



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:52 PM UTC

PDB ID : 7UJA / pdb_00007uja
EMDB ID : EMD-26562
Title : Cryo-EM structure of Human respiratory syncytial virus F variant (construct pXCS847A)
Authors : Lees, J.A.; Ammirati, M.; Han, S.
Deposited on : 2022-03-30
Resolution : 3.70 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:

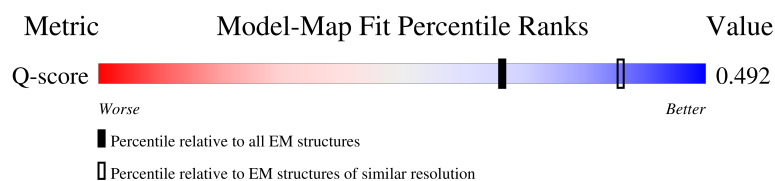
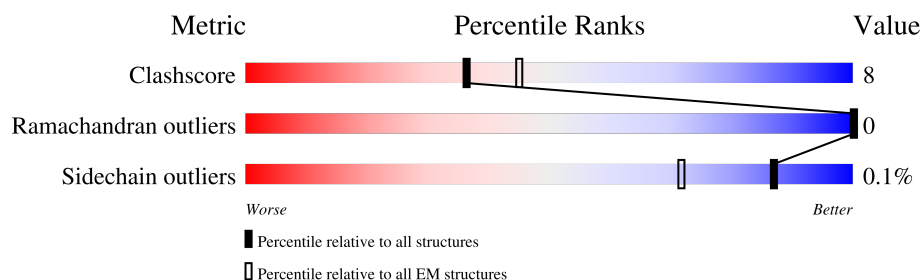
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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.



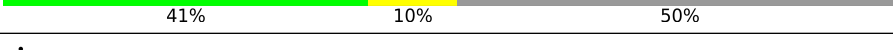
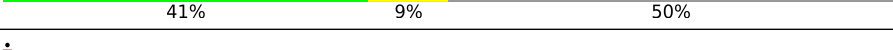
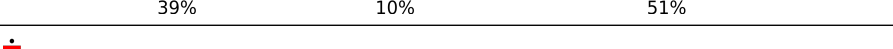
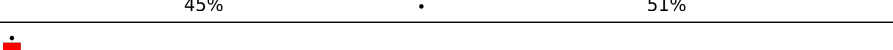
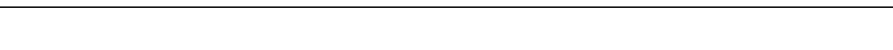
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	410	
1	C	410	
1	K	410	
2	B	245	

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Mol	Chain	Length	Quality of chain
2	G	245	
2	L	245	
3	D	218	
3	H	218	
3	M	218	
4	E	246	
4	I	246	
4	N	246	
5	F	215	
5	J	215	
5	O	215	
6	P	109	
6	Q	109	
6	R	109	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20748 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 RSV variant (construct pXCS847A) F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	372	Total	C	N	O	S	0	0
			2859	1804	474	562	19		
1	C	372	Total	C	N	O	S	0	0
			2859	1804	474	562	19		
1	K	372	Total	C	N	O	S	0	0
			2859	1804	474	562	19		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
A	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
A	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
A	514	SER	-	expression tag	UNP A0A7D5GVC1
A	515	ALA	-	expression tag	UNP A0A7D5GVC1
A	516	ILE	-	expression tag	UNP A0A7D5GVC1
A	517	GLY	-	expression tag	UNP A0A7D5GVC1
A	518	GLY	-	expression tag	UNP A0A7D5GVC1
A	519	TYR	-	expression tag	UNP A0A7D5GVC1
A	520	ILE	-	expression tag	UNP A0A7D5GVC1
A	521	PRO	-	expression tag	UNP A0A7D5GVC1
A	522	GLU	-	expression tag	UNP A0A7D5GVC1
A	523	ALA	-	expression tag	UNP A0A7D5GVC1
A	524	PRO	-	expression tag	UNP A0A7D5GVC1
A	525	ARG	-	expression tag	UNP A0A7D5GVC1
A	526	ASP	-	expression tag	UNP A0A7D5GVC1
A	527	GLY	-	expression tag	UNP A0A7D5GVC1
A	528	GLN	-	expression tag	UNP A0A7D5GVC1
A	529	ALA	-	expression tag	UNP A0A7D5GVC1
A	530	TYR	-	expression tag	UNP A0A7D5GVC1
A	531	VAL	-	expression tag	UNP A0A7D5GVC1
A	532	ARG	-	expression tag	UNP A0A7D5GVC1
A	533	LYS	-	expression tag	UNP A0A7D5GVC1
A	534	ASP	-	expression tag	UNP A0A7D5GVC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLY	-	expression tag	UNP A0A7D5GVC1
A	536	GLU	-	expression tag	UNP A0A7D5GVC1
A	537	TRP	-	expression tag	UNP A0A7D5GVC1
A	538	VAL	-	expression tag	UNP A0A7D5GVC1
A	539	LEU	-	expression tag	UNP A0A7D5GVC1
A	540	LEU	-	expression tag	UNP A0A7D5GVC1
A	541	SER	-	expression tag	UNP A0A7D5GVC1
A	542	THR	-	expression tag	UNP A0A7D5GVC1
A	543	PHE	-	expression tag	UNP A0A7D5GVC1
A	544	LEU	-	expression tag	UNP A0A7D5GVC1
A	545	GLY	-	expression tag	UNP A0A7D5GVC1
A	546	GLY	-	expression tag	UNP A0A7D5GVC1
C	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
C	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
C	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
C	514	SER	-	expression tag	UNP A0A7D5GVC1
C	515	ALA	-	expression tag	UNP A0A7D5GVC1
C	516	ILE	-	expression tag	UNP A0A7D5GVC1
C	517	GLY	-	expression tag	UNP A0A7D5GVC1
C	518	GLY	-	expression tag	UNP A0A7D5GVC1
C	519	TYR	-	expression tag	UNP A0A7D5GVC1
C	520	ILE	-	expression tag	UNP A0A7D5GVC1
C	521	PRO	-	expression tag	UNP A0A7D5GVC1
C	522	GLU	-	expression tag	UNP A0A7D5GVC1
C	523	ALA	-	expression tag	UNP A0A7D5GVC1
C	524	PRO	-	expression tag	UNP A0A7D5GVC1
C	525	ARG	-	expression tag	UNP A0A7D5GVC1
C	526	ASP	-	expression tag	UNP A0A7D5GVC1
C	527	GLY	-	expression tag	UNP A0A7D5GVC1
C	528	GLN	-	expression tag	UNP A0A7D5GVC1
C	529	ALA	-	expression tag	UNP A0A7D5GVC1
C	530	TYR	-	expression tag	UNP A0A7D5GVC1
C	531	VAL	-	expression tag	UNP A0A7D5GVC1
C	532	ARG	-	expression tag	UNP A0A7D5GVC1
C	533	LYS	-	expression tag	UNP A0A7D5GVC1
C	534	ASP	-	expression tag	UNP A0A7D5GVC1
C	535	GLY	-	expression tag	UNP A0A7D5GVC1
C	536	GLU	-	expression tag	UNP A0A7D5GVC1
C	537	TRP	-	expression tag	UNP A0A7D5GVC1
C	538	VAL	-	expression tag	UNP A0A7D5GVC1
C	539	LEU	-	expression tag	UNP A0A7D5GVC1
C	540	LEU	-	expression tag	UNP A0A7D5GVC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	541	SER	-	expression tag	UNP A0A7D5GVC1
C	542	THR	-	expression tag	UNP A0A7D5GVC1
C	543	PHE	-	expression tag	UNP A0A7D5GVC1
C	544	LEU	-	expression tag	UNP A0A7D5GVC1
C	545	GLY	-	expression tag	UNP A0A7D5GVC1
C	546	GLY	-	expression tag	UNP A0A7D5GVC1
K	148	CYS	ILE	engineered mutation	UNP A0A7D5GVC1
K	190	ILE	SER	engineered mutation	UNP A0A7D5GVC1
K	486	SER	ASP	engineered mutation	UNP A0A7D5GVC1
K	514	SER	-	expression tag	UNP A0A7D5GVC1
K	515	ALA	-	expression tag	UNP A0A7D5GVC1
K	516	ILE	-	expression tag	UNP A0A7D5GVC1
K	517	GLY	-	expression tag	UNP A0A7D5GVC1
K	518	GLY	-	expression tag	UNP A0A7D5GVC1
K	519	TYR	-	expression tag	UNP A0A7D5GVC1
K	520	ILE	-	expression tag	UNP A0A7D5GVC1
K	521	PRO	-	expression tag	UNP A0A7D5GVC1
K	522	GLU	-	expression tag	UNP A0A7D5GVC1
K	523	ALA	-	expression tag	UNP A0A7D5GVC1
K	524	PRO	-	expression tag	UNP A0A7D5GVC1
K	525	ARG	-	expression tag	UNP A0A7D5GVC1
K	526	ASP	-	expression tag	UNP A0A7D5GVC1
K	527	GLY	-	expression tag	UNP A0A7D5GVC1
K	528	GLN	-	expression tag	UNP A0A7D5GVC1
K	529	ALA	-	expression tag	UNP A0A7D5GVC1
K	530	TYR	-	expression tag	UNP A0A7D5GVC1
K	531	VAL	-	expression tag	UNP A0A7D5GVC1
K	532	ARG	-	expression tag	UNP A0A7D5GVC1
K	533	LYS	-	expression tag	UNP A0A7D5GVC1
K	534	ASP	-	expression tag	UNP A0A7D5GVC1
K	535	GLY	-	expression tag	UNP A0A7D5GVC1
K	536	GLU	-	expression tag	UNP A0A7D5GVC1
K	537	TRP	-	expression tag	UNP A0A7D5GVC1
K	538	VAL	-	expression tag	UNP A0A7D5GVC1
K	539	LEU	-	expression tag	UNP A0A7D5GVC1
K	540	LEU	-	expression tag	UNP A0A7D5GVC1
K	541	SER	-	expression tag	UNP A0A7D5GVC1
K	542	THR	-	expression tag	UNP A0A7D5GVC1
K	543	PHE	-	expression tag	UNP A0A7D5GVC1
K	544	LEU	-	expression tag	UNP A0A7D5GVC1
K	545	GLY	-	expression tag	UNP A0A7D5GVC1
K	546	GLY	-	expression tag	UNP A0A7D5GVC1

- Molecule 2 is a protein called AM14 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			934	587	162	180	5		
2	G	119	Total	C	N	O	S	0	0
			934	587	162	180	5		
2	L	119	Total	C	N	O	S	0	0
			934	587	162	180	5		

- Molecule 3 is a protein called AM14 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	99	Total	C	N	O	S	0	0
			769	483	129	153	4		
3	H	99	Total	C	N	O	S	0	0
			769	483	129	153	4		
3	M	99	Total	C	N	O	S	0	0
			769	483	129	153	4		

- Molecule 4 is a protein called AM22 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	124	Total	C	N	O	S	0	0
			940	598	155	183	4		
4	I	124	Total	C	N	O	S	0	0
			940	598	155	183	4		
4	N	124	Total	C	N	O	S	0	0
			940	598	155	183	4		

- Molecule 5 is a protein called AM22 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	105	Total	C	N	O	S	0	0
			785	497	135	151	2		
5	J	105	Total	C	N	O	S	0	0
			785	497	135	151	2		
5	O	105	Total	C	N	O	S	0	0
			785	497	135	151	2		

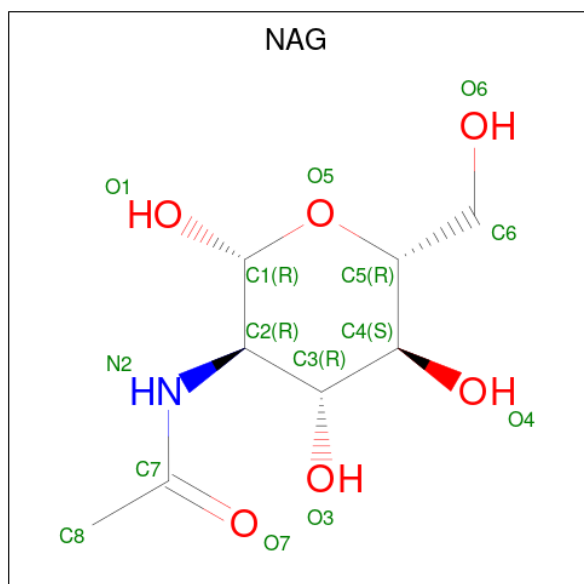
- Molecule 6 is a protein called RSV variant (construct pXCS847A) F2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	79	Total	C	N	O	S	0	0
			615	386	101	124	4		
6	Q	79	Total	C	N	O	S	0	0
			615	386	101	124	4		
6	R	79	Total	C	N	O	S	0	0
			615	386	101	124	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0A7D5GVC1
P	2	GLU	-	expression tag	UNP A0A7D5GVC1
P	3	LEU	-	expression tag	UNP A0A7D5GVC1
P	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1
Q	1	MET	-	initiating methionine	UNP A0A7D5GVC1
Q	2	GLU	-	expression tag	UNP A0A7D5GVC1
Q	3	LEU	-	expression tag	UNP A0A7D5GVC1
Q	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1
R	1	MET	-	initiating methionine	UNP A0A7D5GVC1
R	2	GLU	-	expression tag	UNP A0A7D5GVC1
R	3	LEU	-	expression tag	UNP A0A7D5GVC1
R	103	CYS	ALA	engineered mutation	UNP A0A7D5GVC1

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

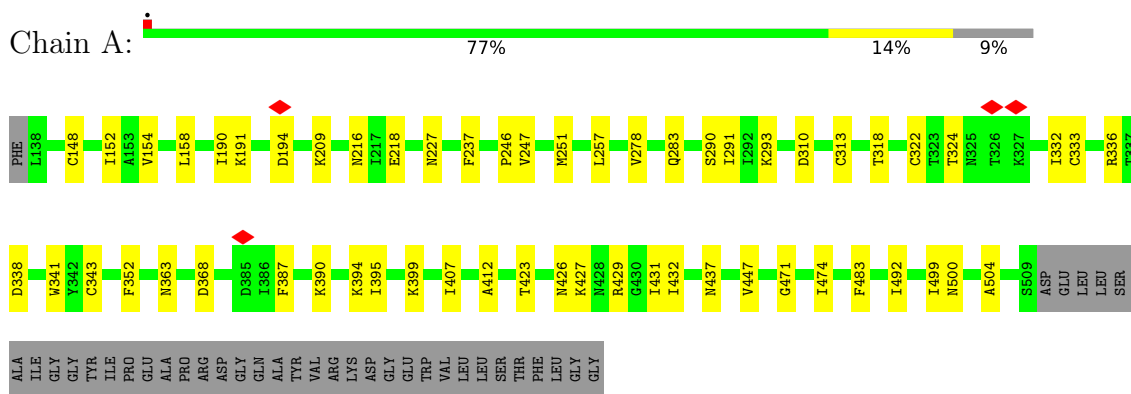


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	K	1	Total 14	C 8	N 1	O 5	0

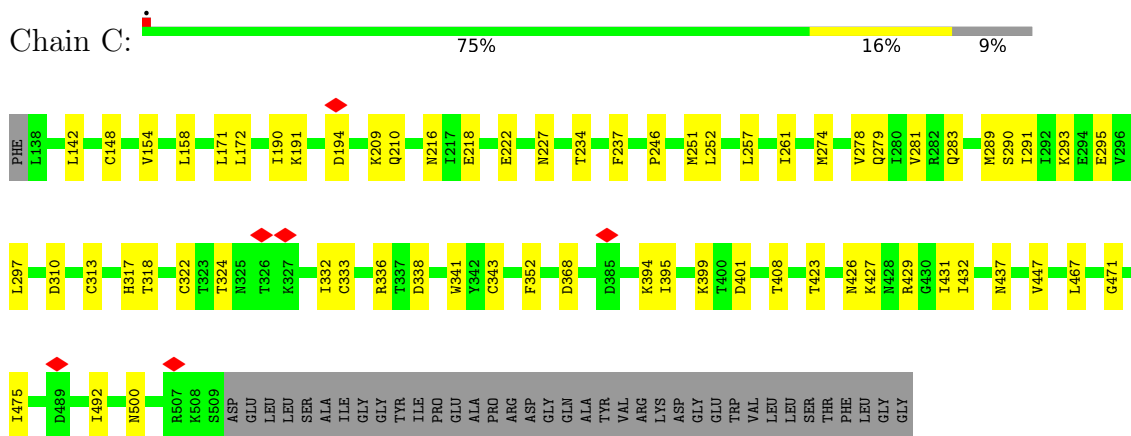
3 Residue-property plots

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

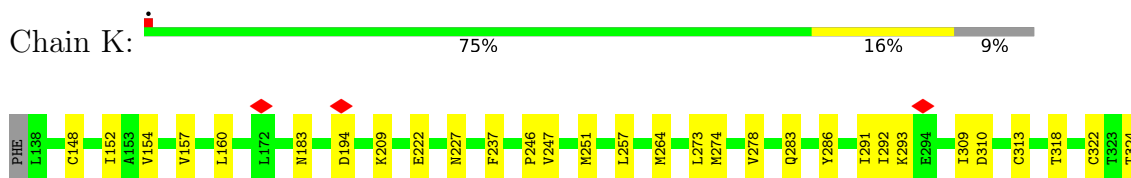
- Molecule 1: RSV variant (construct pXCS847A) F1

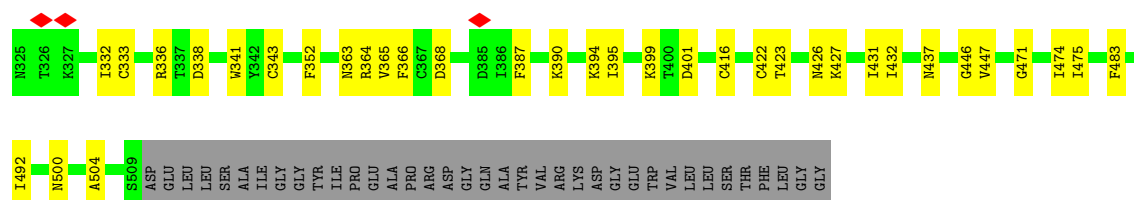


- Molecule 1: RSV variant (construct pXCS847A) F1

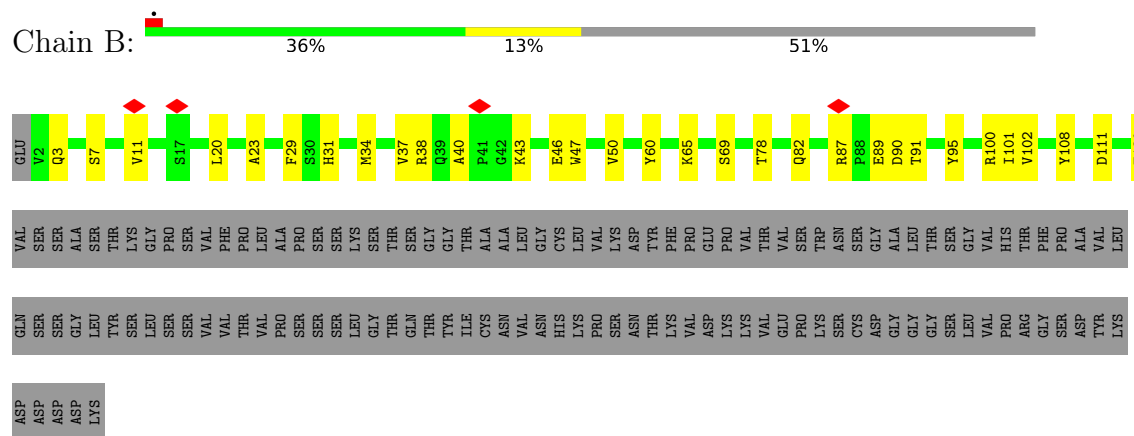


- Molecule 1: RSV variant (construct pXCS847A) F1

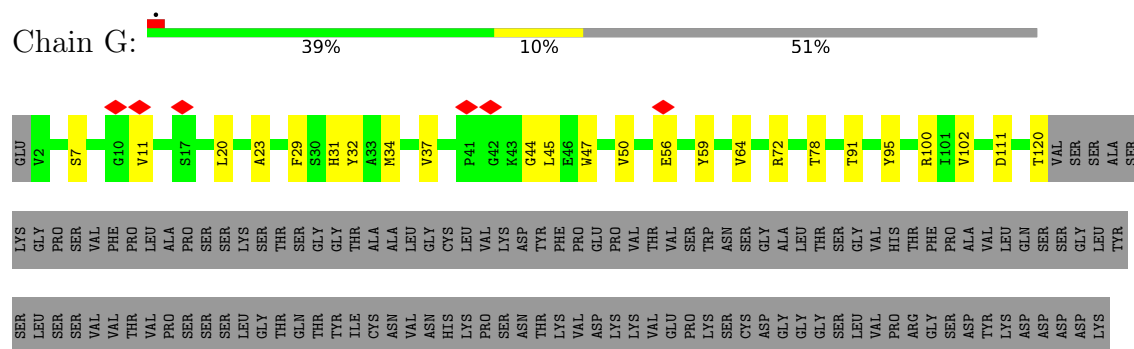




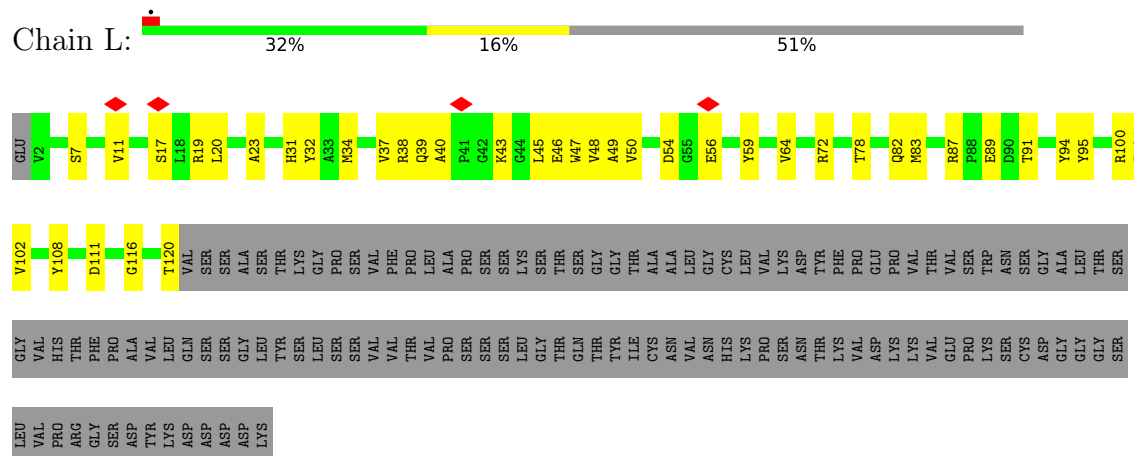
• Molecule 2: AM14 Fab heavy chain



• Molecule 2: AM14 Fab heavy chain



• Molecule 2: AM14 Fab heavy chain



Chain D:

Position	Amino Acid	Information Content (bits)
D1	Asp	0.25
I2	Ile	0.15
Q3	Gln	0.15
S10	Ser	0.25
R18	Arg	0.25
S26	Ser	0.15
K30	Lys	0.15
L33	Leu	0.15
Y36	Tyr	0.15
D50	Asp	0.15
T56	Thr	0.25
S77	Ser	0.25
E81	Glu	0.25
Y87	Tyr	0.15
C88	Cys	0.15
Q89	Gln	0.15
Q90	Gln	0.15
Y91	Tyr	0.15
L94	Leu	0.25
P95	Pro	0.15
P96	Pro	0.15
L97	Leu	0.15
V105	Val	0.25

Chain H:

38% 8% 55%

1 2 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

1 2 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

Chain M:

38% 7% 55%

D1 I2 Q3 Q6 S10 L11 SER ALA SER VAL GLY ASP R18 I21 K30 Y36 H49 D50 E55 T56 G57 S63 T74 E81 Y87 C88 Q89 Q90 Y91 L94 P95 P96 L97 V105 GLU ILE LYS ARG THR VAL ARG THR VAL ALA PRO

VAL PHE ILE PHE PRO PRO ASP SER ASP GLN LEU SER LEU SER GLY THR ALA SER VAL CYS VAL LEU VAL LEU ASN ASH PHE THR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER THR GLN CYS

Chain E:

Sequence logo for Chain E showing amino acid conservation. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows amino acid positions from 1 to 108. A horizontal bar at the top indicates the overall conservation: 6% (red), 38% (green), 12% (yellow), and 50% (grey).

Position	Amino Acid	Information Content (bits)
1	GLN	0.00
2	V2	0.00
3	Q6	0.00
4	S7	0.00
5	G8	0.00
6	K13	0.00
7	V20	0.00
8	S21	0.00
9	C22	0.00
10	K23	0.00
11	I24	0.00
12	S25	0.00
13	G26	0.00
14	H27	0.00
15	T28	0.00
16	L29	0.00
17	I30	0.00
18	H35	0.00
19	W36	0.00
20	A40	0.00
21	P41	0.00
22	G42	0.00
23	K43	0.00
24	G50	0.00
25	Y51	0.00
26	E54	0.00
27	V55	0.00
28	D56	0.00
29	K63	0.00
30	F64	0.00
31	Q65	0.00
32	H66	0.00
33	D73	0.00
34	T74	0.00
35	A75	0.00
36	T76	0.00
37	M81	0.00
38	T87	0.00
39	S88	0.00
40	L89	0.00
41	D89	0.00
42	D90	0.00
43	T91	0.00
44	C96	0.00
45	T102	0.00
46	G107	0.00
47	L108	0.00

GLU ALA ALA LYS VAL GLN TRP LYS VAL VAL ASP ASN ALA LEU GLN SER GLY SER ASN GLN GLU GLU GLN ASP LYS ASP ASP THR THR TYR SER SER LEU LEU LEU LEU LYS ALA ASP TYR GLU LYS HIS HIS HIS GLN GLN GLU VAL VAL THR HIS THR THR LEU

SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

• Molecule 5: AM22 Fab light chain

Chain O: 

GLU
ILE
V3
G9
T10
L11
S12
L13
S14
E17
L21
K40
L47
N77
G78
L79
A80
P81
E82
D83
F84
A85
V86
D93
T103
K104
V105
D106
F107
LYS
ARG
THR
VAL
ALA
ALA
PRO
SER
LEU
SER
PHE
ILE
PHE
PRO
SER
ASP
GLU
GLN
LEU
LYS
GLY
THR

ALA
SER
VAL
VAL
CYS
LEU
LEU
ASN
ASN
GLN
PHE
TYR
GLY
LEU
PRO
ARG
SER
GLU
ALA
VAL
LYS
VAL
GLN
TRP
LYS
VAL
ASP
ASN
GLY
ALA
LEU
GLN
SER
GLY
SER
ASN
SER
GLN
GLU
SER
VAL
THR
GLU
GLN
ASP
SER
LYS
ASP
THR
VAL
TYR
SER
PRO
SER
LEU
SER
PHE
SER
SER
THR
LEU
THR
SER
LYS
SER
ASP
TYR
GLU
LYS
HIS

LYS
VAL
TYR
ALA
CYS
GLU
VAL
THR
HIS
GLN
GLY
LEU
SER
SER
PRO
VAL
THR
SER
PHE
ASN
ARG
GLY
CYS

• Molecule 6: RSV variant (construct pXCS847A) F2

Chain P: 

MET
GLU
LEU
PRO
ILE
LEU
LYS
THR
ASN
ALA
ALA
THR
THR
ILE
LEU
ALA
VAL
THR
LEU
CYS
PHE
PHE
SER
S25
Q26
Q34
L45
S46
T54
T72
D73
V76
E82
E92
S99
T100
P101
A102
C103
ASN
SER
ARG
ALA
ARG
ARG

• Molecule 6: RSV variant (construct pXCS847A) F2

Chain Q: 

MET
GLU
LEU
ILE
LEU
LYS
THR
ASN
ALA
ALA
THR
THR
ILE
LEU
ALA
VAL
THR
LEU
CYS
PHE
PHE
SER
S25
E31
Q34
L45
S46
T54
N63
C69
T72
D73
V76
K77
L78
L93
M97
Q98
C103
ASN
SER
ARG
ALA
ARG
ARG

• Molecule 6: RSV variant (construct pXCS847A) F2

Chain R: 

MET
GLU
LEU
PRO
ILE
LEU
LYS
THR
ASN
ALA
ALA
THR
THR
ILE
LEU
ALA
VAL
THR
LEU
CYS
PHE
PHE
SER
S25
Q34
L45
S46
T54
T72
D73
V76
E82
L83
L93
M97
C103
ASN
SER
ARG
ALA
ARG
ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	183713	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	383.6, 383.6, 383.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: NAG

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	0.11	0/2901	0.30	0/3933
1	C	0.11	0/2901	0.30	0/3933
1	K	0.12	0/2901	0.32	0/3933
2	B	0.12	0/957	0.32	0/1298
2	G	0.12	0/957	0.34	0/1298
2	L	0.13	0/957	0.38	0/1298
3	D	0.15	0/786	0.35	0/1066
3	H	0.13	0/786	0.34	0/1066
3	M	0.14	0/786	0.34	0/1066
4	E	0.12	0/958	0.35	0/1301
4	I	0.11	0/958	0.35	0/1301
4	N	0.11	0/958	0.30	0/1301
5	F	0.10	0/804	0.29	0/1093
5	J	0.11	0/804	0.29	0/1093
5	O	0.12	0/804	0.30	0/1093
6	P	0.10	0/622	0.28	0/839
6	Q	0.10	0/622	0.28	0/839
6	R	0.10	0/622	0.24	0/839
All	All	0.12	0/21084	0.32	0/28590

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 [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	2859	0	2902	41	0
1	C	2859	0	2902	46	0
1	K	2859	0	2902	52	0
2	B	934	0	878	22	0
2	G	934	0	878	18	0
2	L	934	0	878	28	0
3	D	769	0	749	11	0
3	H	769	0	749	13	0
3	M	769	0	749	12	0
4	E	940	0	928	24	0
4	I	940	0	930	15	0
4	N	940	0	930	13	0
5	F	785	0	768	14	0
5	J	785	0	768	8	0
5	O	785	0	768	10	0
6	P	615	0	618	11	0
6	Q	615	0	618	12	0
6	R	615	0	618	15	0
7	A	14	0	13	2	0
7	C	14	0	13	1	0
7	K	14	0	13	2	0
All	All	20748	0	20572	319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (319) 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:C:313:CYS:HA	1:C:343:CYS:HB3	1.44	0.98
5:F:13:LEU:HD11	5:F:79:LEU:HD13	1.49	0.93
4:E:6:GLN:NE2	4:E:96:CYS:SG	2.45	0.90
1:A:313:CYS:HA	1:A:343:CYS:HB3	1.54	0.90
1:K:313:CYS:HA	1:K:343:CYS:HB3	1.57	0.87
5:J:106:ASP:OD1	5:J:107:PHE:N	2.11	0.83
4:I:40:ALA:HB3	4:I:43:LYS:HB2	1.68	0.75
4:I:24:ILE:HD11	4:I:34:ILE:HD11	1.72	0.71
2:L:89:GLU:N	2:L:89:GLU:OE1	2.23	0.70
2:G:47:TRP:HE1	2:G:50:VAL:HG23	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:40:ALA:HB3	4:N:43:LYS:HB2	1.74	0.69
1:C:322:CYS:HA	1:C:333:CYS:HB3	1.72	0.69
2:L:48:VAL:HG12	2:L:49:ALA:H	1.56	0.69
1:C:289:MET:HE1	1:C:297:LEU:HD11	1.76	0.68
4:I:65:GLN:O	4:I:66:HIS:ND1	2.26	0.68
2:L:100:ARG:HB3	2:L:111:ASP:HB2	1.76	0.68
1:K:332:ILE:HG22	1:K:399:LYS:HE2	1.77	0.67
4:E:65:GLN:O	4:E:66:HIS:ND1	2.26	0.67
4:N:65:GLN:O	4:N:66:HIS:ND1	2.28	0.67
3:M:6:GLN:HE21	3:M:21:ILE:HG21	1.60	0.67
2:B:100:ARG:HB3	2:B:111:ASP:HB2	1.78	0.66
1:A:291:ILE:HG12	1:A:293:LYS:H	1.61	0.66
2:L:34:MET:HG2	2:L:72:ARG:HH12	1.60	0.65
4:E:36:TRP:CH2	4:E:96:CYS:SG	2.89	0.65
1:A:148:CYS:N	6:P:103:CYS:SG	2.66	0.65
1:K:291:ILE:HG12	1:K:293:LYS:H	1.61	0.65
2:G:100:ARG:HB3	2:G:111:ASP:HB2	1.78	0.65
1:C:261:ILE:HD13	1:C:274:MET:HB3	1.78	0.65
4:E:20:VAL:HB	4:E:81:MET:HB3	1.79	0.65
4:N:34:ILE:HG21	4:N:79:VAL:HG11	1.79	0.64
3:H:61:ARG:NH2	3:H:82:ASP:OD2	2.31	0.64
2:B:89:GLU:N	2:B:89:GLU:OE2	2.31	0.64
1:C:291:ILE:HG12	1:C:293:LYS:H	1.63	0.64
4:E:40:ALA:HB3	4:E:43:LYS:HB2	1.79	0.63
1:K:423:THR:HG21	1:K:431:ILE:HD12	1.80	0.63
1:A:154:VAL:HG21	6:P:54:THR:HG21	1.81	0.62
1:K:154:VAL:HG21	6:R:54:THR:HG21	1.82	0.62
1:K:324:THR:HG21	1:K:437:ASN:HB3	1.81	0.62
2:B:47:TRP:HE1	2:B:50:VAL:HG23	1.65	0.62
1:C:216:ASN:ND2	1:C:218:GLU:OE1	2.32	0.62
1:C:332:ILE:HG22	1:C:399:LYS:HE2	1.79	0.62
2:G:23:ALA:HA	2:G:78:THR:HG22	1.82	0.62
5:J:106:ASP:CG	5:J:107:PHE:H	2.07	0.62
1:A:216:ASN:ND2	1:A:218:GLU:OE1	2.32	0.61
6:Q:97:MET:SD	6:Q:98:GLN:NE2	2.74	0.61
1:K:310:ASP:HA	6:R:45:LEU:HD12	1.82	0.61
2:G:37:VAL:HG12	2:G:47:TRP:HA	1.82	0.61
1:C:324:THR:HG21	1:C:437:ASN:HB3	1.82	0.61
1:C:310:ASP:HA	6:Q:45:LEU:HD12	1.81	0.61
1:K:148:CYS:HB3	1:K:286:TYR:HD2	1.65	0.61
2:B:37:VAL:HG12	2:B:47:TRP:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:148:CYS:N	6:R:103:CYS:SG	2.68	0.60
2:G:56:GLU:OE2	2:G:56:GLU:N	2.35	0.60
1:A:423:THR:HG21	1:A:431:ILE:HD12	1.83	0.60
1:C:423:THR:HG21	1:C:431:ILE:HD12	1.84	0.59
1:C:471:GLY:H	6:Q:34:GLN:HB3	1.67	0.59
4:E:36:TRP:CZ3	4:E:96:CYS:SG	2.96	0.59
4:E:22:CYS:SG	4:E:36:TRP:CH2	2.94	0.59
2:L:91:THR:HG22	2:L:120:THR:HB	1.85	0.59
5:F:81:PRO:HA	5:F:84:PHE:HE2	1.68	0.58
1:C:234:THR:HG22	6:Q:93:LEU:HD22	1.84	0.58
1:C:429:ARG:NH2	3:M:91:TYR:O	2.36	0.58
5:F:86:VAL:HG22	5:F:104:LYS:HG2	1.85	0.58
1:C:500:ASN:OD1	7:C:601:NAG:N2	2.37	0.57
5:F:13:LEU:HD11	5:F:79:LEU:CD1	2.29	0.57
1:K:471:GLY:H	6:R:34:GLN:HB3	1.68	0.57
2:G:32:TYR:O	2:G:72:ARG:NH2	2.36	0.57
4:E:2:VAL:N	4:E:25:SER:O	2.37	0.57
5:O:40:LYS:NZ	5:O:82:GLU:O	2.37	0.57
1:A:310:ASP:HA	6:P:45:LEU:HD12	1.86	0.57
4:I:2:VAL:N	4:I:25:SER:O	2.38	0.57
1:K:500:ASN:OD1	7:K:601:NAG:N2	2.38	0.57
1:A:324:THR:HG21	1:A:437:ASN:HB3	1.87	0.57
1:A:429:ARG:NH2	3:D:91:TYR:O	2.35	0.56
1:C:279:GLN:NE2	6:P:99:SER:OG	2.39	0.56
1:C:148:CYS:N	6:Q:103:CYS:SG	2.67	0.56
1:A:500:ASN:OD1	7:A:601:NAG:N2	2.39	0.56
4:E:63:LYS:HG3	4:E:64:PHE:CD1	2.41	0.56
4:N:2:VAL:N	4:N:25:SER:O	2.39	0.56
3:D:50:ASP:OD1	3:D:91:TYR:OH	2.23	0.55
1:C:257:LEU:HD22	1:C:278:VAL:HG13	1.89	0.55
4:E:91:THR:HG22	4:E:122:VAL:H	1.72	0.55
1:K:292:ILE:HD12	6:R:93:LEU:HD23	1.89	0.55
5:F:13:LEU:HD21	5:F:19:ALA:HB2	1.88	0.55
2:L:32:TYR:O	2:L:72:ARG:NH2	2.41	0.54
1:C:154:VAL:HG21	6:Q:54:THR:HG21	1.89	0.54
1:K:227:ASN:HD22	6:R:82:GLU:HG3	1.73	0.54
4:N:111:ASP:OD1	4:N:111:ASP:N	2.40	0.54
5:O:13:LEU:HD11	5:O:79:LEU:HD13	1.88	0.54
1:A:313:CYS:CA	1:A:343:CYS:HB3	2.34	0.53
2:B:91:THR:HG22	2:B:120:THR:HB	1.89	0.53
4:E:35:HIS:HA	4:E:50:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:ILE:HD11	6:R:103:CYS:HB2	1.90	0.53
5:O:9:GLY:O	5:O:103:THR:OG1	2.23	0.53
1:C:158:LEU:HD12	1:C:290:SER:OG	2.09	0.53
4:I:72:ALA:HA	4:I:79:VAL:HA	1.91	0.53
5:F:38:GLN:HG2	5:F:48:LEU:HD21	1.91	0.52
1:K:157:VAL:HG21	1:K:183:ASN:HB2	1.90	0.52
4:E:111:ASP:N	4:E:111:ASP:OD1	2.40	0.52
2:B:29:PHE:HE1	2:B:34:MET:HE3	1.74	0.52
1:K:237:PHE:CZ	1:K:251:MET:HE1	2.45	0.52
3:H:35:TRP:CD2	3:H:73:LEU:HD12	2.45	0.52
1:A:313:CYS:SG	1:A:343:CYS:CB	2.97	0.52
4:I:20:VAL:HB	4:I:81:MET:HB3	1.92	0.52
1:C:274:MET:HG2	1:C:281:VAL:HG11	1.92	0.52
2:L:39:GLN:HB2	2:L:45:LEU:HD23	1.92	0.52
3:M:30:LYS:H	3:M:30:LYS:HD2	1.74	0.51
2:G:47:TRP:NE1	2:G:50:VAL:HG23	2.23	0.51
4:I:111:ASP:OD1	4:I:111:ASP:N	2.41	0.51
1:K:222:GLU:HG3	6:Q:78:LEU:HD11	1.91	0.51
1:K:227:ASN:HD22	6:R:82:GLU:CG	2.24	0.51
5:F:11:LEU:HD11	5:F:105:VAL:HG22	1.91	0.51
2:L:82:GLN:NE2	2:L:83:MET:O	2.43	0.51
5:F:33:HIS:HB3	5:F:92:SER:HB3	1.93	0.51
2:B:37:VAL:HG23	2:B:95:TYR:HB2	1.94	0.50
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.93	0.50
2:L:48:VAL:HG12	2:L:49:ALA:N	2.25	0.50
2:B:47:TRP:NE1	2:B:50:VAL:HG23	2.26	0.50
1:C:237:PHE:CZ	1:C:251:MET:HE1	2.46	0.50
6:Q:73:ASP:HB3	6:Q:76:VAL:HG12	1.94	0.50
1:A:426:ASN:OD1	1:A:427:LYS:N	2.45	0.50
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.93	0.50
1:A:338:ASP:HB3	1:A:394:LYS:HE3	1.93	0.50
1:A:341:TRP:HB2	1:A:352:PHE:HD2	1.77	0.50
1:K:322:CYS:HA	1:K:333:CYS:HB3	1.94	0.50
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.92	0.50
2:L:56:GLU:N	2:L:56:GLU:OE1	2.45	0.50
2:L:23:ALA:HA	2:L:78:THR:HG22	1.94	0.49
1:A:247:VAL:HG13	1:A:251:MET:HB2	1.94	0.49
2:G:31:HIS:HB3	2:G:102:VAL:HG13	1.94	0.49
1:K:368:ASP:N	1:K:368:ASP:OD1	2.43	0.49
2:L:37:VAL:HG12	2:L:47:TRP:HA	1.94	0.49
2:B:29:PHE:CE1	2:B:34:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:H	6:P:34:GLN:HB3	1.77	0.49
2:B:69:SER:HB2	2:B:82:GLN:HB3	1.94	0.49
4:E:24:ILE:HD11	4:E:29:LEU:HD13	1.93	0.49
2:B:38:ARG:NH1	2:B:90:ASP:OD2	2.46	0.49
5:O:12:SER:OG	5:O:107:PHE:HB2	2.13	0.49
1:A:152:ILE:HD11	6:P:103:CYS:HB2	1.94	0.48
3:D:3:GLN:HE22	3:D:26:SER:HB2	1.77	0.48
1:C:190:ILE:HG22	1:C:191:LYS:H	1.78	0.48
1:C:368:ASP:OD1	1:C:368:ASP:N	2.45	0.48
6:R:73:ASP:HB3	6:R:76:VAL:HG12	1.95	0.48
1:K:338:ASP:HB3	1:K:394:LYS:HE2	1.96	0.48
1:A:368:ASP:N	1:A:368:ASP:OD1	2.43	0.48
2:G:11:VAL:HG23	2:G:120:THR:HA	1.96	0.48
1:K:194:ASP:N	1:K:194:ASP:OD1	2.47	0.48
1:K:264:MET:HE1	1:K:274:MET:HE1	1.95	0.48
1:C:295:GLU:OE1	1:C:295:GLU:HA	2.14	0.48
4:E:28:THR:HB	4:E:30:ILE:HG12	1.96	0.48
2:L:37:VAL:HG23	2:L:95:TYR:HB2	1.96	0.48
4:I:91:THR:O	4:I:91:THR:OG1	2.31	0.48
5:O:11:LEU:HD11	5:O:105:VAL:HG22	1.95	0.47
1:A:395:ILE:HD13	1:A:492:ILE:HD13	1.96	0.47
2:L:11:VAL:HA	2:L:120:THR:HA	1.95	0.47
1:K:313:CYS:SG	6:R:46:SER:HB3	2.54	0.47
4:N:35:HIS:HA	4:N:50:GLY:HA3	1.97	0.47
5:O:81:PRO:HA	5:O:84:PHE:CE2	2.49	0.47
1:C:194:ASP:OD1	1:C:194:ASP:N	2.46	0.47
2:G:64:VAL:HG23	2:G:64:VAL:O	2.14	0.47
3:H:63:SER:HB2	3:H:74:THR:HG23	1.95	0.47
3:M:63:SER:HB2	3:M:74:THR:HG23	1.97	0.47
6:P:73:ASP:HB3	6:P:76:VAL:HG12	1.96	0.47
1:K:432:ILE:HD11	1:K:447:VAL:HG22	1.96	0.47
5:O:86:VAL:HG22	5:O:104:LYS:HG3	1.97	0.47
1:A:332:ILE:HG22	1:A:399:LYS:HE2	1.96	0.47
1:K:341:TRP:HB2	1:K:352:PHE:HD2	1.80	0.47
2:L:64:VAL:HG23	2:L:64:VAL:O	2.15	0.47
5:O:14:SER:HA	5:O:107:PHE:CD2	2.49	0.47
1:A:194:ASP:N	1:A:194:ASP:OD1	2.47	0.46
1:C:171:LEU:HD13	1:C:191:LYS:HB2	1.95	0.46
2:L:31:HIS:HB3	2:L:102:VAL:HG13	1.97	0.46
5:O:21:LEU:HD22	5:O:103:THR:HG21	1.97	0.46
2:L:38:ARG:NE	2:L:46:GLU:OE1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:LEU:HB3	3:D:96:PRO:HD2	1.97	0.46
1:A:237:PHE:CZ	1:A:251:MET:HE1	2.50	0.46
4:E:81:MET:HE2	4:E:81:MET:HA	1.96	0.46
1:K:426:ASN:OD1	1:K:427:LYS:N	2.49	0.46
3:H:2:ILE:HG12	3:H:27:GLN:HG3	1.98	0.46
2:B:23:ALA:HA	2:B:78:THR:HG22	1.97	0.46
2:G:37:VAL:HG23	2:G:95:TYR:HB2	1.96	0.46
3:M:94:LEU:HB3	3:M:96:PRO:HD2	1.97	0.46
1:C:209:LYS:HE3	4:N:102:THR:HG21	1.98	0.46
4:E:6:GLN:OE1	4:E:22:CYS:SG	2.74	0.46
1:C:252:LEU:HD23	1:C:257:LEU:HD12	1.98	0.46
4:E:6:GLN:CD	4:E:96:CYS:SG	2.99	0.46
3:D:33:LEU:HD12	3:D:33:LEU:HA	1.77	0.46
1:A:209:LYS:HE3	4:E:102:THR:HG21	1.98	0.45
1:A:483:PHE:CD1	1:A:499:ILE:HD11	2.52	0.45
5:J:81:PRO:HA	5:J:84:PHE:CE2	2.51	0.45
5:J:81:PRO:HA	5:J:84:PHE:HE2	1.80	0.45
2:G:45:LEU:H	3:H:87:TYR:HE2	1.64	0.45
4:E:63:LYS:HB2	4:E:63:LYS:HE3	1.76	0.45
1:A:390:LYS:HE2	1:A:390:LYS:HB3	1.82	0.45
2:B:11:VAL:HG23	2:B:120:THR:HA	1.98	0.45
2:B:38:ARG:NE	2:B:46:GLU:OE2	2.30	0.45
3:D:36:TYR:HB2	3:D:87:TYR:HB2	1.98	0.45
4:I:6:GLN:NE2	4:I:6:GLN:HA	2.32	0.45
4:E:24:ILE:CD1	4:E:29:LEU:HD13	2.46	0.45
1:A:322:CYS:HA	1:A:333:CYS:CB	2.47	0.45
2:B:7:SER:O	2:B:20:LEU:HB2	2.17	0.45
3:D:33:LEU:HD12	3:D:89:GLN:O	2.17	0.45
2:G:91:THR:HG22	2:G:120:THR:HB	1.99	0.45
3:M:36:TYR:HB2	3:M:87:TYR:HB2	1.99	0.45
1:C:395:ILE:HD13	1:C:492:ILE:HD13	1.98	0.44
4:I:102:THR:HG21	1:K:209:LYS:HE3	1.99	0.44
2:L:59:TYR:CE2	3:M:95:PRO:HG2	2.52	0.44
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.99	0.44
2:L:38:ARG:HH22	2:L:64:VAL:HG11	1.80	0.44
1:C:426:ASN:OD1	1:C:427:LYS:N	2.50	0.44
4:I:108:LEU:HD21	5:J:32:ASN:HB3	1.99	0.44
1:A:257:LEU:HD22	1:A:278:VAL:HG13	1.99	0.44
1:A:363:ASN:O	6:P:45:LEU:N	2.44	0.44
1:K:257:LEU:HD22	1:K:278:VAL:HG13	1.98	0.44
1:C:218:GLU:O	1:C:222:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:ND2	6:P:82:GLU:OE1	2.51	0.44
1:C:338:ASP:HB3	1:C:394:LYS:HE3	2.00	0.44
1:K:395:ILE:HD13	1:K:492:ILE:HD13	2.00	0.44
2:B:31:HIS:HB3	2:B:102:VAL:HG13	2.00	0.44
4:E:107:GLY:C	4:E:108:LEU:HD23	2.43	0.44
1:K:157:VAL:O	1:K:160:LEU:HG	2.18	0.44
1:K:332:ILE:HD13	1:K:483:PHE:CE2	2.53	0.44
4:N:110:ILE:HD13	5:O:47:LEU:HD11	2.00	0.44
4:I:96:CYS:SG	4:I:97:GLY:N	2.91	0.43
1:K:148:CYS:HB3	1:K:286:TYR:CD2	2.49	0.43
4:I:29:LEU:HD23	4:I:29:LEU:O	2.18	0.43
1:A:313:CYS:SG	6:P:46:SER:HB3	2.59	0.43
5:F:4:LEU:HD23	5:F:23:CYS:SG	2.58	0.43
1:K:387:PHE:HE1	1:K:474:ILE:HD11	1.82	0.43
4:N:87:THR:OG1	4:N:89:ASP:OD1	2.29	0.43
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.89	0.43
2:G:7:SER:O	2:G:20:LEU:HB2	2.17	0.43
2:L:47:TRP:HE1	2:L:50:VAL:HG23	1.84	0.43
1:C:313:CYS:CA	1:C:343:CYS:HB3	2.32	0.43
1:K:365:VAL:HG22	6:R:46:SER:HA	2.01	0.43
1:A:190:ILE:HG22	1:A:191:LYS:H	1.83	0.43
1:K:313:CYS:CA	1:K:343:CYS:HB3	2.37	0.43
1:K:318:THR:HG21	1:K:336:ARG:HB2	2.01	0.43
3:H:35:TRP:CZ3	3:H:88:CYS:HB3	2.53	0.43
4:N:85:ARG:HB2	4:N:85:ARG:NH1	2.35	0.42
1:C:210:GLN:HA	6:Q:69:CYS:HA	2.01	0.42
1:C:313:CYS:SG	6:Q:46:SER:HB3	2.59	0.42
1:C:318:THR:HG21	1:C:336:ARG:HB2	2.00	0.42
5:F:4:LEU:HD21	5:F:91:SER:HB3	2.01	0.42
1:A:504:ALA:HB2	7:A:601:NAG:H82	1.99	0.42
5:F:27:GLN:NE2	5:F:93:ASP:OD2	2.45	0.42
1:K:364:ARG:HD3	1:K:366:PHE:CE2	2.55	0.42
1:A:387:PHE:HE1	1:A:474:ILE:HD11	1.85	0.42
1:K:247:VAL:HG13	1:K:251:MET:HB2	2.02	0.42
2:L:101:ILE:HG13	2:L:108:TYR:CD1	2.54	0.42
2:G:44:GLY:HA2	3:H:87:TYR:OH	2.20	0.42
5:J:106:ASP:CG	5:J:107:PHE:N	2.69	0.42
1:K:246:PRO:HB3	1:K:283:GLN:HA	2.00	0.42
1:K:332:ILE:O	1:K:475:ILE:HD11	2.19	0.42
2:L:7:SER:O	2:L:20:LEU:HB2	2.19	0.42
3:D:3:GLN:NE2	3:D:26:SER:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:13:LEU:C	5:F:13:LEU:HD12	2.45	0.42
1:K:227:ASN:ND2	6:R:82:GLU:HG3	2.35	0.42
3:H:35:TRP:HB2	3:H:48:MET:HG2	2.00	0.42
3:M:49:HIS:ND1	3:M:55:GLU:OE2	2.52	0.42
1:C:332:ILE:HG13	1:C:475:ILE:HD11	2.01	0.42
4:E:51:TYR:HE1	4:E:56:ASP:HA	1.83	0.42
1:C:341:TRP:HB2	1:C:352:PHE:HD2	1.84	0.42
2:B:101:ILE:HG13	2:B:108:TYR:CD1	2.55	0.42
1:K:322:CYS:HA	1:K:333:CYS:CB	2.50	0.42
1:A:318:THR:HG21	1:A:336:ARG:HB2	2.01	0.42
1:C:317:HIS:CG	1:C:408:THR:HG22	2.55	0.42
5:F:39:GLN:HB2	5:F:45:PRO:HB3	2.02	0.42
2:L:54:ASP:OD1	2:L:54:ASP:C	2.63	0.42
4:N:6:GLN:OE1	4:N:6:GLN:HA	2.19	0.42
4:N:96:CYS:SG	4:N:97:GLY:N	2.93	0.42
1:C:227:ASN:O	1:C:227:ASN:ND2	2.53	0.41
1:C:432:ILE:HD11	1:C:447:VAL:HG22	2.01	0.41
1:K:390:LYS:HB3	1:K:390:LYS:HE2	1.81	0.41
4:N:48:MET:HE1	4:N:94:TYR:HE2	1.86	0.41
3:M:50:ASP:OD1	3:M:91:TYR:OH	2.34	0.41
1:A:152:ILE:HG23	6:P:101:PRO:HG2	2.03	0.41
1:A:158:LEU:HD12	1:A:290:SER:HB3	2.03	0.41
2:B:60:TYR:HB2	2:B:65:LYS:HG3	2.01	0.41
1:K:273:LEU:HD22	1:K:309:ILE:HD12	2.03	0.41
1:K:363:ASN:O	6:R:45:LEU:N	2.49	0.41
3:H:94:LEU:HB3	3:H:96:PRO:HD2	2.02	0.41
1:A:246:PRO:HB3	1:A:283:GLN:HA	2.03	0.41
5:F:81:PRO:HA	5:F:84:PHE:CE2	2.52	0.41
2:L:17:SER:HB2	2:L:82:GLN:HE22	1.86	0.41
3:M:89:GLN:NE2	3:M:97:LEU:HD13	2.36	0.41
1:A:407:ILE:HD13	1:A:412:ALA:HB2	2.03	0.41
2:B:87:ARG:H	2:B:87:ARG:HG2	1.67	0.41
1:K:387:PHE:CE1	1:K:474:ILE:HD11	2.56	0.41
1:K:504:ALA:HB2	7:K:601:NAG:H82	2.01	0.41
1:C:401:ASP:OD1	1:C:401:ASP:N	2.54	0.41
2:G:59:TYR:CE1	3:H:95:PRO:HG2	2.56	0.41
3:M:49:HIS:HD2	3:M:50:ASP:OD2	2.02	0.41
2:B:3:GLN:H	2:B:3:GLN:HG3	1.74	0.41
4:I:112:ASP:HB2	4:I:114:TRP:CD1	2.56	0.41
2:L:19:ARG:HH11	2:L:19:ARG:HG2	1.85	0.41
6:R:83:LEU:HD23	6:R:83:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LEU:HB3	6:Q:31:GLU:HG3	2.03	0.41
5:J:12:SER:OG	5:J:107:PHE:HB2	2.21	0.41
1:A:387:PHE:CE1	1:A:474:ILE:HD11	2.55	0.40
2:B:47:TRP:CZ3	3:D:96:PRO:HA	2.56	0.40
2:G:47:TRP:CZ3	3:H:96:PRO:HA	2.56	0.40
4:I:51:TYR:HE1	4:I:56:ASP:HA	1.85	0.40
1:K:292:ILE:HG22	6:R:97:MET:SD	2.62	0.40
1:K:401:ASP:OD1	1:K:401:ASP:N	2.54	0.40
1:K:416:CYS:HB3	1:K:422:CYS:HB3	1.91	0.40
2:L:87:ARG:HD3	2:L:89:GLU:OE2	2.20	0.40
3:M:94:LEU:HD23	3:M:94:LEU:HA	1.85	0.40
1:C:295:GLU:OE2	6:Q:63:ASN:N	2.54	0.40
3:D:95:PRO:O	3:D:97:LEU:HG	2.22	0.40
4:E:28:THR:O	4:E:29:LEU:HB3	2.21	0.40
2:G:29:PHE:CE1	2:G:34:MET:HE3	2.56	0.40
2:L:94:TYR:O	2:L:116:GLY:HA3	2.21	0.40
3:D:30:LYS:H	3:D:30:LYS:HG2	1.60	0.40
1:K:426:ASN:ND2	1:K:446:GLY:O	2.54	0.40
4:E:87:THR:OG1	4:E:89:ASP:OD1	2.34	0.40
5:J:4:LEU:HD23	5:J:23:CYS:SG	2.61	0.40
3:H:36:TYR:HB2	3:H:87:TYR:HB2	2.04	0.40
3:H:39:LYS:HB2	3:H:42:LYS:HB2	2.02	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	370/410 (90%)	355 (96%)	15 (4%)	0	100	100
1	C	370/410 (90%)	352 (95%)	18 (5%)	0	100	100
1	K	370/410 (90%)	355 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	117/245 (48%)	112 (96%)	5 (4%)	0	100	100
2	G	117/245 (48%)	111 (95%)	6 (5%)	0	100	100
2	L	117/245 (48%)	112 (96%)	5 (4%)	0	100	100
3	D	95/218 (44%)	83 (87%)	12 (13%)	0	100	100
3	H	95/218 (44%)	83 (87%)	12 (13%)	0	100	100
3	M	95/218 (44%)	87 (92%)	8 (8%)	0	100	100
4	E	122/246 (50%)	116 (95%)	6 (5%)	0	100	100
4	I	122/246 (50%)	114 (93%)	8 (7%)	0	100	100
4	N	122/246 (50%)	112 (92%)	10 (8%)	0	100	100
5	F	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
5	J	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
5	O	103/215 (48%)	94 (91%)	9 (9%)	0	100	100
6	P	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
6	Q	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
6	R	77/109 (71%)	75 (97%)	2 (3%)	0	100	100
All	All	2652/4329 (61%)	2503 (94%)	149 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	340/369 (92%)	340 (100%)	0	100	100
1	C	340/369 (92%)	339 (100%)	1 (0%)	86	83
1	K	340/369 (92%)	340 (100%)	0	100	100
2	B	98/206 (48%)	98 (100%)	0	100	100
2	G	98/206 (48%)	98 (100%)	0	100	100
2	L	98/206 (48%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	88/194 (45%)	88 (100%)	0	100	100
3	H	88/194 (45%)	88 (100%)	0	100	100
3	M	88/194 (45%)	88 (100%)	0	100	100
4	E	100/205 (49%)	100 (100%)	0	100	100
4	I	100/205 (49%)	100 (100%)	0	100	100
4	N	100/205 (49%)	99 (99%)	1 (1%)	68	74
5	F	86/185 (46%)	85 (99%)	1 (1%)	63	72
5	J	86/185 (46%)	86 (100%)	0	100	100
5	O	86/185 (46%)	86 (100%)	0	100	100
6	P	70/96 (73%)	70 (100%)	0	100	100
6	Q	70/96 (73%)	70 (100%)	0	100	100
6	R	70/96 (73%)	70 (100%)	0	100	100
All	All	2346/3765 (62%)	2343 (100%)	3 (0%)	87	88

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

Mol	Chain	Res	Type
1	C	142	LEU
5	F	96	ILE
4	N	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	202	GLN
1	A	227	ASN
1	A	228	ASN
1	A	254	ASN
1	A	270	GLN
1	C	183	ASN
1	C	202	GLN
1	C	228	ASN
1	C	254	ASN
1	C	270	GLN
1	C	279	GLN
1	C	284	GLN

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Mol	Chain	Res	Type
1	K	165	ASN
1	K	202	GLN
1	K	227	ASN
1	K	254	ASN
1	K	283	GLN
2	L	82	GLN
3	M	6	GLN
3	M	37	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	601	1	14,14,15	0.37	0	17,19,21	0.52	0
7	NAG	C	601	1	14,14,15	0.38	0	17,19,21	0.52	0
7	NAG	K	601	1	14,14,15	0.38	0	17,19,21	0.51	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
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	C	601	1	-	2/6/23/26	0/1/1/1
7	NAG	K	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	NAG	O5-C5-C6-O6
7	K	601	NAG	O5-C5-C6-O6
7	A	601	NAG	O5-C5-C6-O6
7	C	601	NAG	C4-C5-C6-O6
7	K	601	NAG	C4-C5-C6-O6
7	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	NAG	2	0
7	C	601	NAG	1	0
7	K	601	NAG	2	0

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.

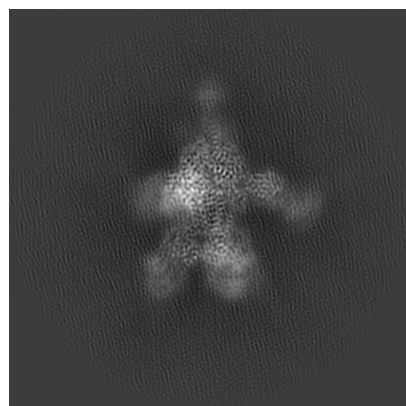
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26562. These allow visual inspection of the internal detail of the map and identification of artifacts.

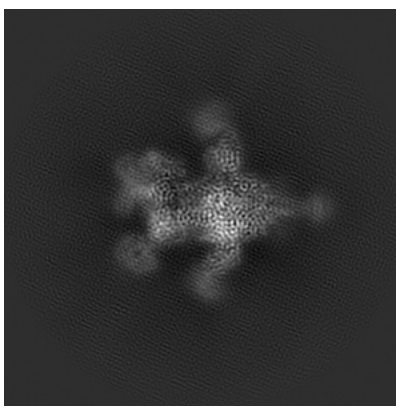
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

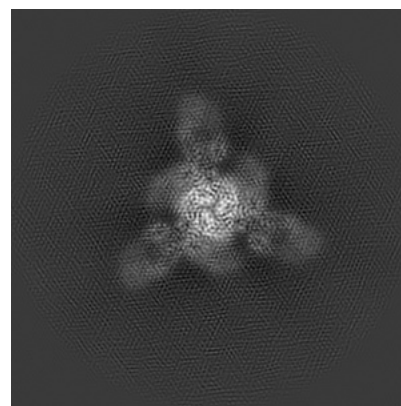
6.1.1 Primary map



X

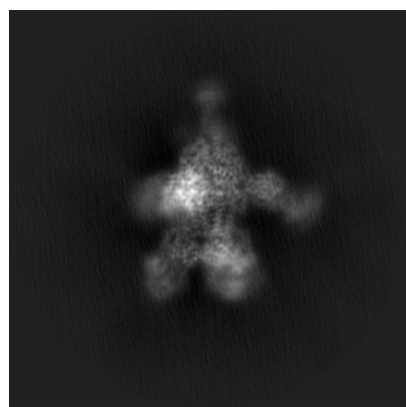


Y

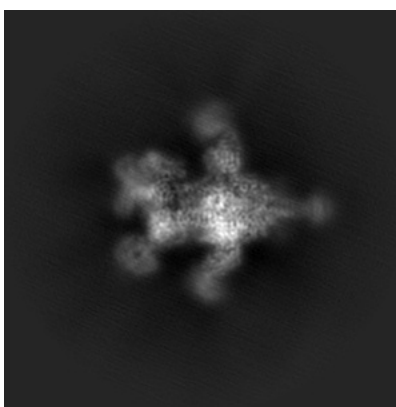


Z

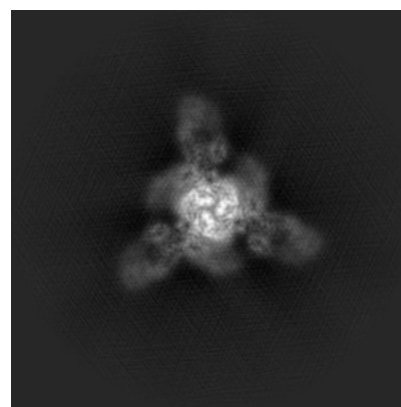
6.1.2 Raw map



X



Y

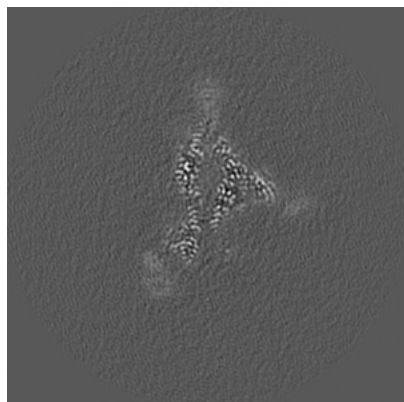


Z

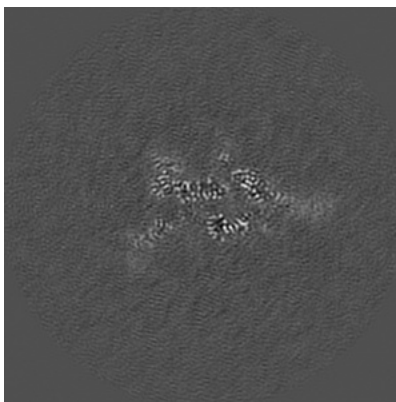
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

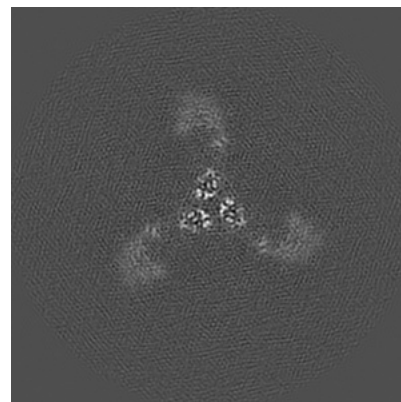
6.2.1 Primary map



X Index: 140

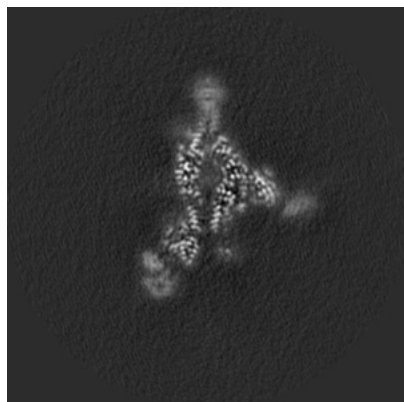


Y Index: 140

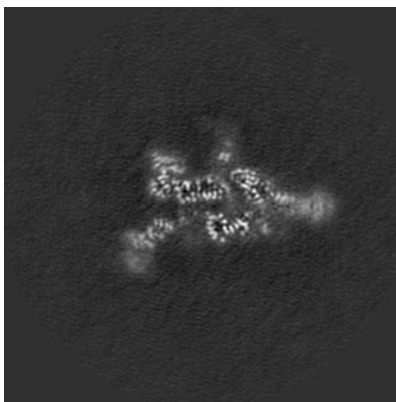


Z Index: 140

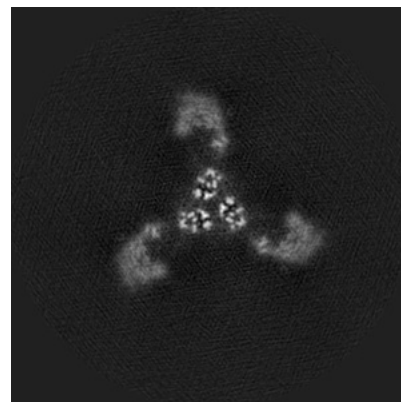
6.2.2 Raw map



X Index: 140



Y Index: 140

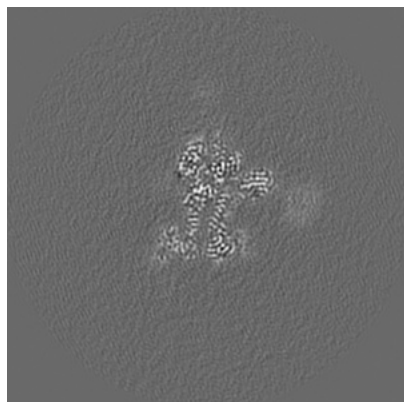


Z Index: 140

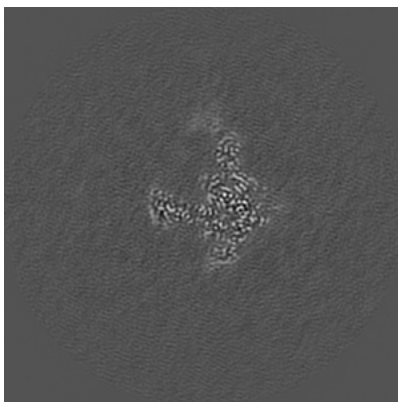
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

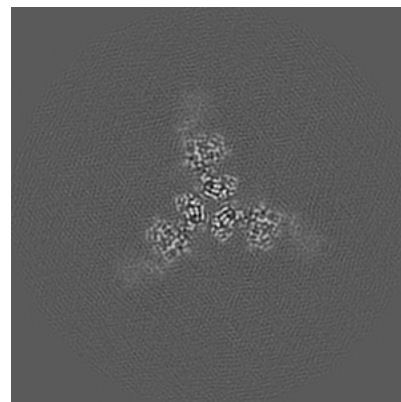
6.3.1 Primary map



X Index: 130

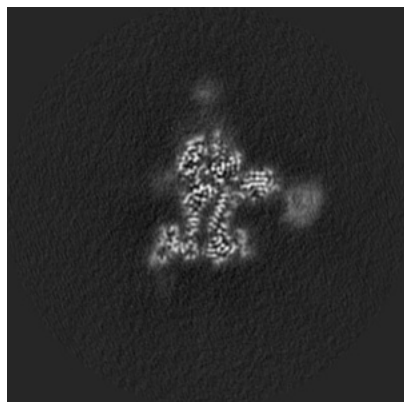


Y Index: 127

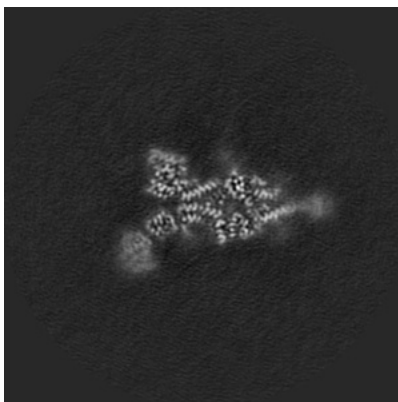


Z Index: 152

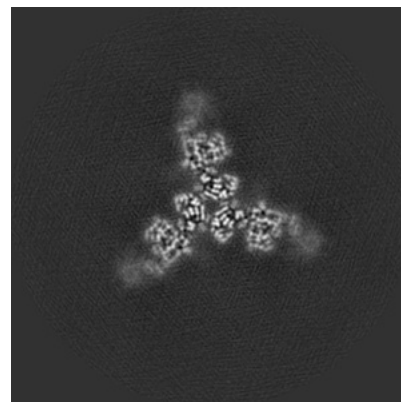
6.3.2 Raw map



X Index: 130



Y Index: 145

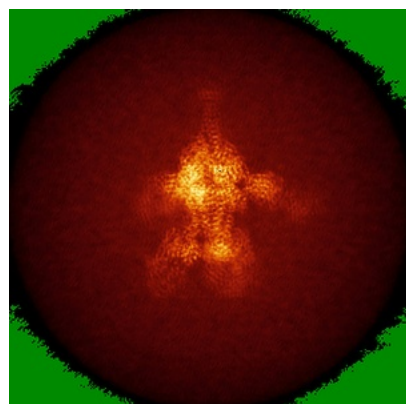


Z Index: 152

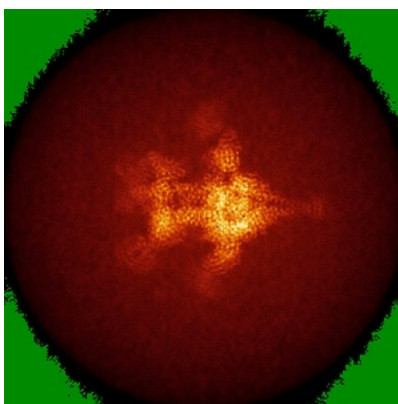
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

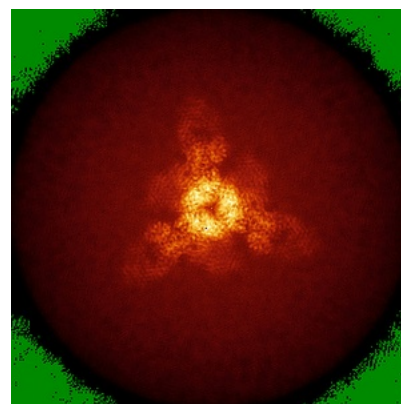
6.4.1 Primary map



X

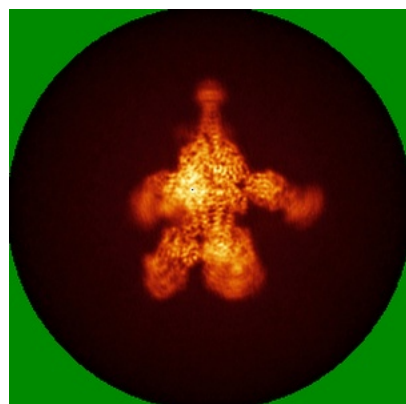


Y

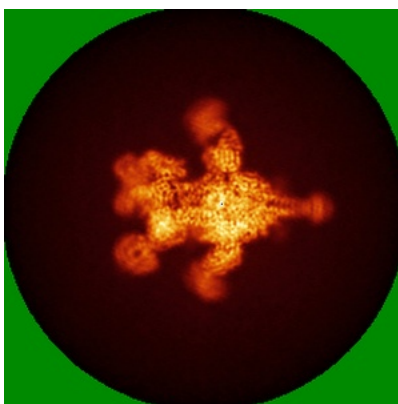


Z

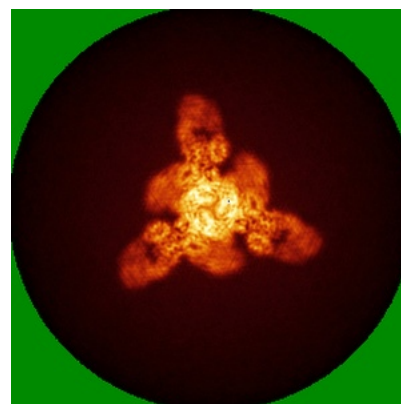
6.4.2 Raw map



X



Y

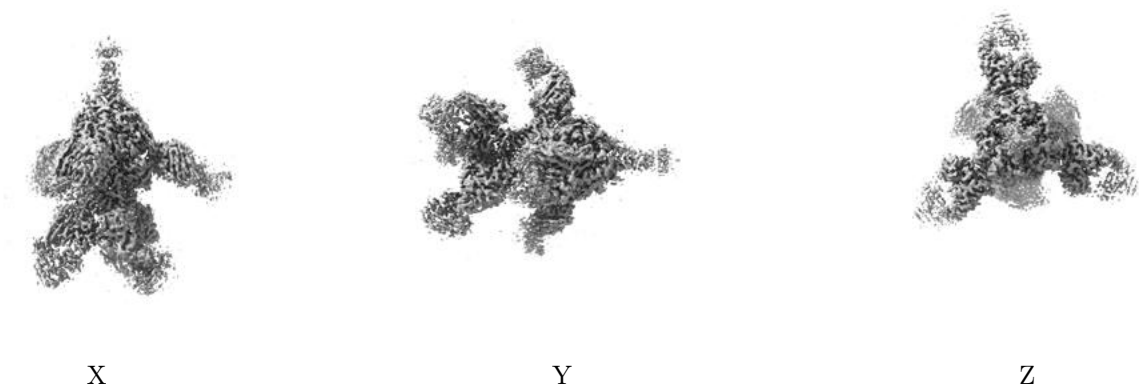


Z

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.

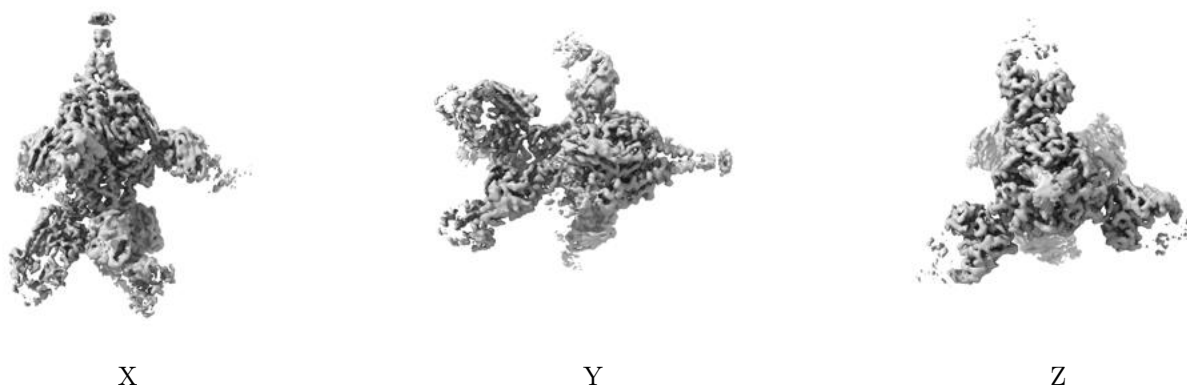
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



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.

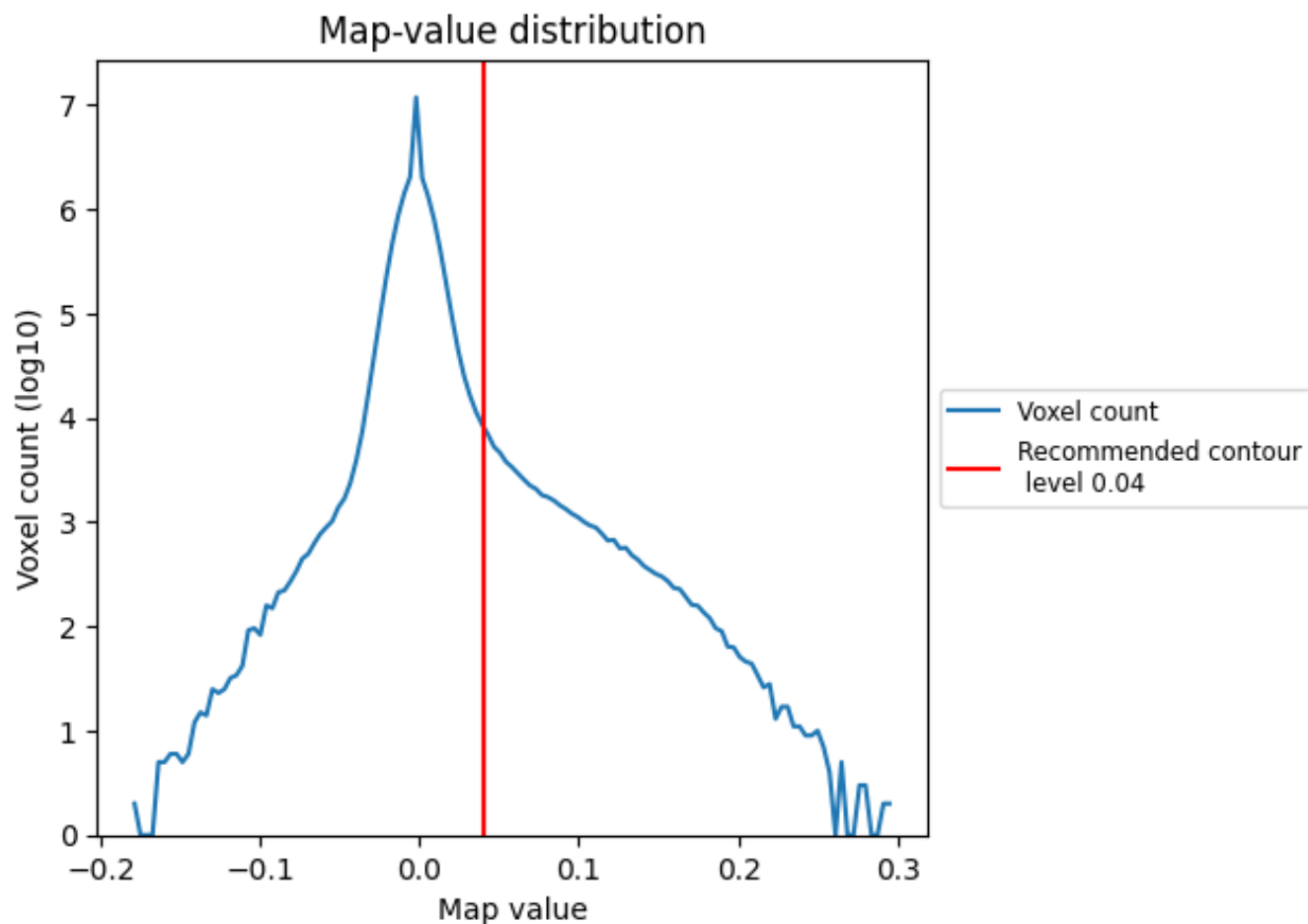
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

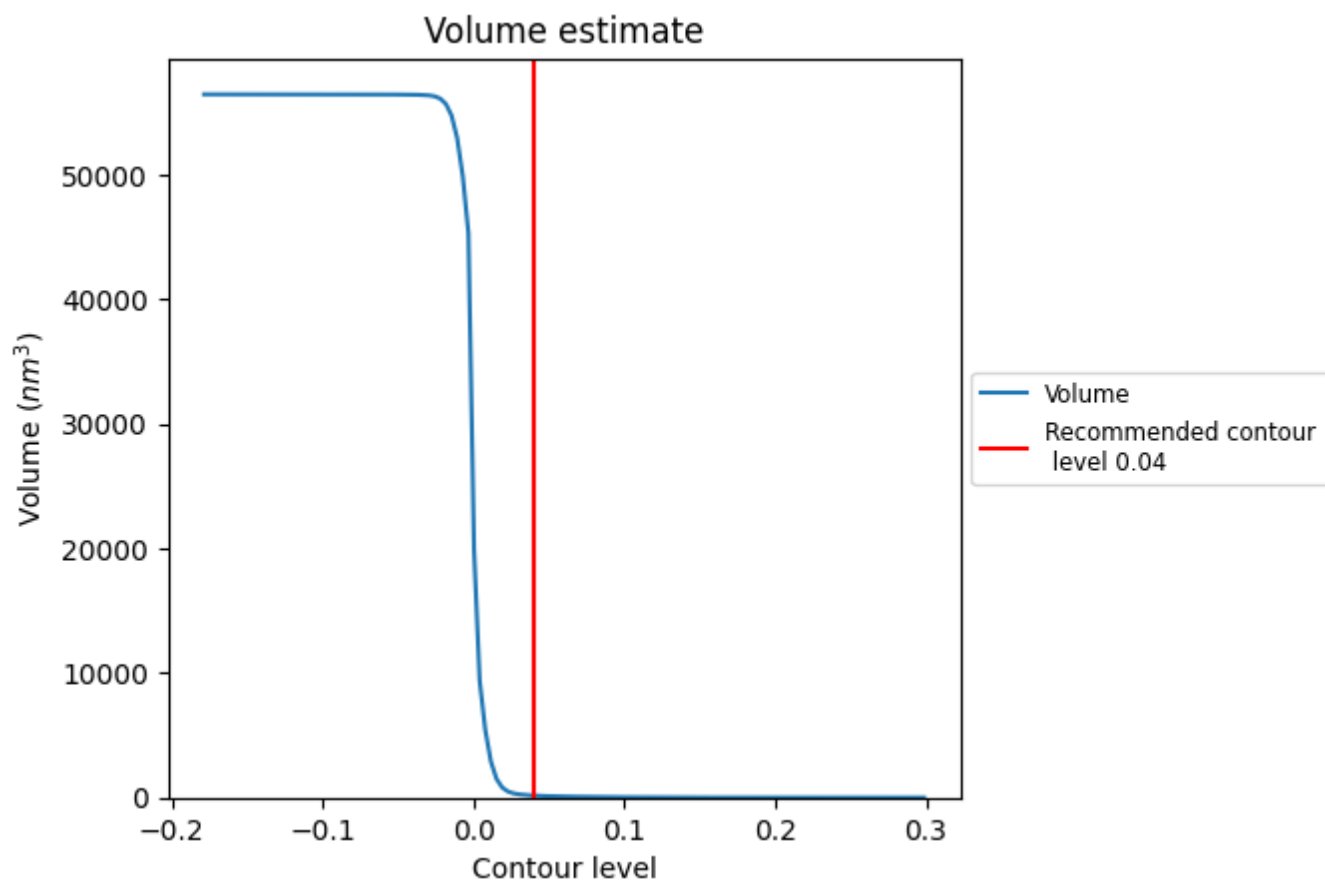
This section contains the results of statistical analysis of the map.

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.

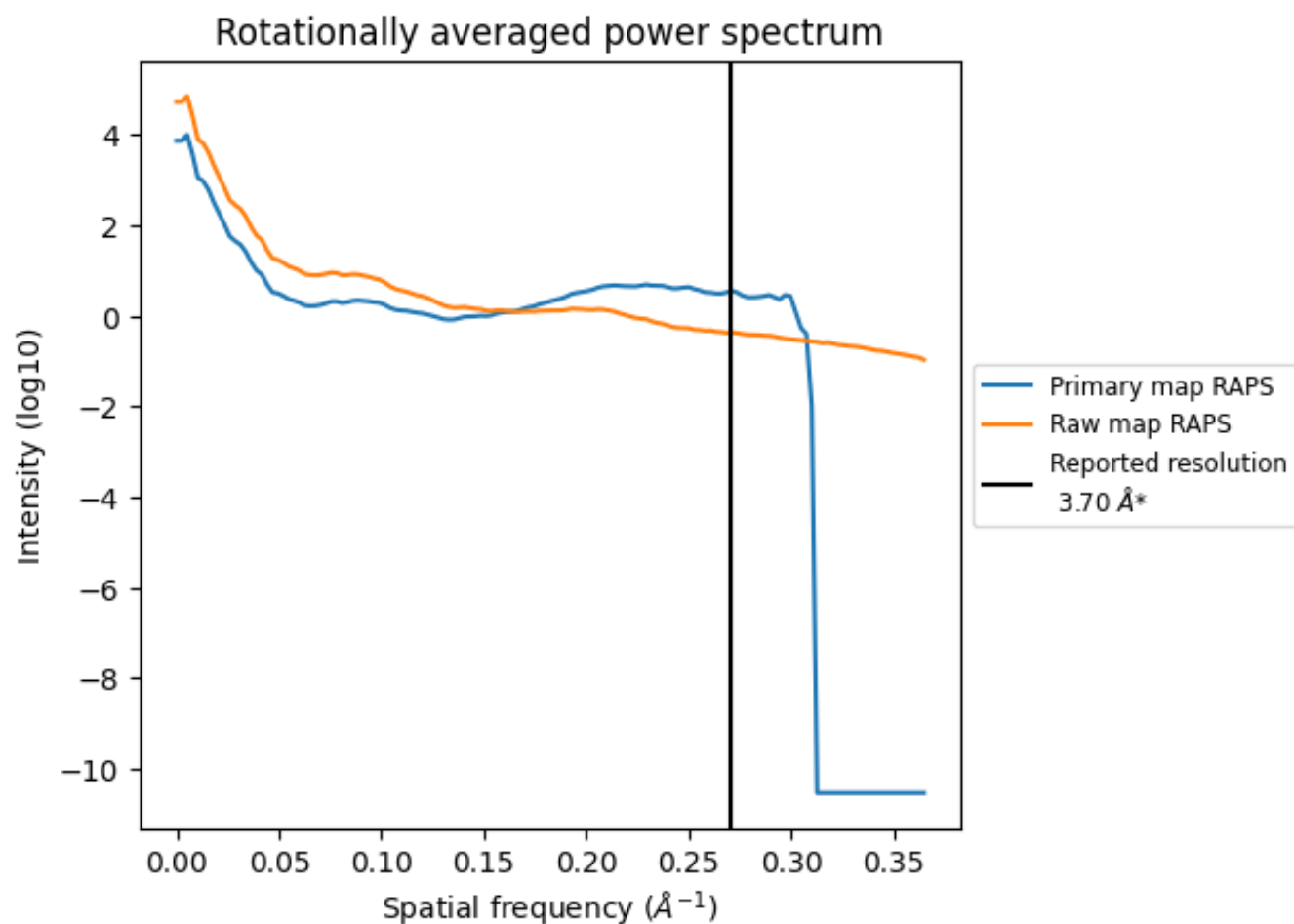
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 ⓘ

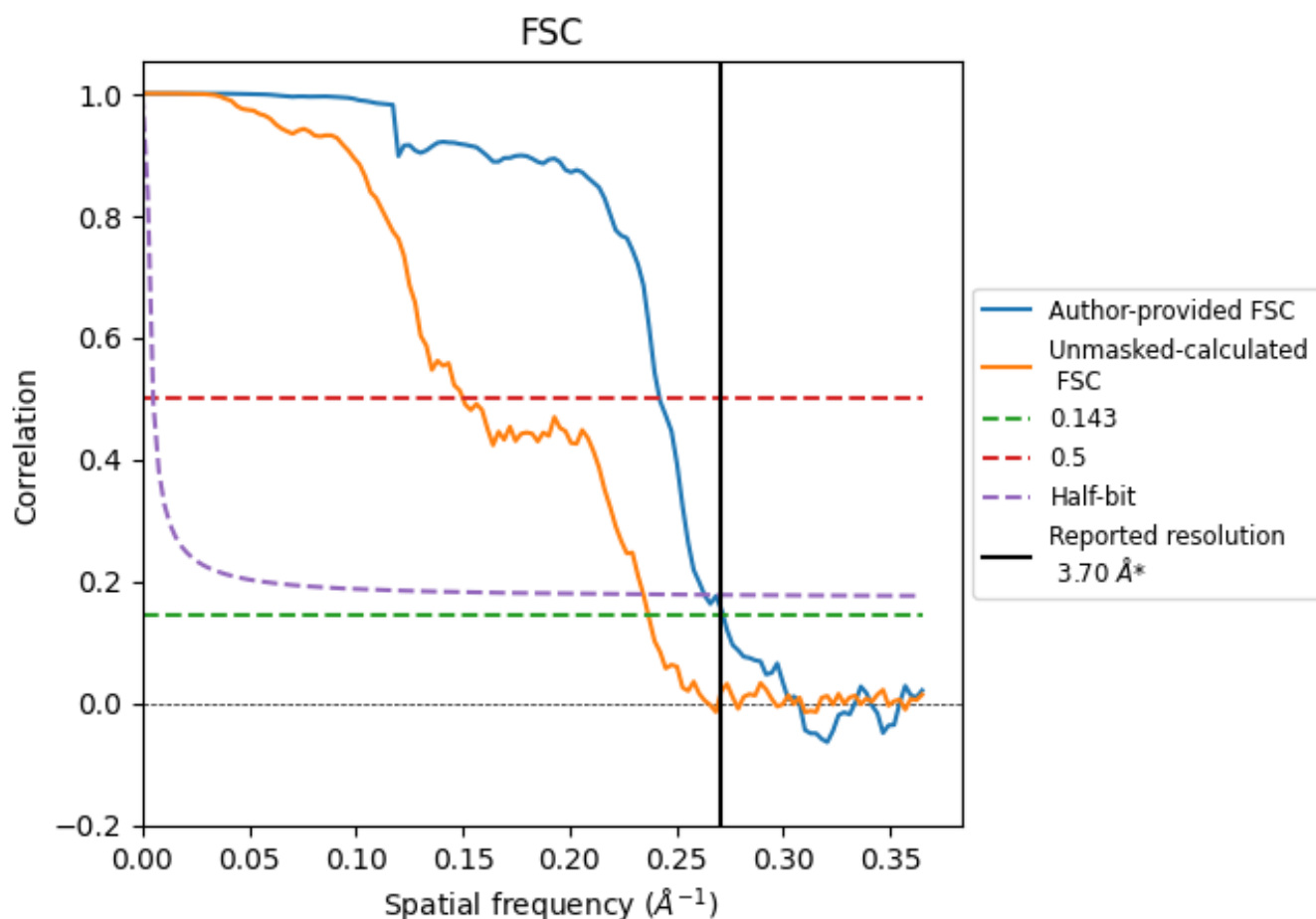


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

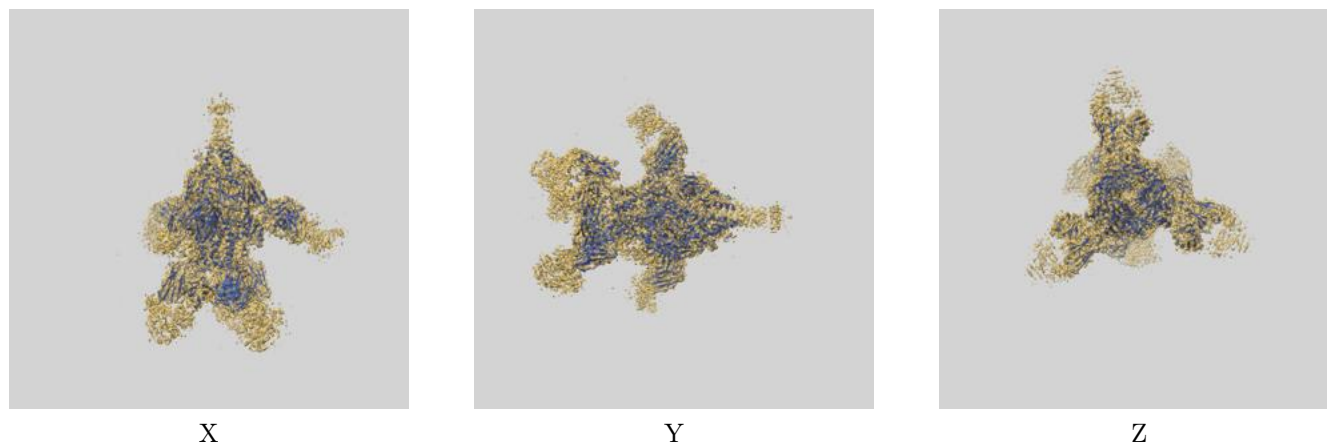
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.13	3.80
Unmasked-calculated*	4.22	6.67	4.26

*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 4.22 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

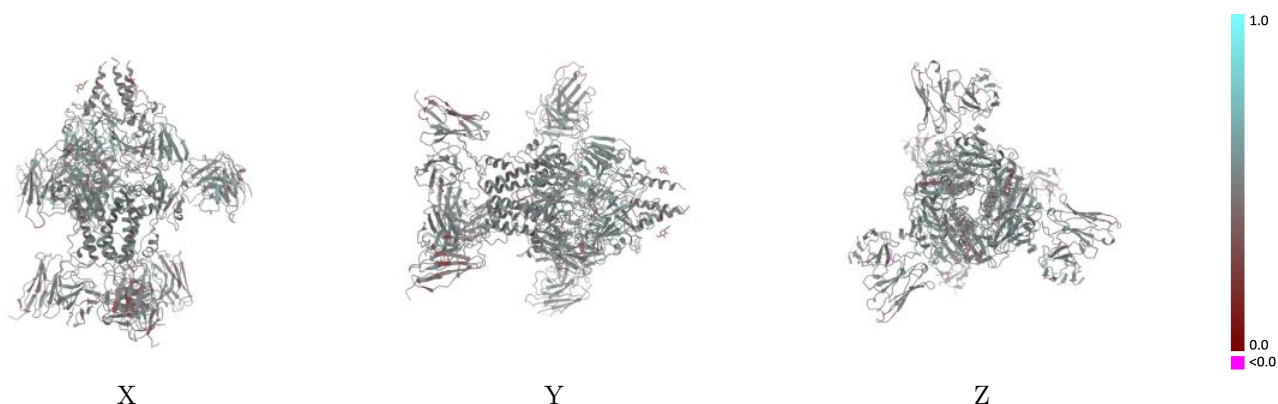
This section contains information regarding the fit between EMDB map EMD-26562 and PDB model 7UJA. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



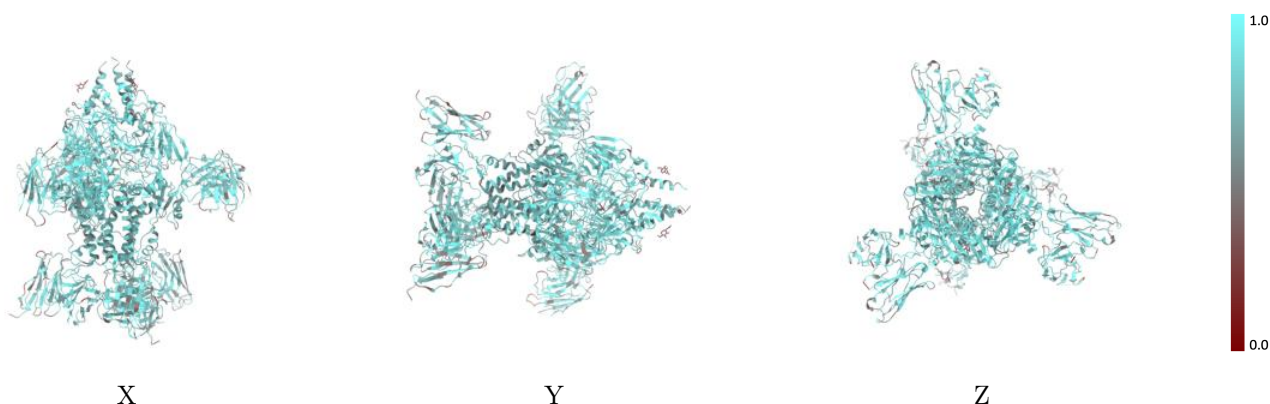
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



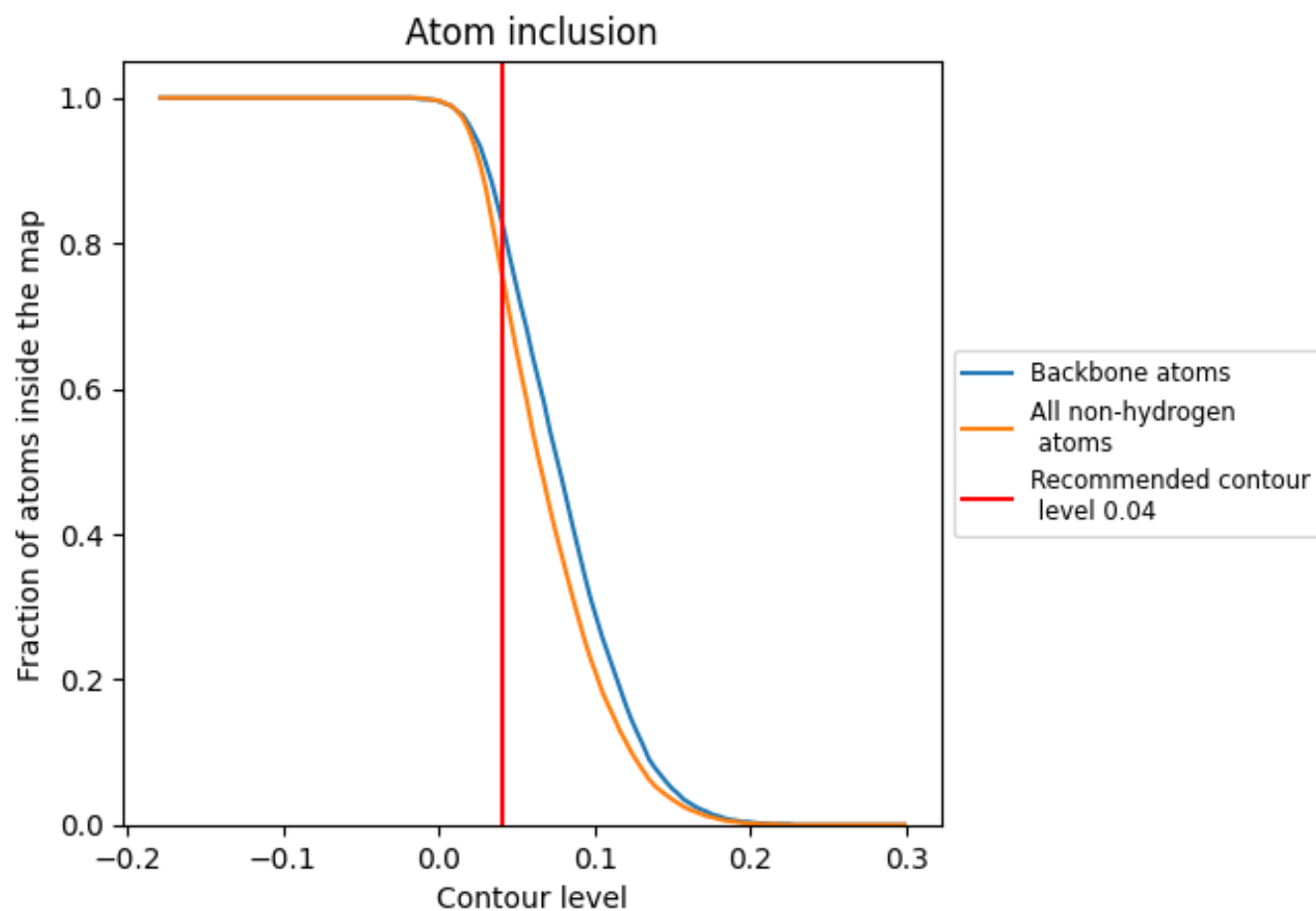
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4920
A	 0.7920	 0.5090
B	 0.7690	 0.4760
C	 0.7880	 0.5100
D	 0.7400	 0.4810
E	 0.6840	 0.4540
F	 0.7530	 0.4960
G	 0.7700	 0.4800
H	 0.7310	 0.4760
I	 0.6920	 0.4630
J	 0.7620	 0.4930
K	 0.7930	 0.5090
L	 0.7650	 0.4750
M	 0.7320	 0.4740
N	 0.6900	 0.4610
O	 0.7570	 0.4970
P	 0.7680	 0.5030
Q	 0.7730	 0.4990
R	 0.7760	 0.5010

