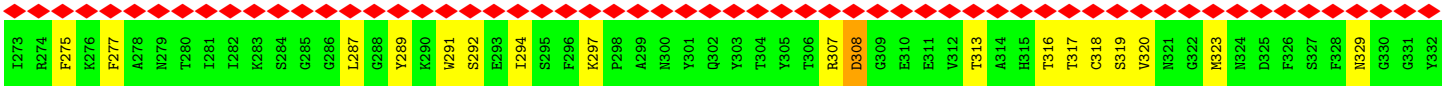
Chain B:

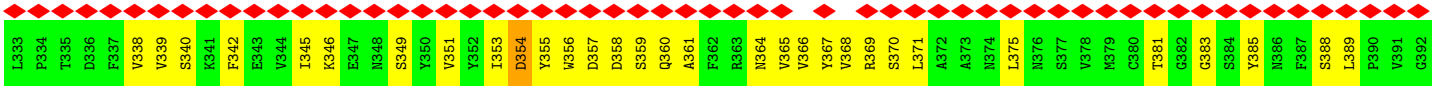


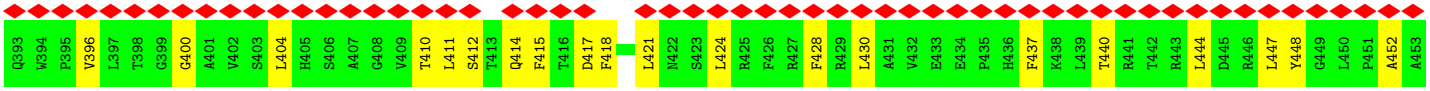


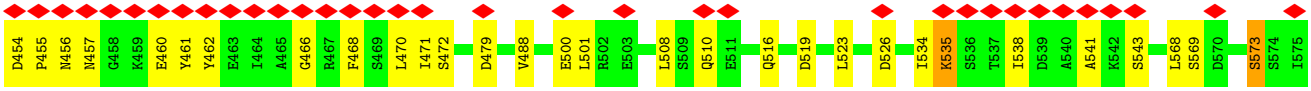


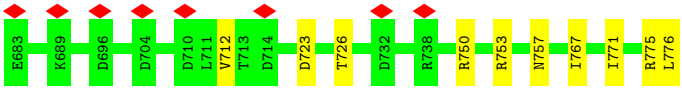






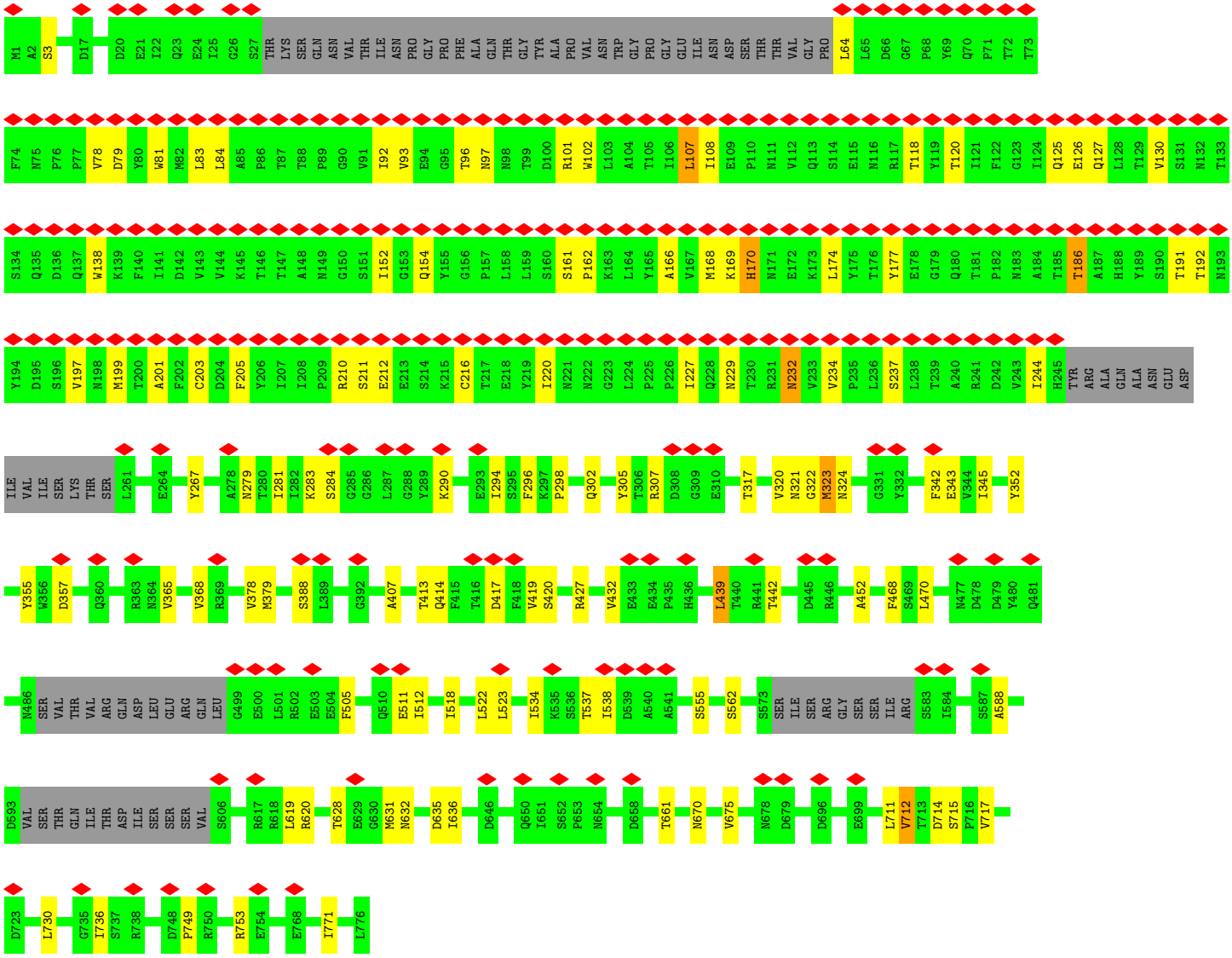




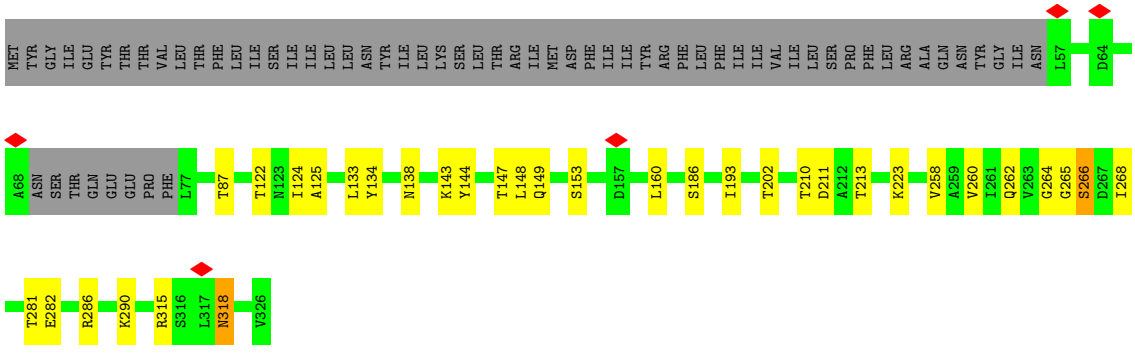


• Molecule 1: Outer capsid protein VP4

Chain C:

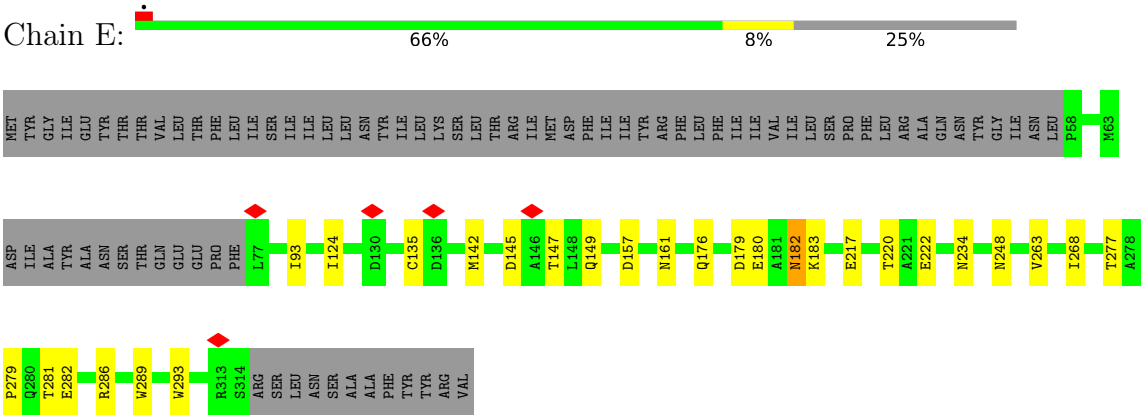


• Molecule 2: Outer capsid glycoprotein VP7



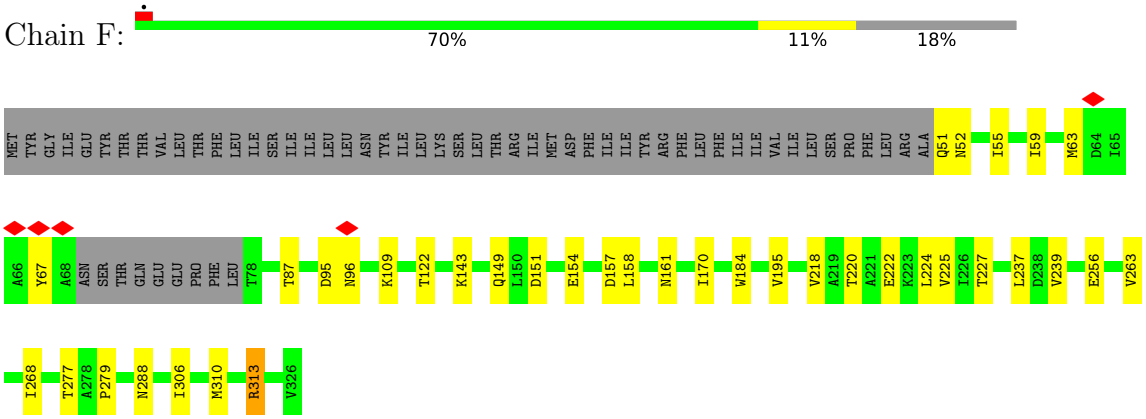
• Molecule 2: Outer capsid glycoprotein VP7

Chain E:



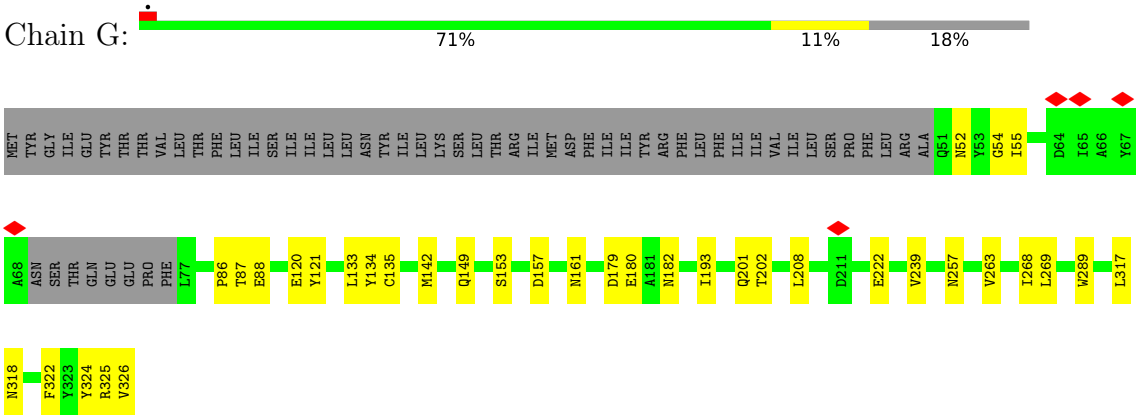
• Molecule 2: Outer capsid glycoprotein VP7

Chain F:



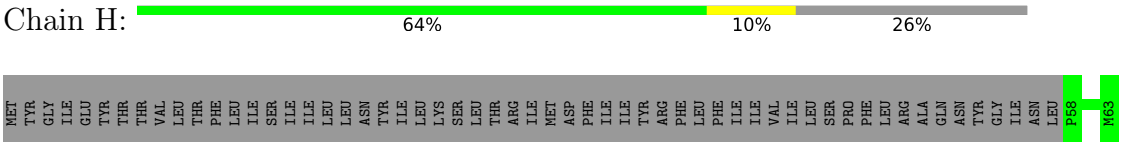
• Molecule 2: Outer capsid glycoprotein VP7

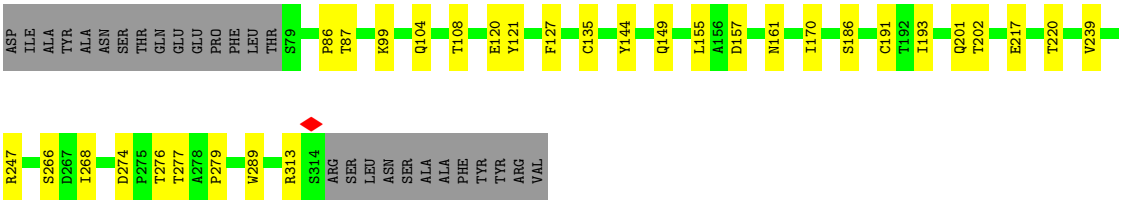
Chain G:



• Molecule 2: Outer capsid glycoprotein VP7

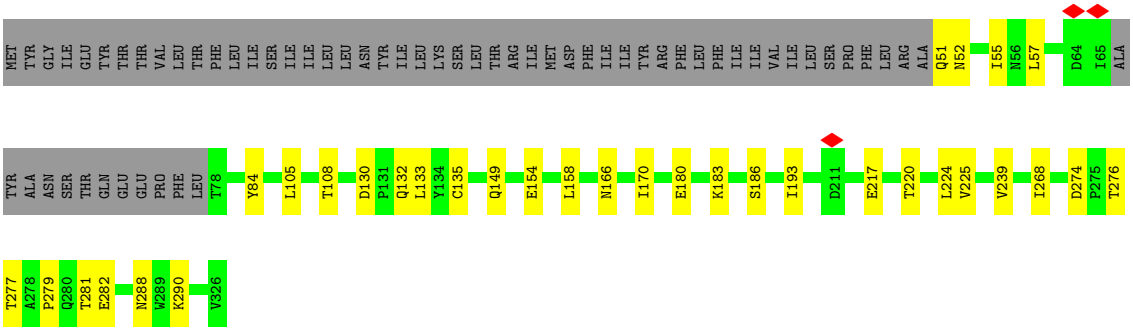
Chain H:





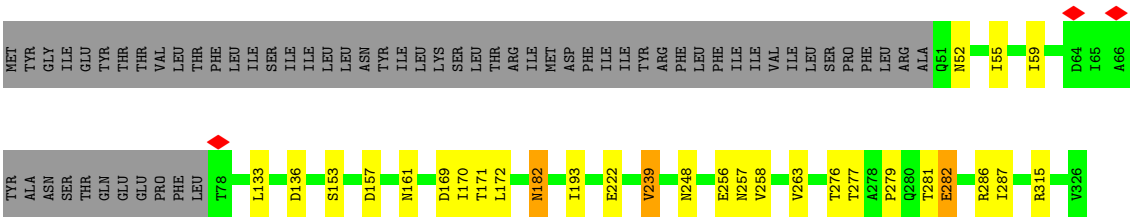
• Molecule 2: Outer capsid glycoprotein VP7

Chain I:



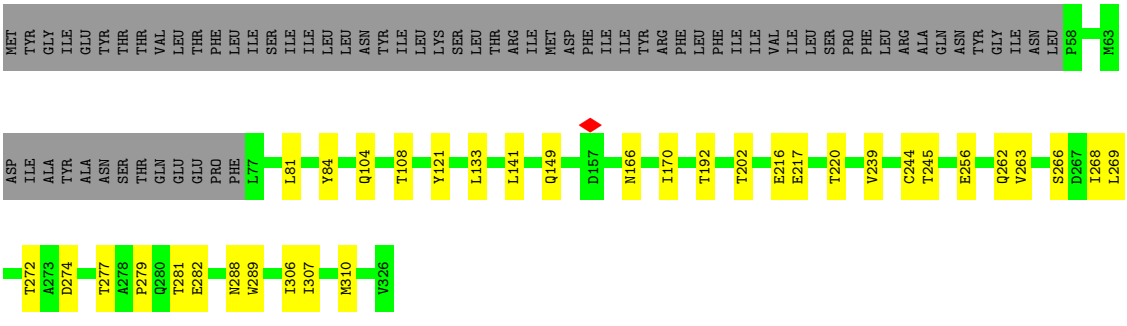
• Molecule 2: Outer capsid glycoprotein VP7

Chain J:



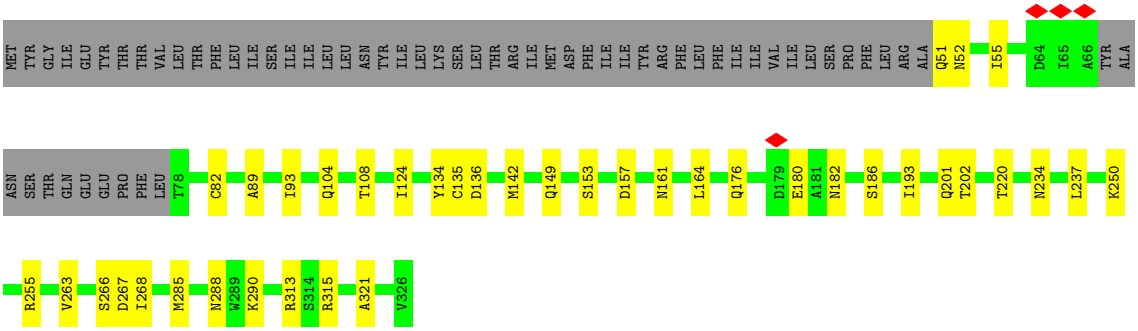
• Molecule 2: Outer capsid glycoprotein VP7

Chain K:

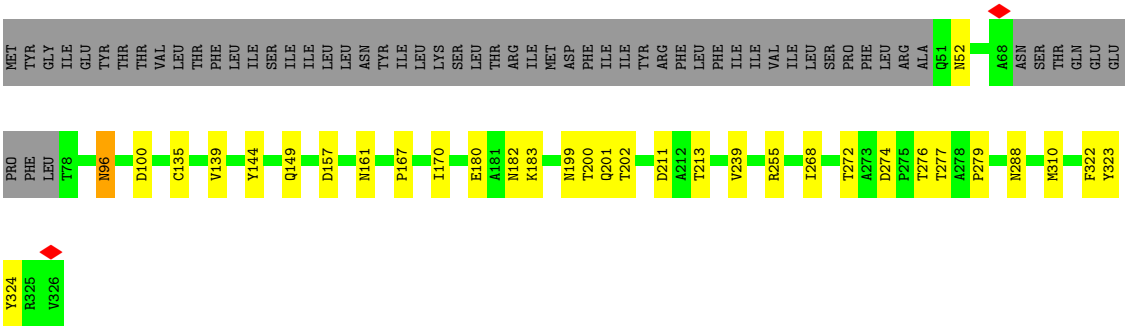


• Molecule 2: Outer capsid glycoprotein VP7

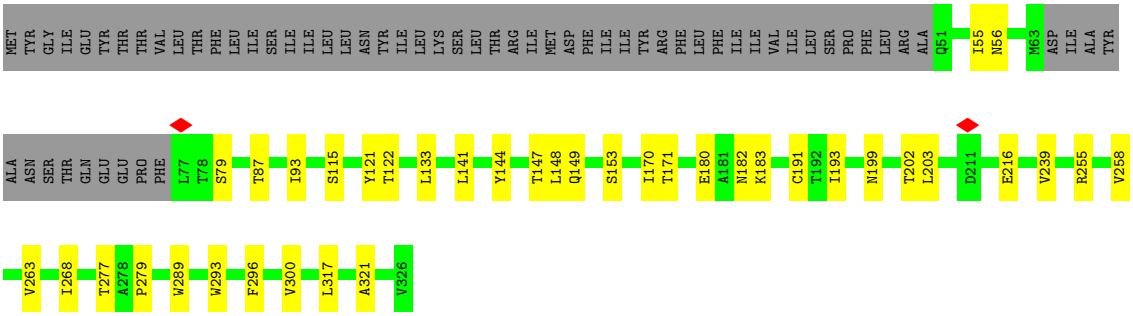
Chain L:



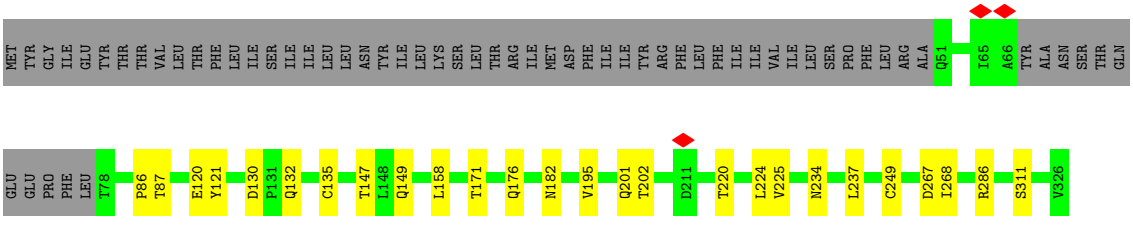
• Molecule 2: Outer capsid glycoprotein VP7



• Molecule 2: Outer capsid glycoprotein VP7

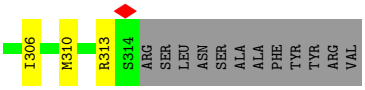


• Molecule 2: Outer capsid glycoprotein VP7



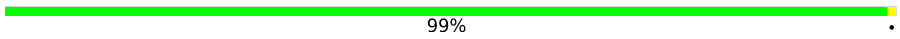
• Molecule 2: Outer capsid glycoprotein VP7

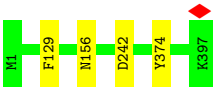
Chain P:



• Molecule 3: Intermediate capsid protein VP6

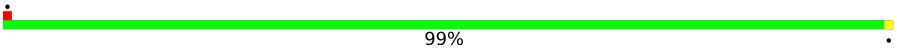
Chain d:





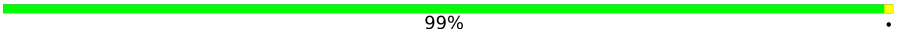
• Molecule 3: Intermediate capsid protein VP6

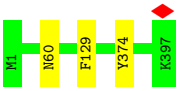
Chain e:



• Molecule 3: Intermediate capsid protein VP6

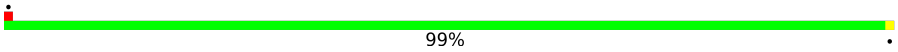
Chain f:

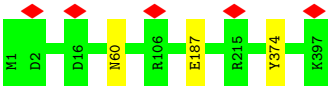




• Molecule 3: Intermediate capsid protein VP6

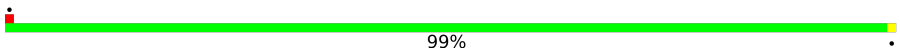
Chain g:

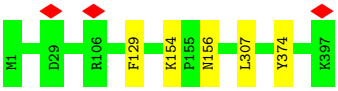




• Molecule 3: Intermediate capsid protein VP6

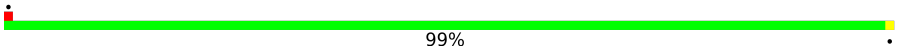
Chain h:

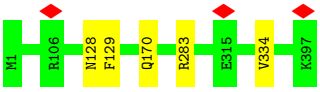




• Molecule 3: Intermediate capsid protein VP6

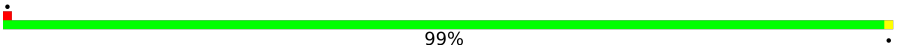
Chain i:

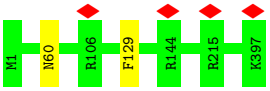




• Molecule 3: Intermediate capsid protein VP6

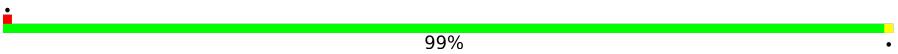
Chain j:

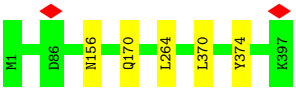




• Molecule 3: Intermediate capsid protein VP6

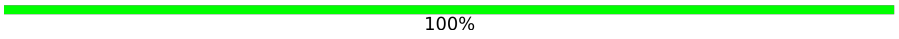
Chain k:

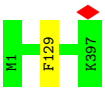




• Molecule 3: Intermediate capsid protein VP6

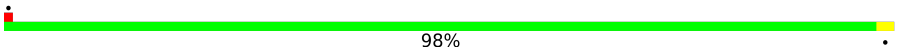
Chain l:





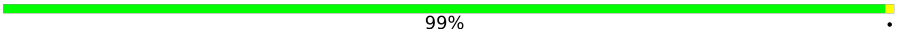
• Molecule 3: Intermediate capsid protein VP6

Chain m:



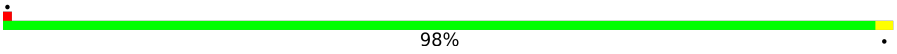
• Molecule 3: Intermediate capsid protein VP6

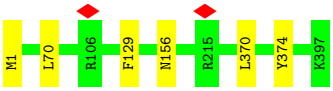
Chain n:



• Molecule 3: Intermediate capsid protein VP6

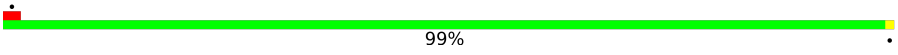
Chain o:

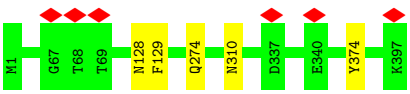




• Molecule 3: Intermediate capsid protein VP6

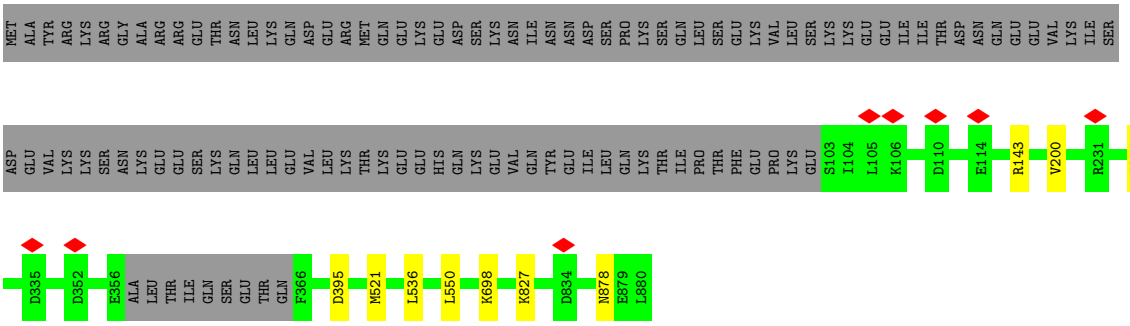
Chain p:





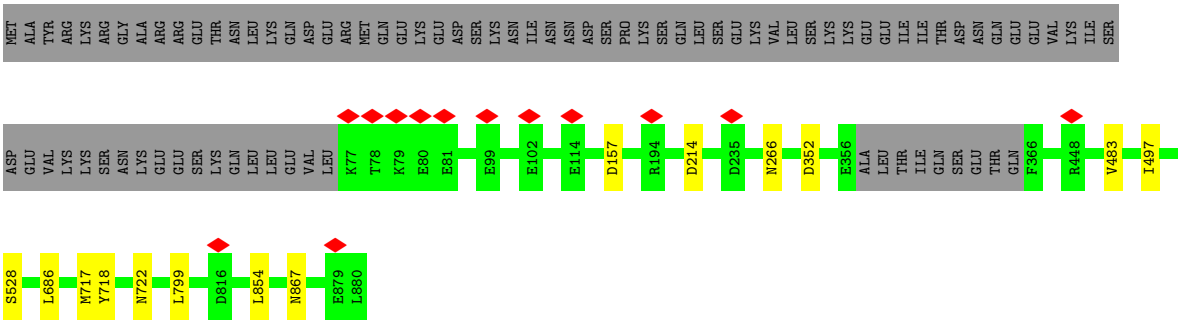
• Molecule 4: Inner capsid protein VP2

Chain q:



• Molecule 4: Inner capsid protein VP2

Chain r:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

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: ZN, CA

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	0.26	0/5832	0.48	0/7925
1	B	0.26	0/5980	0.48	0/8129
1	C	0.27	0/5583	0.48	0/7586
2	D	0.31	0/2119	0.46	0/2893
2	E	0.31	0/1967	0.46	0/2685
2	F	0.32	0/2162	0.47	0/2950
2	G	0.32	0/2169	0.47	0/2961
2	H	0.32	0/1952	0.46	0/2664
2	I	0.33	0/2139	0.47	0/2918
2	J	0.32	0/2143	0.47	0/2925
2	K	0.31	0/2072	0.46	0/2827
2	L	0.31	0/2144	0.47	0/2925
2	M	0.31	0/2162	0.47	0/2950
2	N	0.31	0/2130	0.47	0/2907
2	O	0.32	0/2144	0.46	0/2925
2	P	0.31	0/1952	0.47	0/2664
3	d	0.31	0/3234	0.50	0/4402
3	e	0.31	0/3234	0.50	0/4402
3	f	0.31	0/3234	0.51	0/4402
3	g	0.32	0/3234	0.51	0/4402
3	h	0.32	0/3234	0.51	0/4402
3	i	0.32	0/3234	0.51	0/4402
3	j	0.31	0/3234	0.51	0/4402
3	k	0.32	0/3234	0.51	0/4402
3	l	0.32	0/3234	0.51	0/4402
3	m	0.31	0/3234	0.51	0/4402
3	n	0.32	0/3234	0.51	0/4402
3	o	0.32	0/3234	0.51	0/4402
3	p	0.31	0/3234	0.51	0/4402
4	q	0.31	0/6360	0.49	0/8630
4	r	0.31	0/6590	0.49	0/8939
All	All	0.31	0/99642	0.49	0/135629

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	705	VAL	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	5714	5589	5598	168	0
1	B	5859	5737	5737	188	0
1	C	5470	5343	5345	94	0
2	D	2076	2035	2035	24	0
2	E	1928	1892	1892	16	0
2	F	2118	2067	2067	27	0
2	G	2125	2078	2078	21	0
2	H	1913	1874	1874	18	0
2	I	2096	2048	2048	26	0
2	J	2100	2053	2053	27	0
2	K	2030	1991	1991	23	0
2	L	2101	2053	2053	30	0
2	M	2118	2067	2067	24	0
2	N	2087	2044	2044	28	0
2	O	2101	2053	2053	18	0
2	P	1913	1874	1874	18	0
3	d	3163	3113	3114	0	0
3	e	3163	3113	3114	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	3163	3114	3114	0	0
3	g	3163	3113	3114	0	0
3	h	3163	3114	3114	0	0
3	i	3163	3114	3114	0	0
3	j	3163	3113	3114	0	0
3	k	3163	3113	3114	0	0
3	l	3163	3113	3114	0	0
3	m	3163	3113	3114	0	0
3	n	3163	3113	3114	0	0
3	o	3163	3113	3114	0	0
3	p	3163	3114	3114	0	0
4	q	6247	6273	6276	0	0
4	r	6472	6502	6503	0	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
5	K	3	0	0	0	0
5	L	3	0	0	0	0
5	M	3	0	0	0	0
5	N	3	0	0	0	0
5	O	3	0	0	0	0
5	P	3	0	0	0	0
6	e	1	0	0	0	0
6	g	1	0	0	0	0
6	j	1	0	0	0	0
6	m	1	0	0	0	0
6	p	1	0	0	0	0
All	All	97631	96046	96070	680	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 6.

All (680) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:LEU:HD13	2:D:258:VAL:HG11	1.37	1.05
1:A:280:THR:HG1	1:A:295:SER:HG	1.12	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:O	1:A:340:SER:OG	1.94	0.85
1:B:510:GLN:NE2	2:F:67:TYR:O	2.10	0.84
1:C:320:VAL:HG21	1:C:345:ILE:HG21	1.61	0.82
1:C:439:LEU:O	1:C:442:THR:OG1	1.98	0.82
2:M:274:ASP:OD2	2:M:276:THR:OG1	1.99	0.81
2:H:170:ILE:HD13	2:H:239:VAL:HG22	1.63	0.81
1:A:352:TYR:OH	1:B:54:GLU:OE1	1.98	0.81
1:B:109:GLU:O	1:B:132:ASN:ND2	2.14	0.81
2:H:157:ASP:OD1	2:H:161:ASN:ND2	2.14	0.81
2:K:217:GLU:OE2	2:K:220:THR:OG1	1.98	0.81
1:A:109:GLU:O	1:A:132:ASN:ND2	2.14	0.80
2:J:157:ASP:OD1	2:J:161:ASN:ND2	2.15	0.79
1:B:371:LEU:HD22	1:B:470:LEU:HD22	1.64	0.79
1:B:619:LEU:HD21	1:B:712:VAL:HG13	1.65	0.79
2:L:313:ARG:NH1	2:M:322:PHE:O	2.16	0.78
1:A:715:SER:OG	1:B:750:ARG:NH1	2.17	0.78
1:B:73:THR:HG22	1:B:200:THR:HG22	1.66	0.77
1:C:307:ARG:NH2	1:C:357:ASP:OD2	2.17	0.77
1:B:723:ASP:OD1	1:B:726:THR:OG1	2.01	0.76
1:A:584:ILE:HD12	1:A:615:ILE:HD11	1.66	0.76
1:C:169:LYS:NZ	1:C:199:MET:SD	2.57	0.76
2:F:313:ARG:NH1	2:G:322:PHE:O	2.19	0.76
1:C:97:ASN:ND2	1:C:192:THR:O	2.18	0.76
1:A:83:LEU:HD12	1:A:208:ILE:HD11	1.68	0.75
2:N:255:ARG:NH2	2:N:321:ALA:O	2.19	0.75
1:A:404:LEU:HD22	1:A:428:PHE:HB3	1.67	0.75
1:A:158:LEU:HD22	1:A:165:TYR:CE1	2.23	0.74
1:A:516:GLN:NE2	1:C:588:ALA:O	2.21	0.74
1:A:714:ASP:OD1	1:A:715:SER:N	2.21	0.74
1:A:346:LYS:O	1:A:349:SER:OG	2.05	0.73
1:A:129:THR:O	1:A:154:GLN:NE2	2.22	0.73
1:B:345:ILE:HG23	1:B:430:LEU:HD13	1.69	0.73
1:A:178:GLU:O	1:A:185:THR:N	2.22	0.73
2:M:201:GLN:O	2:M:202:THR:OG1	2.06	0.72
2:P:170:ILE:HD13	2:P:239:VAL:HG12	1.71	0.71
1:C:79:ASP:OD1	1:C:210:ARG:NH2	2.24	0.71
2:J:222:GLU:OE2	2:L:290:LYS:NZ	2.17	0.71
1:B:339:VAL:HG11	1:B:342:PHE:CE2	2.26	0.71
1:B:368:VAL:HG21	1:B:371:LEU:HD21	1.71	0.71
2:F:277:THR:HG22	2:F:279:PRO:HD3	1.73	0.71
2:O:267:ASP:OD1	2:O:286:ARG:NE	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:O	1:A:72:THR:HG23	1.90	0.71
2:N:277:THR:HG22	2:N:279:PRO:HD3	1.71	0.71
1:A:158:LEU:HD11	1:A:177:TYR:O	1.89	0.70
1:B:411:LEU:HD22	1:B:424:LEU:HD22	1.73	0.70
1:A:19:SER:OG	1:A:546:THR:HG21	1.92	0.70
2:L:157:ASP:OD1	2:L:161:ASN:ND2	2.25	0.70
1:A:354:ASP:OD1	1:A:354:ASP:N	2.24	0.69
2:E:145:ASP:OD2	2:E:147:THR:OG1	2.10	0.69
2:I:180:GLU:O	2:I:183:LYS:NZ	2.25	0.69
2:N:170:ILE:HD11	2:N:239:VAL:HG22	1.74	0.69
2:I:217:GLU:OE2	2:I:220:THR:OG1	2.09	0.69
1:B:79:ASP:OD1	1:B:210:ARG:NE	2.25	0.69
2:I:51:GLN:N	2:J:55:ILE:O	2.26	0.69
2:K:216:GLU:N	2:K:216:GLU:OE1	2.25	0.69
1:B:351:VAL:HG23	1:B:430:LEU:HD11	1.75	0.68
1:C:212:GLU:N	1:C:212:GLU:OE1	2.26	0.68
1:A:368:VAL:HG11	1:A:411:LEU:HD13	1.74	0.68
2:E:277:THR:HG22	2:E:279:PRO:HD3	1.73	0.68
1:A:361:ALA:O	1:A:365:VAL:HG23	1.94	0.68
2:N:121:TYR:OH	2:N:141:LEU:O	2.10	0.68
1:A:282:ILE:O	1:A:292:SER:OG	2.12	0.68
2:F:149:GLN:OE1	2:F:268:ILE:HG21	1.94	0.68
2:D:138:ASN:HB2	2:D:258:VAL:HG12	1.76	0.67
1:A:121:ILE:HG22	1:A:122:PHE:CD2	2.29	0.67
1:B:134:SER:HB3	1:B:159:LEU:HD13	1.75	0.67
1:C:120:THR:HG22	1:C:125:GLN:HG2	1.76	0.67
1:B:346:LYS:O	1:B:349:SER:OG	2.12	0.67
1:B:158:LEU:HD13	1:B:165:TYR:CD2	2.30	0.67
2:F:51:GLN:N	2:F:51:GLN:OE1	2.28	0.67
1:B:86:PRO:HB2	1:B:107:LEU:HD11	1.76	0.67
2:M:199:ASN:OD1	2:M:200:THR:N	2.28	0.67
1:A:368:VAL:HG11	1:A:411:LEU:CD1	2.25	0.66
2:K:149:GLN:OE1	2:K:268:ILE:HG21	1.96	0.66
1:B:103:LEU:HD23	1:B:144:VAL:HG22	1.77	0.66
1:A:325:ASP:HB3	1:B:61:VAL:HG13	1.75	0.66
1:B:277:PHE:O	1:B:456:ASN:ND2	2.29	0.66
1:B:272:THR:O	1:B:307:ARG:NH2	2.28	0.66
1:B:360:GLN:N	1:B:360:GLN:OE1	2.29	0.66
1:C:522:LEU:HD21	1:C:749:PRO:CB	2.26	0.66
2:G:222:GLU:OE2	2:I:290:LYS:NZ	2.18	0.66
2:N:180:GLU:O	2:N:183:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD22	1:A:208:ILE:HG12	1.77	0.65
1:A:371:LEU:HD22	1:A:411:LEU:HD11	1.78	0.65
1:A:79:ASP:OD1	1:A:210:ARG:NH2	2.29	0.65
1:C:92:ILE:HD11	1:C:107:LEU:HB2	1.77	0.65
2:E:182:ASN:ND2	2:E:248:ASN:OD1	2.29	0.65
1:A:351:VAL:HG23	1:A:430:LEU:HD11	1.79	0.65
1:C:522:LEU:HD21	1:C:749:PRO:CG	2.26	0.64
1:B:500:GLU:OE2	2:F:109:LYS:NZ	2.19	0.64
1:C:118:THR:HG22	1:C:127:GLN:HG2	1.78	0.64
1:B:619:LEU:HD21	1:B:712:VAL:CG1	2.27	0.64
1:B:444:LEU:CD1	1:B:447:LEU:HD13	2.26	0.64
1:A:44:GLY:O	1:B:369:ARG:NH2	2.30	0.64
1:B:444:LEU:HD13	1:B:447:LEU:HD13	1.78	0.64
2:O:149:GLN:CD	2:O:268:ILE:HG21	2.17	0.64
2:D:211:ASP:OD1	2:D:213:THR:OG1	2.08	0.64
2:J:277:THR:HG22	2:J:279:PRO:HD3	1.80	0.63
1:A:158:LEU:HD21	1:A:178:GLU:HA	1.80	0.63
2:J:52:ASN:O	2:J:55:ILE:HG23	1.97	0.63
2:K:266:SER:HB3	2:L:268:ILE:HD11	1.80	0.63
2:P:134:TYR:O	2:P:313:ARG:NH1	2.31	0.63
2:H:170:ILE:CD1	2:H:239:VAL:HG22	2.27	0.63
1:B:291:TRP:HB2	1:B:339:VAL:HG13	1.79	0.63
2:L:51:GLN:N	2:L:51:GLN:OE1	2.32	0.63
2:L:164:LEU:HD23	2:L:250:LYS:CE	2.29	0.63
1:B:345:ILE:CG2	1:B:430:LEU:HD13	2.29	0.62
1:C:321:ASN:OD1	1:C:322:GLY:N	2.33	0.62
1:A:360:GLN:N	1:A:360:GLN:OE1	2.32	0.62
1:B:214:SER:O	1:B:217:THR:OG1	2.15	0.62
1:C:365:VAL:HG12	1:C:365:VAL:O	1.99	0.62
1:B:88:THR:O	1:B:107:LEU:HD13	1.98	0.62
1:B:159:LEU:HD12	1:B:180:GLN:HG2	1.81	0.62
1:B:292:SER:O	1:B:340:SER:OG	2.17	0.62
1:A:341:LYS:HD3	1:B:61:VAL:HG21	1.80	0.62
1:A:299:ALA:HB1	1:A:301:TYR:CE2	2.35	0.61
2:D:290:LYS:NZ	2:E:222:GLU:OE2	2.28	0.61
1:B:28:THR:O	1:C:321:ASN:ND2	2.33	0.61
2:H:277:THR:HG22	2:H:279:PRO:HD3	1.82	0.61
2:P:200:THR:OG1	2:P:201:GLN:OE1	2.16	0.61
1:A:86:PRO:CG	1:A:107:LEU:HD21	2.31	0.61
1:B:361:ALA:O	1:B:365:VAL:HG23	2.01	0.61
1:B:104:ALA:N	1:B:143:VAL:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:GLN:NE2	2:E:234:ASN:OD1	2.34	0.61
1:B:201:ALA:HB1	1:B:205:PHE:CE1	2.37	0.60
2:G:325:ARG:HG3	2:G:326:VAL:HG23	1.83	0.60
1:A:72:THR:HG21	1:A:333:LEU:CD1	2.32	0.60
2:I:158:LEU:HD22	2:I:224:LEU:HD11	1.82	0.60
1:A:273:ILE:HD12	1:A:375:LEU:HD21	1.81	0.60
1:B:346:LYS:N	1:B:349:SER:OG	2.34	0.60
1:B:370:SER:O	1:B:371:LEU:HD23	2.01	0.60
2:O:268:ILE:O	2:O:268:ILE:HG22	2.00	0.60
1:B:177:TYR:HE2	1:B:217:THR:HG22	1.67	0.60
1:B:111:ASN:ND2	1:B:135:GLN:O	2.34	0.60
1:B:568:LEU:HD12	1:C:523:LEU:HD22	1.84	0.59
2:L:136:ASP:OD1	2:L:315:ARG:NH1	2.32	0.59
2:H:149:GLN:CD	2:H:268:ILE:HG21	2.21	0.59
1:C:296:PHE:N	1:C:343:GLU:OE2	2.31	0.59
2:M:180:GLU:O	2:M:183:LYS:NZ	2.31	0.59
1:A:705:VAL:HG13	1:A:705:VAL:O	2.02	0.59
1:B:381:THR:OG1	1:B:457:ASN:ND2	2.35	0.59
2:M:139:VAL:HG22	2:M:310:MET:CE	2.32	0.59
1:B:307:ARG:NH1	1:B:357:ASP:OD2	2.35	0.59
1:B:108:ILE:HD12	1:B:139:LYS:HB3	1.85	0.59
1:B:568:LEU:CD1	1:C:523:LEU:HD22	2.32	0.59
1:C:92:ILE:HG22	1:C:93:VAL:HG23	1.85	0.58
2:D:149:GLN:OE1	2:D:268:ILE:HG21	2.03	0.58
1:A:414:GLN:HB3	1:B:410:THR:HG22	1.84	0.58
2:D:160:LEU:HD21	2:D:260:VAL:HG23	1.84	0.58
2:L:180:GLU:OE1	2:L:180:GLU:N	2.35	0.58
1:B:71:PRO:HA	1:B:201:ALA:HB3	1.86	0.58
2:L:164:LEU:HD23	2:L:250:LYS:HE2	1.86	0.58
2:E:180:GLU:O	2:E:183:LYS:NZ	2.35	0.58
2:G:135:CYS:O	2:G:257:ASN:ND2	2.35	0.58
1:A:73:THR:HG22	1:A:200:THR:HG22	1.85	0.58
1:C:64:LEU:N	1:C:229:ASN:O	2.36	0.58
1:C:632:ASN:O	1:C:636:ILE:HD12	2.04	0.58
1:A:714:ASP:OD1	1:B:750:ARG:NH1	2.36	0.58
1:A:589:SER:OG	1:B:519:ASP:OD2	2.21	0.58
2:L:201:GLN:O	2:L:202:THR:OG1	2.15	0.58
1:B:775:ARG:O	1:B:776:LEU:HB2	2.04	0.57
2:I:57:LEU:HD21	2:J:59:ILE:HG23	1.85	0.57
1:A:250:ALA:O	1:B:270:ASP:N	2.35	0.57
1:A:256:ILE:HD11	1:B:266:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HD21	1:A:749:PRO:CB	2.34	0.57
2:I:149:GLN:OE1	2:I:268:ILE:HG21	2.04	0.57
2:O:176:GLN:NE2	2:O:234:ASN:OD1	2.37	0.57
1:C:305:TYR:HH	1:C:355:TYR:HH	1.49	0.57
1:C:168:MET:SD	1:C:170:HIS:NE2	2.78	0.57
2:G:179:ASP:OD1	2:G:180:GLU:N	2.37	0.57
1:A:72:THR:HG21	1:A:333:LEU:HD11	1.86	0.57
1:B:10:LEU:HD12	1:B:624:MET:HE2	1.87	0.57
1:B:516:GLN:OE1	1:B:516:GLN:N	2.36	0.57
1:C:267:TYR:HB2	1:C:470:LEU:HD21	1.86	0.57
2:K:268:ILE:C	2:K:269:LEU:HD12	2.24	0.56
1:B:137:GLN:OE1	1:B:181:THR:OG1	2.23	0.56
2:K:81:LEU:HD13	2:K:307:ILE:HD11	1.87	0.56
1:A:172:GLU:O	1:A:194:TYR:OH	2.22	0.56
1:B:753:ARG:O	1:B:757:ASN:ND2	2.38	0.56
2:E:217:GLU:OE2	2:E:220:THR:OG1	2.18	0.56
2:M:170:ILE:HD13	2:M:239:VAL:HG12	1.86	0.56
1:C:730:LEU:HD23	1:C:736:ILE:HD11	1.86	0.56
2:H:274:ASP:OD1	2:H:276:THR:OG1	2.23	0.56
2:M:277:THR:HG22	2:M:279:PRO:HD3	1.88	0.56
1:C:237:SER:OG	1:C:417:ASP:OD1	2.22	0.56
2:I:166:ASN:OD1	2:J:315:ARG:NH2	2.38	0.56
2:M:288:ASN:ND2	2:N:153:SER:OG	2.39	0.56
1:B:84:LEU:HD21	1:B:205:PHE:CZ	2.41	0.56
1:A:584:ILE:CD1	1:A:615:ILE:HD11	2.35	0.56
1:B:81:TRP:HA	1:B:168:MET:HG2	1.87	0.56
1:B:116:ASN:OD1	1:B:129:THR:HG22	2.05	0.56
1:A:92:ILE:HD13	1:A:140:PHE:CD2	2.40	0.56
1:A:687:ASP:OD1	1:A:688:GLY:N	2.39	0.56
1:B:479:ASP:O	2:G:208:LEU:HD21	2.05	0.56
2:F:195:VAL:HG12	2:F:237:LEU:HD22	1.88	0.56
1:C:323:MET:SD	1:C:323:MET:N	2.72	0.56
1:C:468:PHE:HE1	1:C:470:LEU:HD22	1.70	0.56
2:L:149:GLN:OE1	2:L:268:ILE:HG21	2.05	0.56
2:O:195:VAL:HG12	2:O:237:LEU:HD23	1.87	0.56
1:B:101:ARG:NE	1:B:191:THR:OG1	2.38	0.55
2:H:313:ARG:NH2	2:P:166:ASN:OD1	2.37	0.55
1:C:83:LEU:HD21	1:C:216:CYS:SG	2.46	0.55
2:L:176:GLN:NE2	2:L:234:ASN:OD1	2.39	0.55
2:O:224:LEU:HD23	2:O:225:VAL:N	2.20	0.55
2:J:153:SER:OG	2:L:288:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:149:GLN:CD	2:M:268:ILE:HG21	2.26	0.55
1:B:329:ASN:OD1	1:B:338:VAL:HG13	2.07	0.55
2:I:277:THR:HG22	2:I:279:PRO:HD3	1.87	0.55
1:C:211:SER:OG	1:C:212:GLU:OE1	2.18	0.55
2:G:153:SER:OG	2:I:288:ASN:ND2	2.40	0.55
2:D:202:THR:O	2:D:202:THR:HG22	2.07	0.55
2:L:149:GLN:NE2	2:L:268:ILE:HD13	2.22	0.55
2:N:149:GLN:OE1	2:N:268:ILE:HG21	2.06	0.55
1:A:86:PRO:HG3	1:A:107:LEU:HD21	1.87	0.54
1:A:134:SER:OG	1:A:137:GLN:O	2.25	0.54
2:D:262:GLN:NE2	2:D:266:SER:O	2.39	0.54
1:B:86:PRO:CB	1:B:107:LEU:HD11	2.38	0.54
1:A:325:ASP:HB2	1:B:61:VAL:HG22	1.90	0.54
2:N:216:GLU:N	2:N:216:GLU:OE1	2.40	0.54
2:N:268:ILE:HG22	2:N:268:ILE:O	2.08	0.54
2:I:149:GLN:CD	2:I:268:ILE:HG21	2.27	0.54
1:A:19:SER:CB	1:A:546:THR:HG21	2.38	0.54
2:M:211:ASP:OD1	2:M:213:THR:OG1	2.21	0.54
1:A:381:THR:O	1:A:457:ASN:ND2	2.37	0.54
1:A:715:SER:HG	1:B:750:ARG:NH1	2.05	0.54
1:B:121:ILE:HG22	1:B:122:PHE:CD2	2.43	0.54
2:N:149:GLN:CD	2:N:268:ILE:HG21	2.28	0.54
1:A:101:ARG:NH2	1:A:192:THR:O	2.39	0.54
2:D:318:ASN:N	2:D:318:ASN:OD1	2.40	0.54
1:A:116:ASN:OD1	1:A:129:THR:HG22	2.08	0.53
1:A:66:ASP:O	1:A:290:LYS:NZ	2.24	0.53
1:A:404:LEU:HD22	1:A:428:PHE:CB	2.38	0.53
2:M:149:GLN:NE2	2:M:268:ILE:HD13	2.23	0.53
1:B:77:PRO:HG2	1:B:287:LEU:HD22	1.90	0.53
1:B:351:VAL:HG21	1:B:404:LEU:HD21	1.90	0.53
2:D:87:THR:HG23	2:D:122:THR:HA	1.91	0.53
2:M:323:TYR:O	2:M:324:TYR:CG	2.61	0.53
2:P:170:ILE:HD13	2:P:239:VAL:CG1	2.37	0.53
1:A:85:ALA:HB2	1:A:164:LEU:CD2	2.39	0.53
1:B:52:PRO:HB3	1:B:317:THR:HG21	1.90	0.53
1:A:410:THR:HG22	1:B:414:GLN:HG2	1.89	0.53
2:D:265:GLY:O	2:D:286:ARG:NH1	2.40	0.53
1:A:143:VAL:HG22	1:A:154:GLN:HG2	1.91	0.53
1:A:584:ILE:HD11	1:A:594:VAL:HG11	1.90	0.53
1:B:133:THR:OG1	1:B:159:LEU:HD11	2.09	0.53
2:F:95:ASP:OD1	2:F:96:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:158:LEU:HD22	2:O:224:LEU:HD11	1.91	0.53
1:B:103:LEU:HD23	1:B:144:VAL:CG2	2.39	0.53
1:B:277:PHE:N	1:B:456:ASN:OD1	2.41	0.53
2:J:286:ARG:HH12	2:K:268:ILE:HG23	1.74	0.53
2:O:149:GLN:OE1	2:O:268:ILE:HG21	2.09	0.53
1:A:341:LYS:HA	1:B:61:VAL:HG11	1.90	0.52
2:D:149:GLN:CD	2:D:268:ILE:HG21	2.30	0.52
2:H:201:GLN:O	2:H:202:THR:OG1	2.22	0.52
2:L:149:GLN:CD	2:L:268:ILE:HG21	2.29	0.52
2:I:170:ILE:HD13	2:I:239:VAL:HG22	1.91	0.52
1:A:72:THR:OG1	1:A:333:LEU:HD22	2.09	0.52
2:H:274:ASP:OD1	2:H:276:THR:N	2.41	0.52
2:J:276:THR:HG22	2:L:285:MET:CE	2.39	0.52
2:O:87:THR:HG22	2:O:120:GLU:OE2	2.08	0.52
1:B:101:ARG:NH1	1:B:174:LEU:HD11	2.25	0.52
2:H:144:TYR:HE1	2:H:268:ILE:HD12	1.75	0.52
1:B:73:THR:HG22	1:B:200:THR:CG2	2.38	0.52
1:B:92:ILE:HD11	1:B:107:LEU:HG	1.91	0.52
1:C:244:ILE:HG23	1:C:413:THR:HG21	1.91	0.52
1:B:108:ILE:HD11	1:B:141:ILE:HD12	1.91	0.52
1:B:388:SER:O	1:B:389:LEU:HD23	2.10	0.52
2:I:55:ILE:HD12	2:J:59:ILE:HG21	1.91	0.52
1:A:326:PHE:CZ	1:A:447:LEU:HD13	2.45	0.52
1:B:625:ALA:O	1:B:626:THR:OG1	2.28	0.51
1:C:512:ILE:HD11	1:C:771:ILE:CG2	2.40	0.51
1:A:345:ILE:N	1:A:450:LEU:O	2.43	0.51
2:E:149:GLN:OE1	2:E:268:ILE:HG21	2.10	0.51
2:N:170:ILE:CD1	2:N:239:VAL:HG22	2.38	0.51
1:C:619:LEU:HD11	1:C:712:VAL:HG21	1.92	0.51
1:A:256:ILE:HD11	1:B:471:ILE:HG12	1.91	0.51
1:A:325:ASP:CB	1:B:61:VAL:HG22	2.40	0.51
1:C:177:TYR:HD2	1:C:220:ILE:HD13	1.74	0.51
1:A:57:ASP:O	1:A:58:SER:OG	2.21	0.51
1:A:407:ALA:HB2	1:A:429:ARG:HG3	1.93	0.51
1:B:375:LEU:HD21	1:B:468:PHE:CZ	2.46	0.51
2:I:52:ASN:HB3	2:I:55:ILE:HD11	1.92	0.51
1:A:51:GLY:N	1:A:52:PRO:CD	2.73	0.51
2:F:222:GLU:HG2	2:F:225:VAL:HG22	1.92	0.51
1:A:93:VAL:HG13	1:A:201:ALA:HB2	1.93	0.51
1:A:164:LEU:HD12	1:A:223:GLY:HA2	1.93	0.51
1:A:339:VAL:HG13	1:A:342:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:VAL:HG11	1:A:448:TYR:HB3	1.92	0.51
1:A:568:LEU:HD12	1:B:523:LEU:HD13	1.93	0.50
1:C:468:PHE:CE1	1:C:470:LEU:HD22	2.45	0.50
1:A:411:LEU:HD12	1:B:415:PHE:CE1	2.46	0.50
2:O:220:THR:HG23	2:O:220:THR:O	2.10	0.50
1:A:351:VAL:CG2	1:A:430:LEU:HD11	2.41	0.50
2:E:157:ASP:OD1	2:E:161:ASN:ND2	2.44	0.50
2:J:182:ASN:ND2	2:J:248:ASN:OD1	2.39	0.50
1:B:158:LEU:HD13	1:B:165:TYR:CE2	2.45	0.50
2:P:124:ILE:H	2:P:124:ILE:HD12	1.76	0.50
1:C:126:GLU:OE1	1:C:152:ILE:HD12	2.10	0.50
1:B:190:SER:O	1:B:191:THR:HG23	2.12	0.50
1:B:294:ILE:HD12	1:B:342:PHE:CE1	2.46	0.50
1:C:512:ILE:HD11	1:C:771:ILE:HG21	1.94	0.50
2:D:133:LEU:HD13	2:D:258:VAL:CG1	2.26	0.50
1:A:59:THR:OG1	1:B:323:MET:O	2.08	0.50
1:A:345:ILE:HG23	1:A:430:LEU:HD13	1.92	0.50
1:A:369:ARG:N	1:A:471:ILE:O	2.42	0.50
1:B:455:PRO:O	1:B:462:TYR:OH	2.29	0.50
1:A:522:LEU:HD21	1:A:749:PRO:CG	2.42	0.50
1:B:158:LEU:HD11	1:B:177:TYR:O	2.12	0.50
2:D:153:SER:OG	2:F:288:ASN:ND2	2.45	0.50
1:A:74:PHE:CE1	1:A:333:LEU:HD13	2.47	0.49
1:A:159:LEU:HD12	1:A:180:GLN:HG2	1.94	0.49
1:B:289:TYR:CD2	1:B:389:LEU:HD22	2.47	0.49
1:B:437:PHE:N	1:B:447:LEU:O	2.29	0.49
1:C:470:LEU:HD23	1:C:470:LEU:H	1.77	0.49
1:A:21:GLU:O	1:A:25:ILE:HG23	2.12	0.49
1:C:675:VAL:HG11	1:C:711:LEU:HB3	1.94	0.49
2:H:266:SER:HB3	2:I:268:ILE:HD11	1.95	0.49
1:A:353:ILE:HD12	1:A:428:PHE:CE1	2.47	0.49
1:C:169:LYS:HZ3	1:C:197:VAL:CG1	2.25	0.49
1:C:283:LYS:NZ	1:C:388:SER:OG	2.31	0.49
2:P:184:TRP:CZ3	2:P:237:LEU:HD21	2.47	0.49
1:A:404:LEU:HD21	1:A:430:LEU:CD2	2.42	0.49
1:B:108:ILE:HD13	1:B:130:VAL:HG13	1.94	0.49
2:D:268:ILE:HG22	2:D:268:ILE:O	2.12	0.49
1:A:407:ALA:HB2	1:A:429:ARG:CG	2.42	0.49
1:C:714:ASP:OD1	1:C:715:SER:N	2.45	0.49
1:A:775:ARG:O	1:A:776:LEU:HB2	2.13	0.49
1:B:83:LEU:CD1	1:B:208:ILE:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HD12	1:B:254:ILE:H	1.77	0.49
1:C:3:SER:N	1:C:635:ASP:OD1	2.38	0.49
2:G:268:ILE:HG22	2:G:268:ILE:O	2.13	0.49
2:I:224:LEU:HD23	2:I:225:VAL:N	2.27	0.49
1:A:532:SER:OG	1:C:562:SER:OG	2.16	0.49
1:C:227:ILE:HD12	1:C:227:ILE:H	1.78	0.49
2:D:147:THR:C	2:D:148:LEU:HD12	2.33	0.49
2:J:281:THR:HG22	2:J:282:GLU:H	1.78	0.49
2:P:141:LEU:HD23	2:P:261:ILE:HB	1.94	0.49
1:A:108:ILE:HD11	1:A:141:ILE:HD12	1.95	0.49
1:A:414:GLN:CB	1:B:410:THR:HG22	2.43	0.49
2:G:88:GLU:N	2:G:88:GLU:OE1	2.46	0.49
1:A:289:TYR:OH	1:A:391:VAL:O	2.24	0.48
2:J:256:GLU:OE1	2:J:256:GLU:N	2.44	0.48
1:B:73:THR:CG2	1:B:200:THR:HG22	2.40	0.48
2:I:274:ASP:OD1	2:I:276:THR:OG1	2.28	0.48
1:B:371:LEU:HD11	1:B:411:LEU:HD11	1.95	0.48
1:A:134:SER:HB3	1:A:159:LEU:HD13	1.96	0.48
2:P:281:THR:HG22	2:P:282:GLU:N	2.28	0.48
1:A:73:THR:HG22	1:A:200:THR:CG2	2.44	0.48
1:C:79:ASP:HA	1:C:210:ARG:HE	1.79	0.48
2:N:149:GLN:NE2	2:N:268:ILE:HD13	2.28	0.48
2:N:202:THR:O	2:N:202:THR:HG22	2.14	0.48
2:E:281:THR:HG22	2:E:282:GLU:N	2.29	0.48
2:F:224:LEU:HD23	2:F:225:VAL:N	2.28	0.48
2:J:193:ILE:N	2:J:193:ILE:HD12	2.29	0.48
2:K:170:ILE:HD13	2:K:239:VAL:HG22	1.94	0.48
1:B:10:LEU:HD12	1:B:624:MET:CE	2.43	0.48
1:B:108:ILE:HG21	1:B:132:ASN:OD1	2.13	0.48
1:B:169:LYS:NZ	1:B:194:TYR:O	2.45	0.48
1:C:522:LEU:HD21	1:C:749:PRO:HB3	1.94	0.48
2:J:171:THR:HG23	2:J:172:LEU:HG	1.94	0.48
1:A:137:GLN:OE1	1:A:181:THR:OG1	2.32	0.48
1:B:84:LEU:HD13	1:B:92:ILE:HG21	1.96	0.48
1:B:320:VAL:HG22	1:B:351:VAL:HG22	1.96	0.48
2:F:157:ASP:OD1	2:F:161:ASN:ND2	2.45	0.48
1:B:400:GLY:HA3	1:B:437:PHE:CE2	2.48	0.48
2:G:157:ASP:OD1	2:G:161:ASN:ND2	2.47	0.48
2:N:144:TYR:CE1	2:N:268:ILE:HD12	2.49	0.48
2:N:55:ILE:HG22	2:N:56:ASN:N	2.29	0.47
1:B:308:ASP:OD1	1:B:308:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD12	1:B:421:LEU:N	2.29	0.47
2:K:170:ILE:CD1	2:K:239:VAL:HG22	2.44	0.47
2:L:104:GLN:O	2:L:108:THR:HG23	2.14	0.47
2:M:161:ASN:O	2:M:255:ARG:NH1	2.48	0.47
1:C:84:LEU:HD13	1:C:93:VAL:HG21	1.95	0.47
1:A:190:SER:O	1:A:191:THR:HG23	2.14	0.47
1:A:52:PRO:HG3	1:A:421:LEU:HD22	1.96	0.47
1:B:375:LEU:HD23	1:B:466:GLY:HA3	1.97	0.47
2:P:296:PHE:O	2:P:300:VAL:HG23	2.14	0.47
1:A:346:LYS:N	1:A:349:SER:OG	2.46	0.47
1:B:269:ARG:NH1	1:B:359:SER:OG	2.47	0.47
1:B:294:ILE:HG22	1:B:452:ALA:HB3	1.96	0.47
1:B:541:ALA:O	1:B:543:SER:N	2.44	0.47
2:H:247:ARG:NH2	2:P:134:TYR:OH	2.48	0.47
2:O:149:GLN:NE2	2:O:268:ILE:HD13	2.29	0.47
2:P:106:PHE:CE2	2:P:300:VAL:HG22	2.50	0.47
1:B:275:PHE:CE2	1:B:316:THR:HB	2.50	0.47
2:K:262:GLN:OE1	2:K:269:LEU:HD11	2.15	0.47
1:A:73:THR:CG2	1:A:200:THR:HG22	2.45	0.47
1:A:158:LEU:HD21	1:A:178:GLU:CA	2.43	0.47
1:B:55:ILE:HD13	1:B:319:SER:CB	2.45	0.47
1:C:379:MET:HG2	2:D:210:THR:HG21	1.97	0.47
2:D:144:TYR:HB3	2:D:264:GLY:HA3	1.97	0.47
1:C:522:LEU:HD21	1:C:749:PRO:HG2	1.95	0.47
1:A:108:ILE:CD1	1:A:141:ILE:HD12	2.45	0.46
1:A:396:VAL:HG12	1:A:397:LEU:N	2.30	0.46
2:G:201:GLN:O	2:G:202:THR:OG1	2.20	0.46
2:I:224:LEU:HD23	2:I:224:LEU:C	2.35	0.46
2:O:171:THR:O	2:O:171:THR:HG22	2.15	0.46
1:C:279:ASN:ND2	1:C:452:ALA:O	2.48	0.46
1:C:294:ILE:HD12	1:C:342:PHE:CZ	2.50	0.46
2:J:281:THR:HG22	2:J:282:GLU:N	2.30	0.46
2:N:193:ILE:HD12	2:N:193:ILE:N	2.31	0.46
2:F:87:THR:HG23	2:F:122:THR:HA	1.98	0.46
1:A:584:ILE:HG21	1:A:705:VAL:HG22	1.96	0.46
1:B:207:ILE:HD13	1:B:287:LEU:CD2	2.45	0.46
2:M:96:ASN:OD1	2:M:96:ASN:N	2.49	0.46
2:E:179:ASP:N	2:E:179:ASP:OD1	2.49	0.46
2:M:139:VAL:HG22	2:M:310:MET:HE1	1.97	0.46
1:B:508:LEU:HD11	1:B:648:SER:HB3	1.97	0.46
2:F:170:ILE:HG12	2:F:237:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:286:ARG:NH1	2:K:268:ILE:HG23	2.31	0.46
2:N:144:TYR:HE1	2:N:268:ILE:HD12	1.81	0.46
1:B:128:LEU:CD1	1:B:152:ILE:HG21	2.45	0.46
2:G:324:TYR:O	2:G:325:ARG:HB2	2.15	0.46
1:A:471:ILE:HG23	1:B:256:ILE:CD1	2.46	0.46
1:A:502:ARG:HD3	1:A:776:LEU:HD23	1.98	0.46
1:C:317:THR:HG22	1:C:414:GLN:OE1	2.16	0.46
2:J:169:ASP:OD1	2:J:171:THR:HG22	2.16	0.46
1:A:81:TRP:CE3	1:A:166:ALA:HB1	2.50	0.46
1:A:101:ARG:HH11	1:A:174:LEU:HD11	1.81	0.46
1:A:280:THR:HG22	1:A:297:LYS:HG3	1.97	0.46
2:F:313:ARG:NH2	2:G:54:GLY:O	2.44	0.46
2:J:170:ILE:CD1	2:J:239:VAL:HG22	2.46	0.46
2:M:100:ASP:N	2:M:100:ASP:OD1	2.49	0.46
1:C:107:LEU:HD21	1:C:138:TRP:CZ3	2.51	0.45
2:L:55:ILE:HG22	2:M:52:ASN:O	2.16	0.45
2:M:272:THR:OG1	2:M:277:THR:O	2.33	0.45
1:A:60:THR:HG22	1:A:293:GLU:OE1	2.16	0.45
1:B:158:LEU:HD22	1:B:165:TYR:HE2	1.80	0.45
1:B:584:ILE:HD13	1:B:611:GLN:HB3	1.98	0.45
2:P:183:LYS:NZ	2:P:228:ASP:OD1	2.45	0.45
1:C:161:SER:N	1:C:162:PRO:CD	2.80	0.45
1:C:320:VAL:HG21	1:C:345:ILE:CG2	2.39	0.45
2:F:220:THR:O	2:F:220:THR:HG23	2.16	0.45
1:B:411:LEU:HD13	1:B:424:LEU:HD22	1.98	0.45
2:N:171:THR:HG22	2:N:171:THR:O	2.17	0.45
1:A:81:TRP:HE3	1:A:166:ALA:HB1	1.82	0.45
1:A:584:ILE:HD11	1:A:594:VAL:CG1	2.46	0.45
1:C:267:TYR:CB	1:C:470:LEU:HD21	2.46	0.45
2:D:149:GLN:NE2	2:D:268:ILE:HD13	2.32	0.45
2:F:170:ILE:HG21	2:F:239:VAL:CG1	2.46	0.45
2:G:317:LEU:O	2:G:318:ASN:HB3	2.17	0.45
1:A:164:LEU:HD13	1:A:219:TYR:HB3	1.98	0.45
1:A:710:ASP:O	1:A:713:THR:HG22	2.17	0.45
2:F:306:ILE:HG22	2:F:310:MET:HE2	1.98	0.45
2:G:142:MET:CE	2:G:269:LEU:HD11	2.47	0.45
1:A:404:LEU:HD21	1:A:430:LEU:HG	1.99	0.45
1:B:213:GLU:O	1:B:217:THR:HG23	2.16	0.45
1:C:108:ILE:HD12	1:C:130:VAL:HG11	1.98	0.45
2:G:52:ASN:HB3	2:G:55:ILE:HD11	1.98	0.45
2:K:121:TYR:OH	2:K:141:LEU:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ALA:HB1	1:B:516:GLN:HG2	1.98	0.45
2:F:218:VAL:HG11	2:F:227:THR:HG23	1.99	0.45
2:G:149:GLN:NE2	2:G:268:ILE:HD13	2.31	0.45
2:H:87:THR:HG22	2:H:120:GLU:HG2	1.98	0.45
2:O:182:ASN:ND2	2:O:249:CYS:O	2.50	0.45
1:B:139:LYS:HG3	1:B:159:LEU:HD21	1.99	0.44
1:B:313:THR:OG1	1:B:358:ASP:OD2	2.34	0.44
1:B:368:VAL:HG23	1:B:472:SER:HB3	1.98	0.44
1:C:232:ASN:O	1:C:234:VAL:N	2.45	0.44
2:G:86:PRO:HA	2:G:121:TYR:O	2.17	0.44
2:I:281:THR:HG22	2:I:282:GLU:N	2.32	0.44
2:M:170:ILE:HD13	2:M:239:VAL:CG1	2.47	0.44
2:H:127:PHE:HD2	2:H:155:LEU:HD21	1.81	0.44
1:A:273:ILE:HD11	1:A:468:PHE:HZ	1.82	0.44
1:B:417:ASP:OD1	1:B:418:PHE:N	2.50	0.44
2:D:281:THR:HG22	2:D:282:GLU:N	2.32	0.44
2:E:263:VAL:HG12	2:E:289:TRP:CD1	2.53	0.44
2:K:277:THR:HG22	2:K:279:PRO:HD3	2.00	0.44
1:C:201:ALA:HB1	1:C:205:PHE:CZ	2.53	0.44
1:C:305:TYR:OH	1:C:355:TYR:OH	2.26	0.44
2:K:263:VAL:HG12	2:K:289:TRP:CD1	2.52	0.44
1:B:78:VAL:HG12	1:B:79:ASP:OD1	2.17	0.44
2:D:125:ALA:HB1	2:D:223:LYS:HG3	1.99	0.44
2:F:184:TRP:CZ3	2:F:237:LEU:HD21	2.53	0.44
2:L:220:THR:O	2:L:220:THR:HG22	3.39	0.44
2:M:144:TYR:HE1	2:M:268:ILE:HD12	1.82	0.44
1:A:345:ILE:CG2	1:A:430:LEU:HD13	2.47	0.44
1:B:366:VAL:HG12	1:B:367:TYR:CD1	2.53	0.44
1:B:655:THR:HG22	1:B:655:THR:O	2.17	0.44
1:C:174:LEU:HD12	1:C:191:THR:HG21	2.00	0.44
1:C:378:VAL:HG22	1:C:379:MET:N	2.33	0.44
1:A:201:ALA:HB3	1:A:205:PHE:CZ	2.53	0.44
1:C:227:ILE:HG21	1:C:298:PRO:CG	2.48	0.44
2:M:157:ASP:OD1	2:M:161:ASN:ND2	2.51	0.44
1:A:345:ILE:HG12	1:A:430:LEU:HD13	2.00	0.44
1:C:81:TRP:CZ3	1:C:166:ALA:HB1	2.52	0.44
1:C:518:ILE:HD12	1:C:631:MET:HE2	1.99	0.44
1:A:256:ILE:HD12	1:B:471:ILE:HG23	2.00	0.43
1:A:275:PHE:CZ	1:A:316:THR:HB	2.52	0.43
1:A:325:ASP:CB	1:B:61:VAL:HG13	2.47	0.43
1:A:707:LYS:O	1:A:711:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD11	1:B:174:LEU:HD13	2.00	0.43
2:K:306:ILE:HG22	2:K:310:MET:HE2	1.98	0.43
1:A:584:ILE:HD13	1:A:611:GLN:HB3	1.99	0.43
1:A:498:LEU:O	1:A:502:ARG:HG3	2.17	0.43
2:I:105:LEU:O	2:I:108:THR:OG1	2.27	0.43
2:L:164:LEU:HD23	2:L:250:LYS:HE3	2.00	0.43
1:A:92:ILE:HG22	1:A:93:VAL:HG23	2.00	0.43
1:A:280:THR:CG2	1:A:297:LYS:HG3	2.47	0.43
1:A:291:TRP:HE1	1:A:389:LEU:HD21	1.83	0.43
1:A:471:ILE:HG23	1:B:256:ILE:HD12	1.99	0.43
1:B:656:ILE:N	1:B:657:PRO:HD2	2.33	0.43
2:O:130:ASP:OD1	2:O:132:GLN:NE2	2.49	0.43
1:A:2:ALA:O	1:A:5:ILE:HG22	2.19	0.43
1:B:55:ILE:HD13	1:B:319:SER:HB3	2.01	0.43
1:C:177:TYR:CE1	1:C:186:THR:HG22	2.53	0.43
2:J:136:ASP:O	2:J:257:ASN:OD1	2.37	0.43
2:N:133:LEU:HD13	2:N:258:VAL:HG21	2.00	0.43
1:A:5:ILE:HG23	1:A:6:TYR:N	2.34	0.43
1:A:280:THR:HB	1:A:282:ILE:HD11	2.00	0.43
1:B:404:LEU:HD22	1:B:428:PHE:HB2	2.01	0.43
1:B:460:GLU:O	1:B:461:TYR:CG	2.71	0.43
1:C:101:ARG:HD2	1:C:191:THR:HG22	2.01	0.43
2:K:202:THR:O	2:K:202:THR:HG22	2.18	0.43
1:A:168:MET:SD	1:A:170:HIS:CE1	3.12	0.43
1:B:569:SER:O	1:B:573:SER:OG	2.29	0.43
1:C:78:VAL:HG12	1:C:79:ASP:N	2.33	0.43
1:C:232:ASN:OD1	1:C:232:ASN:N	2.51	0.43
1:B:584:ILE:HD11	1:B:594:VAL:CG1	2.49	0.43
2:F:154:GLU:HB3	2:F:224:LEU:HD22	2.01	0.43
2:N:79:SER:O	2:N:115:SER:OG	2.36	0.43
1:A:345:ILE:O	1:A:449:GLY:HA3	2.19	0.42
1:A:368:VAL:HG13	1:B:415:PHE:CZ	2.54	0.42
1:A:419:VAL:HG12	1:A:420:SER:N	2.34	0.42
2:O:195:VAL:HG12	2:O:237:LEU:CD2	2.49	0.42
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.86	0.42
1:C:368:VAL:O	1:C:537:THR:HG22	2.18	0.42
2:O:201:GLN:O	2:O:202:THR:OG1	2.27	0.42
1:A:272:THR:HG1	1:A:305:TYR:HD2	1.63	0.42
1:B:84:LEU:O	1:B:164:LEU:HD23	2.19	0.42
1:C:555:SER:CB	1:C:661:THR:HG23	2.48	0.42
2:G:87:THR:HG22	2:G:120:GLU:CD	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:263:VAL:HG12	2:J:287:ILE:HD11	2.01	0.42
2:L:52:ASN:O	2:L:55:ILE:HG23	2.19	0.42
2:L:186:SER:OG	2:L:193:ILE:HD11	2.18	0.42
1:A:169:LYS:O	1:A:170:HIS:ND1	2.53	0.42
1:B:275:PHE:CE2	1:B:353:ILE:CG2	3.02	0.42
2:K:288:ASN:ND2	2:L:153:SER:OG	2.52	0.42
1:B:97:ASN:CG	1:B:197:VAL:HG22	2.40	0.42
1:C:365:VAL:O	1:C:365:VAL:CG1	2.66	0.42
1:C:537:THR:HG22	1:C:538:ILE:H	1.84	0.42
2:G:193:ILE:HD12	2:G:239:VAL:HG22	2.01	0.42
2:K:281:THR:HG22	2:K:282:GLU:N	2.34	0.42
2:O:147:THR:O	2:O:147:THR:HG22	2.19	0.42
1:A:120:THR:HG22	1:A:125:GLN:HG2	2.00	0.42
1:B:264:GLU:OE2	1:B:369:ARG:NE	2.52	0.42
1:C:511:GLU:N	1:C:511:GLU:OE1	2.52	0.42
2:I:154:GLU:HB3	2:I:224:LEU:HD22	2.02	0.42
2:N:182:ASN:OD1	2:N:183:LYS:N	2.53	0.42
1:A:52:PRO:HG3	1:A:421:LEU:HB3	2.01	0.42
1:B:69:TYR:HB2	1:B:205:PHE:HB2	2.02	0.42
1:B:488:VAL:HA	1:C:432:VAL:HG23	2.00	0.42
1:C:108:ILE:CD1	1:C:130:VAL:HG11	2.50	0.42
1:C:628:THR:HG22	1:C:717:VAL:HG23	2.01	0.42
2:D:160:LEU:HD23	2:D:258:VAL:HG23	2.01	0.42
2:F:143:LYS:HA	2:F:263:VAL:HG22	2.02	0.42
2:K:272:THR:HG22	2:K:274:ASP:H	1.83	0.42
1:B:501:LEU:HD21	1:B:659:ILE:HD11	2.02	0.42
2:J:263:VAL:O	2:J:263:VAL:HG23	2.19	0.42
2:L:82:CYS:N	2:L:135:CYS:SG	2.93	0.42
2:M:149:GLN:OE1	2:M:268:ILE:HG21	2.20	0.42
2:P:272:THR:HG23	2:P:272:THR:O	4.00	0.42
1:A:111:ASN:ND2	1:A:135:GLN:O	2.53	0.42
1:B:767:ILE:O	1:B:771:ILE:HG12	2.19	0.42
1:C:419:VAL:HG22	1:C:420:SER:N	2.35	0.42
2:P:202:THR:O	2:P:202:THR:HG22	2.20	0.42
1:A:457:ASN:OD1	1:A:457:ASN:N	2.53	0.42
1:C:81:TRP:CH2	1:C:177:TYR:CE1	3.08	0.42
2:H:217:GLU:OE2	2:H:220:THR:OG1	2.22	0.42
2:I:55:ILE:HD13	2:J:59:ILE:HD13	2.02	0.42
2:I:130:ASP:OD1	2:I:132:GLN:NE2	2.52	0.42
2:L:263:VAL:O	2:L:263:VAL:HG23	2.20	0.42
2:N:199:ASN:OD1	2:N:203:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:263:VAL:HG12	2:N:289:TRP:CD1	2.55	0.42
1:C:169:LYS:HZ3	1:C:197:VAL:HG12	1.84	0.41
1:C:407:ALA:O	1:C:427:ARG:NH2	2.52	0.41
2:E:286:ARG:NH1	2:F:268:ILE:HG23	2.35	0.41
2:K:84:TYR:OH	2:K:133:LEU:HA	2.20	0.41
1:A:407:ALA:HB3	1:A:427:ARG:O	2.19	0.41
1:B:101:ARG:HH11	1:B:174:LEU:HD11	1.84	0.41
1:B:120:THR:HG22	1:B:125:GLN:HG2	2.01	0.41
1:B:396:VAL:N	1:B:440:THR:OG1	2.45	0.41
1:B:643:THR:HG22	1:B:647:LYS:HE2	2.02	0.41
2:K:104:GLN:O	2:K:108:THR:HG23	2.21	0.41
2:N:87:THR:HG23	2:N:122:THR:HA	2.01	0.41
2:P:82:CYS:N	2:P:135:CYS:SG	2.93	0.41
1:A:85:ALA:HB2	1:A:164:LEU:HD23	2.01	0.41
1:B:83:LEU:HD12	1:B:208:ILE:HD12	2.01	0.41
1:B:208:ILE:CG2	1:B:212:GLU:HB2	2.50	0.41
1:B:354:ASP:OD1	1:B:354:ASP:N	2.51	0.41
1:B:411:LEU:HD22	1:B:424:LEU:CD2	2.46	0.41
1:B:526:ASP:OD1	1:B:526:ASP:N	2.52	0.41
1:B:534:ILE:HG22	1:B:535:LYS:N	2.36	0.41
1:C:81:TRP:CD2	1:C:168:MET:CG	3.03	0.41
2:D:124:ILE:HD11	2:D:143:LYS:O	2.19	0.41
2:D:186:SER:OG	2:D:193:ILE:HD11	2.20	0.41
2:F:256:GLU:OE1	2:F:256:GLU:N	2.50	0.41
2:L:134:TYR:HB3	2:M:167:PRO:HG3	2.02	0.41
2:L:237:LEU:HD12	2:L:237:LEU:N	2.35	0.41
1:B:76:PRO:HA	1:B:77:PRO:HD3	1.97	0.41
1:C:96:THR:HG21	1:C:102:TRP:CE3	2.56	0.41
1:C:201:ALA:HB1	1:C:205:PHE:CE1	2.55	0.41
1:C:284:SER:OG	1:C:290:LYS:O	2.35	0.41
2:E:124:ILE:HD11	2:E:142:MET:HG2	2.02	0.41
2:N:191:CYS:SG	2:N:193:ILE:HD11	2.60	0.41
1:A:412:SER:HA	1:B:412:SER:HA	2.03	0.41
1:B:207:ILE:HD13	1:B:287:LEU:HD21	2.01	0.41
2:F:52:ASN:O	2:F:55:ILE:HG23	2.20	0.41
2:H:191:CYS:SG	2:H:193:ILE:HD11	2.60	0.41
2:K:244:CYS:SG	2:K:245:THR:N	2.93	0.41
2:N:147:THR:C	2:N:148:LEU:HD12	2.40	0.41
1:A:268:ASN:OD1	1:B:254:ILE:HD11	2.20	0.41
1:A:294:ILE:HD12	1:A:342:PHE:CZ	2.55	0.41
1:A:402:VAL:HG11	1:A:430:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.95	0.41
1:C:518:ILE:HG21	1:C:753:ARG:HG3	2.03	0.41
1:C:534:ILE:HG23	1:C:534:ILE:O	2.20	0.41
2:H:86:PRO:HA	2:H:121:TYR:O	2.21	0.41
2:I:57:LEU:HD11	2:J:59:ILE:CG2	2.51	0.41
2:L:89:ALA:O	2:L:93:ILE:HG12	2.21	0.41
1:A:278:ALA:HB2	1:A:299:ALA:HB2	2.03	0.41
1:A:501:LEU:HD21	1:A:651:ILE:HD12	2.03	0.41
1:B:649:THR:HG22	1:B:649:THR:O	2.21	0.41
2:F:149:GLN:CD	2:F:268:ILE:HG21	2.40	0.41
2:G:263:VAL:HG22	2:G:289:TRP:CD1	2.55	0.41
2:L:124:ILE:HD11	2:L:142:MET:HG2	2.02	0.41
2:P:306:ILE:HG22	2:P:310:MET:HE2	2.02	0.41
1:A:166:ALA:HB3	1:A:177:TYR:CD1	2.55	0.41
1:A:256:ILE:CD1	1:B:471:ILE:HG23	2.51	0.41
1:B:351:VAL:CG2	1:B:430:LEU:HD11	2.47	0.41
1:B:355:TYR:CD1	1:B:355:TYR:N	2.88	0.41
2:J:170:ILE:HD13	2:J:239:VAL:HG22	2.03	0.41
1:A:31:GLN:HB3	1:B:35:ILE:HD13	2.03	0.41
1:A:64:LEU:C	1:A:65:LEU:HD23	2.42	0.41
1:A:294:ILE:HD12	1:A:342:PHE:CE2	2.56	0.41
1:A:388:SER:O	1:A:389:LEU:HD23	2.20	0.41
1:B:134:SER:OG	1:B:159:LEU:HD22	2.21	0.41
1:B:383:GLY:N	1:B:457:ASN:OD1	2.54	0.41
1:B:582:ARG:O	1:B:594:VAL:HG22	2.21	0.41
1:B:651:ILE:HG22	1:B:652:SER:N	2.35	0.41
1:C:281:ILE:N	1:C:281:ILE:HD12	2.36	0.41
2:L:255:ARG:NH2	2:L:321:ALA:O	2.50	0.41
1:C:203:CYS:O	1:C:205:PHE:CZ	2.74	0.41
2:E:281:THR:HG22	2:E:282:GLU:H	1.85	0.41
2:O:86:PRO:HA	2:O:121:TYR:O	2.21	0.41
1:A:266:GLN:HB3	1:B:254:ILE:HD12	2.02	0.40
1:A:341:LYS:CB	1:B:61:VAL:HG11	2.51	0.40
1:B:606:SER:O	1:B:609:SER:OG	2.29	0.40
1:C:81:TRP:CD2	1:C:168:MET:HG3	2.56	0.40
2:E:93:ILE:HG23	2:E:293:TRP:NE1	2.36	0.40
2:F:158:LEU:HD22	2:F:224:LEU:HD11	2.03	0.40
1:A:177:TYR:OH	1:A:217:THR:HG23	2.21	0.40
1:B:101:ARG:HD3	1:B:174:LEU:HD11	2.04	0.40
2:I:84:TYR:CZ	2:I:133:LEU:HD22	2.56	0.40
2:N:296:PHE:O	2:N:300:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:187:MET:HG2	2:P:224:LEU:HD13	2.03	0.40
1:A:726:THR:HG21	1:A:766:ARG:HB2	2.03	0.40
1:B:27:SER:O	1:C:352:TYR:OH	2.38	0.40
1:B:106:ILE:HG22	1:B:107:LEU:N	2.37	0.40
1:B:271:ILE:HD12	1:B:468:PHE:CD1	2.57	0.40
1:B:421:LEU:HD12	1:B:421:LEU:H	1.86	0.40
1:B:775:ARG:O	1:B:776:LEU:CB	2.67	0.40
2:H:104:GLN:O	2:H:108:THR:HG23	2.21	0.40
2:I:193:ILE:N	2:I:193:ILE:HD12	2.36	0.40
2:J:133:LEU:HD13	2:J:258:VAL:HG21	2.03	0.40
1:A:60:THR:HG21	1:A:282:ILE:HD13	2.04	0.40
1:A:161:SER:N	1:A:162:PRO:CD	2.84	0.40
1:A:271:ILE:HG23	1:A:307:ARG:CZ	2.52	0.40
1:A:522:LEU:HD21	1:A:749:PRO:HG2	2.02	0.40
1:B:5:ILE:HG23	1:B:6:TYR:N	2.35	0.40
1:B:50:TRP:HB3	1:B:356:TRP:CE3	2.56	0.40
1:B:367:TYR:CD1	1:B:367:TYR:N	2.89	0.40
1:C:302:GLN:OE1	1:C:302:GLN:N	2.55	0.40
2:K:192:THR:O	2:K:239:VAL:HA	2.21	0.40
2:N:93:ILE:HG23	2:N:293:TRP:CE2	2.55	0.40
1:A:775:ARG:HG3	1:A:776:LEU:N	2.36	0.40
1:B:15:THR:O	1:B:15:THR:HG22	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 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	718/776 (92%)	653 (91%)	65 (9%)	0	100	100
1	B	738/776 (95%)	684 (93%)	54 (7%)	0	100	100
1	C	680/776 (88%)	646 (95%)	34 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	258/326 (79%)	248 (96%)	10 (4%)	0	100	100
2	E	240/326 (74%)	234 (98%)	6 (2%)	0	100	100
2	F	263/326 (81%)	255 (97%)	8 (3%)	0	100	100
2	G	264/326 (81%)	253 (96%)	11 (4%)	0	100	100
2	H	238/326 (73%)	230 (97%)	8 (3%)	0	100	100
2	I	260/326 (80%)	252 (97%)	8 (3%)	0	100	100
2	J	261/326 (80%)	253 (97%)	8 (3%)	0	100	100
2	K	252/326 (77%)	241 (96%)	11 (4%)	0	100	100
2	L	261/326 (80%)	257 (98%)	4 (2%)	0	100	100
2	M	263/326 (81%)	251 (95%)	12 (5%)	0	100	100
2	N	259/326 (79%)	248 (96%)	11 (4%)	0	100	100
2	O	261/326 (80%)	253 (97%)	8 (3%)	0	100	100
2	P	238/326 (73%)	230 (97%)	8 (3%)	0	100	100
3	d	395/397 (100%)	383 (97%)	12 (3%)	0	100	100
3	e	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	f	395/397 (100%)	384 (97%)	11 (3%)	0	100	100
3	g	395/397 (100%)	379 (96%)	16 (4%)	0	100	100
3	h	395/397 (100%)	376 (95%)	19 (5%)	0	100	100
3	i	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	j	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	k	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	l	395/397 (100%)	373 (94%)	22 (6%)	0	100	100
3	m	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	n	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	o	395/397 (100%)	376 (95%)	19 (5%)	0	100	100
3	p	395/397 (100%)	378 (96%)	17 (4%)	0	100	100
4	q	765/882 (87%)	742 (97%)	23 (3%)	0	100	100
4	r	791/882 (90%)	762 (96%)	29 (4%)	0	100	100
All	All	12145/13491 (90%)	11629 (96%)	516 (4%)	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 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	642/689 (93%)	627 (98%)	15 (2%)	50 78
1	B	659/689 (96%)	640 (97%)	19 (3%)	42 71
1	C	613/689 (89%)	601 (98%)	12 (2%)	55 81
2	D	235/296 (79%)	231 (98%)	4 (2%)	60 84
2	E	221/296 (75%)	219 (99%)	2 (1%)	78 92
2	F	239/296 (81%)	235 (98%)	4 (2%)	60 84
2	G	240/296 (81%)	237 (99%)	3 (1%)	69 87
2	H	219/296 (74%)	215 (98%)	4 (2%)	59 83
2	I	238/296 (80%)	236 (99%)	2 (1%)	81 93
2	J	238/296 (80%)	235 (99%)	3 (1%)	69 87
2	K	231/296 (78%)	229 (99%)	2 (1%)	78 92
2	L	238/296 (80%)	235 (99%)	3 (1%)	69 87
2	M	239/296 (81%)	236 (99%)	3 (1%)	69 87
2	N	237/296 (80%)	236 (100%)	1 (0%)	91 97
2	O	238/296 (80%)	236 (99%)	2 (1%)	81 93
2	P	219/296 (74%)	218 (100%)	1 (0%)	88 96
3	d	351/351 (100%)	347 (99%)	4 (1%)	73 90
3	e	351/351 (100%)	346 (99%)	5 (1%)	67 86
3	f	351/351 (100%)	348 (99%)	3 (1%)	78 92
3	g	351/351 (100%)	348 (99%)	3 (1%)	78 92
3	h	351/351 (100%)	346 (99%)	5 (1%)	67 86
3	i	351/351 (100%)	346 (99%)	5 (1%)	67 86
3	j	351/351 (100%)	349 (99%)	2 (1%)	86 95
3	k	351/351 (100%)	346 (99%)	5 (1%)	67 86
3	l	351/351 (100%)	350 (100%)	1 (0%)	92 98
3	m	351/351 (100%)	345 (98%)	6 (2%)	60 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	n	351/351 (100%)	346 (99%)	5 (1%)	67 86
3	o	351/351 (100%)	345 (98%)	6 (2%)	60 84
3	p	351/351 (100%)	346 (99%)	5 (1%)	67 86
4	q	698/809 (86%)	688 (99%)	10 (1%)	67 86
4	r	724/809 (90%)	710 (98%)	14 (2%)	57 82
All	All	10931/12096 (90%)	10772 (98%)	159 (2%)	66 86

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	96	THR
1	A	107	LEU
1	A	168	MET
1	A	275	PHE
1	A	354	ASP
1	A	437	PHE
1	A	454	ASP
1	A	457	ASN
1	A	470	LEU
1	A	577	ARG
1	A	620	ARG
1	A	647	LYS
1	A	674	ARG
1	A	776	LEU
1	B	72	THR
1	B	77	PRO
1	B	169	LYS
1	B	206	TYR
1	B	254	ILE
1	B	297	LYS
1	B	308	ASP
1	B	318	CYS
1	B	354	ASP
1	B	364	ASN
1	B	385	TYR
1	B	448	TYR
1	B	454	ASP
1	B	535	LYS
1	B	538	ILE

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Mol	Chain	Res	Type
1	B	573	SER
1	B	582	ARG
1	B	620	ARG
1	B	654	ASN
1	C	107	LEU
1	C	154	GLN
1	C	170	HIS
1	C	186	THR
1	C	232	ASN
1	C	323	MET
1	C	324	ASN
1	C	439	LEU
1	C	505	PHE
1	C	620	ARG
1	C	670	ASN
1	C	712	VAL
2	D	134	TYR
2	D	266	SER
2	D	315	ARG
2	D	318	ASN
2	E	135	CYS
2	E	182	ASN
2	F	59	ILE
2	F	63	MET
2	F	151	ASP
2	F	313	ARG
2	G	133	LEU
2	G	134	TYR
2	G	182	ASN
2	H	99	LYS
2	H	135	CYS
2	H	186	SER
2	H	289	TRP
2	I	135	CYS
2	I	186	SER
2	J	182	ASN
2	J	239	VAL
2	J	282	GLU
2	K	166	ASN
2	K	256	GLU
2	L	182	ASN
2	L	266	SER

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Mol	Chain	Res	Type
2	L	267	ASP
2	M	96	ASN
2	M	135	CYS
2	M	182	ASN
2	N	317	LEU
2	O	135	CYS
2	O	311	SER
2	P	182	ASN
3	d	129	PHE
3	d	156	ASN
3	d	242	ASP
3	d	374	TYR
3	e	60	ASN
3	e	129	PHE
3	e	143	ASN
3	e	156	ASN
3	e	374	TYR
3	f	60	ASN
3	f	129	PHE
3	f	374	TYR
3	g	60	ASN
3	g	187	GLU
3	g	374	TYR
3	h	129	PHE
3	h	154	LYS
3	h	156	ASN
3	h	307	LEU
3	h	374	TYR
3	i	128	ASN
3	i	129	PHE
3	i	170	GLN
3	i	283	ARG
3	i	334	VAL
3	j	60	ASN
3	j	129	PHE
3	k	156	ASN
3	k	170	GLN
3	k	264	LEU
3	k	370	LEU
3	k	374	TYR
3	l	129	PHE
3	m	93	ASP

Continued on next page...

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Mol	Chain	Res	Type
3	m	129	PHE
3	m	142	GLN
3	m	145	ARG
3	m	156	ASN
3	m	189	GLN
3	n	60	ASN
3	n	129	PHE
3	n	296	ARG
3	n	325	ARG
3	n	374	TYR
3	o	1	MET
3	o	70	LEU
3	o	129	PHE
3	o	156	ASN
3	o	370	LEU
3	o	374	TYR
3	p	128	ASN
3	p	129	PHE
3	p	274	GLN
3	p	310	ASN
3	p	374	TYR
4	q	143	ARG
4	q	200	VAL
4	q	271	PHE
4	q	395	ASP
4	q	521	MET
4	q	536	LEU
4	q	550	LEU
4	q	698	LYS
4	q	827	LYS
4	q	878	ASN
4	r	157	ASP
4	r	214	ASP
4	r	266	ASN
4	r	352	ASP
4	r	483	VAL
4	r	497	ILE
4	r	528	SER
4	r	686	LEU
4	r	717	MET
4	r	718	TYR
4	r	722	ASN

Continued on next page...

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Mol	Chain	Res	Type
4	r	799	LEU
4	r	854	LEU
4	r	867	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
2	F	51	GLN
2	F	288	ASN
2	J	235	HIS
2	L	56	ASN
2	L	288	ASN
2	N	288	ASN
3	m	173	HIS
3	m	189	GLN

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

Of 44 ligands modelled in this entry, 44 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.

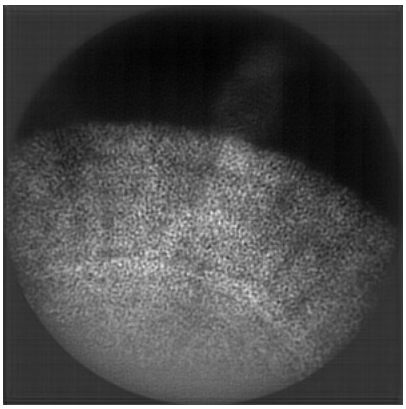
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16146. These allow visual inspection of the internal detail of the map and identification of artifacts.

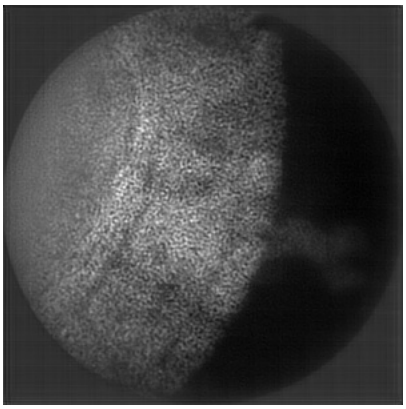
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

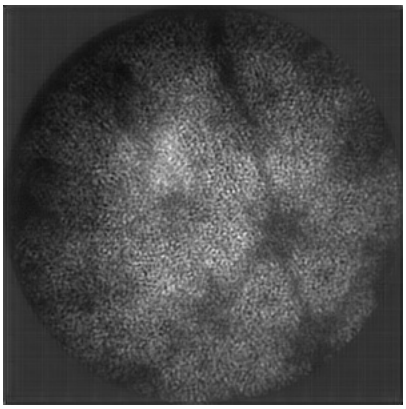
6.1.1 Primary map



X

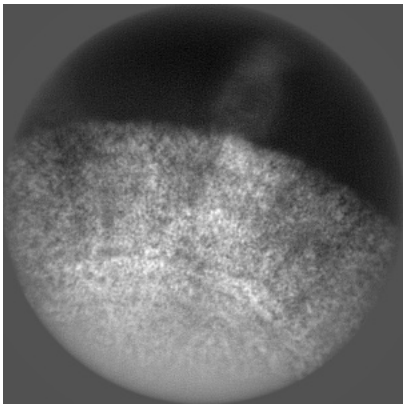


Y

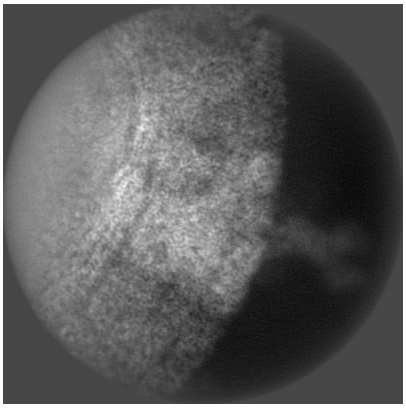


Z

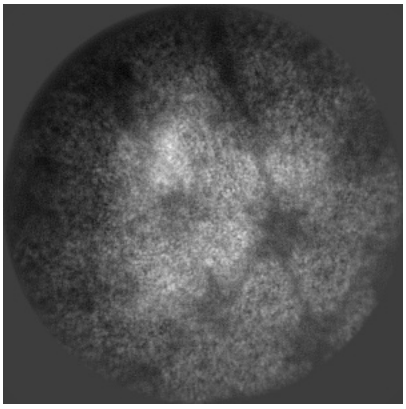
6.1.2 Raw map



X



Y

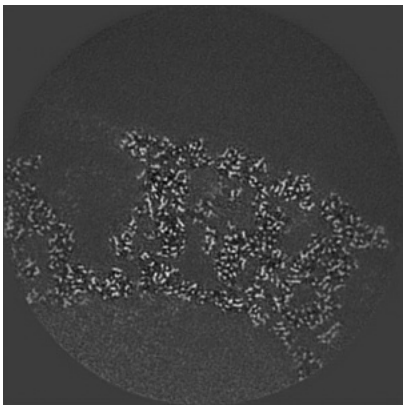


Z

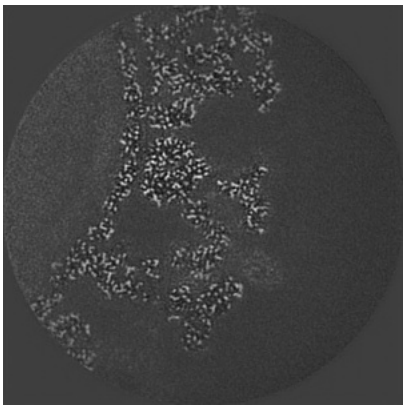
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

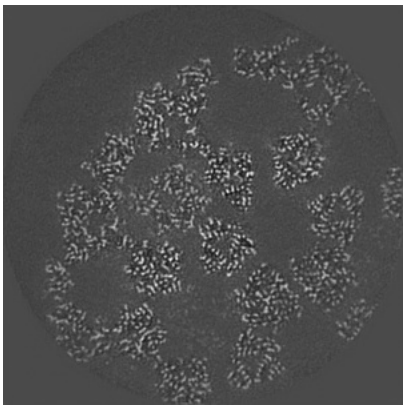
6.2.1 Primary map



X Index: 224

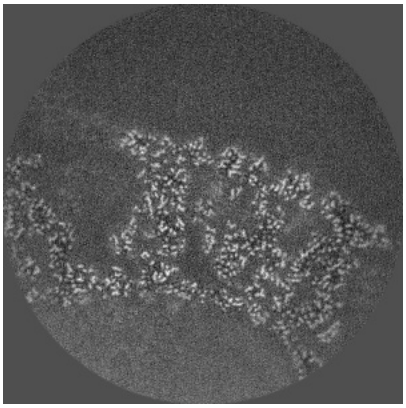


Y Index: 224

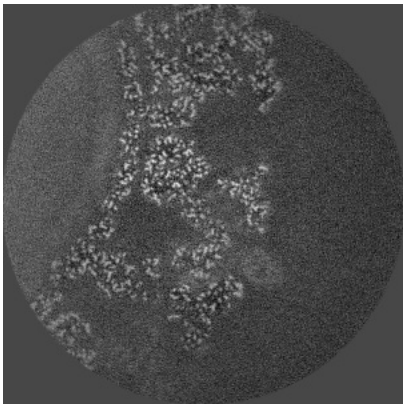


Z Index: 224

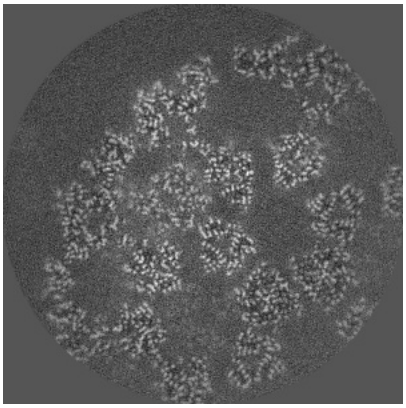
6.2.2 Raw map



X Index: 224



Y Index: 224

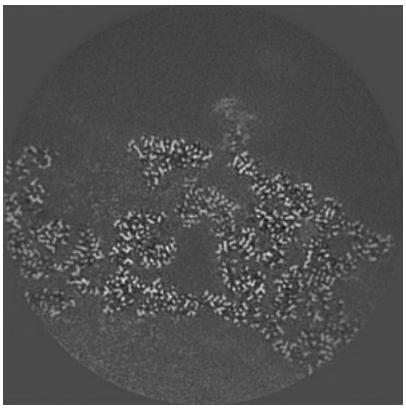


Z Index: 224

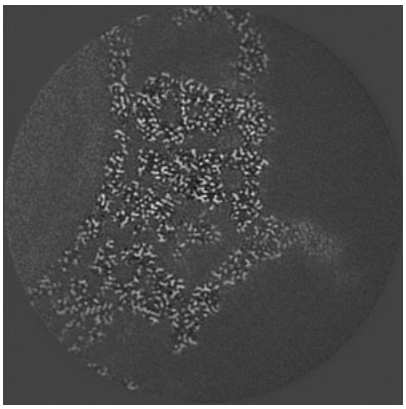
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

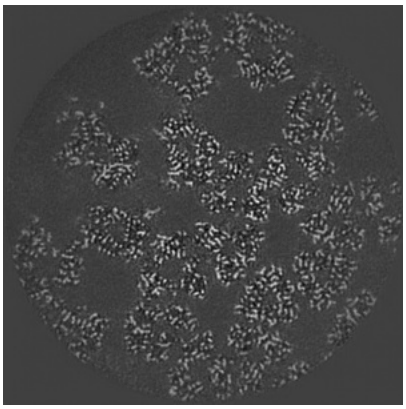
6.3.1 Primary map



X Index: 205

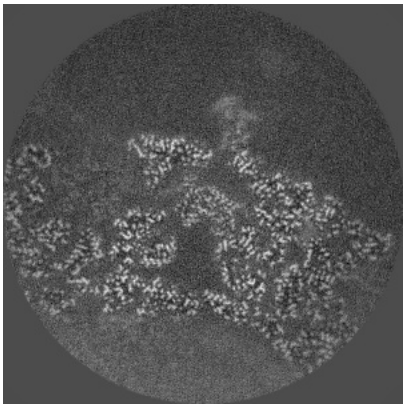


Y Index: 261

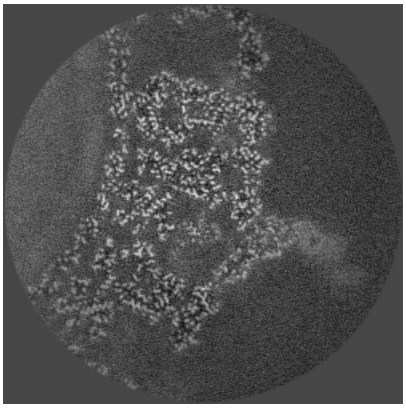


Z Index: 183

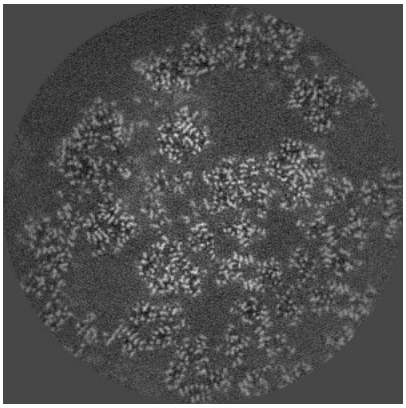
6.3.2 Raw map



X Index: 205



Y Index: 262

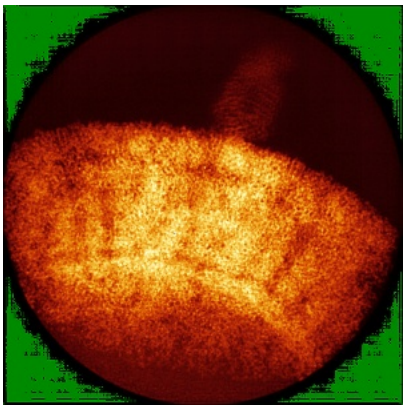


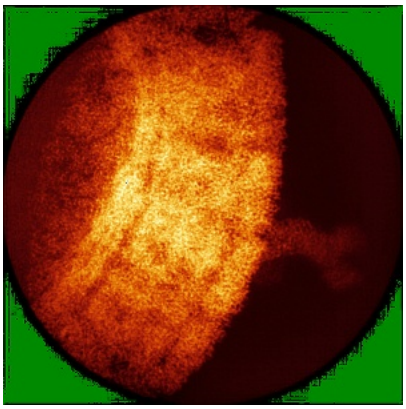
Z Index: 200

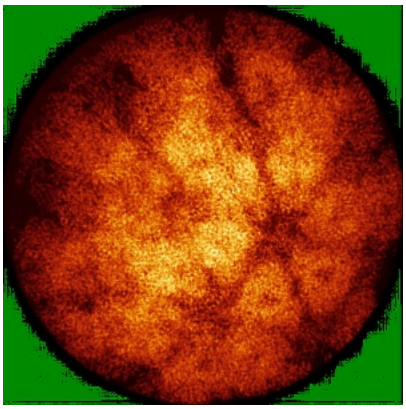
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

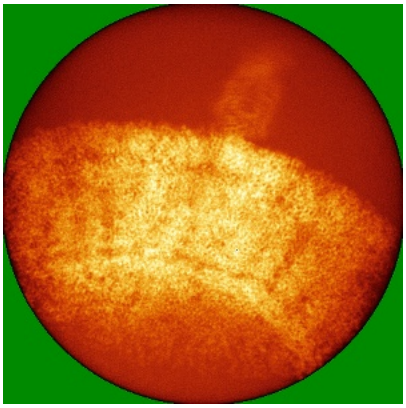
6.4.1 Primary map

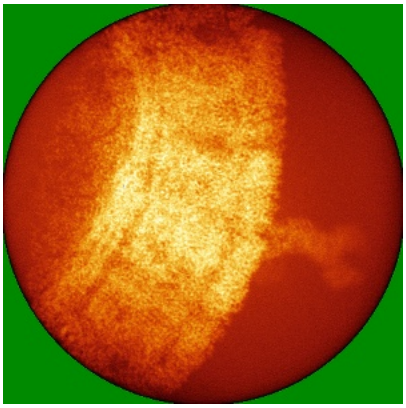

X

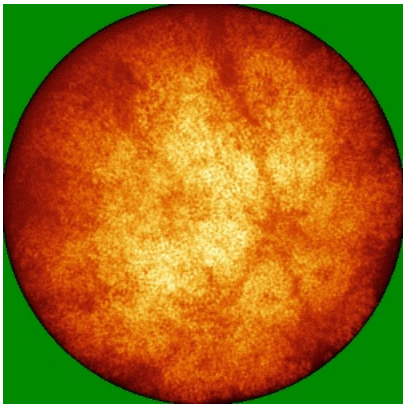

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

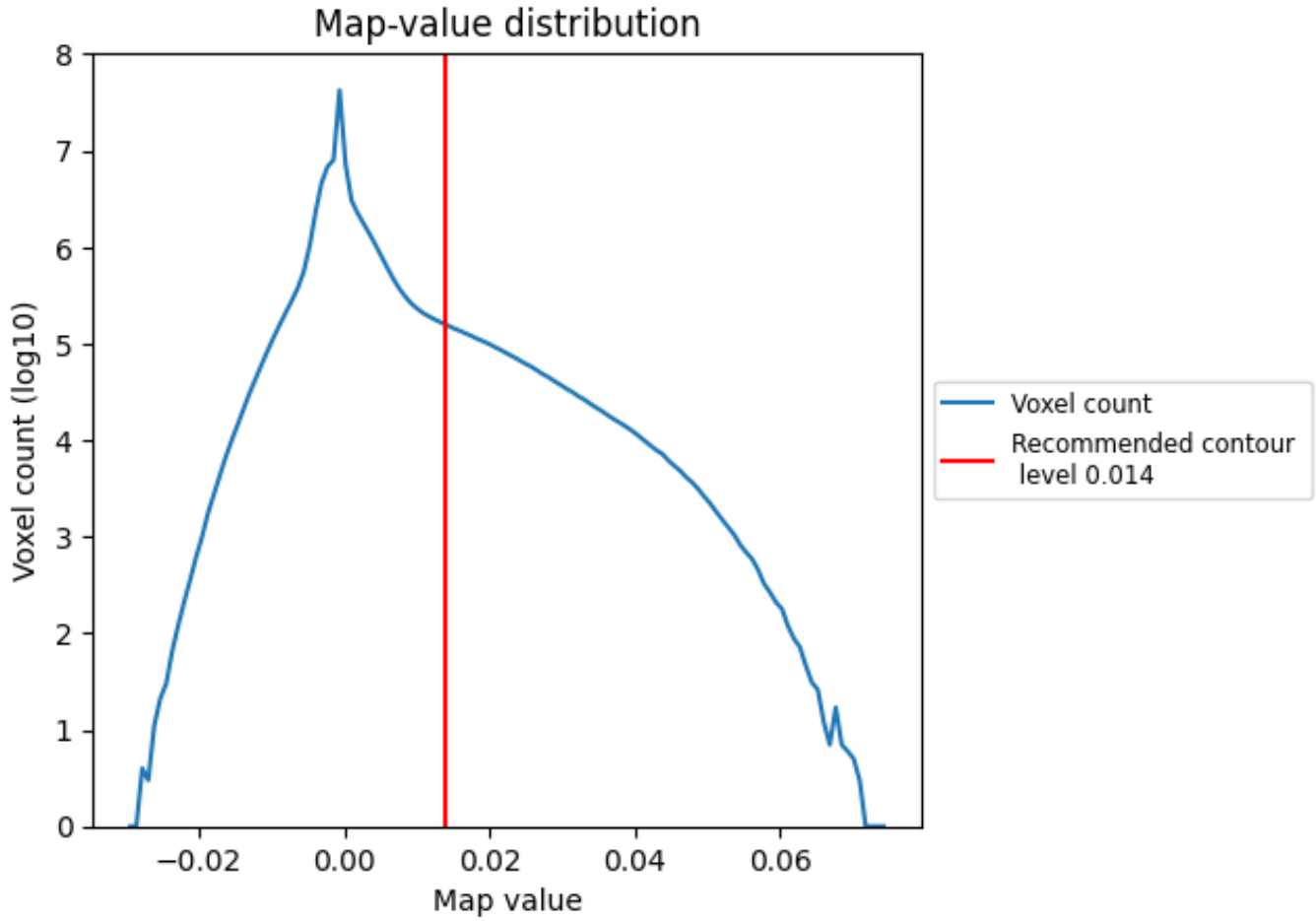
6.6 Mask visualisation (i)

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

7 Map analysis

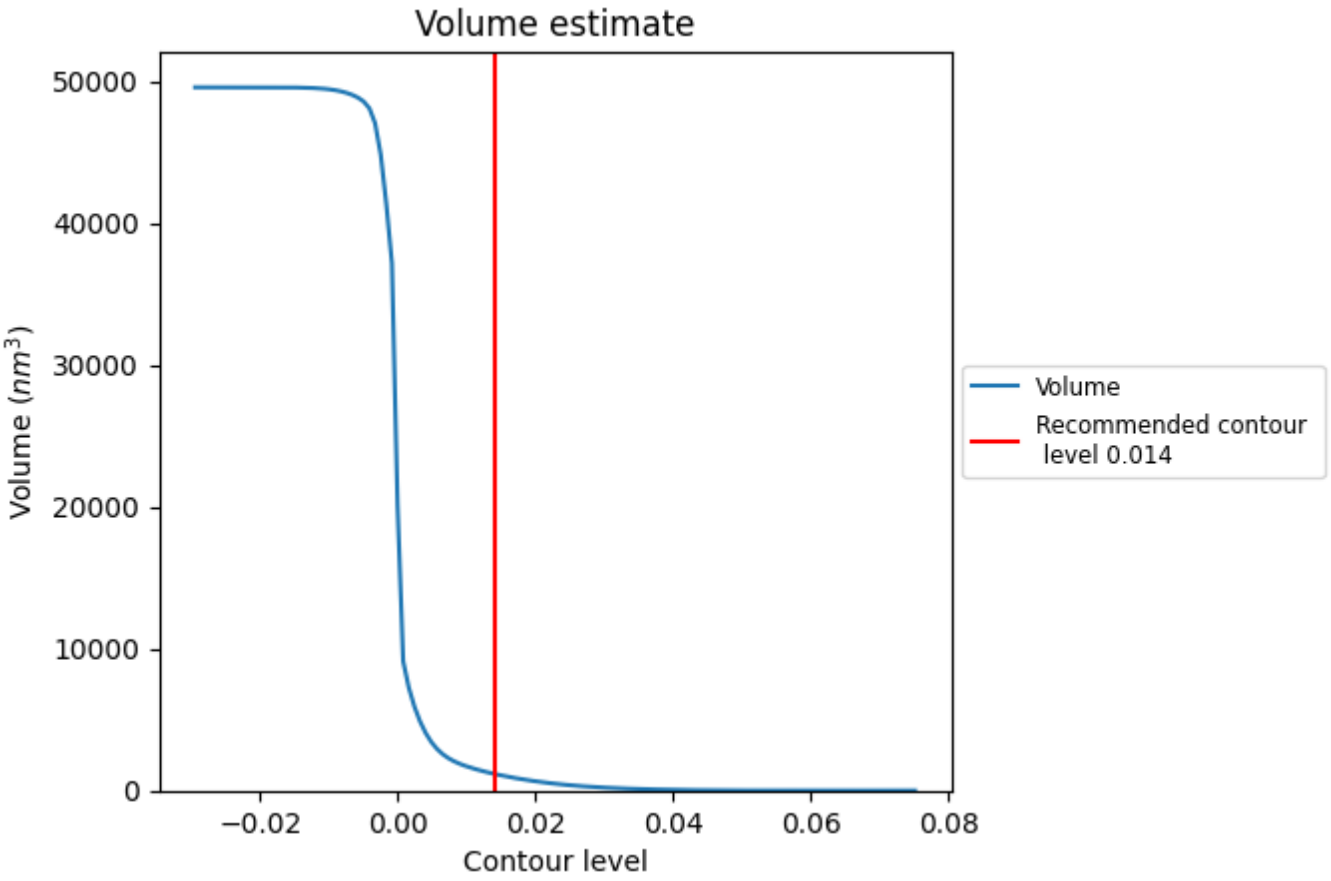
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

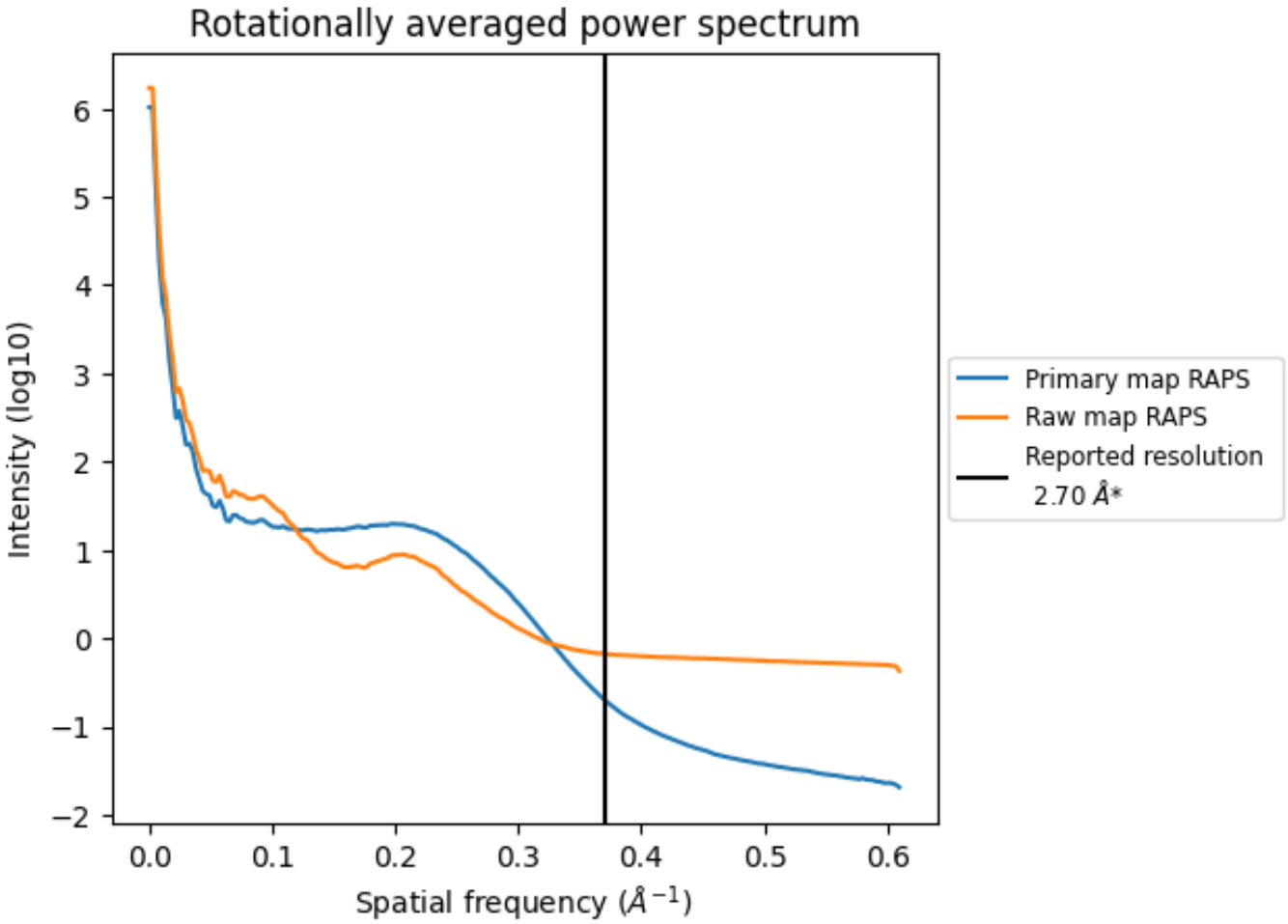
7.2 Volume estimate



The volume at the recommended contour level is 1176 nm^3; this corresponds to an approximate mass of 1063 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)

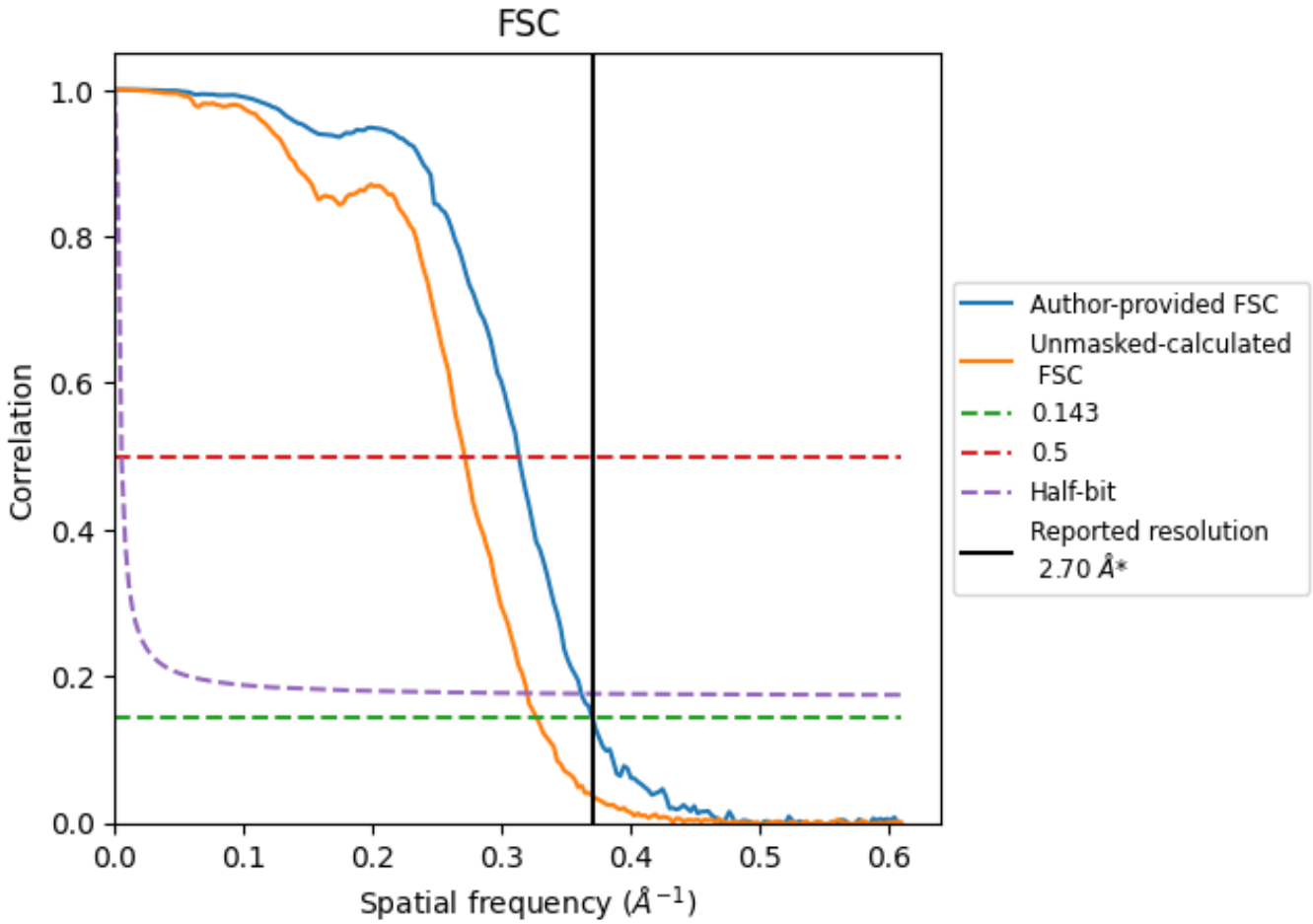


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

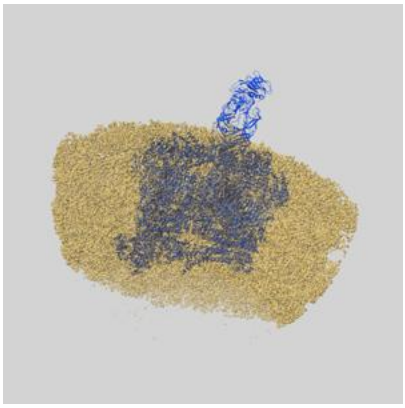
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.19	2.76
Unmasked-calculated*	3.06	3.69	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.7 by more than 10 %

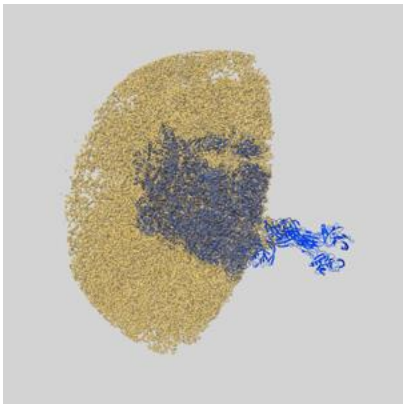
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16146 and PDB model 8BP8. Per-residue inclusion information can be found in section 3 on page 10.

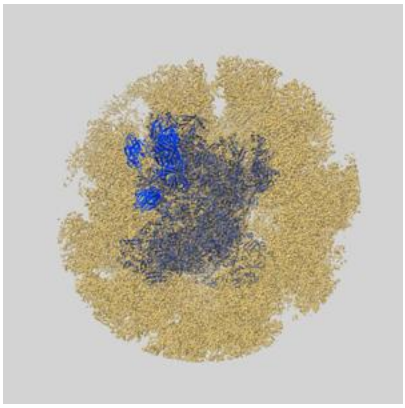
9.1 Map-model overlay



X



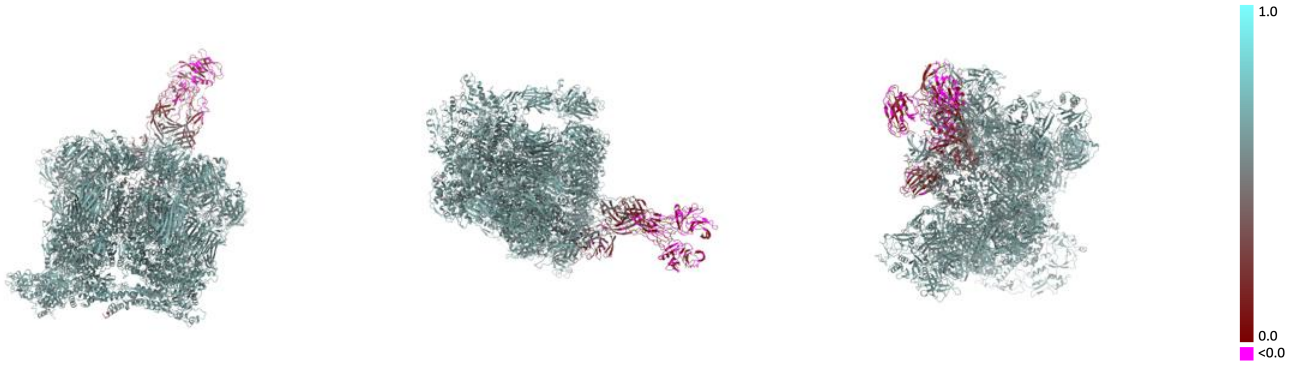
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

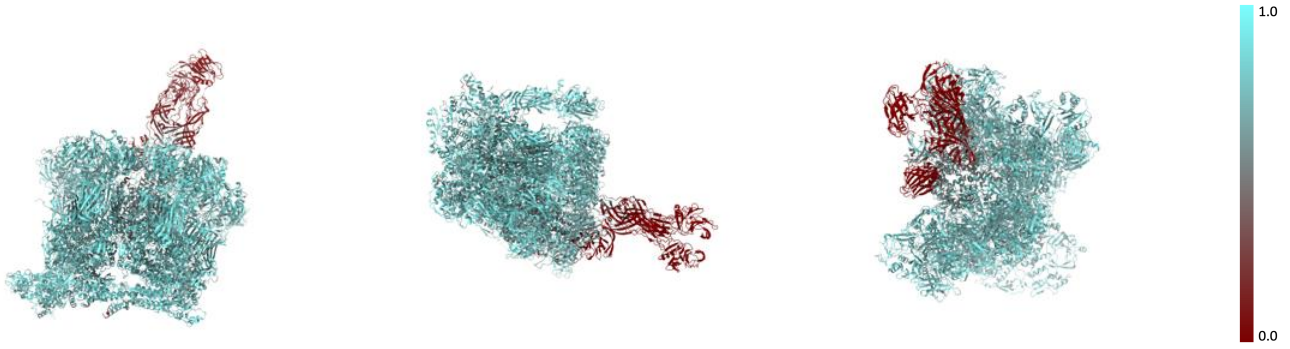
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

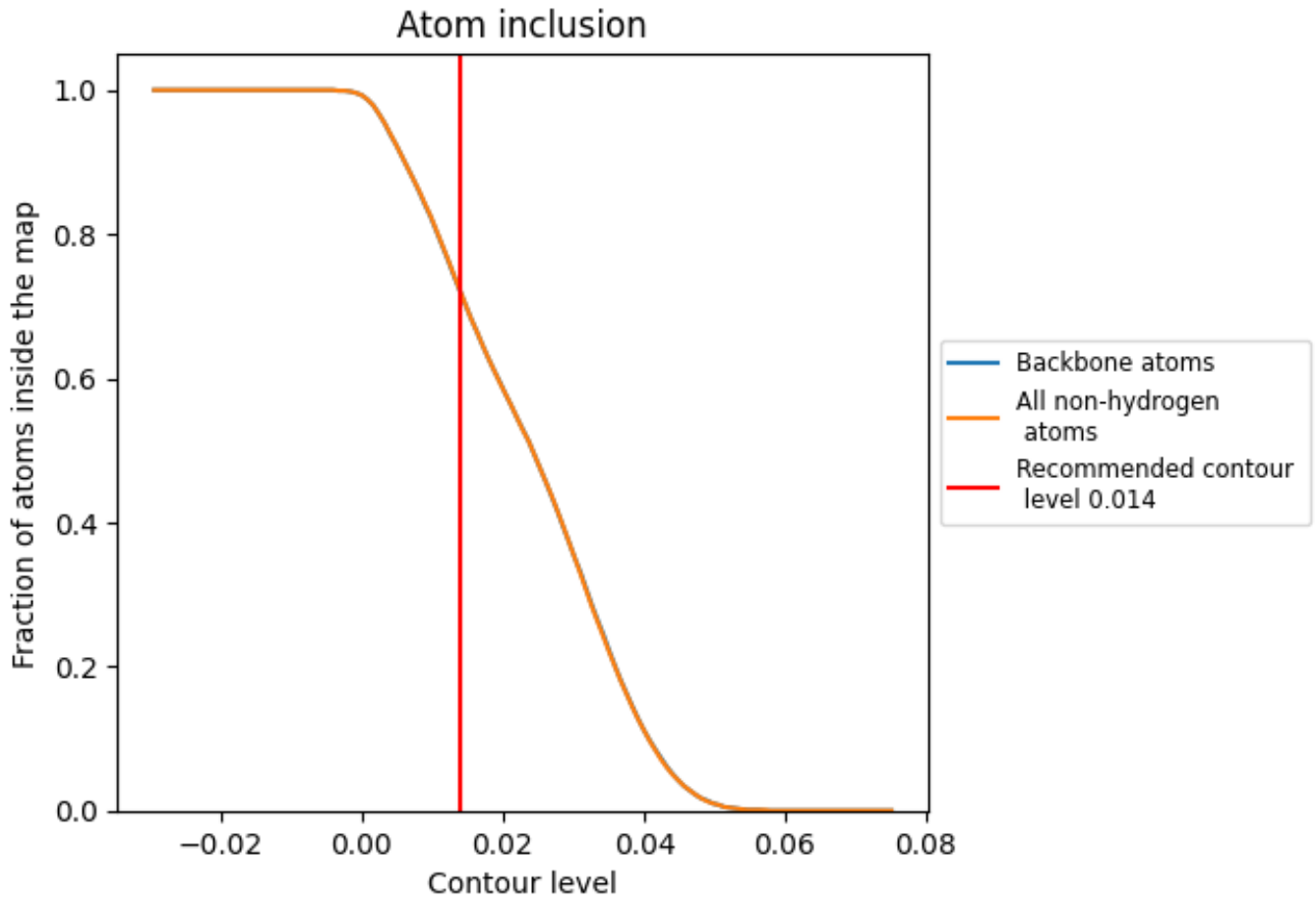
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.5670
A	0.3020	0.3240
B	0.3100	0.3360
C	0.4610	0.4860
D	0.7630	0.5940
E	0.7650	0.5950
F	0.7910	0.5960
G	0.7980	0.6000
H	0.7840	0.6020
I	0.8080	0.6060
J	0.7930	0.6040
K	0.7790	0.5940
L	0.7950	0.6030
M	0.7790	0.6000
N	0.7710	0.5920
O	0.7890	0.5960
P	0.7630	0.5910
d	0.8090	0.6080
e	0.7970	0.6070
f	0.8250	0.6140
g	0.8240	0.6160
h	0.8210	0.6160
i	0.8330	0.6210
j	0.8220	0.6160
k	0.8300	0.6180
l	0.8240	0.6170
m	0.8270	0.6150
n	0.8120	0.6100
o	0.8070	0.6110
p	0.7850	0.6060
q	0.7920	0.5980
r	0.7950	0.6000