



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 01:58 AM EST

PDB ID : 5U1F
EMDB ID : EMD-8427
Title : Initial contact of HIV-1 Env with CD4: Cryo-EM structure of BG505 DS-SOSIP trimer in complex with CD4 and antibody PGT145
Authors : Acharya, P.; Kwong, P.D.; Potter, C.S.; Carragher, B.
Deposited on : 2016-11-28
Resolution : 6.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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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:

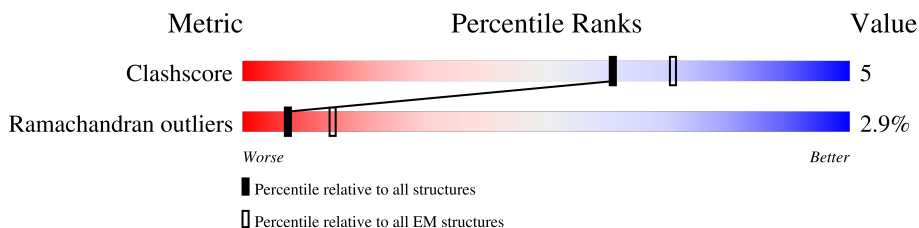
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (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 6.80 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

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	501	
1	C	501	
1	D	501	
2	B	178	
2	E	178	
2	F	178	
3	H	267	
4	L	239	
5	M	363	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12578 atoms, of which 0 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 BG505 DS-SOSIP gp120.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	C	447	2210	1316	447	447	0	0
1	D	447	2210	1316	447	447	0	0
1	A	447	2210	1316	447	447	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	SER	-	expression tag	UNP Q2N0S6
C	4	ARG	-	expression tag	UNP Q2N0S6
C	5	ALA	-	expression tag	UNP Q2N0S6
C	6	THR	-	expression tag	UNP Q2N0S6
C	7	MET	-	expression tag	UNP Q2N0S6
C	8	PRO	-	expression tag	UNP Q2N0S6
C	9	MET	-	expression tag	UNP Q2N0S6
C	10	GLY	-	expression tag	UNP Q2N0S6
C	11	SER	-	expression tag	UNP Q2N0S6
C	12	LEU	-	expression tag	UNP Q2N0S6
C	13	GLN	-	expression tag	UNP Q2N0S6
C	14	PRO	-	expression tag	UNP Q2N0S6
C	15	LEU	-	expression tag	UNP Q2N0S6
C	16	ALA	-	expression tag	UNP Q2N0S6
C	17	THR	-	expression tag	UNP Q2N0S6
C	18	LEU	-	expression tag	UNP Q2N0S6
C	19	TYR	-	expression tag	UNP Q2N0S6
C	20	LEU	-	expression tag	UNP Q2N0S6
C	21	LEU	-	expression tag	UNP Q2N0S6
C	22	GLY	-	expression tag	UNP Q2N0S6
C	23	MET	-	expression tag	UNP Q2N0S6
C	24	LEU	-	expression tag	UNP Q2N0S6
C	25	VAL	-	expression tag	UNP Q2N0S6
C	26	ALA	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	27	SER	-	expression tag	UNP Q2N0S6
C	28	VAL	-	expression tag	UNP Q2N0S6
C	29	LEU	-	expression tag	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
D	3	SER	-	expression tag	UNP Q2N0S6
D	4	ARG	-	expression tag	UNP Q2N0S6
D	5	ALA	-	expression tag	UNP Q2N0S6
D	6	THR	-	expression tag	UNP Q2N0S6
D	7	MET	-	expression tag	UNP Q2N0S6
D	8	PRO	-	expression tag	UNP Q2N0S6
D	9	MET	-	expression tag	UNP Q2N0S6
D	10	GLY	-	expression tag	UNP Q2N0S6
D	11	SER	-	expression tag	UNP Q2N0S6
D	12	LEU	-	expression tag	UNP Q2N0S6
D	13	GLN	-	expression tag	UNP Q2N0S6
D	14	PRO	-	expression tag	UNP Q2N0S6
D	15	LEU	-	expression tag	UNP Q2N0S6
D	16	ALA	-	expression tag	UNP Q2N0S6
D	17	THR	-	expression tag	UNP Q2N0S6
D	18	LEU	-	expression tag	UNP Q2N0S6
D	19	TYR	-	expression tag	UNP Q2N0S6
D	20	LEU	-	expression tag	UNP Q2N0S6
D	21	LEU	-	expression tag	UNP Q2N0S6
D	22	GLY	-	expression tag	UNP Q2N0S6
D	23	MET	-	expression tag	UNP Q2N0S6
D	24	LEU	-	expression tag	UNP Q2N0S6
D	25	VAL	-	expression tag	UNP Q2N0S6
D	26	ALA	-	expression tag	UNP Q2N0S6
D	27	SER	-	expression tag	UNP Q2N0S6
D	28	VAL	-	expression tag	UNP Q2N0S6
D	29	LEU	-	expression tag	UNP Q2N0S6
D	201	CYS	ILE	conflict	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	433	CYS	ALA	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6
A	3	SER	-	expression tag	UNP Q2N0S6
A	4	ARG	-	expression tag	UNP Q2N0S6
A	5	ALA	-	expression tag	UNP Q2N0S6
A	6	THR	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q2N0S6
A	8	PRO	-	expression tag	UNP Q2N0S6
A	9	MET	-	expression tag	UNP Q2N0S6
A	10	GLY	-	expression tag	UNP Q2N0S6
A	11	SER	-	expression tag	UNP Q2N0S6
A	12	LEU	-	expression tag	UNP Q2N0S6
A	13	GLN	-	expression tag	UNP Q2N0S6
A	14	PRO	-	expression tag	UNP Q2N0S6
A	15	LEU	-	expression tag	UNP Q2N0S6
A	16	ALA	-	expression tag	UNP Q2N0S6
A	17	THR	-	expression tag	UNP Q2N0S6
A	18	LEU	-	expression tag	UNP Q2N0S6
A	19	TYR	-	expression tag	UNP Q2N0S6
A	20	LEU	-	expression tag	UNP Q2N0S6
A	21	LEU	-	expression tag	UNP Q2N0S6
A	22	GLY	-	expression tag	UNP Q2N0S6
A	23	MET	-	expression tag	UNP Q2N0S6
A	24	LEU	-	expression tag	UNP Q2N0S6
A	25	VAL	-	expression tag	UNP Q2N0S6
A	26	ALA	-	expression tag	UNP Q2N0S6
A	27	SER	-	expression tag	UNP Q2N0S6
A	28	VAL	-	expression tag	UNP Q2N0S6
A	29	LEU	-	expression tag	UNP Q2N0S6
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	132	Total	C	N	O	0	0
			650	386	132	132		
2	E	132	Total	C	N	O	0	0
			650	386	132	132		
2	F	132	Total	C	N	O	0	0
			650	386	132	132		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	504	VAL	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	505	GLY	-	expression tag	UNP Q2N0S6
B	506	ARG	-	expression tag	UNP Q2N0S6
B	507	ARG	-	expression tag	UNP Q2N0S6
B	508	ARG	-	expression tag	UNP Q2N0S6
B	509	ARG	-	expression tag	UNP Q2N0S6
B	510	ARG	-	expression tag	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
B	665	GLY	-	expression tag	UNP Q2N0S6
B	666	SER	-	expression tag	UNP Q2N0S6
B	667	ALA	-	expression tag	UNP Q2N0S6
B	668	PRO	-	expression tag	UNP Q2N0S6
B	669	THR	-	expression tag	UNP Q2N0S6
B	670	LYS	-	expression tag	UNP Q2N0S6
B	671	ALA	-	expression tag	UNP Q2N0S6
B	672	LYS	-	expression tag	UNP Q2N0S6
B	673	ARG	-	expression tag	UNP Q2N0S6
B	674	ARG	-	expression tag	UNP Q2N0S6
B	675	VAL	-	expression tag	UNP Q2N0S6
B	676	VAL	-	expression tag	UNP Q2N0S6
B	677	GLN	-	expression tag	UNP Q2N0S6
B	678	ARG	-	expression tag	UNP Q2N0S6
B	679	GLU	-	expression tag	UNP Q2N0S6
B	680	LYS	-	expression tag	UNP Q2N0S6
B	681	ARG	-	expression tag	UNP Q2N0S6
E	504	VAL	-	expression tag	UNP Q2N0S6
E	505	GLY	-	expression tag	UNP Q2N0S6
E	506	ARG	-	expression tag	UNP Q2N0S6
E	507	ARG	-	expression tag	UNP Q2N0S6
E	508	ARG	-	expression tag	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
E	665	GLY	-	expression tag	UNP Q2N0S6
E	666	SER	-	expression tag	UNP Q2N0S6
E	667	ALA	-	expression tag	UNP Q2N0S6
E	668	PRO	-	expression tag	UNP Q2N0S6
E	669	THR	-	expression tag	UNP Q2N0S6
E	670	LYS	-	expression tag	UNP Q2N0S6
E	671	ALA	-	expression tag	UNP Q2N0S6
E	672	LYS	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	673	ARG	-	expression tag	UNP Q2N0S6
E	674	ARG	-	expression tag	UNP Q2N0S6
E	675	VAL	-	expression tag	UNP Q2N0S6
E	676	VAL	-	expression tag	UNP Q2N0S6
E	677	GLN	-	expression tag	UNP Q2N0S6
E	678	ARG	-	expression tag	UNP Q2N0S6
E	679	GLU	-	expression tag	UNP Q2N0S6
E	680	LYS	-	expression tag	UNP Q2N0S6
E	681	ARG	-	expression tag	UNP Q2N0S6
F	504	VAL	-	expression tag	UNP Q2N0S6
F	505	GLY	-	expression tag	UNP Q2N0S6
F	506	ARG	-	expression tag	UNP Q2N0S6
F	507	ARG	-	expression tag	UNP Q2N0S6
F	508	ARG	-	expression tag	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6
F	665	GLY	-	expression tag	UNP Q2N0S6
F	666	SER	-	expression tag	UNP Q2N0S6
F	667	ALA	-	expression tag	UNP Q2N0S6
F	668	PRO	-	expression tag	UNP Q2N0S6
F	669	THR	-	expression tag	UNP Q2N0S6
F	670	LYS	-	expression tag	UNP Q2N0S6
F	671	ALA	-	expression tag	UNP Q2N0S6
F	672	LYS	-	expression tag	UNP Q2N0S6
F	673	ARG	-	expression tag	UNP Q2N0S6
F	674	ARG	-	expression tag	UNP Q2N0S6
F	675	VAL	-	expression tag	UNP Q2N0S6
F	676	VAL	-	expression tag	UNP Q2N0S6
F	677	GLN	-	expression tag	UNP Q2N0S6
F	678	ARG	-	expression tag	UNP Q2N0S6
F	679	GLU	-	expression tag	UNP Q2N0S6
F	680	LYS	-	expression tag	UNP Q2N0S6
F	681	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called PGT145 heavy chain.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N	O	
3	H	235	1151	681	235	235	0

- Molecule 4 is a protein called PGT145 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L	214	1055	627	214	214	0	0


- Molecule 5 is a protein called T-cell surface glycoprotein CD4.

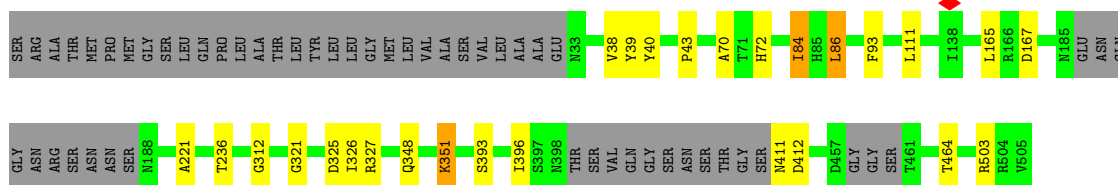
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	363	1792	1066	363	363	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

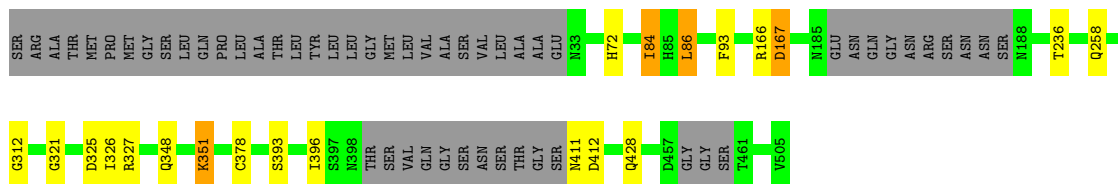
- Molecule 1: BG505 DS-SOSIP gp120

Chain C: 




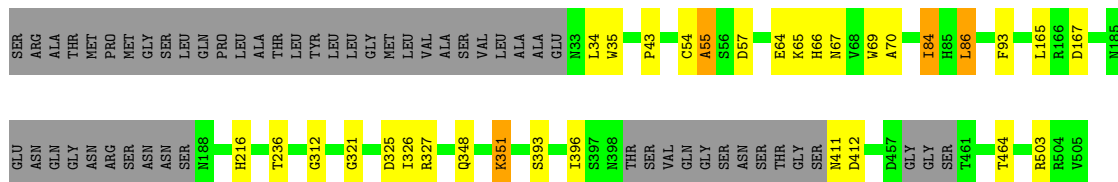
- Molecule 1: BG505 DS-SOSIP gp120

Chain D: 



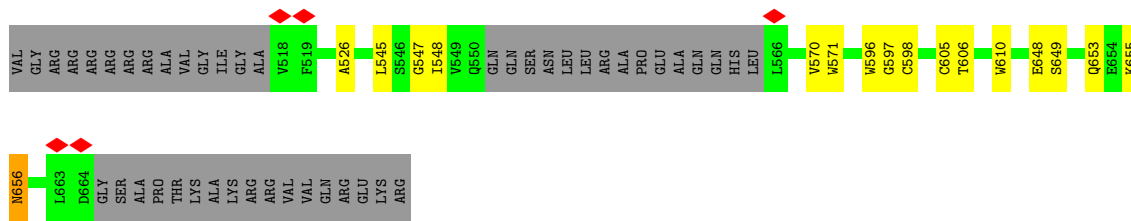
- Molecule 1: BG505 DS-SOSIP gp120

Chain A: 

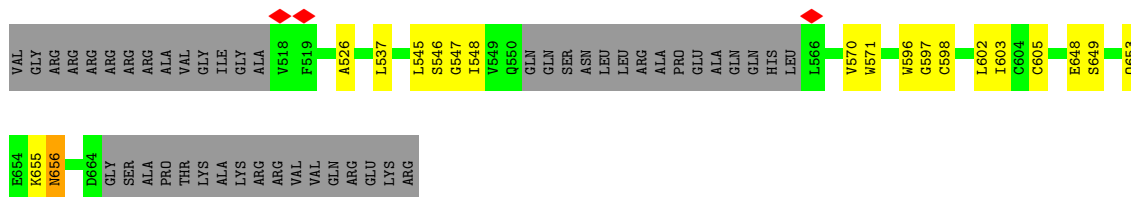


- Molecule 2: BG505 SOSIP gp41

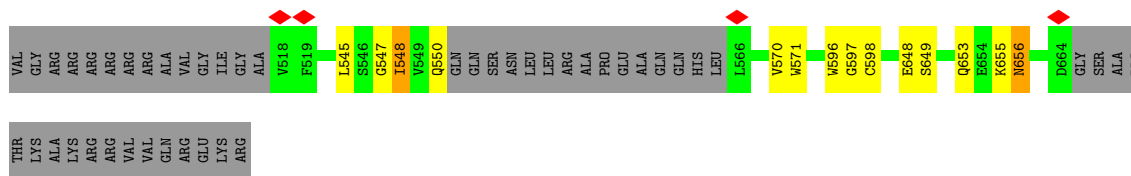
Chain B: 



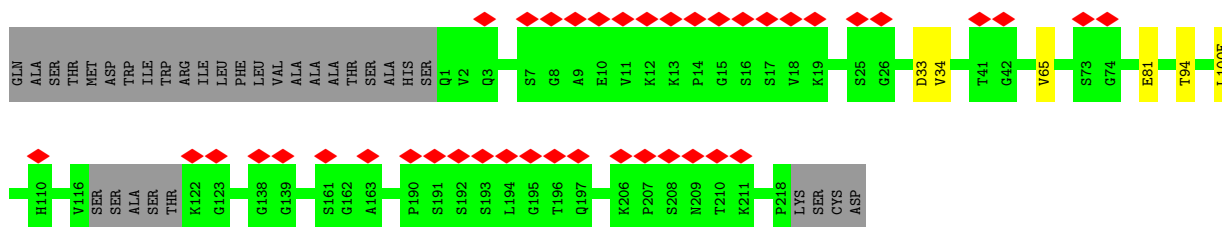
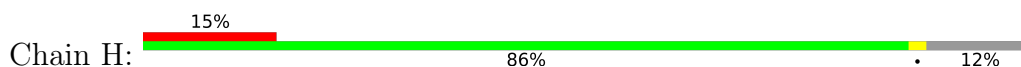
• Molecule 2: BG505 SOSIP gp41



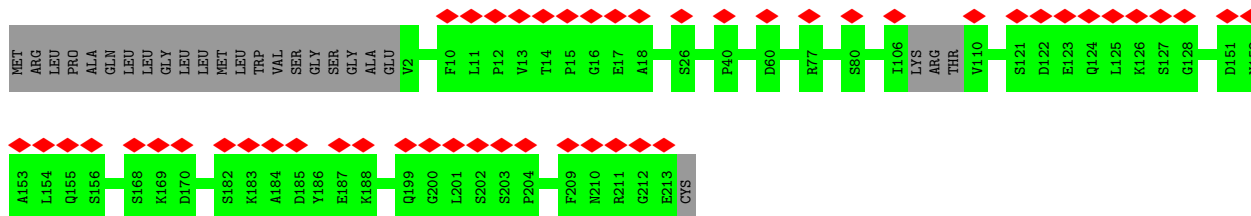
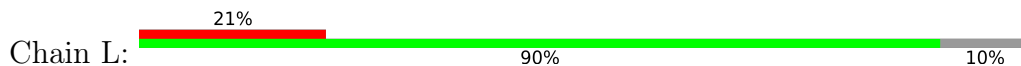
• Molecule 2: BG505 SOSIP gp41



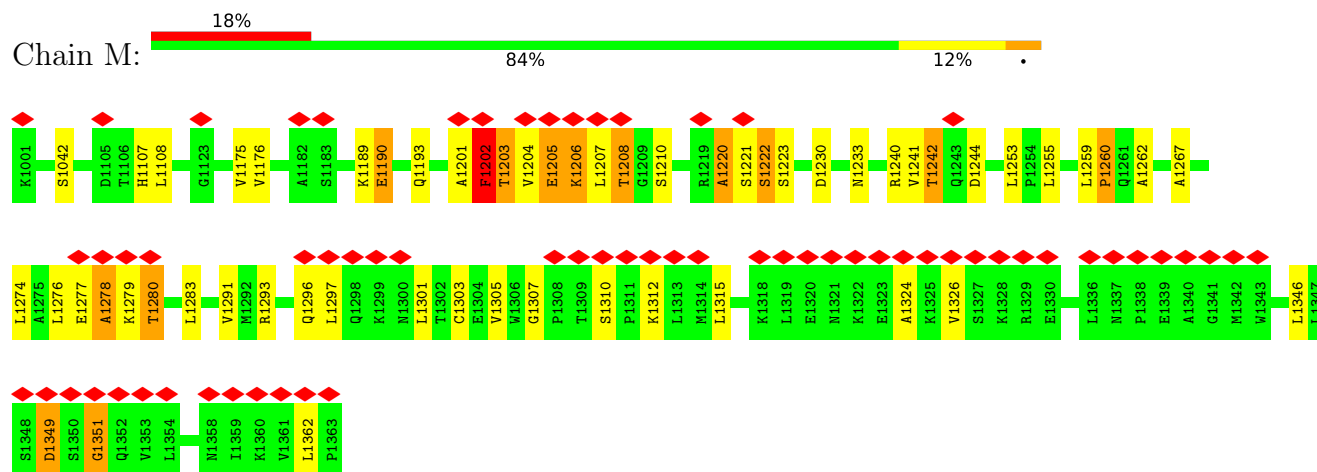
• Molecule 3: PGT145 heavy chain



• Molecule 4: PGT145 light chain



- Molecule 5: T-cell surface glycoprotein CD4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.033	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: TYS

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	0.38	1/2206 (0.0%)	0.84	16/3067 (0.5%)
1	C	0.38	2/2206 (0.1%)	0.83	15/3067 (0.5%)
1	D	0.38	1/2206 (0.0%)	0.84	15/3067 (0.5%)
2	B	0.27	0/648	0.84	3/898 (0.3%)
2	E	0.27	0/648	0.84	3/898 (0.3%)
2	F	0.27	0/648	0.84	3/898 (0.3%)
3	H	0.39	0/1137	0.60	1/1571 (0.1%)
4	L	0.39	0/1053	0.58	0/1462
5	M	0.52	1/1791 (0.1%)	0.96	6/2492 (0.2%)
All	All	0.39	5/12543 (0.0%)	0.82	62/17420 (0.4%)

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
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ILE	C-N	6.01	1.47	1.34
1	C	84	ILE	C-N	5.96	1.47	1.34
1	D	84	ILE	C-N	5.95	1.47	1.34
5	M	1202	PHE	C-O	-5.23	1.13	1.23
1	C	393	SER	C-N	5.02	1.45	1.34

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	648	GLU	N-CA-C	14.21	149.38	111.00
2	E	648	GLU	N-CA-C	14.16	149.24	111.00
2	F	648	GLU	N-CA-C	14.12	149.13	111.00
1	C	84	ILE	O-C-N	12.81	143.20	122.70
1	D	86	LEU	O-C-N	-12.72	102.35	122.70
1	D	84	ILE	O-C-N	12.69	143.00	122.70
1	A	84	ILE	O-C-N	12.69	143.00	122.70
1	C	86	LEU	O-C-N	-12.64	102.47	122.70
1	A	86	LEU	O-C-N	-12.58	102.58	122.70
1	A	393	SER	O-C-N	11.26	140.72	122.70
1	D	393	SER	O-C-N	11.17	140.57	122.70
1	C	393	SER	O-C-N	11.08	140.43	122.70
1	C	84	ILE	CA-C-N	-10.77	93.51	117.20
1	A	84	ILE	CA-C-N	-10.73	93.59	117.20
1	D	84	ILE	CA-C-N	-10.71	93.63	117.20
1	C	348	GLN	O-C-N	10.59	139.65	122.70
1	D	348	GLN	O-C-N	10.54	139.57	122.70
1	A	348	GLN	O-C-N	10.53	139.55	122.70
1	C	351	LYS	O-C-N	-10.17	106.43	122.70
1	A	351	LYS	O-C-N	-10.14	106.47	122.70
1	D	351	LYS	O-C-N	-10.14	106.48	122.70
1	C	84	ILE	C-N-CA	-8.90	99.44	121.70
1	A	84	ILE	C-N-CA	-8.90	99.44	121.70
1	D	84	ILE	C-N-CA	-8.86	99.55	121.70
1	D	393	SER	CA-C-N	-8.39	98.75	117.20
1	A	393	SER	CA-C-N	-8.38	98.77	117.20
1	C	393	SER	CA-C-N	-8.34	98.86	117.20
1	C	348	GLN	CA-C-N	-8.03	99.53	117.20
1	D	348	GLN	CA-C-N	-8.03	99.54	117.20
1	A	348	GLN	CA-C-N	-8.02	99.56	117.20
5	M	1208	THR	N-CA-C	7.57	131.45	111.00
1	C	351	LYS	CA-C-N	7.30	133.25	117.20
1	A	351	LYS	CA-C-N	7.26	133.18	117.20
1	D	351	LYS	CA-C-N	7.23	133.12	117.20
2	B	648	GLU	N-CA-CB	-7.02	97.96	110.60
2	E	648	GLU	N-CA-CB	-6.97	98.06	110.60
2	F	648	GLU	N-CA-CB	-6.92	98.14	110.60
5	M	1277	GLU	O-C-N	6.87	133.69	122.70
1	D	86	LEU	CA-C-N	6.78	132.12	117.20
1	C	86	LEU	CA-C-N	6.77	132.09	117.20
1	C	348	GLN	C-N-CA	-6.74	104.85	121.70
1	A	86	LEU	CA-C-N	6.74	132.03	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	GLN	C-N-CA	-6.74	104.85	121.70
1	D	348	GLN	C-N-CA	-6.71	104.91	121.70
1	D	86	LEU	C-N-CA	6.66	138.35	121.70
1	C	86	LEU	C-N-CA	6.61	138.22	121.70
1	A	86	LEU	C-N-CA	6.54	138.06	121.70
3	H	34	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	393	SER	C-N-CA	-5.87	107.02	121.70
1	D	393	SER	C-N-CA	-5.84	107.10	121.70
1	C	393	SER	C-N-CA	-5.80	107.20	121.70
5	M	1202	PHE	N-CA-C	5.78	126.61	111.00
2	B	653	GLN	N-CA-C	5.71	126.41	111.00
2	E	653	GLN	N-CA-C	5.69	126.35	111.00
2	F	653	GLN	N-CA-C	5.65	126.25	111.00
1	C	351	LYS	C-N-CA	5.49	135.43	121.70
5	M	1278	ALA	O-C-N	5.48	131.47	122.70
1	A	351	LYS	C-N-CA	5.48	135.39	121.70
1	D	351	LYS	C-N-CA	5.47	135.38	121.70
5	M	1277	GLU	CA-C-N	-5.46	105.19	117.20
1	A	66	HIS	N-CA-CB	5.35	120.23	110.60
5	M	1242	THR	N-CA-C	-5.12	97.19	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	LYS	Mainchain
1	A	86	LEU	Mainchain
1	C	86	LEU	Mainchain
1	D	86	LEU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2210	0	953	18	0
1	C	2210	0	953	18	0
1	D	2210	0	953	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	650	0	295	14	0
2	E	650	0	295	16	0
2	F	650	0	295	5	0
3	H	1151	0	525	3	0
4	L	1055	0	468	0	0
5	M	1792	0	781	28	0
All	All	12578	0	5518	84	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 5.

All (84) 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:35:TRP:HA	2:B:610:TRP:CB	1.87	1.04
1:C:43:PRO:CB	2:E:526:ALA:HA	1.89	1.02
1:A:43:PRO:CB	2:B:526:ALA:CB	2.42	0.98
1:A:43:PRO:CB	2:B:526:ALA:HA	1.93	0.97
1:A:503:ARG:CB	2:B:605:CYS:CB	2.45	0.94
1:C:40:TYR:O	2:E:537:LEU:CB	2.18	0.91
1:C:43:PRO:CB	2:E:526:ALA:CA	2.52	0.88
1:A:43:PRO:CB	2:B:526:ALA:CA	2.52	0.87
1:A:43:PRO:CB	2:B:526:ALA:HB1	2.06	0.84
1:C:38:VAL:O	2:E:603:ILE:HA	1.80	0.82
1:D:428:GLN:CB	5:M:1042:SER:CB	2.62	0.78
1:A:93:PHE:O	1:A:236:THR:HA	1.85	0.77
1:A:35:TRP:CA	2:B:610:TRP:CB	2.62	0.77
1:D:93:PHE:O	1:D:236:THR:HA	1.85	0.77
1:C:93:PHE:O	1:C:236:THR:HA	1.85	0.75
1:A:503:ARG:CB	2:B:606:THR:O	2.36	0.74
1:C:70:ALA:CB	1:C:111:LEU:CB	2.67	0.72
1:C:43:PRO:CB	2:E:526:ALA:CB	2.68	0.72
5:M:1108:LEU:O	5:M:1176:VAL:HA	1.90	0.72
5:M:1193:GLN:HA	5:M:1260:PRO:O	1.91	0.70
1:C:221:ALA:HB2	2:E:546:SER:CB	2.22	0.70
1:C:43:PRO:CB	2:E:526:ALA:HB2	2.21	0.70
1:C:40:TYR:CB	2:E:602:LEU:HA	2.21	0.69
1:C:503:ARG:CB	2:E:605:CYS:CB	2.72	0.67
5:M:1108:LEU:O	5:M:1176:VAL:CA	2.43	0.66
1:C:39:TYR:HA	2:E:602:LEU:O	1.95	0.65
1:A:55:ALA:O	1:A:216:HIS:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1108:LEU:O	5:M:1176:VAL:CB	2.46	0.63
5:M:1208:THR:O	5:M:1276:LEU:CB	2.46	0.63
5:M:1107:HIS:HA	5:M:1175:VAL:O	2.00	0.62
2:B:596:TRP:O	2:B:598:CYS:N	2.36	0.59
2:F:596:TRP:O	2:F:598:CYS:N	2.36	0.59
2:E:596:TRP:O	2:E:598:CYS:N	2.35	0.59
2:F:570:VAL:O	2:F:571:TRP:CB	2.51	0.58
2:E:570:VAL:O	2:E:571:TRP:CB	2.51	0.57
1:C:70:ALA:HB2	1:C:111:LEU:CB	2.35	0.57
2:B:570:VAL:O	2:B:571:TRP:CB	2.51	0.57
5:M:1315:LEU:HA	5:M:1346:LEU:O	2.04	0.56
5:M:1279:LYS:O	5:M:1280:THR:O	2.24	0.56
5:M:1274:LEU:O	5:M:1283:LEU:N	2.39	0.55
1:C:221:ALA:CB	2:E:546:SER:CB	2.87	0.53
5:M:1259:LEU:O	5:M:1260:PRO:O	2.26	0.53
1:A:54:CYS:O	1:A:55:ALA:HB2	2.10	0.52
5:M:1204:VAL:O	5:M:1205:GLU:CB	2.59	0.51
1:D:167:ASP:HA	3:H:100(E):LEU:HA	1.92	0.50
1:D:411:ASN:CB	1:D:412:ASP:HA	2.42	0.50
5:M:1291:VAL:O	5:M:1305:VAL:HA	2.11	0.50
5:M:1221:SER:O	5:M:1223:SER:N	2.45	0.50
1:A:411:ASN:CB	1:A:412:ASP:HA	2.42	0.50
5:M:1206:LYS:O	5:M:1208:THR:N	2.44	0.50
1:C:411:ASN:CB	1:C:412:ASP:HA	2.42	0.49
5:M:1220:ALA:C	5:M:1222:SER:H	2.17	0.48
5:M:1293:ARG:O	5:M:1303:CYS:HA	2.14	0.47
5:M:1190:GLU:HA	5:M:1262:ALA:O	2.16	0.46
5:M:1296:GLN:HA	5:M:1301:LEU:HA	1.98	0.46
5:M:1202:PHE:O	5:M:1203:THR:O	2.33	0.46
1:D:411:ASN:CB	1:D:412:ASP:CA	2.94	0.46
5:M:1267:ALA:HB1	5:M:1307:GLY:CA	2.46	0.46
1:A:411:ASN:CB	1:A:412:ASP:CA	2.94	0.46
2:B:655:LYS:O	2:B:656:ASN:CB	2.64	0.45
1:C:411:ASN:CB	1:C:412:ASP:CA	2.94	0.45
2:E:655:LYS:O	2:E:656:ASN:CB	2.65	0.45
5:M:1310:SER:C	5:M:1312:LYS:H	2.19	0.45
2:F:655:LYS:O	2:F:656:ASN:CB	2.64	0.45
1:A:54:CYS:O	1:A:55:ALA:CB	2.65	0.44
1:A:35:TRP:C	2:B:610:TRP:CB	2.86	0.44
5:M:1210:SER:CB	5:M:1230:ASP:HA	2.47	0.44
1:C:325:ASP:O	1:C:327:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ASP:O	1:D:327:ARG:N	2.52	0.43
1:A:325:ASP:O	1:A:327:ARG:N	2.51	0.43
5:M:1220:ALA:C	5:M:1222:SER:N	2.72	0.43
5:M:1189:LYS:O	5:M:1190:GLU:C	2.56	0.43
1:A:34:LEU:O	2:B:610:TRP:CB	2.67	0.42
5:M:1267:ALA:HB1	5:M:1307:GLY:HA3	2.01	0.42
2:F:545:LEU:O	2:F:547:GLY:N	2.53	0.41
3:H:65:VAL:HA	3:H:81:GLU:O	2.20	0.41
2:B:545:LEU:O	2:B:547:GLY:N	2.53	0.41
2:E:545:LEU:O	2:E:547:GLY:N	2.54	0.41
2:F:548:ILE:O	2:F:550:GLN:N	2.54	0.41
3:H:33:ASP:O	3:H:94:THR:HA	2.21	0.41
5:M:1349:ASP:O	5:M:1351:GLY:N	2.53	0.41
1:C:38:VAL:O	2:E:603:ILE:CA	2.61	0.41
5:M:1296:GLN:HA	5:M:1301:LEU:CB	2.51	0.41
1:A:411:ASN:N	1:A:412:ASP:HA	2.36	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	439/501 (88%)	391 (89%)	33 (8%)	15 (3%)	3	26
1	C	439/501 (88%)	398 (91%)	31 (7%)	10 (2%)	6	34
1	D	439/501 (88%)	388 (88%)	40 (9%)	11 (2%)	5	32
2	B	128/178 (72%)	103 (80%)	21 (16%)	4 (3%)	4	27
2	E	128/178 (72%)	103 (80%)	21 (16%)	4 (3%)	4	27
2	F	128/178 (72%)	103 (80%)	21 (16%)	4 (3%)	4	27
3	H	229/267 (86%)	219 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	210/239 (88%)	207 (99%)	3 (1%)	0	100	100
5	M	361/363 (99%)	298 (82%)	38 (10%)	25 (7%)	1	15
All	All	2501/2906 (86%)	2210 (88%)	218 (9%)	73 (3%)	7	29

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	396	ILE
1	D	396	ILE
1	A	55	ALA
1	A	396	ILE
5	M	1190	GLU
5	M	1202	PHE
5	M	1203	THR
5	M	1205	GLU
5	M	1222	SER
5	M	1241	VAL
5	M	1242	THR
5	M	1244	ASP
5	M	1255	LEU
5	M	1260	PRO
5	M	1280	THR
5	M	1349	ASP
1	C	72	HIS
1	C	165	LEU
1	C	464	THR
1	D	72	HIS
1	A	70	ALA
1	A	464	THR
2	B	597	GLY
2	E	597	GLY
2	E	649	SER
2	F	597	GLY
2	F	649	SER
5	M	1207	LEU
5	M	1278	ALA
1	C	167	ASP
1	D	167	ASP
1	D	258	GLN
1	D	312	GLY
1	A	64	GLU

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Mol	Chain	Res	Type
1	A	69	TRP
1	A	167	ASP
2	B	548	ILE
2	B	649	SER
2	E	548	ILE
2	F	548	ILE
5	M	1233	ASN
5	M	1253	LEU
5	M	1297	LEU
5	M	1324	ALA
1	C	321	GLY
1	D	321	GLY
1	D	378	CYS
1	A	57	ASP
1	A	67	ASN
1	A	165	LEU
1	A	321	GLY
2	B	656	ASN
2	E	656	ASN
2	F	656	ASN
5	M	1201	ALA
5	M	1206	LYS
5	M	1240	ARG
5	M	1351	GLY
1	C	351	LYS
1	D	84	ILE
1	D	351	LYS
1	A	84	ILE
1	A	351	LYS
5	M	1220	ALA
5	M	1326	VAL
1	C	84	ILE
1	D	166	ARG
1	C	312	GLY
1	A	326	ILE
1	C	326	ILE
1	D	326	ILE
1	A	312	GLY
5	M	1362	LEU

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYS	H	100(I)	3	3,4,17	0.93	0	2,4,24	0.98	0
3	TYS	H	100(F)	3	3,4,17	0.95	0	2,4,24	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	H	100(I)	3	-	0/0/2/13	-
3	TYS	H	100(F)	3	-	0/0/2/13	-

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

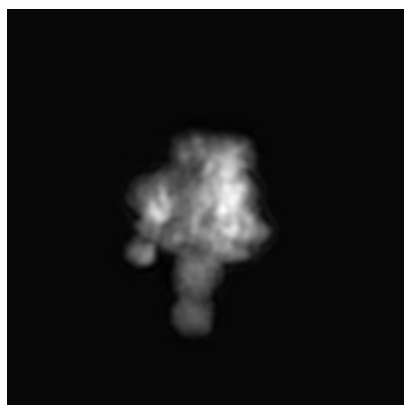
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8427. These allow visual inspection of the internal detail of the map and identification of artifacts.

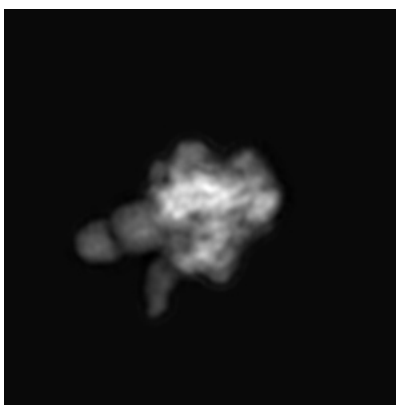
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

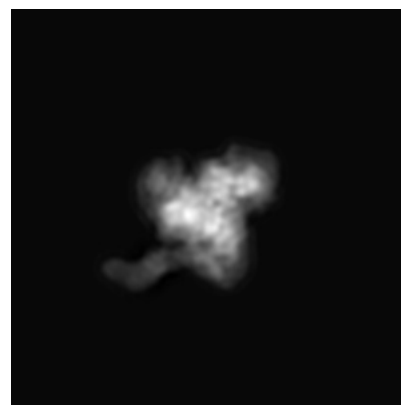
6.1.1 Primary map



X



Y



Z

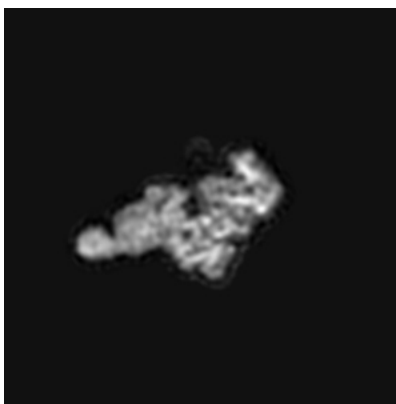
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

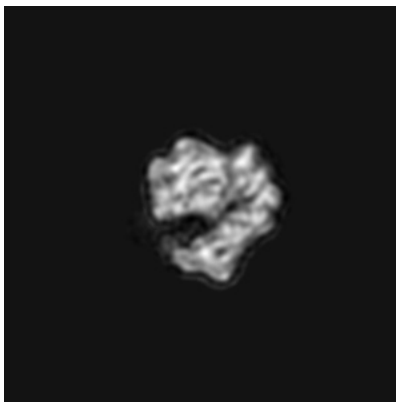
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 165



Y Index: 180

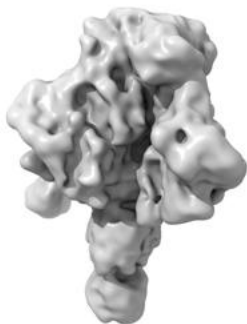


Z Index: 157

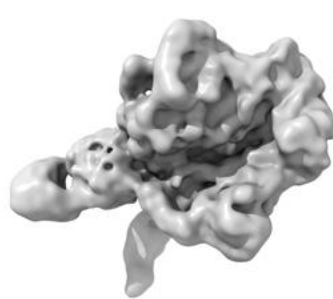
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

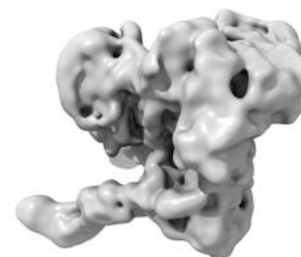
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

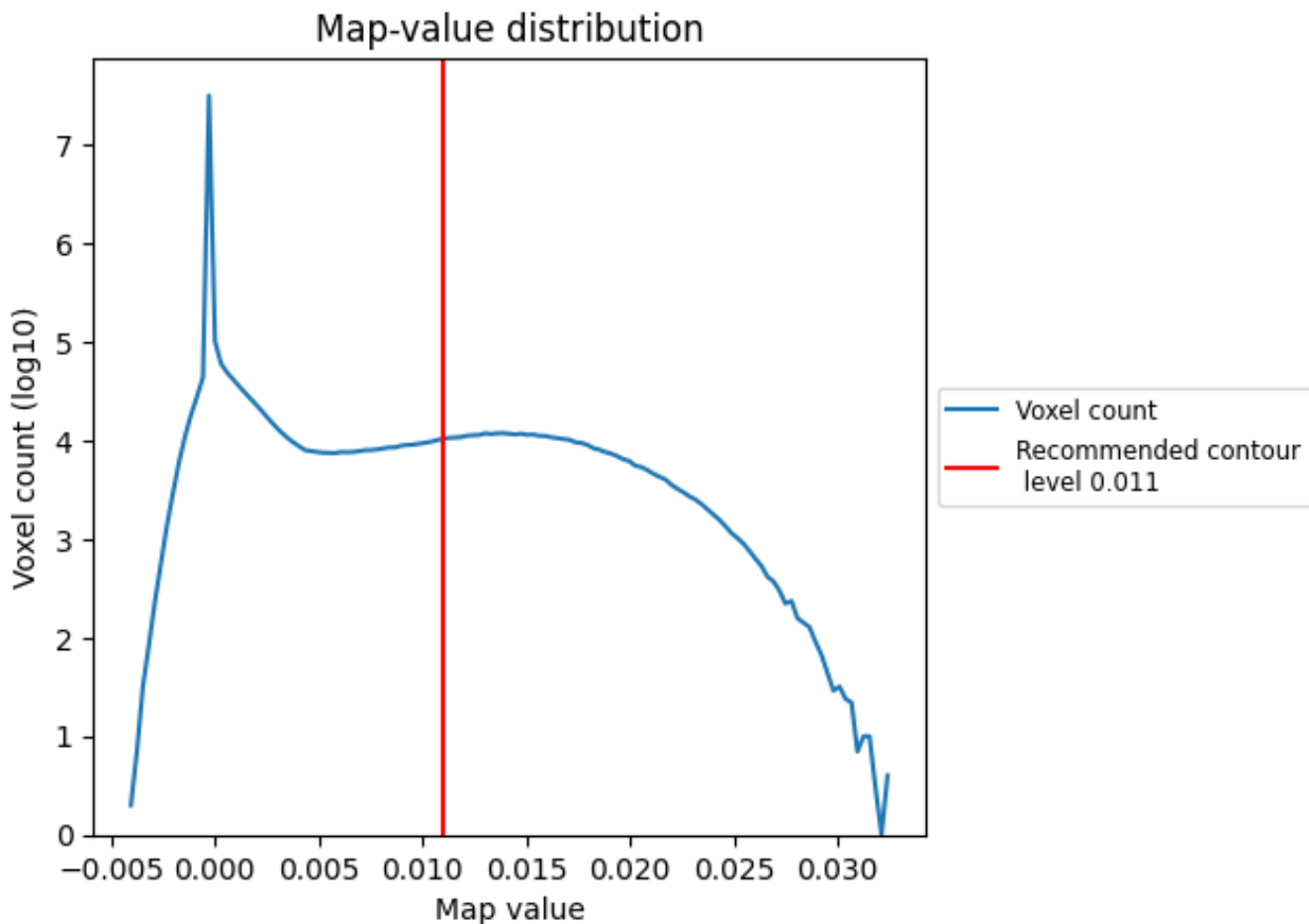
6.5 Mask visualisation

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

7 Map analysis [i](#)

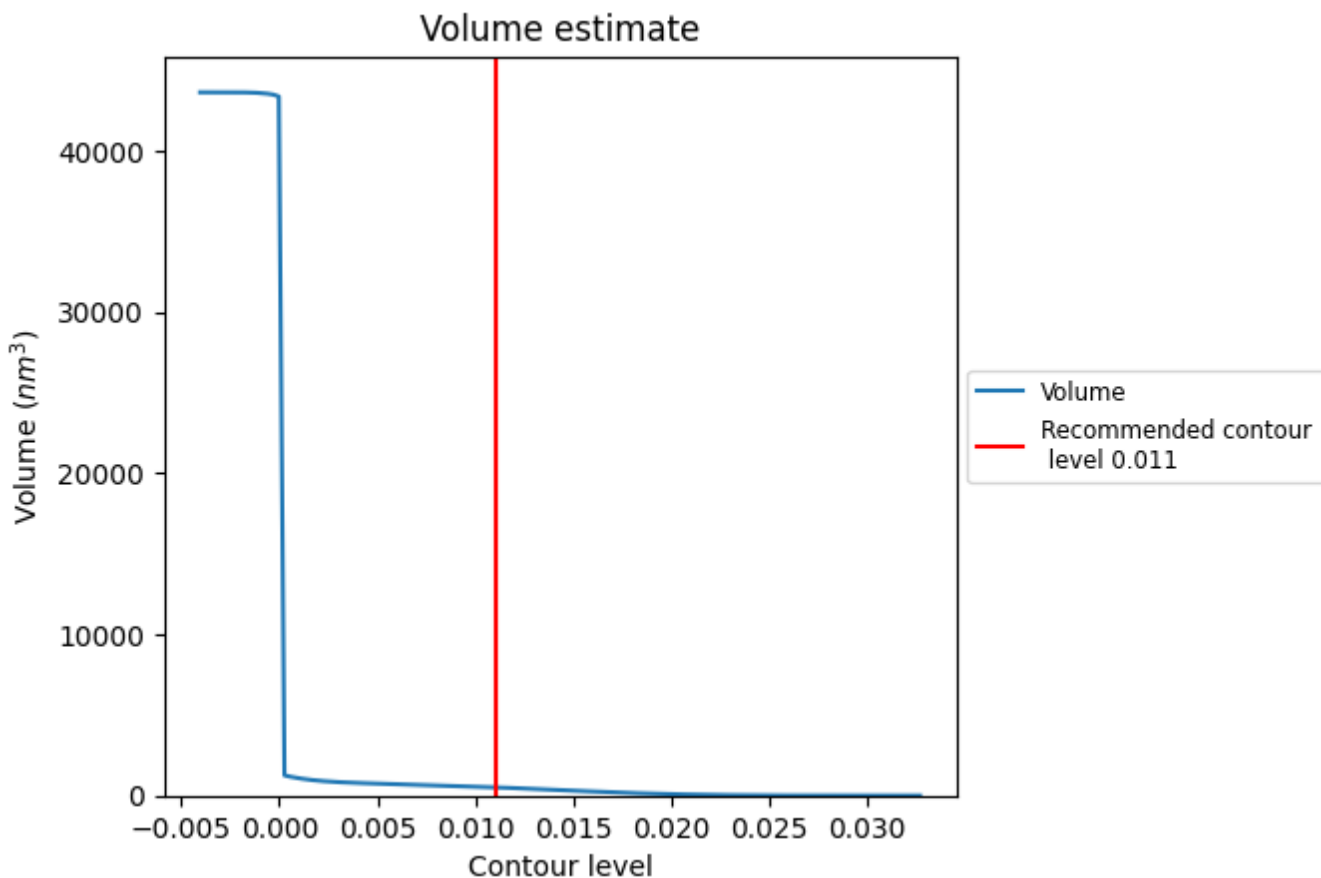
This section contains the results of statistical analysis of the map.

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.

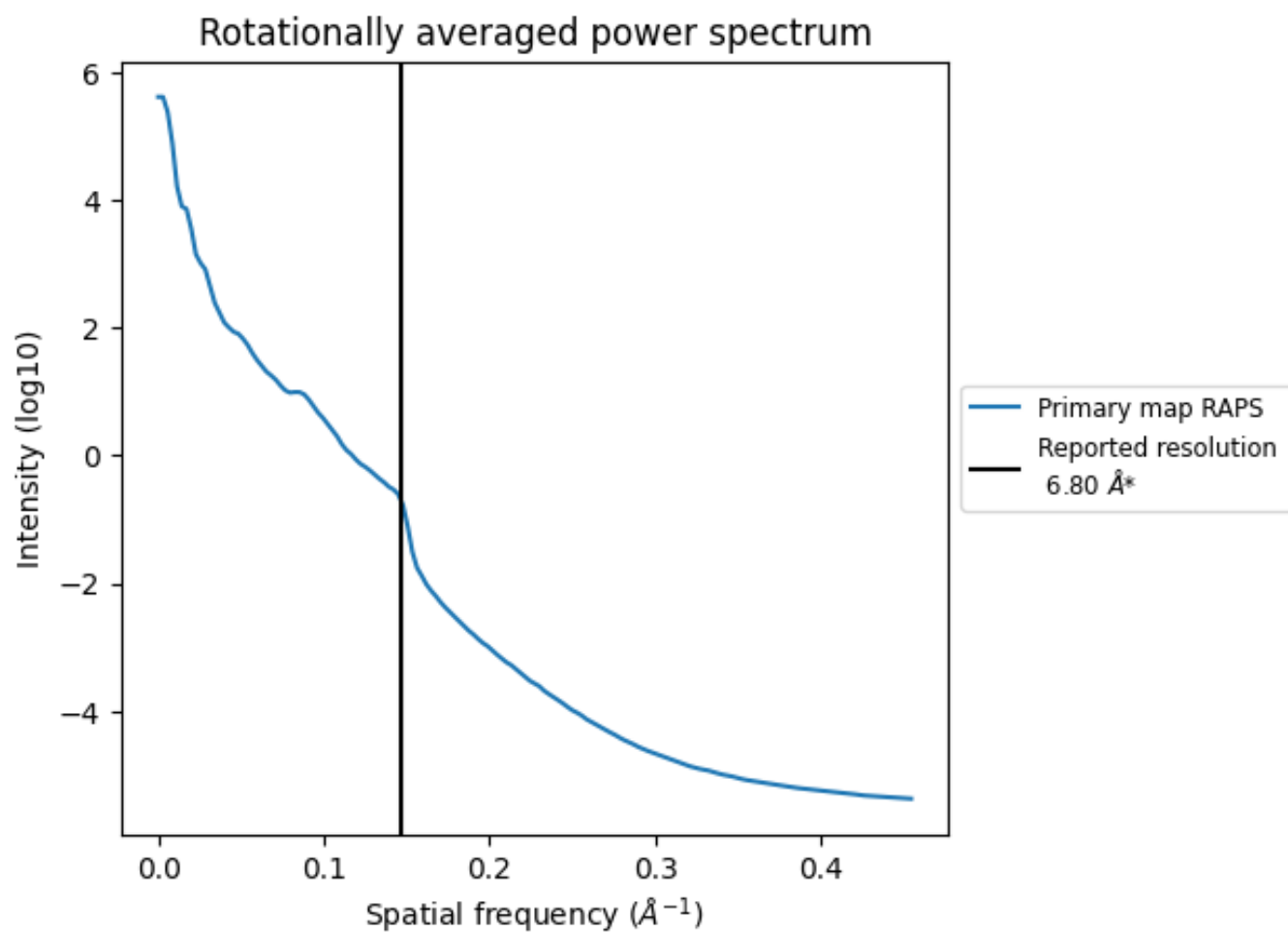
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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](#)

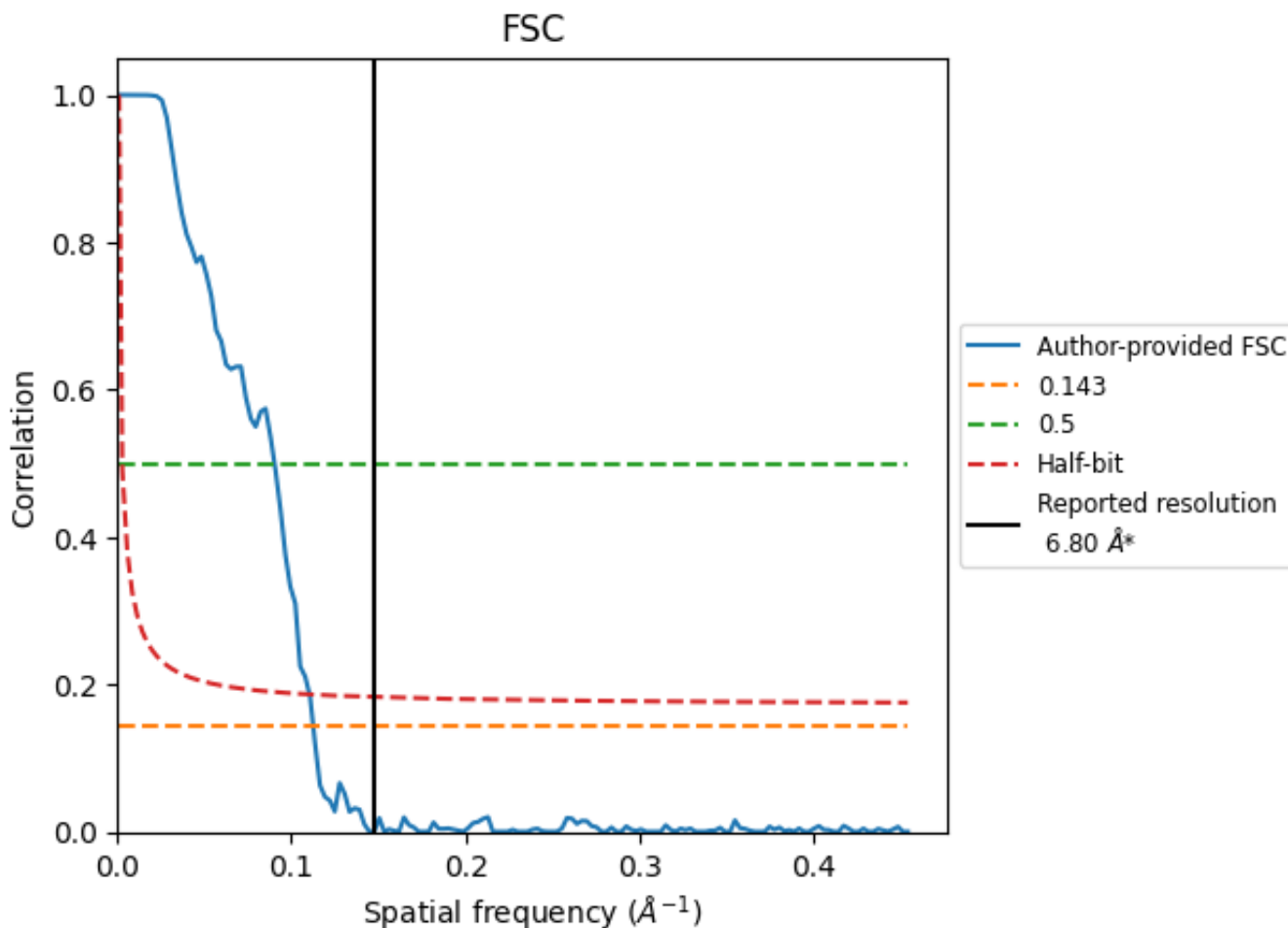


*Reported resolution corresponds to spatial frequency of 0.147\AA^{-1}

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 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

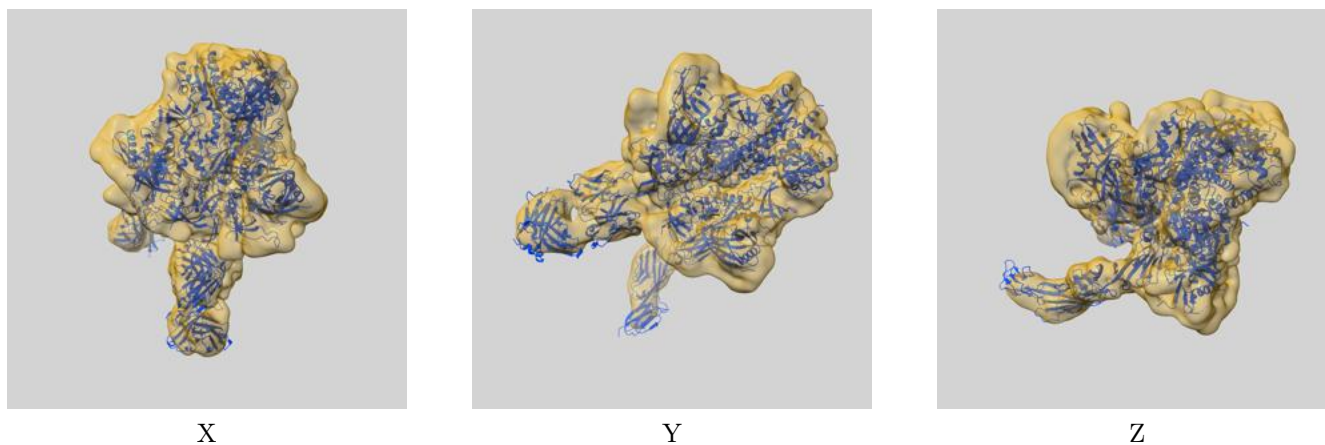
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	8.88	11.07	9.05
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.88 differs from the reported value 6.8 by more than 10 %

9 Map-model fit [i](#)

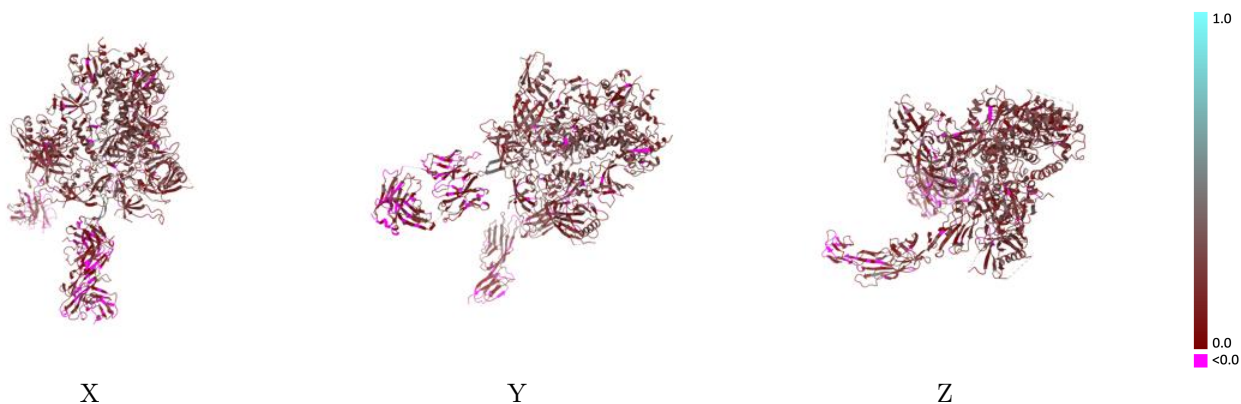
This section contains information regarding the fit between EMDB map EMD-8427 and PDB model 5U1F. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



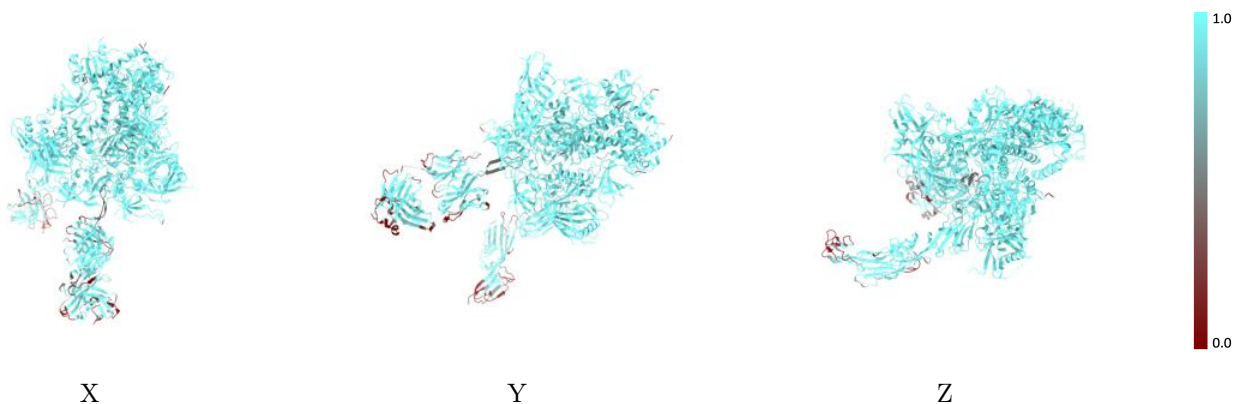
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



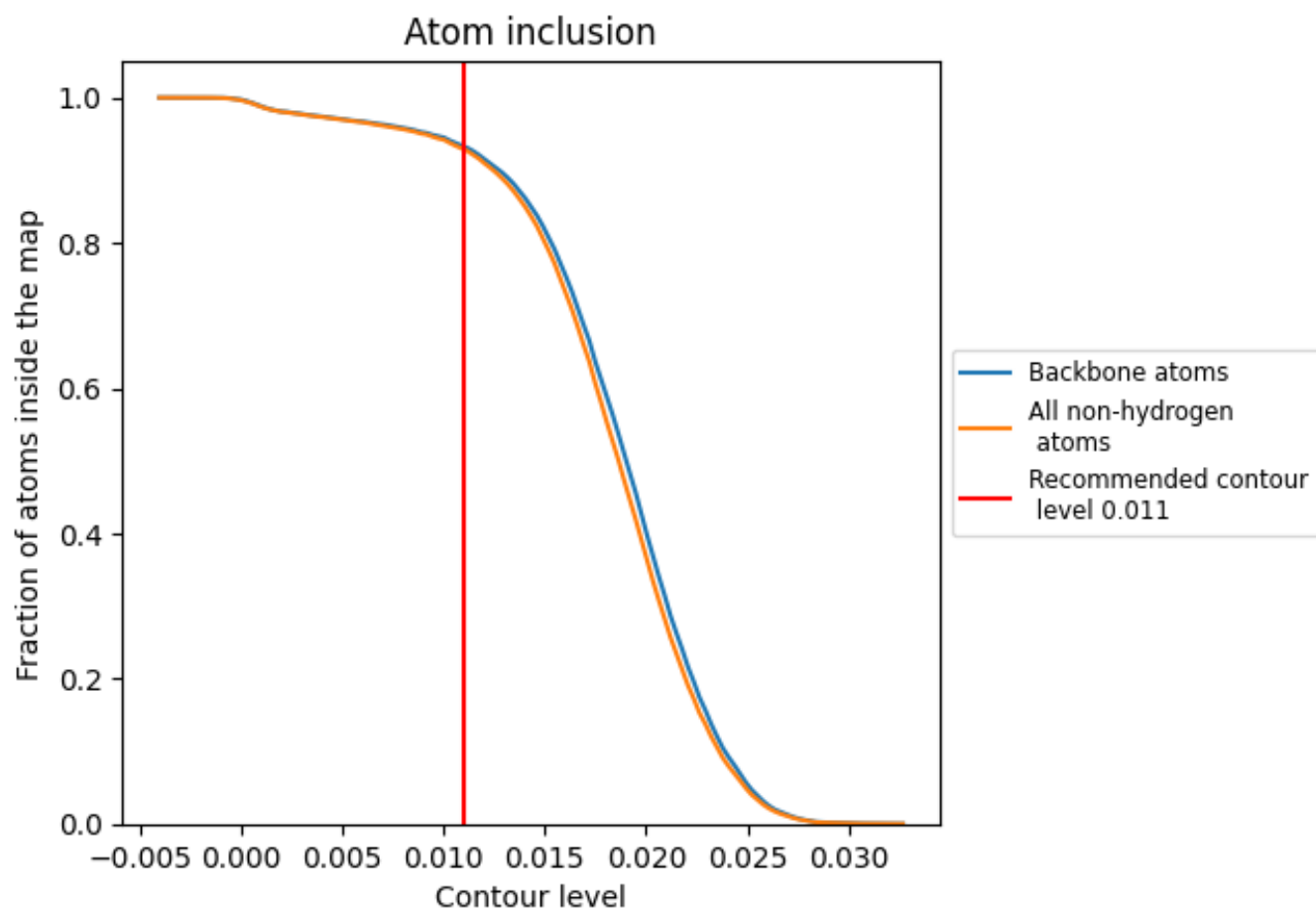
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9288	 0.1800
A	 0.9941	 0.2040
B	 0.9646	 0.2340
C	 0.9959	 0.2080
D	 0.9955	 0.2150
E	 0.9708	 0.2210
F	 0.9769	 0.2240
H	 0.8228	 0.0950
L	 0.7678	 0.0770
M	 0.8002	 0.1390

