wwPDB EM Validation Summary Report

Dec 5, 2022 – 02:11 PM EST

PDB ID	:	8D5C
EMDB ID	:	EMD-27208
Title	:	anti-HIV-1 gp120-sCD4 complex antibody CG10 Fab in complex with B41-sCD4
Authors	:	Yang, Z.; Bjorkman, P.J.; Gershoni, J.M.
Deposited on	:	2022-06-04
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

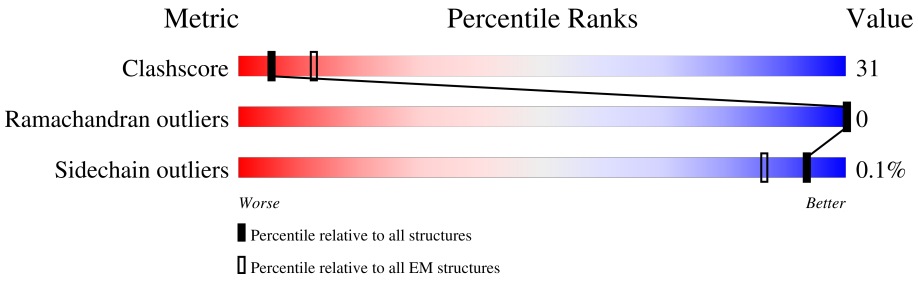
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	X	153	5% 49% 35% 16%
1	Y	153	48% 37% 16%
1	Z	153	43% 41% 16%
2	A	516	37% 36% 27%
2	B	516	41% 32% 27%
2	C	516	27% 46% 27%
3	D	183	16% 29% 67%
3	E	183	16% 48% 48%

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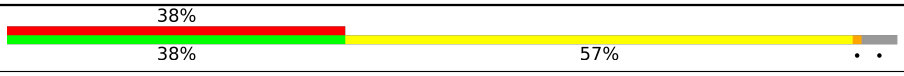
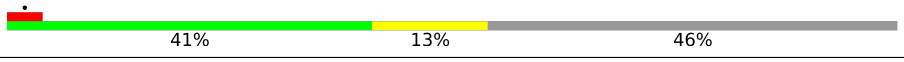
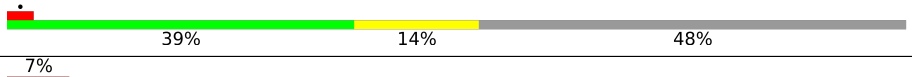
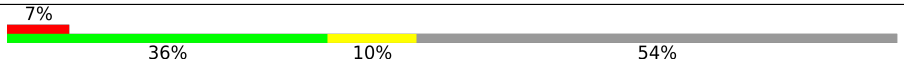
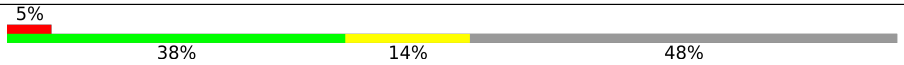
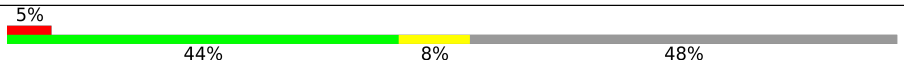
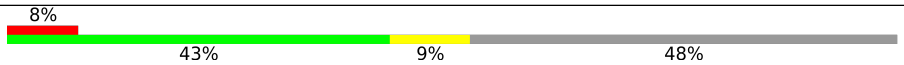
Mol	Chain	Length	Quality of chain
3	F	183	
4	H	228	
4	I	228	
4	P	228	
5	J	218	
5	L	218	
5	Q	218	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26109 atoms, of which 4739 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	129	Total	C	N	O	S	0	0
			1042	661	177	196	8		
1	Y	129	Total	C	N	O	S	0	0
			1042	661	177	196	8		
1	Z	129	Total	C	N	O	S	0	0
			1042	661	177	196	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	559	PRO	ILE	engineered mutation	UNP B3UEZ6
X	605	CYS	THR	engineered mutation	UNP B3UEZ6
Y	559	PRO	ILE	engineered mutation	UNP B3UEZ6
Y	605	CYS	THR	engineered mutation	UNP B3UEZ6
Z	559	PRO	ILE	engineered mutation	UNP B3UEZ6
Z	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	377	Total	C	N	O	S	0	0
			2952	1855	519	554	24		
2	B	377	Total	C	N	O	S	0	0
			2952	1855	519	554	24		
2	C	377	Total	C	N	O	S	0	0
			2952	1855	519	554	24		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP B3UES2
A	-3	ASP	-	expression tag	UNP B3UES2
A	-2	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP B3UES2
A	0	LYS	-	expression tag	UNP B3UES2
A	1	ARG	-	expression tag	UNP B3UES2
A	2	GLY	-	expression tag	UNP B3UES2
A	3	LEU	-	expression tag	UNP B3UES2
A	4	CYS	-	expression tag	UNP B3UES2
A	5	CYS	-	expression tag	UNP B3UES2
A	6	VAL	-	expression tag	UNP B3UES2
A	7	LEU	-	expression tag	UNP B3UES2
A	8	LEU	-	expression tag	UNP B3UES2
A	9	LEU	-	expression tag	UNP B3UES2
A	10	CYS	-	expression tag	UNP B3UES2
A	11	GLY	-	expression tag	UNP B3UES2
A	12	ALA	-	expression tag	UNP B3UES2
A	13	VAL	-	expression tag	UNP B3UES2
A	14	PHE	-	expression tag	UNP B3UES2
A	15	VAL	-	expression tag	UNP B3UES2
A	16	SER	-	expression tag	UNP B3UES2
A	17	PRO	-	expression tag	UNP B3UES2
A	18	SER	-	expression tag	UNP B3UES2
A	19	GLN	-	expression tag	UNP B3UES2
A	20	GLU	-	expression tag	UNP B3UES2
A	21	ILE	-	expression tag	UNP B3UES2
A	22	HIS	-	expression tag	UNP B3UES2
A	23	ALA	-	expression tag	UNP B3UES2
A	24	ARG	-	expression tag	UNP B3UES2
A	25	PHE	-	expression tag	UNP B3UES2
A	26	ARG	-	expression tag	UNP B3UES2
A	27	ARG	-	expression tag	UNP B3UES2
A	28	GLY	-	expression tag	UNP B3UES2
A	29	ALA	-	expression tag	UNP B3UES2
A	30	ARG	-	expression tag	UNP B3UES2
A	501	CYS	ALA	conflict	UNP B3UES2
B	-4	MET	-	expression tag	UNP B3UES2
B	-3	ASP	-	expression tag	UNP B3UES2
B	-2	ALA	-	expression tag	UNP B3UES2
B	-1	MET	-	expression tag	UNP B3UES2
B	0	LYS	-	expression tag	UNP B3UES2
B	1	ARG	-	expression tag	UNP B3UES2
B	2	GLY	-	expression tag	UNP B3UES2
B	3	LEU	-	expression tag	UNP B3UES2
B	4	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	CYS	-	expression tag	UNP B3UES2
B	6	VAL	-	expression tag	UNP B3UES2
B	7	LEU	-	expression tag	UNP B3UES2
B	8	LEU	-	expression tag	UNP B3UES2
B	9	LEU	-	expression tag	UNP B3UES2
B	10	CYS	-	expression tag	UNP B3UES2
B	11	GLY	-	expression tag	UNP B3UES2
B	12	ALA	-	expression tag	UNP B3UES2
B	13	VAL	-	expression tag	UNP B3UES2
B	14	PHE	-	expression tag	UNP B3UES2
B	15	VAL	-	expression tag	UNP B3UES2
B	16	SER	-	expression tag	UNP B3UES2
B	17	PRO	-	expression tag	UNP B3UES2
B	18	SER	-	expression tag	UNP B3UES2
B	19	GLN	-	expression tag	UNP B3UES2
B	20	GLU	-	expression tag	UNP B3UES2
B	21	ILE	-	expression tag	UNP B3UES2
B	22	HIS	-	expression tag	UNP B3UES2
B	23	ALA	-	expression tag	UNP B3UES2
B	24	ARG	-	expression tag	UNP B3UES2
B	25	PHE	-	expression tag	UNP B3UES2
B	26	ARG	-	expression tag	UNP B3UES2
B	27	ARG	-	expression tag	UNP B3UES2
B	28	GLY	-	expression tag	UNP B3UES2
B	29	ALA	-	expression tag	UNP B3UES2
B	30	ARG	-	expression tag	UNP B3UES2
B	501	CYS	ALA	conflict	UNP B3UES2
C	-4	MET	-	expression tag	UNP B3UES2
C	-3	ASP	-	expression tag	UNP B3UES2
C	-2	ALA	-	expression tag	UNP B3UES2
C	-1	MET	-	expression tag	UNP B3UES2
C	0	LYS	-	expression tag	UNP B3UES2
C	1	ARG	-	expression tag	UNP B3UES2
C	2	GLY	-	expression tag	UNP B3UES2
C	3	LEU	-	expression tag	UNP B3UES2
C	4	CYS	-	expression tag	UNP B3UES2
C	5	CYS	-	expression tag	UNP B3UES2
C	6	VAL	-	expression tag	UNP B3UES2
C	7	LEU	-	expression tag	UNP B3UES2
C	8	LEU	-	expression tag	UNP B3UES2
C	9	LEU	-	expression tag	UNP B3UES2
C	10	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	expression tag	UNP B3UES2
C	12	ALA	-	expression tag	UNP B3UES2
C	13	VAL	-	expression tag	UNP B3UES2
C	14	PHE	-	expression tag	UNP B3UES2
C	15	VAL	-	expression tag	UNP B3UES2
C	16	SER	-	expression tag	UNP B3UES2
C	17	PRO	-	expression tag	UNP B3UES2
C	18	SER	-	expression tag	UNP B3UES2
C	19	GLN	-	expression tag	UNP B3UES2
C	20	GLU	-	expression tag	UNP B3UES2
C	21	ILE	-	expression tag	UNP B3UES2
C	22	HIS	-	expression tag	UNP B3UES2
C	23	ALA	-	expression tag	UNP B3UES2
C	24	ARG	-	expression tag	UNP B3UES2
C	25	PHE	-	expression tag	UNP B3UES2
C	26	ARG	-	expression tag	UNP B3UES2
C	27	ARG	-	expression tag	UNP B3UES2
C	28	GLY	-	expression tag	UNP B3UES2
C	29	ALA	-	expression tag	UNP B3UES2
C	30	ARG	-	expression tag	UNP B3UES2
C	501	CYS	ALA	conflict	UNP B3UES2

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
3	E	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
3	F	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		

- Molecule 4 is a protein called CG10 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	122	Total	C	H	N	O	S	0	0
			1790	617	832	150	186	5		
4	I	119	Total	C	H	N	O	S	0	0
			1766	608	825	150	178	5		
4	P	104	Total	C	H	N	O	S	0	0
			1523	512	721	132	153	5		

- Molecule 5 is a protein called CG10 Fab light chain.

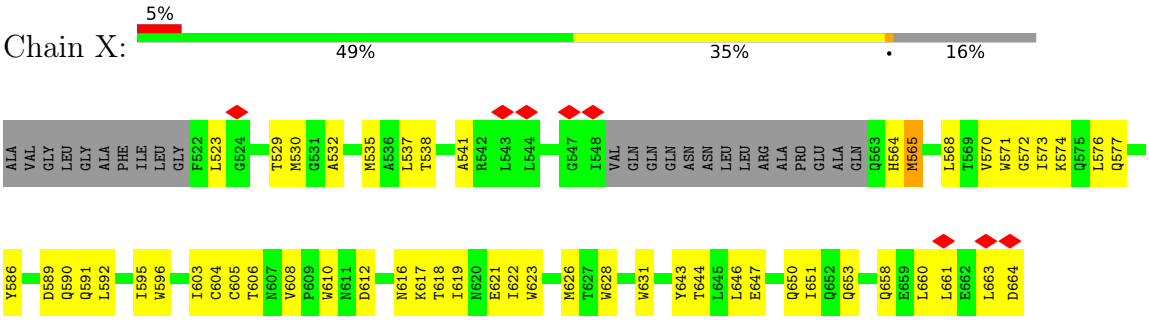
Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	113	Total	C	H	N	O	S	0	0
			1646	537	787	143	175	4		
5	J	113	Total	C	H	N	O	S	0	0
			1646	537	787	143	175	4		
5	Q	113	Total	C	H	N	O	S	0	0
			1646	537	787	143	175	4		

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.

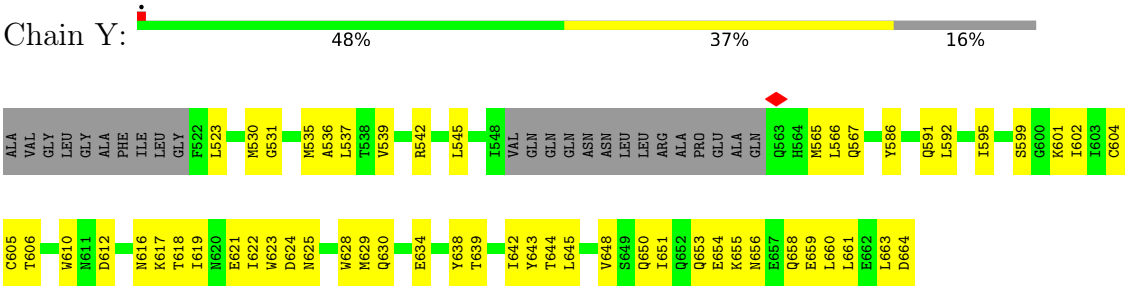
• Molecule 1: Envelope glycoprotein gp41

Chain X:



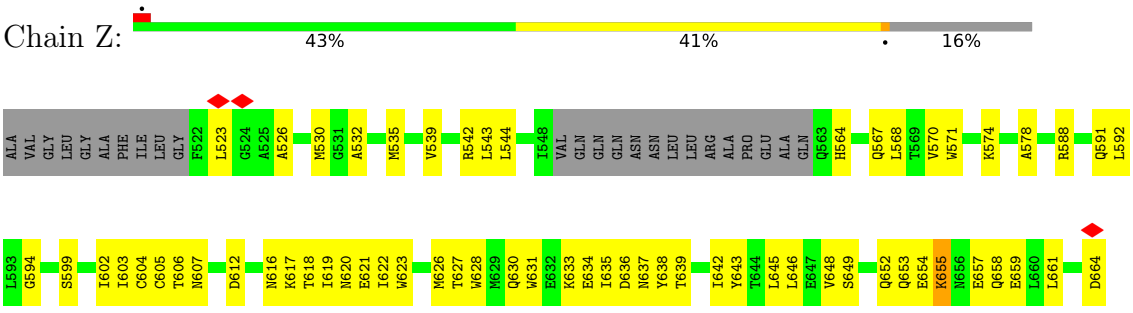
• Molecule 1: Envelope glycoprotein gp41

Chain Y:



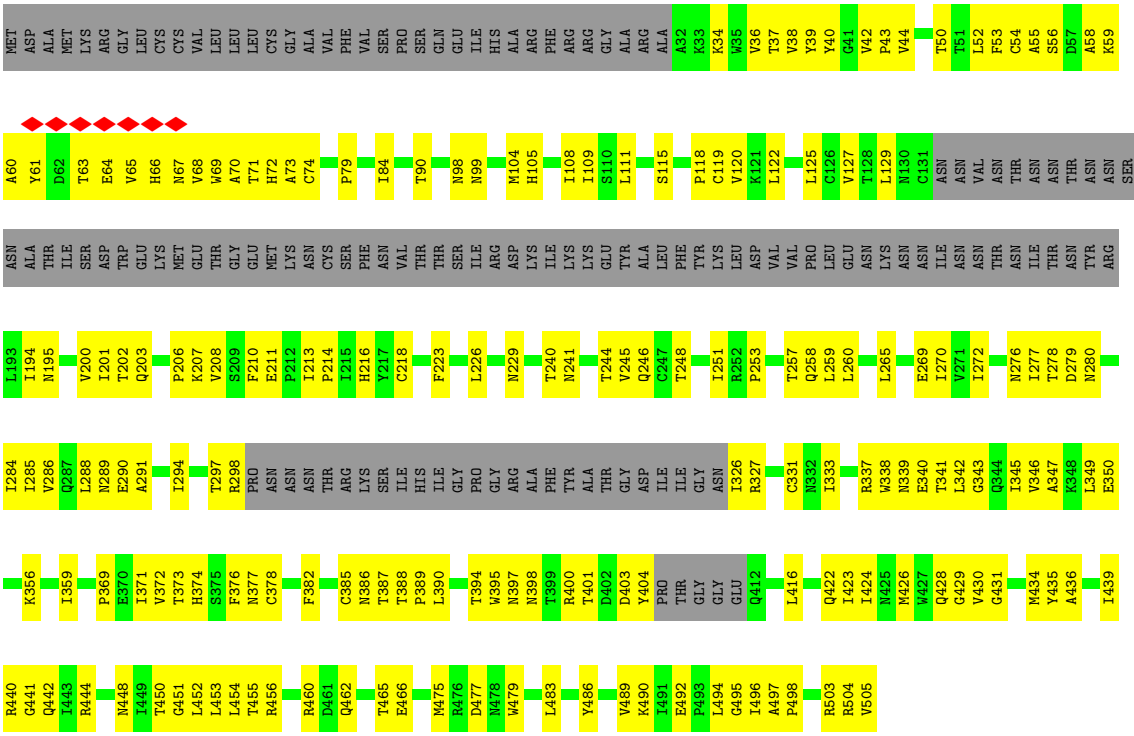
• Molecule 1: Envelope glycoprotein gp41

Chain Z:



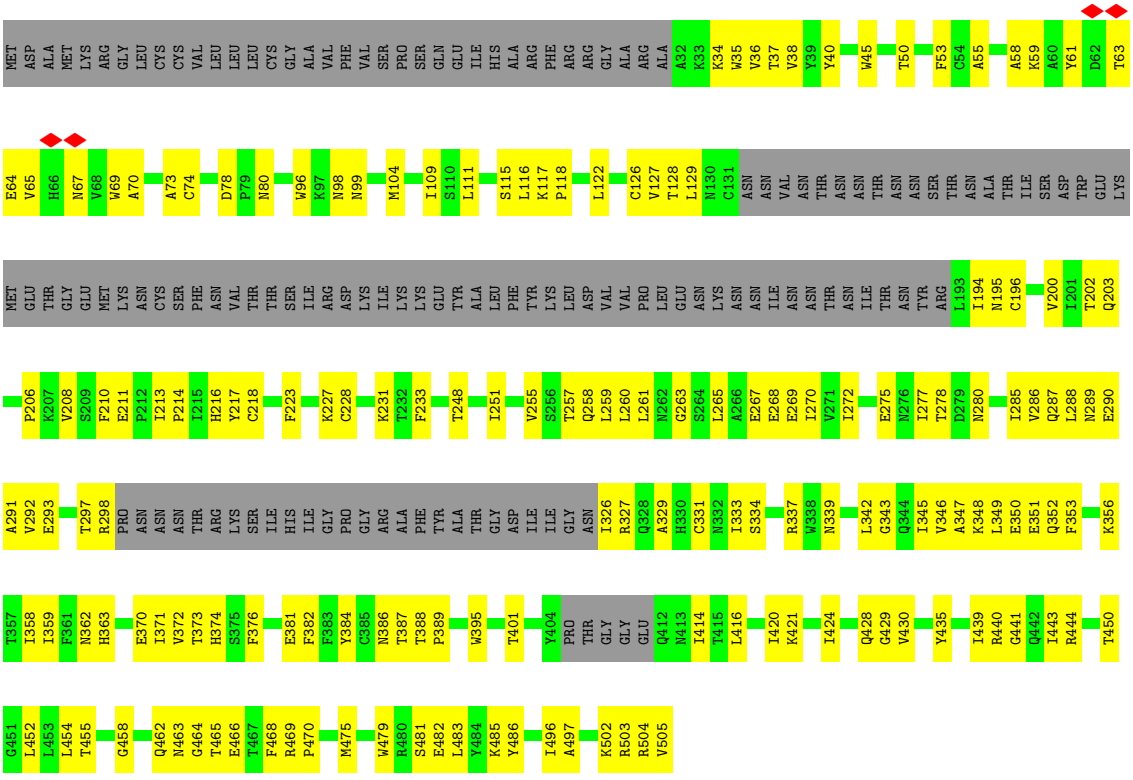
• Molecule 2: Envelope glycoprotein gp160

Chain A:

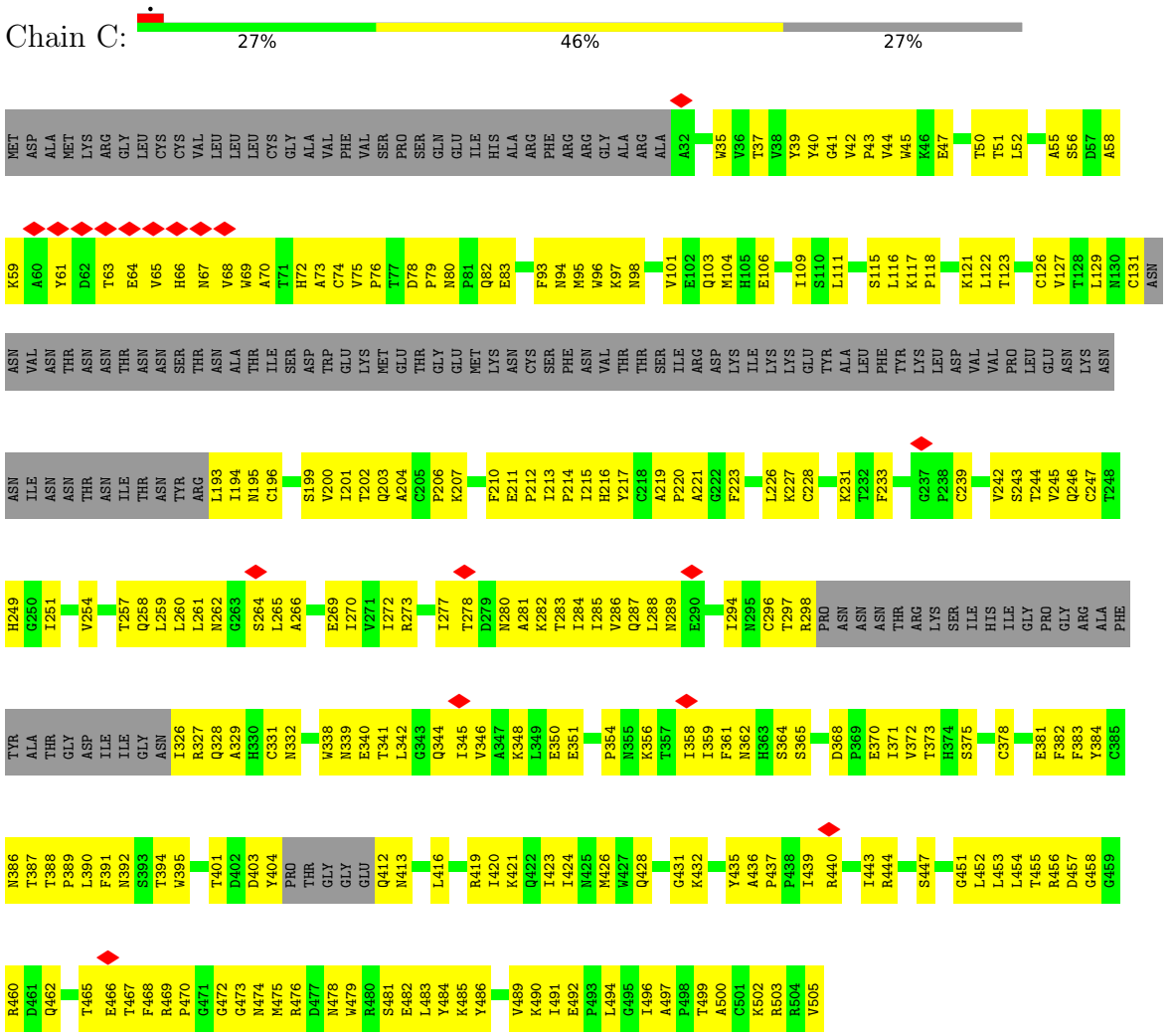


• Molecule 2: Envelope glycoprotein gp160

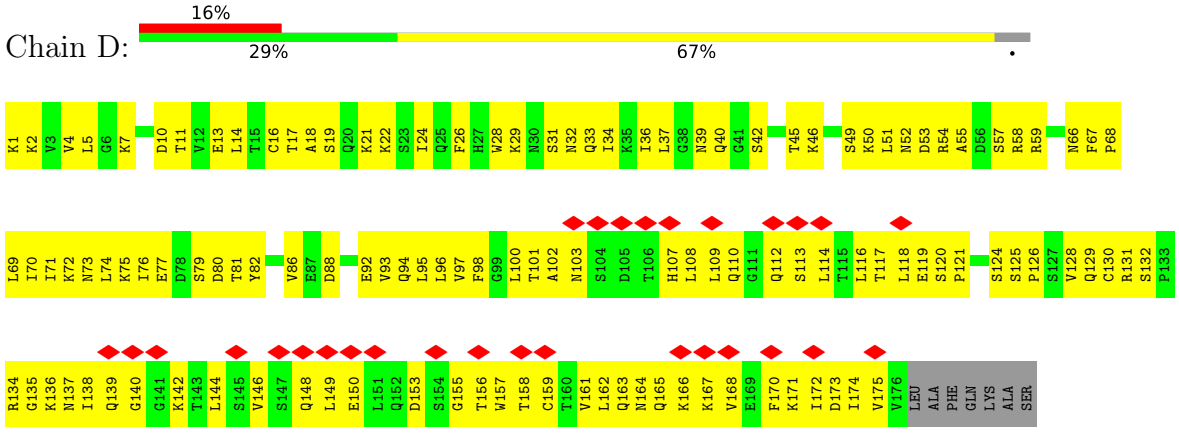
Chain B:



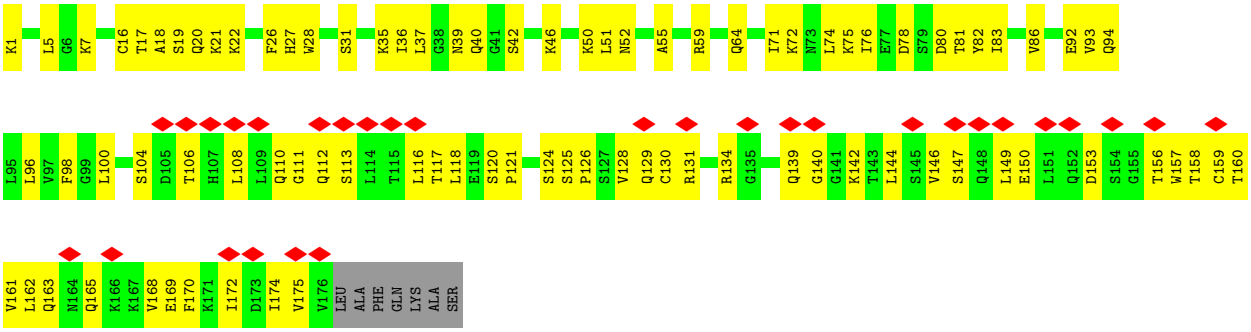
• Molecule 2: Envelope glycoprotein gp160



• Molecule 3: T-cell surface glycoprotein CD4

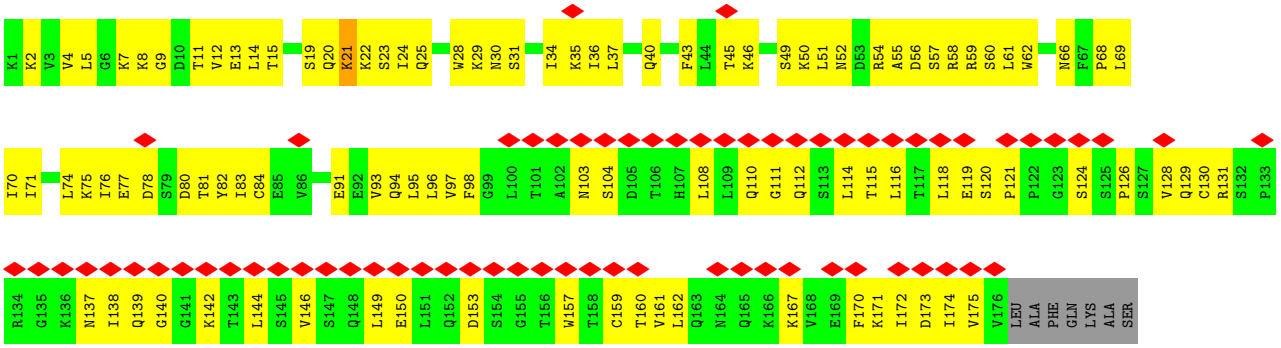


• Molecule 3: T-cell surface glycoprotein CD4



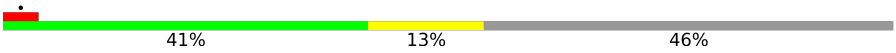
• Molecule 3: T-cell surface glycoprotein CD4

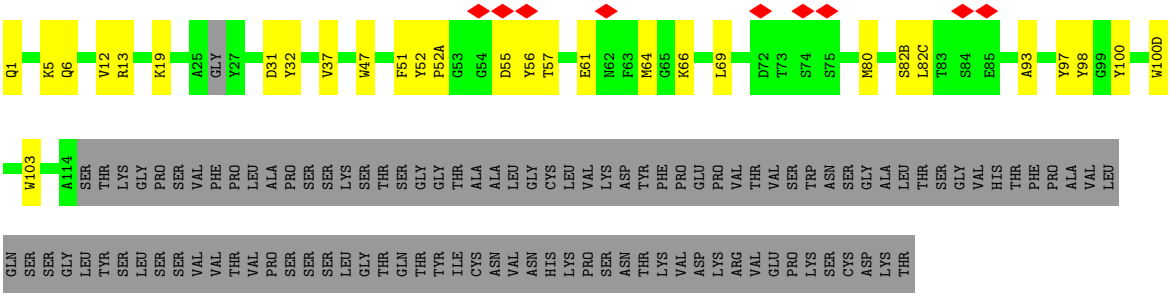
Chain F:



• Molecule 4: CG10 Fab heavy chain

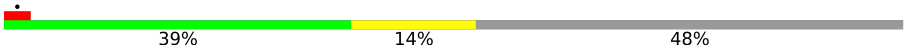
Chain H:

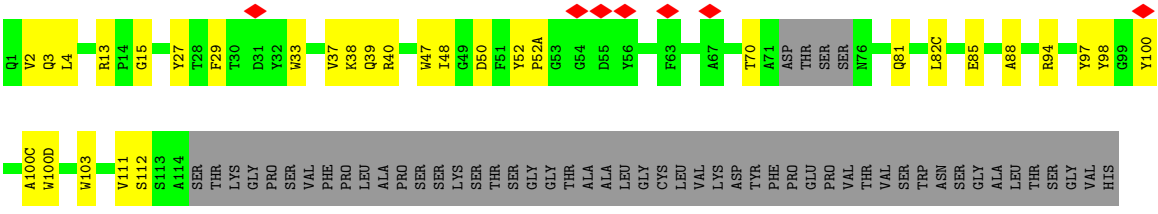




• Molecule 4: CG10 Fab heavy chain

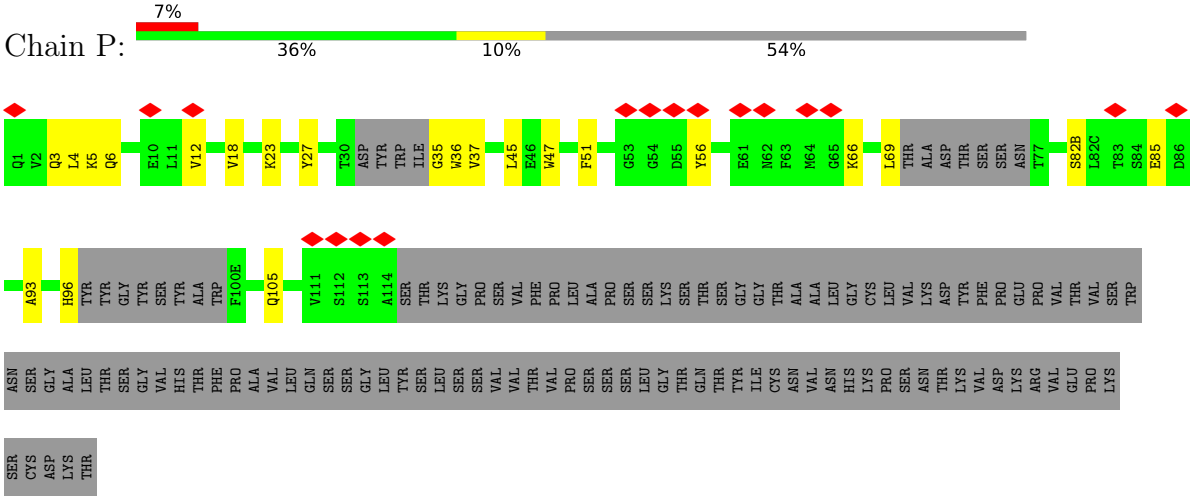
Chain I:





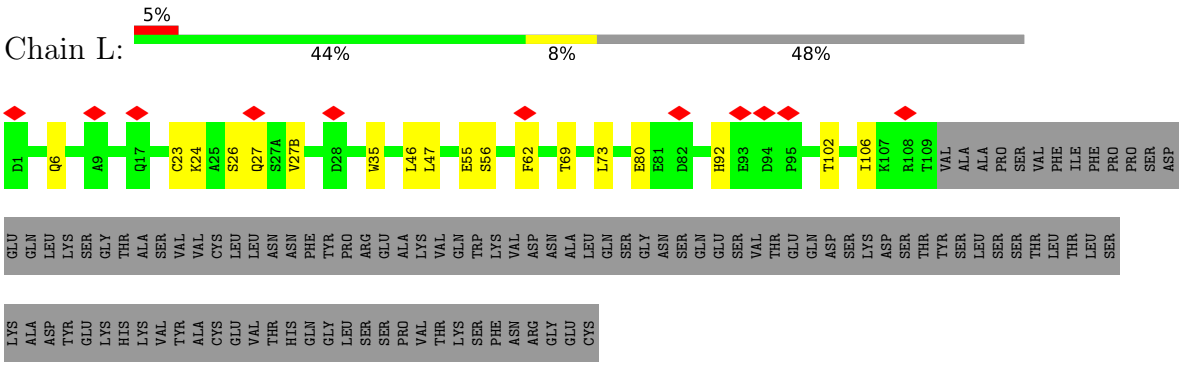
• Molecule 4: CG10 Fab heavy chain

Chain P:



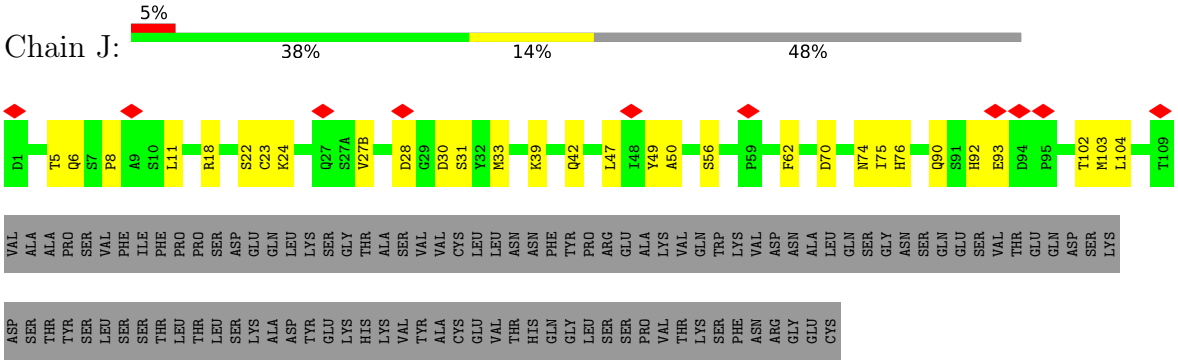
• Molecule 5: CG10 Fab light chain

Chain L:



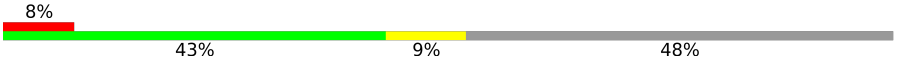
• Molecule 5: CG10 Fab light chain

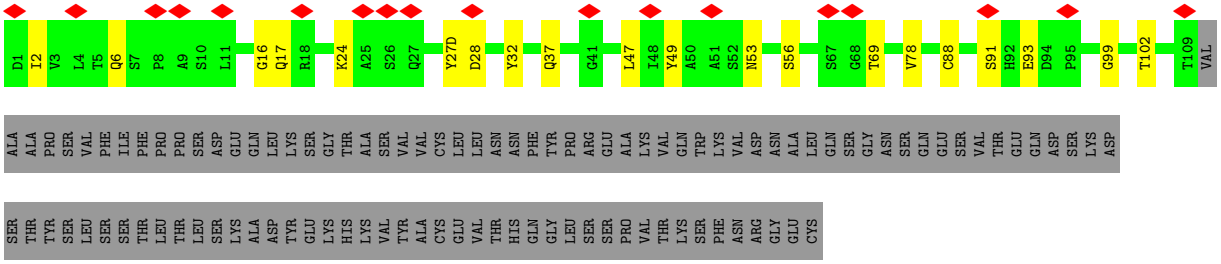
Chain J:



• Molecule 5: CG10 Fab light chain

Chain Q:




D1 I2 V3 L4 T5 Q6 S7 P8 A9 S10 L11 G16 Q17 R18 K24 A25 S26 Q27 Y27D D28 Y32 Q37 G41 L47 I48 Y49 A50 A51 S52 N53 S56 S67 G68 T69 V78 C88 S91 H92 E93 D94 P95 G99 T102 T109 VAL
ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP
SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134746	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.161	Depositor
Minimum map value	-0.715	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.105	Depositor
Map size (Å)	333.0, 333.0, 333.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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	X	0.23	0/1061	0.41	0/1437
1	Y	0.23	0/1061	0.41	0/1437
1	Z	0.23	0/1061	0.43	0/1437
2	A	0.24	0/3015	0.48	0/4100
2	B	0.23	0/3015	0.47	0/4100
2	C	0.24	0/3015	0.48	0/4100
3	D	0.23	0/1389	0.47	0/1873
3	E	0.24	0/1389	0.47	0/1873
3	F	0.23	0/1389	0.45	0/1873
4	H	0.26	0/988	0.50	0/1344
4	I	0.26	0/971	0.50	0/1319
4	P	0.25	0/821	0.47	0/1107
5	J	0.25	0/880	0.47	0/1197
5	L	0.25	0/880	0.48	0/1197
5	Q	0.25	0/880	0.48	0/1197
All	All	0.24	0/21815	0.47	0/29591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1042	0	1026	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1042	0	1026	59	0
1	Z	1042	0	1025	86	0
2	A	2952	0	2895	198	0
2	B	2952	0	2895	169	0
2	C	2952	0	2894	296	0
3	D	1370	0	1398	166	0
3	E	1370	0	1398	100	0
3	F	1370	0	1398	176	0
4	H	958	832	882	28	0
4	I	941	825	875	23	0
4	P	802	721	762	20	0
5	J	859	787	812	26	0
5	L	859	787	812	11	0
5	Q	859	787	812	20	0
All	All	21370	4739	20910	1322	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 31.

The worst 5 of 1322 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:C:131:CYS:HG	2:C:193:LEU:N	1.44	1.12
3:E:140:GLY:HA3	3:E:144:LEU:HD21	1.30	1.10
2:A:260:LEU:HD12	2:A:451:GLY:HA3	1.38	1.05
3:E:130:CYS:HA	3:E:159:CYS:HA	1.40	1.04
3:D:129:GLN:HG2	3:D:139:GLN:HE22	1.23	1.03

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	X	125/153 (82%)	120 (96%)	5 (4%)	0	100	100
1	Y	125/153 (82%)	120 (96%)	5 (4%)	0	100	100
1	Z	125/153 (82%)	119 (95%)	6 (5%)	0	100	100
2	A	369/516 (72%)	344 (93%)	25 (7%)	0	100	100
2	B	369/516 (72%)	340 (92%)	29 (8%)	0	100	100
2	C	369/516 (72%)	340 (92%)	29 (8%)	0	100	100
3	D	174/183 (95%)	162 (93%)	12 (7%)	0	100	100
3	E	174/183 (95%)	157 (90%)	17 (10%)	0	100	100
3	F	174/183 (95%)	165 (95%)	9 (5%)	0	100	100
4	H	118/228 (52%)	107 (91%)	11 (9%)	0	100	100
4	I	115/228 (50%)	102 (89%)	13 (11%)	0	100	100
4	P	96/228 (42%)	93 (97%)	3 (3%)	0	100	100
5	J	111/218 (51%)	101 (91%)	10 (9%)	0	100	100
5	L	111/218 (51%)	102 (92%)	9 (8%)	0	100	100
5	Q	111/218 (51%)	107 (96%)	4 (4%)	0	100	100
All	All	2666/3894 (68%)	2479 (93%)	187 (7%)	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	X	113/130 (87%)	112 (99%)	1 (1%)	78	87
1	Y	113/130 (87%)	113 (100%)	0	100	100
1	Z	113/130 (87%)	112 (99%)	1 (1%)	78	87
2	A	332/453 (73%)	332 (100%)	0	100	100
2	B	332/453 (73%)	332 (100%)	0	100	100
2	C	332/453 (73%)	332 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	160/165 (97%)	160 (100%)	0	100 100
3	E	160/165 (97%)	160 (100%)	0	100 100
3	F	160/165 (97%)	159 (99%)	1 (1%)	86 91
4	H	98/191 (51%)	98 (100%)	0	100 100
4	I	95/191 (50%)	95 (100%)	0	100 100
4	P	83/191 (44%)	83 (100%)	0	100 100
5	J	93/187 (50%)	93 (100%)	0	100 100
5	L	93/187 (50%)	93 (100%)	0	100 100
5	Q	93/187 (50%)	93 (100%)	0	100 100
All	All	2370/3378 (70%)	2367 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	565	MET
1	Z	655	LYS
3	F	21	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	96	HIS
4	I	81	GLN
2	C	67	ASN
5	L	27	GLN
2	B	280	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

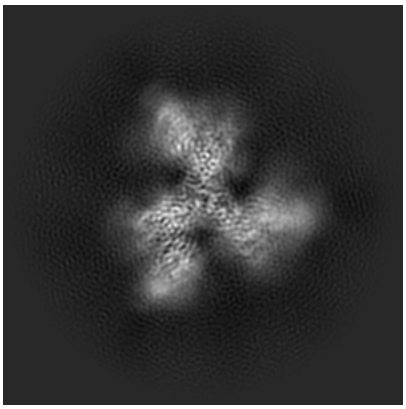
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27208. These allow visual inspection of the internal detail of the map and identification of artifacts.

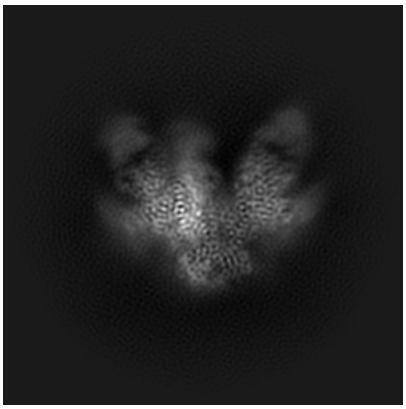
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

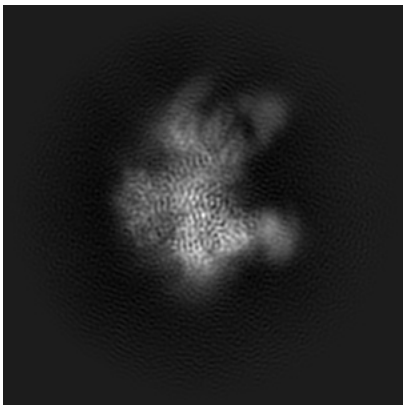
6.1.1 Primary map



X

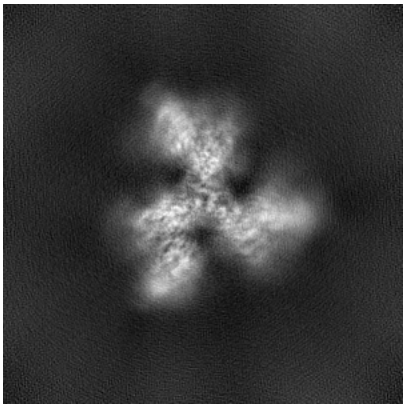


Y

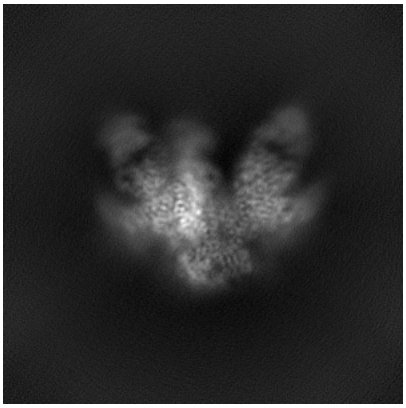


Z

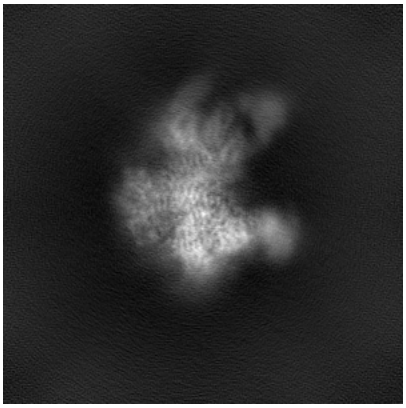
6.1.2 Raw map



X



Y

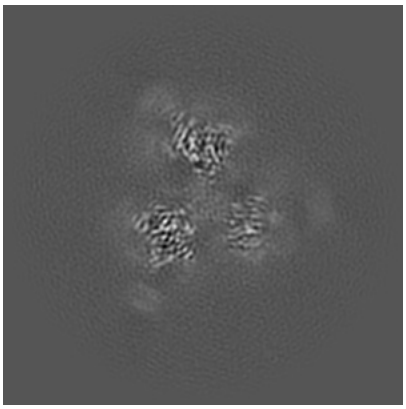


Z

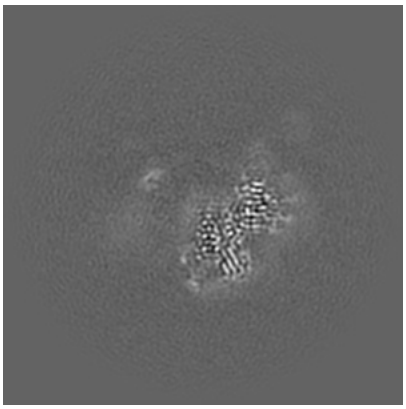
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

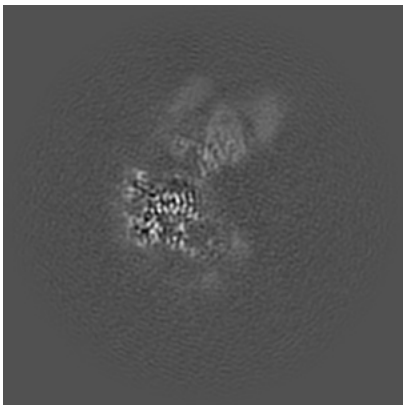
6.2.1 Primary map



X Index: 150

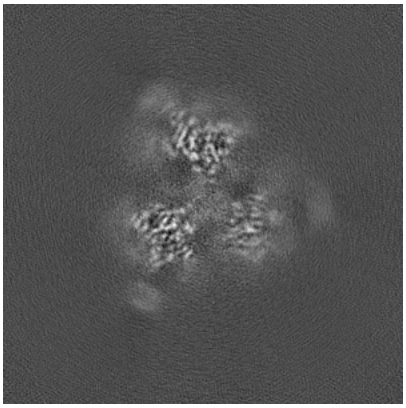


Y Index: 150

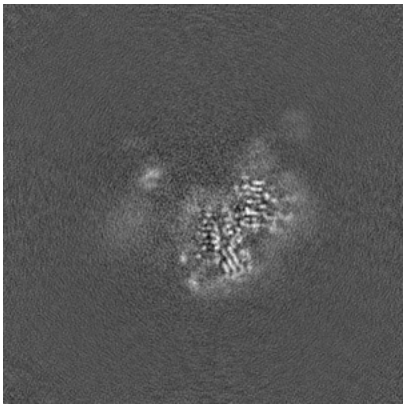


Z Index: 150

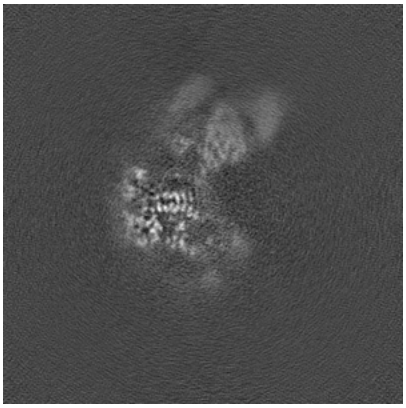
6.2.2 Raw map



X Index: 150



Y Index: 150

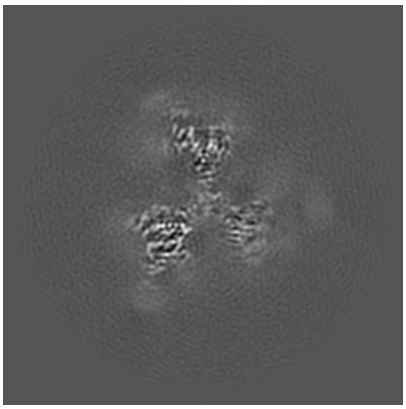


Z Index: 150

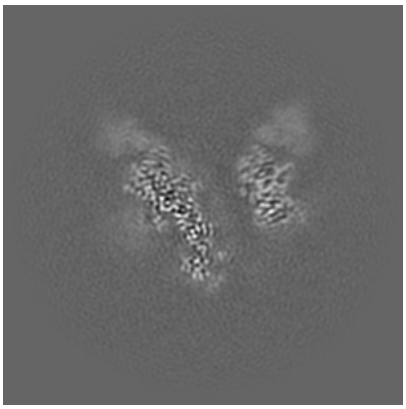
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

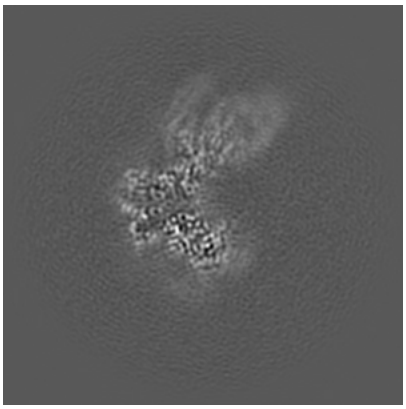
6.3.1 Primary map



X Index: 146

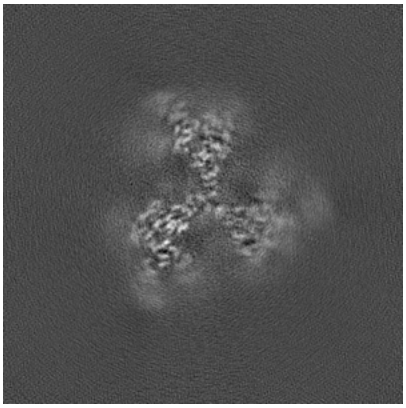


Y Index: 132

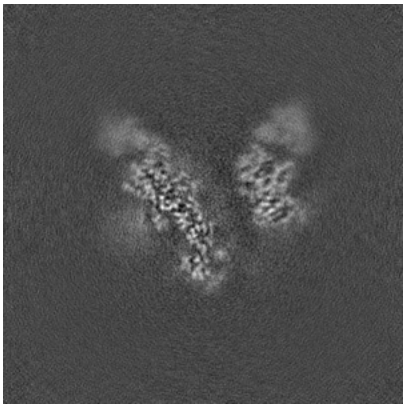


Z Index: 142

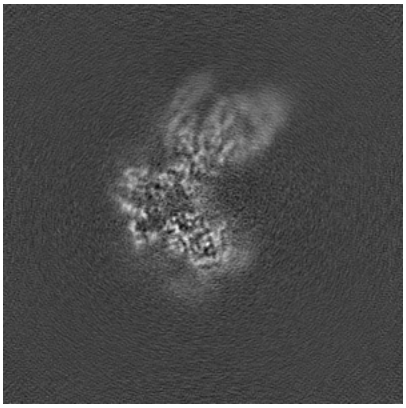
6.3.2 Raw map



X Index: 142



Y Index: 132



Z Index: 142

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 0.105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

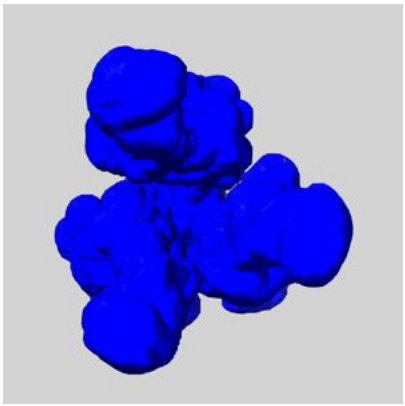
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

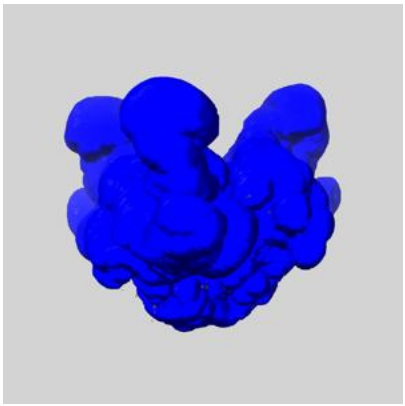
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

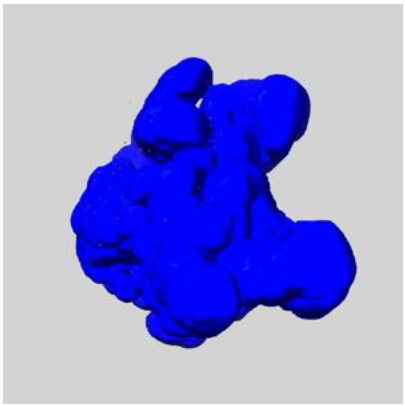
6.5.1 emd_27208_msk_1.map (i)



X



Y

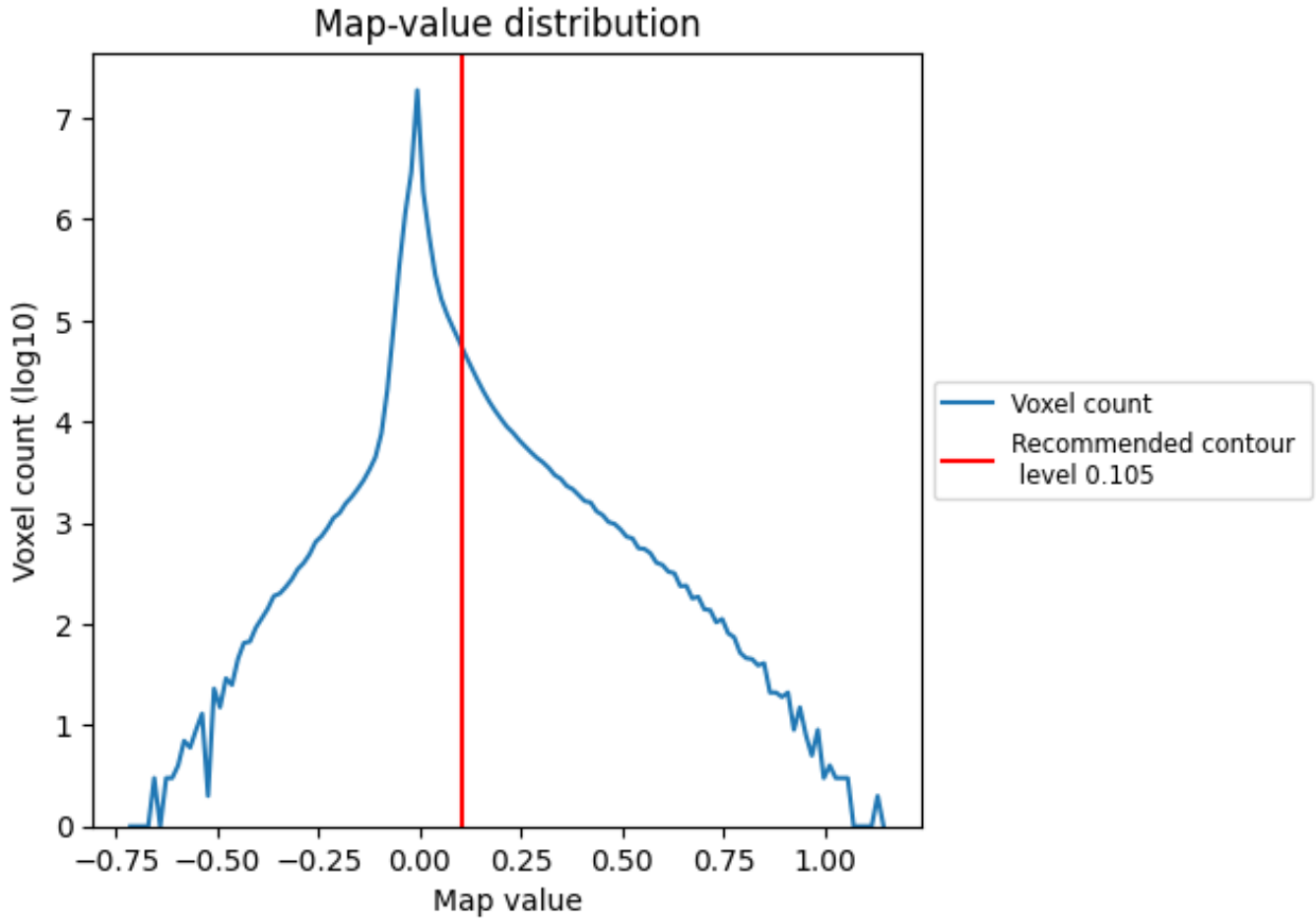


Z

7 Map analysis

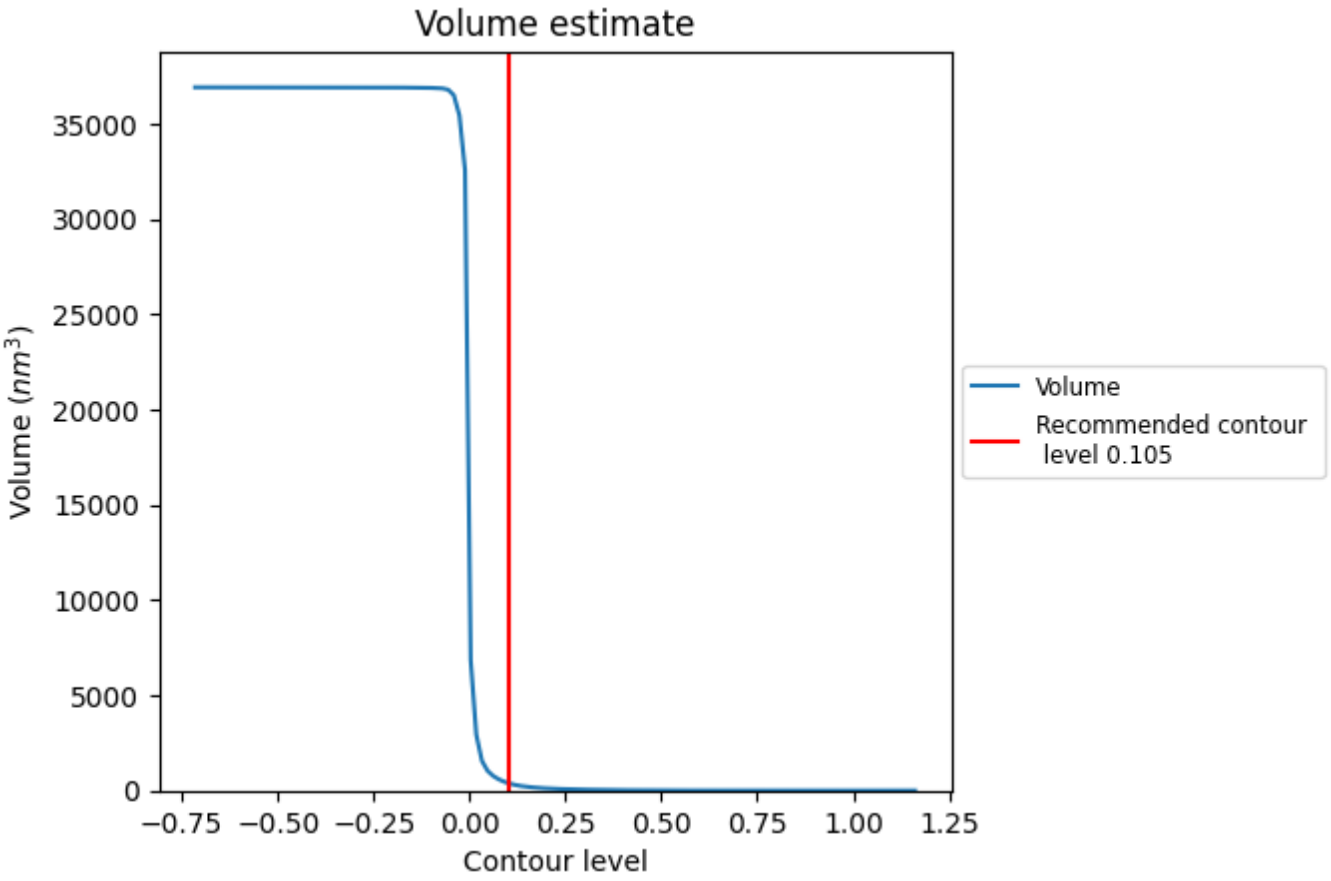
This section contains the results of statistical analysis of the map.

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.

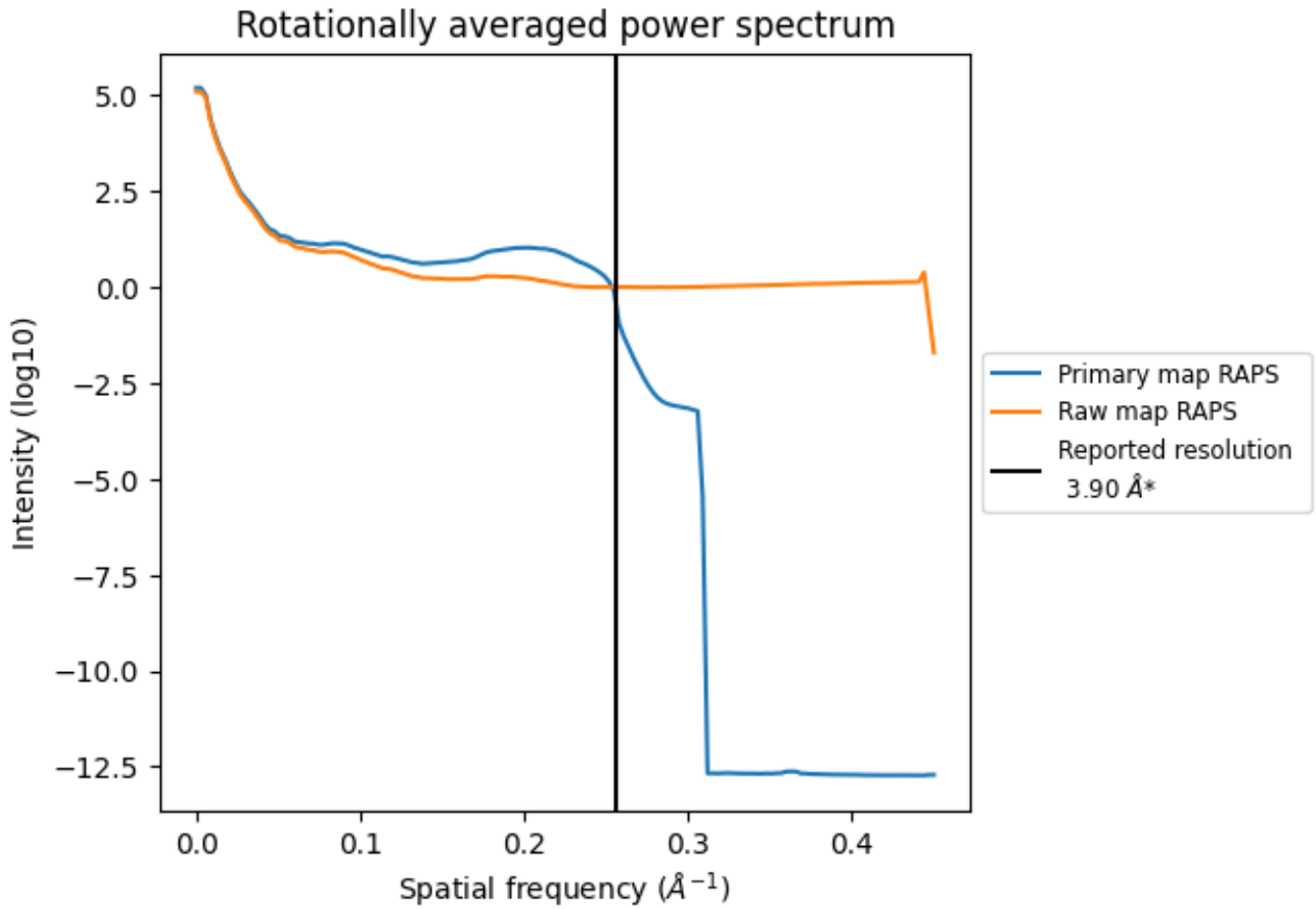
7.2 Volume estimate (i)



The volume at the recommended contour level is 368 nm^3; this corresponds to an approximate mass of 333 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)

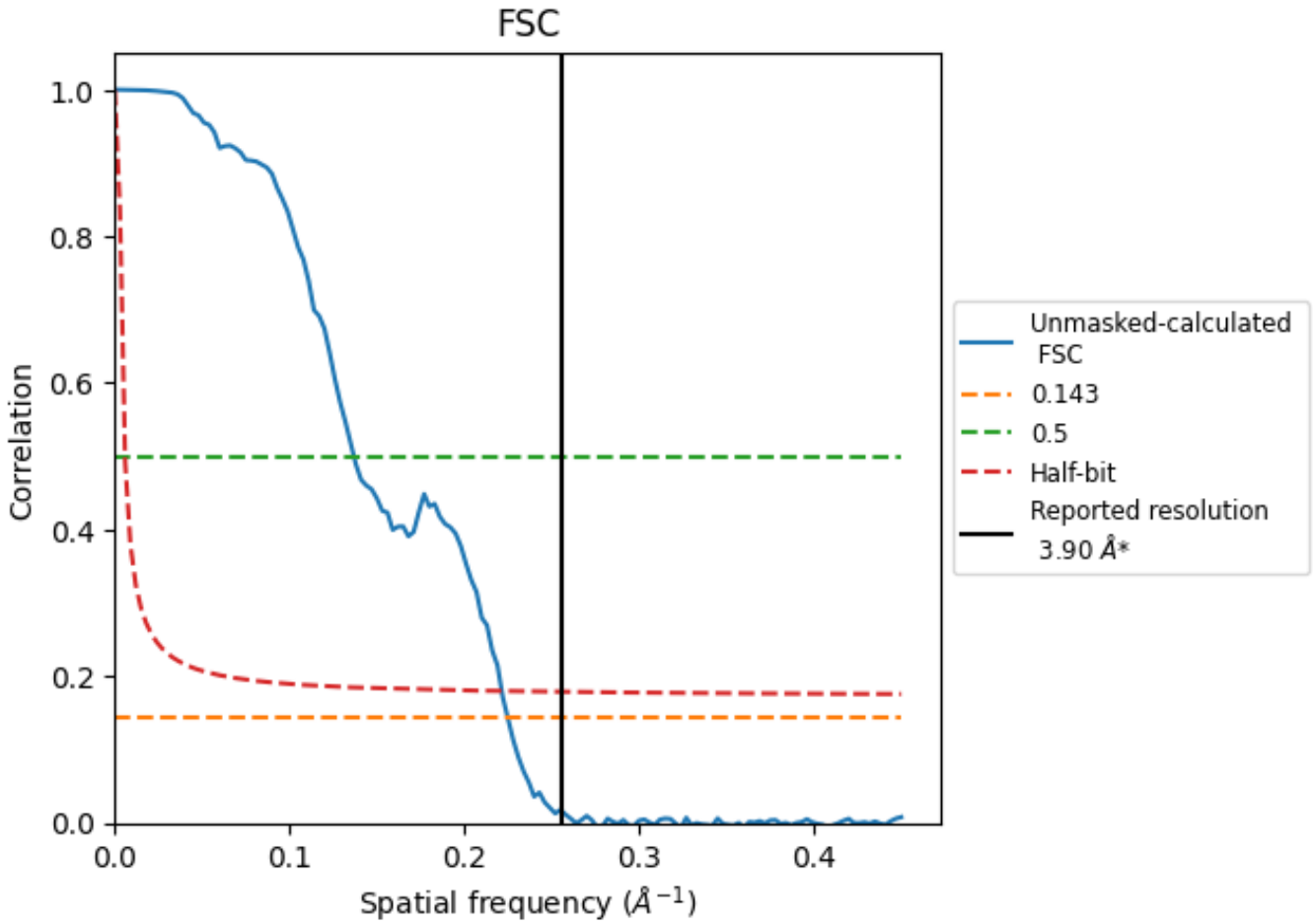


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

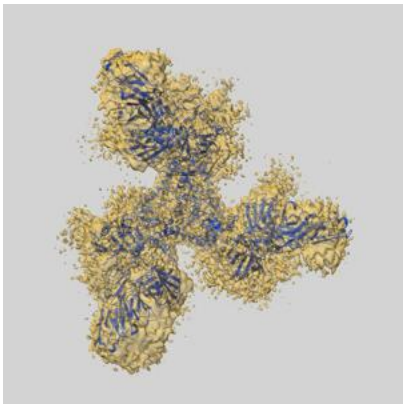
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	7.30	4.51

*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 4.44 differs from the reported value 3.9 by more than 10 %

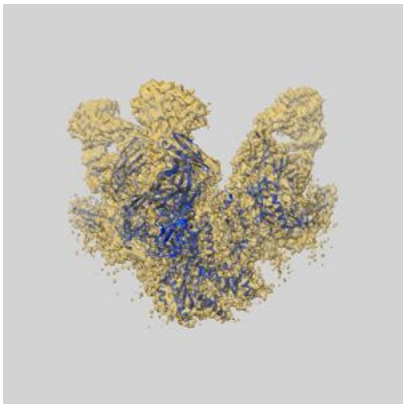
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27208 and PDB model 8D5C. Per-residue inclusion information can be found in section 3 on page 9.

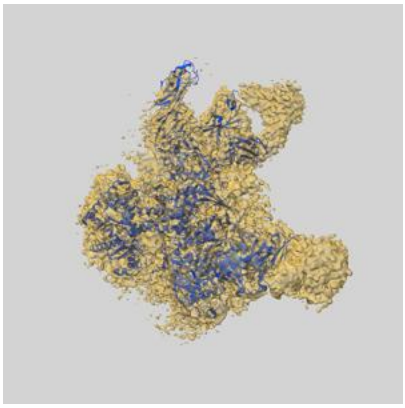
9.1 Map-model overlay



X



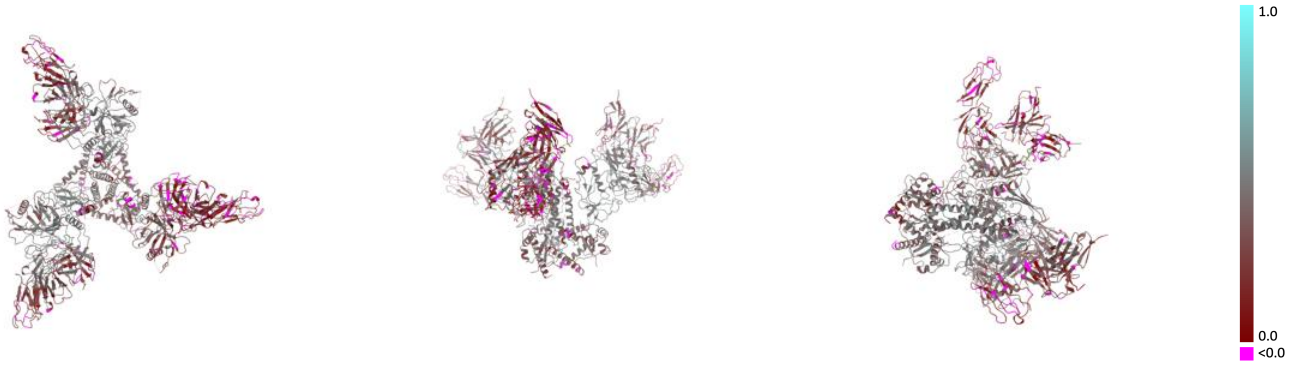
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.105 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.

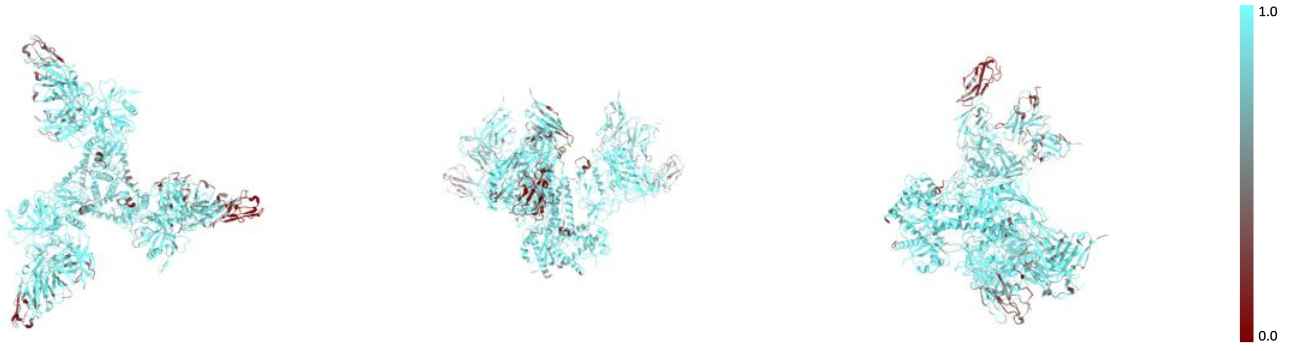
9.2 Q-score mapped to coordinate model



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.

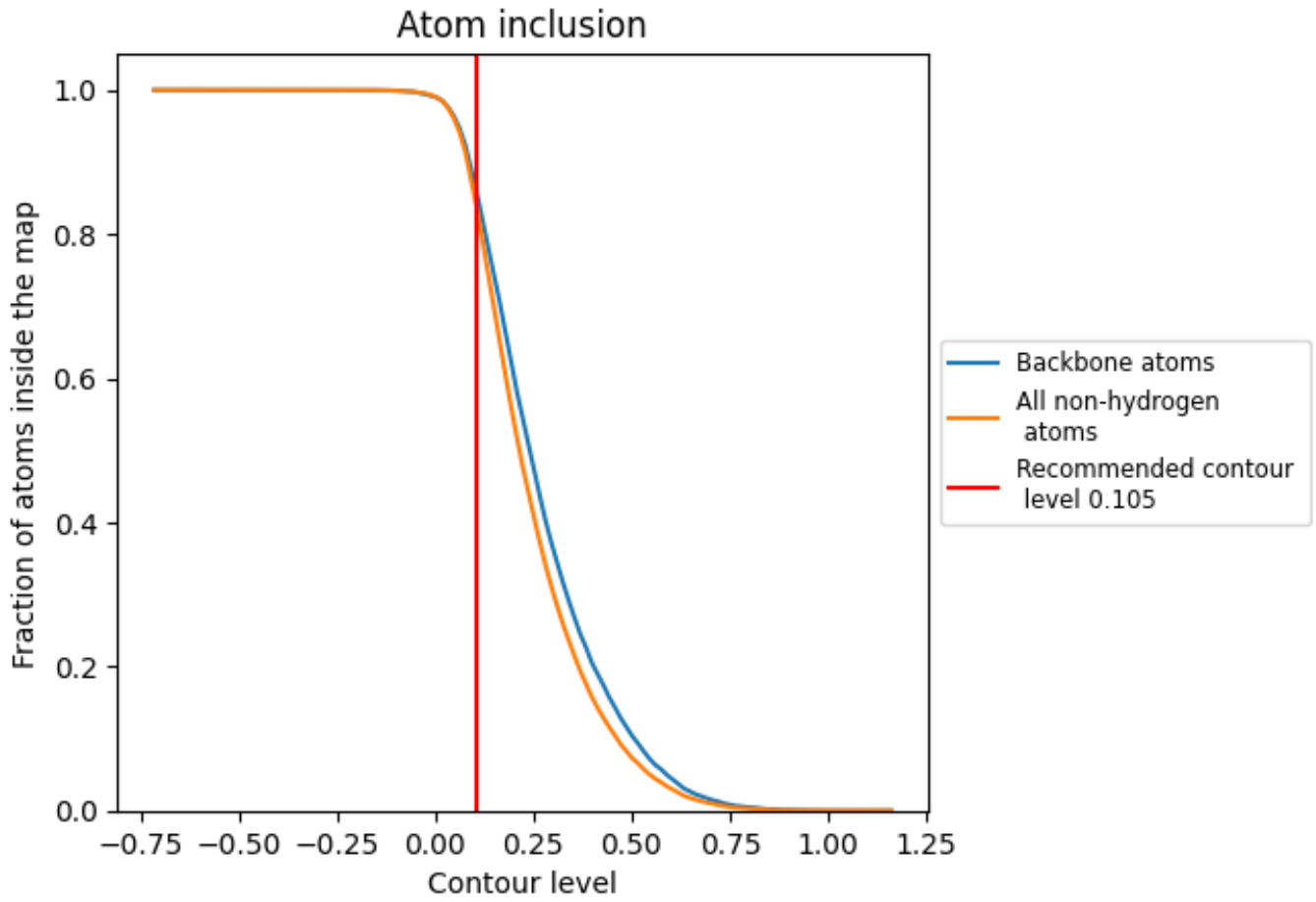
9.3 Atom inclusion mapped to coordinate model



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 (0.105).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8387	0.3360
A	0.9352	0.4460
B	0.9397	0.4390
C	0.8715	0.3350
D	0.7375	0.3140
E	0.7640	0.3610
F	0.5288	0.1740
H	0.8013	0.2790
I	0.8255	0.2910
J	0.8142	0.2830
L	0.7751	0.2520
P	0.7045	0.1730
Q	0.7231	0.1270
X	0.8809	0.3640
Y	0.9189	0.4050
Z	0.9004	0.3510