



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:14 AM UTC

PDB ID : 9JY4 / pdb\_00009jy4  
EMDB ID : EMD-61887  
Title : gamma epsilon/gamma epsilon Fab-TCR tetramer  
Authors : Wang, L.; Li, J.; Li, Z.  
Deposited on : 2024-10-12  
Resolution : 3.29 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
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



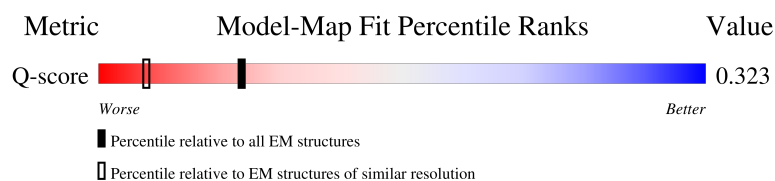
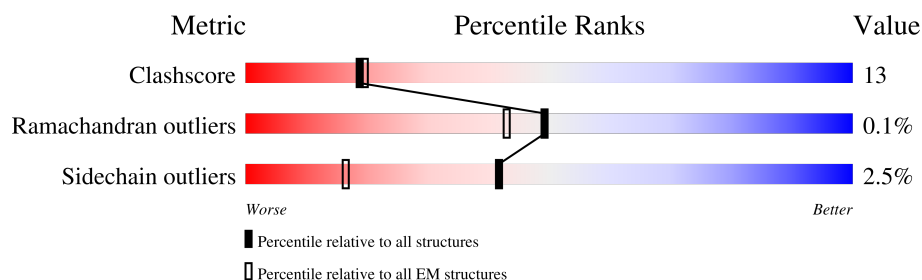
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





The reported resolution of this entry is 3.29 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	14466 ( 2.79 - 3.79 )

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  $\geq 3$ , 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	166	
1	B	166	
1	a	166	
1	b	166	

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Mol	Chain	Length	Quality of chain
2	D	171	
2	d	171	
3	E	207	
3	F	207	
3	e	207	
3	f	207	
4	G	182	
4	g	182	
5	M	292	
5	m	292	
6	N	315	
6	n	315	
7	P	222	
7	R	222	
8	O	212	
8	Q	212	



## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15642 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 T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
1	b	29	Total	C	N	O	S	0	0
			237	166	34	36	1		
1	A	31	Total	C	N	O	S	0	0
			251	175	36	39	1		
1	B	29	Total	C	N	O	S	0	0
			237	166	34	36	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	165	SER	-	expression tag	UNP P20963
a	166	ALA	-	expression tag	UNP P20963
b	165	SER	-	expression tag	UNP P20963
b	166	ALA	-	expression tag	UNP P20963
A	165	SER	-	expression tag	UNP P20963
A	166	ALA	-	expression tag	UNP P20963
B	165	SER	-	expression tag	UNP P20963
B	166	ALA	-	expression tag	UNP P20963

- Molecule 2 is a protein called T-cell surface glycoprotein CD3 delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	105	Total	C	N	O	S	0	0
			817	521	135	155	6		
2	D	105	Total	C	N	O	S	0	0
			817	521	135	155	6		

- Molecule 3 is a protein called T-cell surface glycoprotein CD3 epsilon chain.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
3	f	122	Total	C	N	O	S	0	0
			967	613	153	193	8		
3	E	121	Total	C	N	O	S	0	0
			959	609	151	191	8		
3	F	122	Total	C	N	O	S	0	0
			967	613	153	193	8		

- Molecule 4 is a protein called T-cell surface glycoprotein CD3 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	115	Total	C	N	O	S	0	0
			907	582	150	168	7		
4	G	115	Total	C	N	O	S	0	0
			907	582	150	168	7		

- Molecule 5 is a protein called T cell receptor delta variable 2, T cell receptor delta constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	36	Total	C	N	O	S	0	0
			285	191	46	45	3		
5	M	36	Total	C	N	O	S	0	0
			285	191	46	45	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	114	LEU	VAL	conflict	UNP B7Z8B9
m	115	GLY	TYR	conflict	UNP B7Z8B9
m	116	MET	TRP	conflict	UNP B7Z8B9
m	?	-	ILE	deletion	UNP B7Z8B9
m	118	GLY	SER	conflict	UNP B7Z8B9
m	119	GLU	ARG	conflict	UNP B7Z8B9
M	114	LEU	VAL	conflict	UNP B7Z8B9
M	115	GLY	TYR	conflict	UNP B7Z8B9
M	116	MET	TRP	conflict	UNP B7Z8B9
M	?	-	ILE	deletion	UNP B7Z8B9
M	118	GLY	SER	conflict	UNP B7Z8B9
M	119	GLU	ARG	conflict	UNP B7Z8B9

- Molecule 6 is a protein called T cell receptor gamma variable 9,T cell receptor gamma constant 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	38	Total 310	C 207	N 47	O 53	S 3	0	0
6	N	38	Total 310	C 207	N 47	O 53	S 3	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	104	ALA	-	linker	UNP Q99603
n	105	GLN	-	linker	UNP Q99603
n	106	GLN	-	linker	UNP Q99603
n	107	GLU	-	linker	UNP Q99603
n	108	LEU	-	linker	UNP Q99603
n	109	GLY	-	linker	UNP Q99603
n	110	LYS	-	linker	UNP Q99603
n	111	LYS	-	linker	UNP Q99603
n	112	ILE	-	linker	UNP Q99603
n	113	LYS	-	linker	UNP Q99603
n	114	VAL	-	linker	UNP Q99603
n	115	PHE	-	linker	UNP Q99603
n	116	GLY	-	linker	UNP Q99603
n	117	PRO	-	linker	UNP Q99603
n	118	GLY	-	linker	UNP Q99603
n	119	THR	-	linker	UNP Q99603
n	120	LYS	-	linker	UNP Q99603
n	121	LEU	-	linker	UNP Q99603
n	122	ILE	-	linker	UNP Q99603
n	123	ILE	-	linker	UNP Q99603
n	124	THR	-	linker	UNP Q99603
n	171	GLU	GLN	conflict	UNP P0CF51
N	104	ALA	-	linker	UNP Q99603
N	105	GLN	-	linker	UNP Q99603
N	106	GLN	-	linker	UNP Q99603
N	107	GLU	-	linker	UNP Q99603
N	108	LEU	-	linker	UNP Q99603
N	109	GLY	-	linker	UNP Q99603
N	110	LYS	-	linker	UNP Q99603
N	111	LYS	-	linker	UNP Q99603
N	112	ILE	-	linker	UNP Q99603
N	113	LYS	-	linker	UNP Q99603
N	114	VAL	-	linker	UNP Q99603
N	115	PHE	-	linker	UNP Q99603
N	116	GLY	-	linker	UNP Q99603

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Chain	Residue	Modelled	Actual	Comment	Reference
N	117	PRO	-	linker	UNP Q99603
N	118	GLY	-	linker	UNP Q99603
N	119	THR	-	linker	UNP Q99603
N	120	LYS	-	linker	UNP Q99603
N	121	LEU	-	linker	UNP Q99603
N	122	ILE	-	linker	UNP Q99603
N	123	ILE	-	linker	UNP Q99603
N	124	THR	-	linker	UNP Q99603
N	171	GLU	GLN	conflict	UNP P0CF51

- Molecule 7 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	195	Total	C	N	O	S	0	0
			1505	969	236	291	9		
7	R	195	Total	C	N	O	S	0	0
			1505	969	236	291	9		

- Molecule 8 is a protein called Fab light chain.

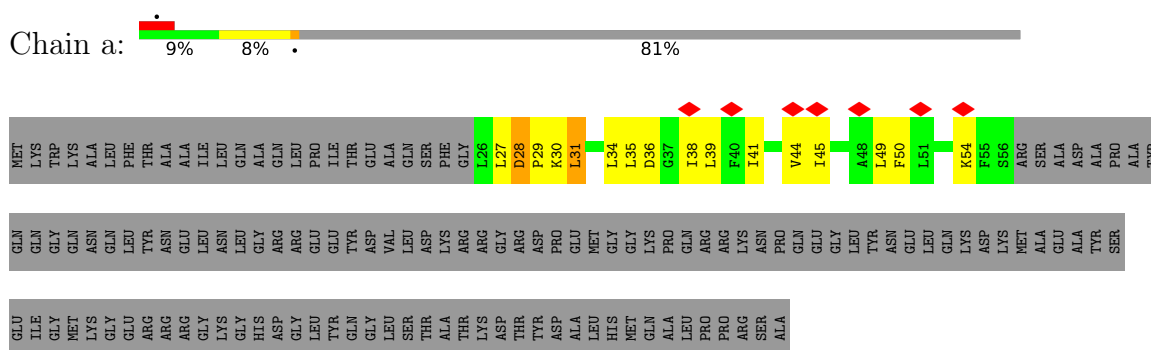
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	209	Total	C	N	O	S	0	0
			1583	988	268	321	6		
8	Q	209	Total	C	N	O	S	0	0
			1583	988	268	321	6		



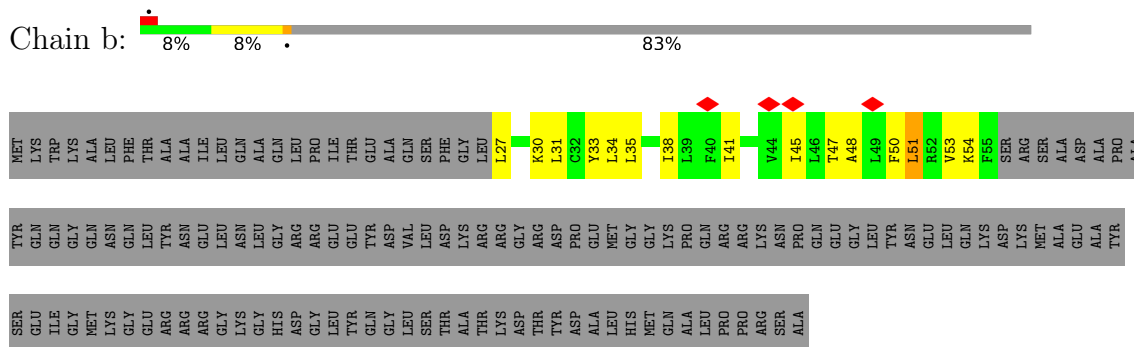
### 3 Residue-property plots

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.

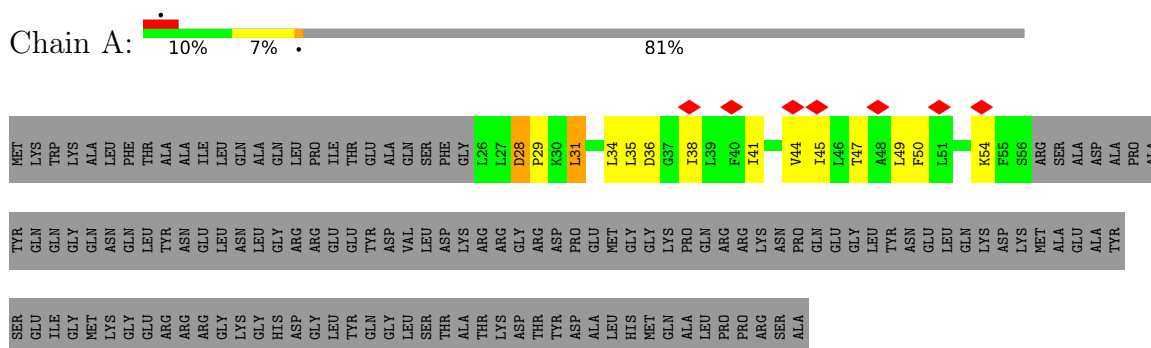
- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



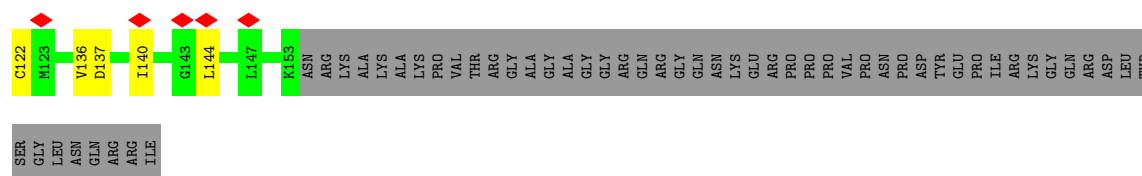
- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



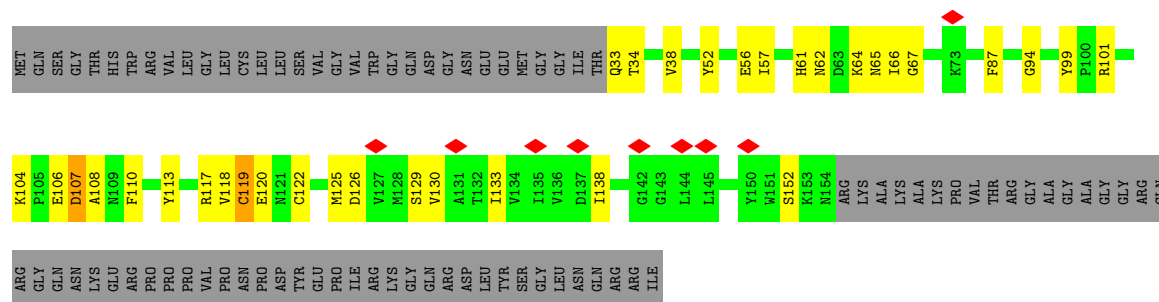


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| N62 | D63 | K64 | N65 | I66 | G67 | G68 | D69 | E70 | D71 | D72 | K73 | N74 | I75 | G76 | S77 | D78 | E79 | D80 | H81 | L82 | S83 | L84 | K85 | E86 | F87 | S88 | E89 | E90 | Q92 | S93 | G94 | Y95 | Y96 | Y97 | C98 | Y99 | P100 | R101 | G102 | S103 | K104 | P105 | E106 | D107 | A108 | N109 | F110 | Y111 | L112 | Y113 | L114 | R115 | A116 | R117 | V118 | C119 | E120 | N121 |
| MET | GLN | SER | GLY | THR | HIS | TRP | ARG | VAL | LEU | GLY | LEU | CYS | LEU | LEU | SER | GLY | VAL | TRP | GLY | GLN | ASP | GLY | ASN | GLU | GLU | MET | GLY | GLY | ILE | THR | Q33 | T34 | P35 | V36 | K37 | V38 | S39  | L40  | S41  | G42  | V45  | I46  | L47  | T48  | C49  | P50  | Q51  | Y52  | P53  | G54  | S55  | E56  | I57  | L58  | W59  | Q60  | H61  |      |

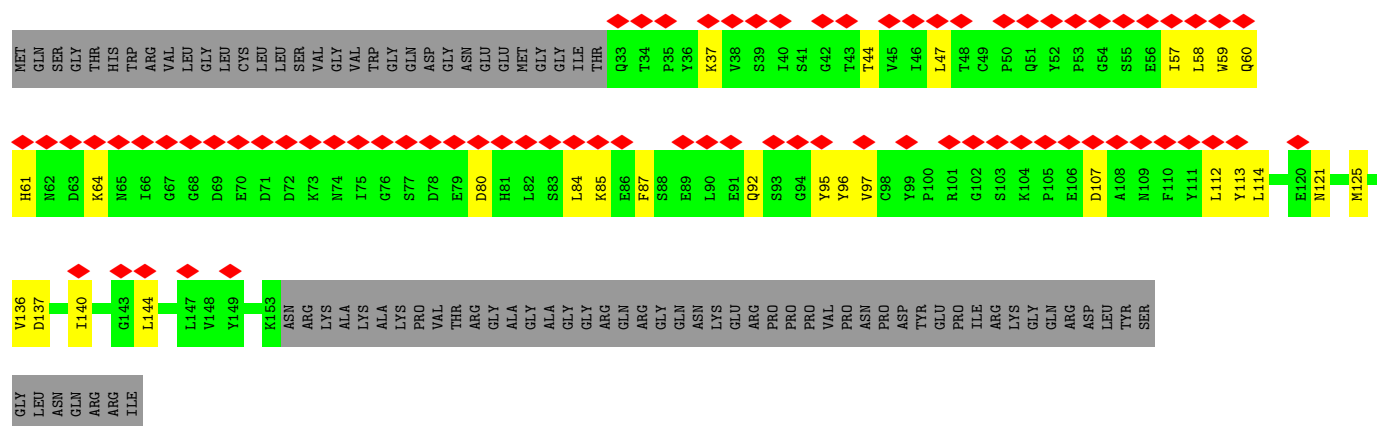
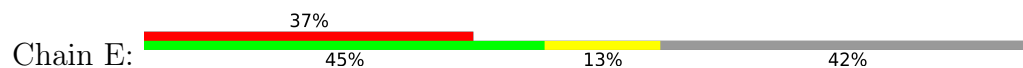




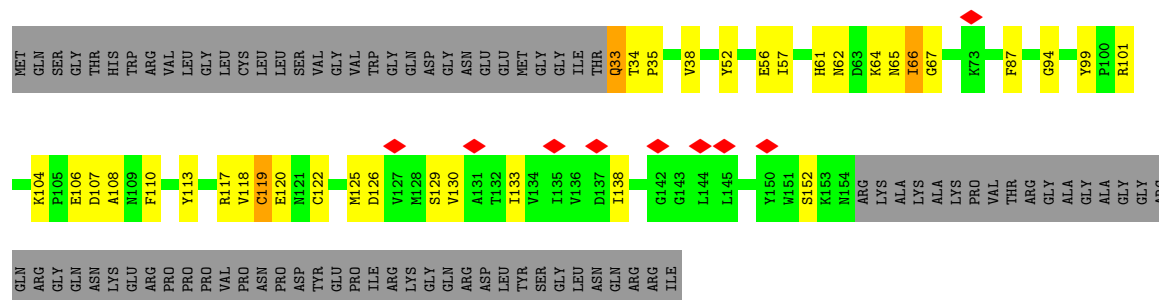
• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain



• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain



• Molecule 3: T-cell surface glycoprotein CD3 epsilon chain





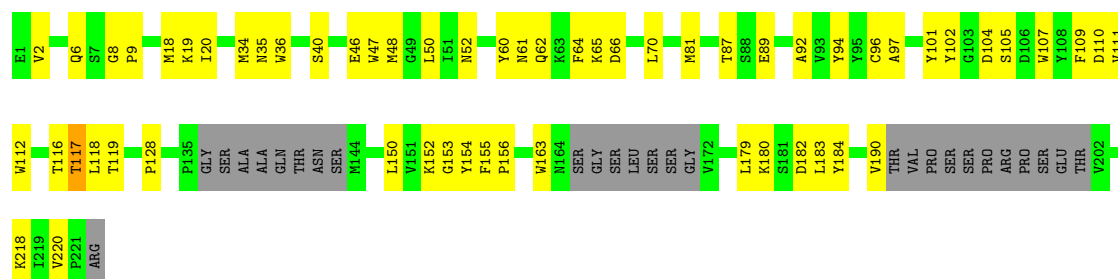






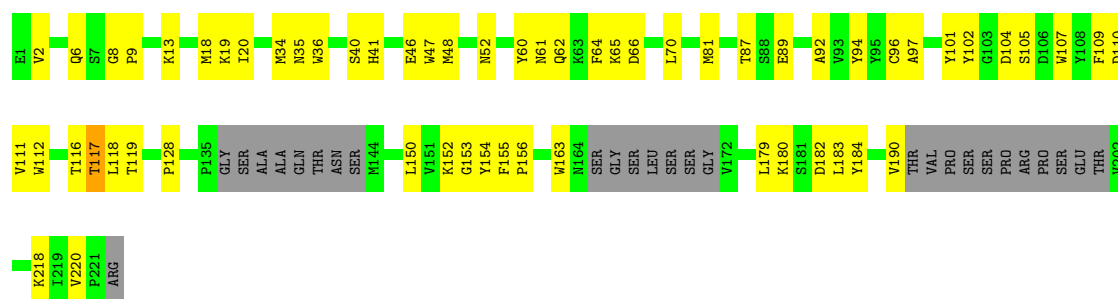


Chain P: 




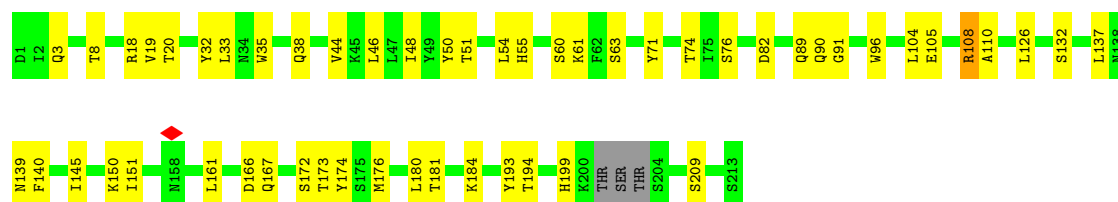
• Molecule 7: Fab heavy chain

Chain R: 



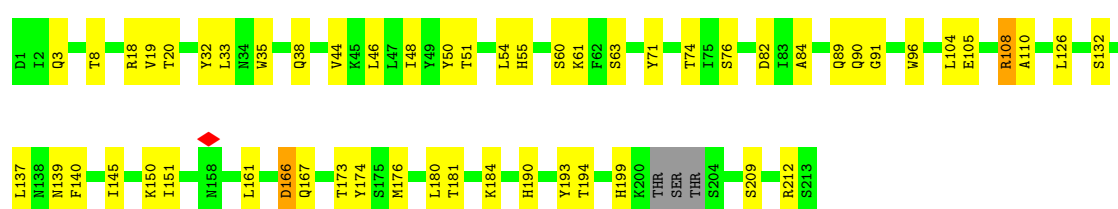
• Molecule 8: Fab light chain

Chain O: 



• Molecule 8: Fab light chain

Chain Q: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.133	Depositor
Minimum map value	-0.736	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.074	Depositor
Map size (Å)	421.888, 421.888, 421.888	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.20	0/256	0.61	0/346
1	B	0.15	0/242	0.45	0/327
1	a	0.21	0/256	0.61	0/346
1	b	0.15	0/242	0.47	0/327
2	D	0.11	0/829	0.31	0/1127
2	d	0.11	0/829	0.30	0/1127
3	E	0.11	0/980	0.27	0/1331
3	F	0.18	0/988	0.42	0/1342
3	e	0.12	0/980	0.32	0/1331
3	f	0.16	0/988	0.39	0/1342
4	G	0.16	0/925	0.46	0/1244
4	g	0.15	0/925	0.46	0/1244
5	M	0.18	0/289	0.55	0/388
5	m	0.20	0/289	0.75	2/388 (0.5%)
6	N	0.15	0/314	0.45	0/427
6	n	0.16	0/314	0.45	0/427
7	P	0.15	0/1545	0.34	0/2105
7	R	0.15	0/1545	0.34	0/2105
8	O	0.16	0/1616	0.41	2/2197 (0.1%)
8	Q	0.16	0/1616	0.40	2/2197 (0.1%)
All	All	0.15	0/15968	0.40	6/21668 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	108	ARG	CA-C-N	5.97	132.45	121.70
8	O	108	ARG	C-N-CA	5.97	132.45	121.70
8	Q	108	ARG	CA-C-N	5.95	132.41	121.70
8	Q	108	ARG	C-N-CA	5.95	132.41	121.70
5	m	260	ASN	CA-C-N	-5.18	113.65	122.56
5	m	260	ASN	C-N-CA	-5.18	113.65	122.56



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	A	251	0	276	11	0
1	B	237	0	260	10	0
1	a	251	0	276	13	0
1	b	237	0	260	10	0
2	D	817	0	828	29	0
2	d	817	0	828	35	0
3	E	959	0	921	19	0
3	F	967	0	925	29	0
3	e	959	0	921	19	0
3	f	967	0	925	27	0
4	G	907	0	897	24	0
4	g	907	0	897	29	0
5	M	285	0	312	17	0
5	m	285	0	312	23	0
6	N	310	0	336	12	0
6	n	310	0	336	11	0
7	P	1505	0	1473	45	0
7	R	1505	0	1473	46	0
8	O	1583	0	1497	35	0
8	Q	1583	0	1497	36	0
All	All	15642	0	15450	402	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 13.

All (402) 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)
3:F:33:GLN:HE21	3:F:33:GLN:N	1.20	1.38
3:F:33:GLN:N	3:F:33:GLN:NE2	2.05	1.05
2:d:99:LEU:HA	5:m:261:MET:HE1	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:31:LEU:HD21	5:m:267:LEU:HD11	1.64	0.79
1:A:31:LEU:HD21	5:M:267:LEU:HD11	1.65	0.79
3:f:62:ASN:HD21	3:f:94:GLY:HA3	1.49	0.77
3:F:62:ASN:HD21	3:F:94:GLY:HA3	1.49	0.77
3:f:67:GLY:O	7:P:102:TYR:OH	2.02	0.75
7:R:153:GLY:HA2	7:R:183:LEU:HD13	1.69	0.75
7:P:180:LYS:HD3	8:O:161:LEU:HD11	1.69	0.75
7:P:153:GLY:HA2	7:P:183:LEU:HD13	1.69	0.75
4:G:56:PHE:HB2	4:G:86:GLN:HB2	1.69	0.74
7:R:180:LYS:HD3	8:Q:161:LEU:HD11	1.69	0.74
4:g:56:PHE:HB2	4:g:86:GLN:HB2	1.68	0.73
3:f:33:GLN:N	3:f:33:GLN:OE1	2.21	0.72
2:D:32:ARG:HE	2:D:33:VAL:H	1.39	0.71
2:d:32:ARG:HE	2:d:33:VAL:H	1.39	0.70
8:Q:137:LEU:HB2	8:Q:176:MET:HB3	1.73	0.69
8:O:137:LEU:HB2	8:O:176:MET:HB3	1.73	0.69
5:m:261:MET:O	5:m:265:THR:HG23	1.93	0.68
5:m:261:MET:HA	5:m:264:LEU:HB2	1.76	0.67
3:F:138:ILE:HD12	6:N:271:LEU:HD11	1.76	0.67
3:E:47:LEU:HD21	3:E:114:LEU:HD11	1.78	0.66
3:F:67:GLY:O	7:R:102:TYR:OH	2.12	0.66
2:D:119:ALA:HB2	3:E:144:LEU:HD21	1.79	0.65
3:F:104:LYS:NZ	8:Q:91:GLY:O	2.24	0.65
3:f:138:ILE:HD12	6:n:271:LEU:HD11	1.78	0.64
2:d:119:ALA:HB2	3:e:144:LEU:HD21	1.79	0.64
2:D:36:ASN:ND2	2:D:56:THR:O	2.31	0.64
3:f:117:ARG:HG3	4:g:103:MET:SD	2.37	0.64
3:f:61:HIS:HD2	3:f:64:LYS:HE3	1.63	0.64
3:f:104:LYS:NZ	8:O:91:GLY:O	2.24	0.64
3:F:106:GLU:OE1	3:F:106:GLU:N	2.31	0.64
3:F:117:ARG:HG3	4:G:103:MET:SD	2.38	0.64
7:P:180:LYS:HB3	8:O:161:LEU:HD21	1.79	0.64
3:F:61:HIS:HD2	3:F:64:LYS:HE3	1.62	0.64
3:e:47:LEU:HD21	3:e:114:LEU:HD11	1.79	0.63
1:A:54:LYS:HE2	1:B:53:VAL:HG21	1.81	0.63
2:d:36:ASN:ND2	2:d:56:THR:O	2.31	0.63
3:F:101:ARG:NH2	7:R:101:TYR:O	2.22	0.63
3:f:106:GLU:OE1	3:f:106:GLU:N	2.31	0.63
1:a:54:LYS:HE2	1:b:53:VAL:HG21	1.80	0.63
5:M:270:ARG:HG3	5:M:271:MET:HE2	1.81	0.63
7:P:128:PRO:HB3	7:P:154:TYR:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:180:LYS:HB3	8:Q:161:LEU:HD21	1.79	0.63
7:R:179:LEU:HD12	7:R:184:TYR:HE2	1.64	0.63
7:P:179:LEU:HD12	7:P:184:TYR:HE2	1.64	0.62
8:Q:48:ILE:HG22	8:Q:54:LEU:HD23	1.81	0.62
3:f:101:ARG:NH2	7:P:101:TYR:O	2.22	0.62
8:O:150:LYS:HB2	8:O:194:THR:HB	1.82	0.62
4:G:88:LYS:HD2	4:G:93:LYS:HB3	1.82	0.62
7:P:97:ALA:HB1	7:P:109:PHE:HB3	1.81	0.62
7:R:97:ALA:HB1	7:R:109:PHE:HB3	1.81	0.62
8:O:48:ILE:HG22	8:O:54:LEU:HD23	1.81	0.62
4:g:88:LYS:HD2	4:g:93:LYS:HB3	1.82	0.61
8:Q:150:LYS:HB2	8:Q:194:THR:HB	1.82	0.61
5:M:261:MET:O	5:M:265:THR:HG23	2.01	0.61
7:R:150:LEU:HD22	7:R:152:LYS:HG2	1.82	0.61
5:m:270:ARG:HG3	5:m:271:MET:HE2	1.81	0.61
3:F:119:CYS:SG	3:F:120:GLU:N	2.73	0.61
5:M:256:THR:O	5:M:260:ASN:ND2	2.33	0.61
3:f:125:MET:N	3:f:125:MET:SD	2.73	0.61
7:R:128:PRO:HB3	7:R:154:TYR:HB3	1.81	0.61
7:P:150:LEU:HD22	7:P:152:LYS:HG2	1.82	0.60
5:m:273:PHE:O	5:m:277:VAL:HG12	2.01	0.60
3:f:119:CYS:SG	3:f:120:GLU:N	2.74	0.60
5:M:273:PHE:O	5:M:277:VAL:HG12	2.02	0.59
2:D:99:LEU:HA	5:M:261:MET:HE3	1.85	0.59
8:Q:108:ARG:HA	8:Q:110:ALA:HB3	1.83	0.59
2:D:70:ILE:HD12	2:D:87:GLN:HG2	1.85	0.58
4:G:44:LEU:HG	4:G:74:LEU:HD11	1.86	0.58
4:g:110:LEU:HB3	4:g:115:ILE:HD11	1.84	0.58
3:F:125:MET:SD	3:F:125:MET:N	2.76	0.58
3:F:56:GLU:OE2	7:R:52:ASN:ND2	2.30	0.58
1:a:50:PHE:HD1	1:b:50:PHE:HD1	1.52	0.58
5:m:261:MET:HG2	5:m:264:LEU:HD22	1.86	0.58
2:d:70:ILE:HD12	2:d:87:GLN:HG2	1.86	0.58
4:G:110:LEU:HB3	4:G:115:ILE:HD11	1.84	0.58
8:O:108:ARG:HA	8:O:110:ALA:HB3	1.85	0.57
2:D:109:VAL:O	2:D:113:ILE:HG12	2.03	0.57
4:g:44:LEU:HG	4:g:74:LEU:HD11	1.86	0.56
3:E:60:GLN:HB3	3:E:97:VAL:HG13	1.87	0.56
2:d:93:CYS:SG	3:e:117:ARG:NH1	2.78	0.56
3:e:60:GLN:HB3	3:e:97:VAL:HG13	1.87	0.56
3:F:65:ASN:HB3	7:R:102:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HA	1:B:30:LYS:HE2	1.86	0.56
1:B:50:PHE:CZ	1:B:54:LYS:HD2	2.40	0.56
8:Q:89:GLN:NE2	8:Q:90:GLN:O	2.38	0.56
8:O:105:GLU:OE2	8:O:174:TYR:OH	2.20	0.56
7:P:182:ASP:O	7:P:183:LEU:HD23	2.05	0.56
1:b:27:LEU:HA	1:b:30:LYS:HE2	1.85	0.56
2:D:97:VAL:HB	5:M:261:MET:HE2	1.88	0.55
7:R:182:ASP:O	7:R:183:LEU:HD23	2.05	0.55
8:O:89:GLN:NE2	8:O:90:GLN:O	2.38	0.55
1:A:50:PHE:HD1	1:B:50:PHE:HD1	1.54	0.55
3:E:58:LEU:HD12	3:E:59:TRP:H	1.71	0.55
4:g:115:ILE:O	4:g:119:LEU:HG	2.07	0.55
1:a:35:LEU:HD12	1:a:36:ASP:N	2.22	0.55
3:f:56:GLU:OE2	7:P:52:ASN:ND2	2.31	0.55
3:e:58:LEU:HD12	3:e:59:TRP:H	1.71	0.55
3:F:125:MET:SD	4:G:106:ASN:HB2	2.47	0.55
1:A:35:LEU:HD12	1:A:36:ASP:N	2.23	0.54
4:G:115:ILE:O	4:G:119:LEU:HG	2.07	0.54
3:F:99:TYR:HB3	3:F:108:ALA:HB2	1.90	0.54
3:E:87:PHE:HA	3:E:92:GLN:HE21	1.71	0.54
3:e:136:VAL:O	3:e:140:ILE:HG23	2.08	0.54
2:D:24:ILE:HG21	2:D:35:VAL:HG23	1.88	0.54
2:d:97:VAL:HB	5:m:261:MET:CE	2.38	0.54
7:R:34:MET:C	7:R:35:ASN:HD22	2.16	0.54
2:D:68:ARG:HG2	2:D:89:HIS:HD2	1.73	0.54
2:d:24:ILE:HG21	2:d:35:VAL:HG23	1.89	0.53
3:e:61:HIS:O	3:e:64:LYS:HG3	2.09	0.53
3:e:87:PHE:HA	3:e:92:GLN:HE21	1.73	0.53
3:F:126:ASP:O	3:F:130:VAL:HG12	2.08	0.53
8:Q:61:LYS:HE3	8:Q:82:ASP:OD1	2.09	0.53
7:P:34:MET:C	7:P:35:ASN:HD22	2.16	0.53
3:f:125:MET:SD	4:g:106:ASN:HB2	2.49	0.53
8:O:50:TYR:O	8:O:51:THR:HG22	2.09	0.53
8:O:194:THR:HG23	8:O:209:SER:HB2	1.91	0.53
3:E:61:HIS:O	3:E:64:LYS:HG3	2.09	0.53
8:Q:89:GLN:HE21	8:Q:96:TRP:HB3	1.73	0.53
3:f:126:ASP:O	3:f:130:VAL:HG12	2.08	0.53
7:R:65:LYS:HG3	7:R:66:ASP:OD2	2.09	0.53
8:O:89:GLN:HE21	8:O:96:TRP:HB3	1.73	0.52
3:f:99:TYR:HB3	3:f:108:ALA:HB2	1.90	0.52
3:f:122:CYS:HB3	4:g:109:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:35:ASN:HB3	7:R:47:TRP:HE1	1.74	0.52
1:a:41:ILE:HA	1:a:44:VAL:HG12	1.91	0.52
4:g:42:VAL:HG23	4:g:74:LEU:HD13	1.90	0.52
8:Q:151:ILE:HG22	8:Q:193:TYR:HD1	1.74	0.52
7:P:35:ASN:HD22	7:P:35:ASN:N	2.08	0.52
7:P:110:ASP:OD2	7:P:111:VAL:HG23	2.10	0.52
4:G:42:VAL:HG23	4:G:74:LEU:HD13	1.90	0.52
8:Q:50:TYR:O	8:Q:51:THR:HG22	2.09	0.52
1:b:50:PHE:CZ	1:b:54:LYS:HD2	2.45	0.52
8:Q:194:THR:HG23	8:Q:209:SER:HB2	1.91	0.52
2:d:97:VAL:HB	5:m:261:MET:HE2	1.91	0.52
7:R:110:ASP:OD2	7:R:111:VAL:HG23	2.10	0.52
8:Q:166:ASP:OD2	8:Q:166:ASP:N	2.32	0.52
8:O:38:GLN:HG3	8:O:44:VAL:HG22	1.92	0.52
8:Q:38:GLN:HG3	8:Q:44:VAL:HG22	1.92	0.52
2:D:24:ILE:O	3:E:95:TYR:OH	2.18	0.52
3:E:137:ASP:O	3:E:140:ILE:HG12	2.10	0.52
7:R:35:ASN:HD22	7:R:35:ASN:N	2.08	0.52
7:P:65:LYS:HG3	7:P:66:ASP:OD2	2.09	0.51
8:O:151:ILE:HG22	8:O:193:TYR:HD1	1.74	0.51
2:d:99:LEU:O	3:e:121:ASN:ND2	2.44	0.51
2:d:109:VAL:O	2:d:113:ILE:HG12	2.09	0.51
8:O:61:LYS:HE3	8:O:82:ASP:OD2	2.09	0.51
1:A:41:ILE:HA	1:A:44:VAL:HG12	1.92	0.51
6:n:269:LEU:O	6:n:272:LYS:HG3	2.11	0.51
6:N:253:LEU:O	6:N:257:LEU:HD23	2.11	0.51
8:O:35:TRP:HB2	8:O:48:ILE:HG12	1.93	0.50
4:g:80:ASP:HB3	4:g:82:ARG:HH12	1.75	0.50
5:m:261:MET:HB3	5:m:264:LEU:HB2	1.93	0.50
7:P:35:ASN:HB3	7:P:47:TRP:HE1	1.75	0.50
2:D:32:ARG:CZ	2:D:59:ASP:HB2	2.41	0.50
1:a:35:LEU:HD12	1:a:36:ASP:H	1.77	0.50
2:d:32:ARG:CZ	2:d:59:ASP:HB2	2.41	0.50
4:G:80:ASP:HB3	4:G:82:ARG:HH12	1.75	0.50
7:R:9:PRO:HB3	7:R:117:THR:HG23	1.93	0.50
2:d:68:ARG:HG2	2:d:89:HIS:HD2	1.76	0.50
7:P:9:PRO:HB3	7:P:117:THR:HG23	1.93	0.50
2:D:24:ILE:HB	2:D:86:VAL:HG11	1.94	0.50
7:R:40:SER:HB2	7:R:92:ALA:HB2	1.93	0.50
7:P:104:ASP:OD2	7:P:105:SER:N	2.45	0.50
3:f:152:SER:HB3	4:g:134:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:40:SER:HB2	7:P:92:ALA:HB2	1.94	0.50
2:D:90:TYR:HE1	3:E:113:TYR:HE2	1.60	0.50
1:b:34:LEU:O	1:b:38:ILE:HG23	2.12	0.50
4:G:118:PHE:O	4:G:122:GLU:HG2	2.12	0.50
8:Q:35:TRP:HB2	8:Q:48:ILE:HG12	1.93	0.50
3:e:57:ILE:HD11	3:e:80:ASP:HA	1.94	0.50
3:F:152:SER:HB3	4:G:134:TYR:CD1	2.47	0.50
4:G:129:LEU:HD13	6:N:272:LYS:HZ1	1.77	0.50
1:A:41:ILE:O	1:A:45:ILE:HG12	2.13	0.49
2:d:45:GLU:H	2:d:70:ILE:HB	1.78	0.49
6:N:269:LEU:O	6:N:272:LYS:HG3	2.11	0.49
3:F:122:CYS:HB3	4:G:109:GLU:HA	1.94	0.49
5:m:261:MET:HA	5:m:264:LEU:H	1.77	0.49
7:P:48:MET:HE1	7:P:81:MET:SD	2.53	0.49
2:d:63:ARG:HH21	2:d:92:MET:HE3	1.77	0.49
5:m:257:GLU:CD	5:m:257:GLU:H	2.19	0.49
3:F:104:LYS:HD3	8:Q:32:TYR:CZ	2.48	0.49
4:g:118:PHE:O	4:g:122:GLU:HG2	2.12	0.49
1:a:34:LEU:O	1:a:38:ILE:HG12	2.12	0.49
2:D:44:VAL:HG12	2:D:45:GLU:HG3	1.94	0.49
8:Q:126:LEU:O	8:Q:184:LYS:NZ	2.33	0.49
3:f:65:ASN:HB3	7:P:102:TYR:CE1	2.48	0.49
3:f:104:LYS:HD3	8:O:32:TYR:CZ	2.48	0.49
2:D:99:LEU:O	3:E:121:ASN:ND2	2.46	0.49
4:G:61:MET:HE2	4:G:61:MET:HA	1.95	0.49
2:d:44:VAL:HG12	2:d:45:GLU:HG3	1.93	0.48
3:E:57:ILE:HD11	3:E:80:ASP:HA	1.94	0.48
5:M:257:GLU:CD	5:M:257:GLU:H	2.21	0.48
2:d:32:ARG:NH2	2:d:61:GLY:O	2.46	0.48
1:A:47:THR:OG1	1:B:42:TYR:OH	2.30	0.48
7:R:48:MET:HE1	7:R:81:MET:SD	2.53	0.48
2:d:90:TYR:HE1	3:e:113:TYR:HE2	1.61	0.48
8:Q:151:ILE:HG22	8:Q:193:TYR:CD1	2.49	0.48
1:a:41:ILE:O	1:a:45:ILE:HG12	2.13	0.48
3:e:137:ASP:O	3:e:140:ILE:HG12	2.14	0.48
4:g:61:MET:HE2	4:g:61:MET:HA	1.95	0.48
1:A:34:LEU:O	1:A:38:ILE:HG12	2.13	0.48
8:O:151:ILE:HG22	8:O:193:TYR:CD1	2.49	0.48
2:D:32:ARG:NH2	2:D:61:GLY:O	2.46	0.48
1:b:38:ILE:O	1:b:41:ILE:HG22	2.13	0.48
2:d:24:ILE:HB	2:d:86:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:20:ILE:HD11	7:P:118:LEU:HD21	1.95	0.48
3:F:94:GLY:HA2	3:F:113:TYR:CE1	2.49	0.48
7:R:20:ILE:HD11	7:R:118:LEU:HD21	1.95	0.48
6:n:253:LEU:O	6:n:257:LEU:HD23	2.13	0.48
4:G:107:CYS:O	6:N:257:LEU:HD13	2.14	0.48
4:g:43:LEU:HD13	4:g:71:LYS:HE3	1.96	0.47
3:f:94:GLY:HA2	3:f:113:TYR:CE1	2.49	0.47
1:A:35:LEU:HD12	1:A:36:ASP:H	1.79	0.47
3:F:129:SER:O	3:F:133:ILE:HG12	2.15	0.47
1:B:38:ILE:O	1:B:41:ILE:HG22	2.14	0.47
2:D:43:TRP:NE1	2:D:45:GLU:O	2.47	0.47
2:D:45:GLU:H	2:D:70:ILE:HB	1.79	0.47
3:f:65:ASN:HB3	7:P:102:TYR:CZ	2.50	0.47
4:g:106:ASN:OD1	4:g:106:ASN:N	2.39	0.47
7:R:104:ASP:OD1	7:R:105:SER:N	2.48	0.47
3:f:129:SER:O	3:f:133:ILE:HG12	2.14	0.47
1:A:35:LEU:HD22	5:M:270:ARG:HG2	1.96	0.47
2:d:43:TRP:NE1	2:d:45:GLU:O	2.47	0.47
3:e:96:TYR:HB2	3:e:112:LEU:HB2	1.97	0.47
2:d:97:VAL:HG12	5:m:260:ASN:HB2	1.97	0.47
5:m:262:MET:HE2	5:m:262:MET:HA	1.97	0.47
7:P:104:ASP:O	7:P:107:TRP:NE1	2.47	0.47
4:G:43:LEU:HD13	4:G:71:LYS:HE3	1.96	0.47
3:E:96:TYR:HB2	3:E:112:LEU:HB2	1.97	0.47
8:Q:105:GLU:OE1	8:Q:174:TYR:OH	2.23	0.47
8:O:140:PHE:CD2	8:O:145:ILE:HD13	2.50	0.46
3:F:65:ASN:HB3	7:R:102:TYR:CE1	2.50	0.46
5:m:273:PHE:CZ	6:n:269:LEU:HD12	2.50	0.46
4:g:63:GLY:HA2	4:g:72:TRP:CH2	2.50	0.46
7:R:13:LYS:HB2	7:R:13:LYS:HE2	1.78	0.46
3:e:119:CYS:SG	3:e:120:GLU:N	2.89	0.46
5:m:271:MET:O	5:m:275:LYS:HG2	2.16	0.46
7:R:94:TYR:CE2	7:R:118:LEU:HD12	2.51	0.46
2:D:30:GLU:OE1	2:D:31:ASP:HB2	2.16	0.46
8:Q:63:SER:OG	8:Q:74:THR:OG1	2.32	0.46
2:d:93:CYS:H	3:e:117:ARG:NH1	2.14	0.46
7:P:218:LYS:HG2	7:P:220:VAL:HG23	1.98	0.46
4:G:63:GLY:HA2	4:G:72:TRP:CH2	2.50	0.46
7:P:6:GLN:HE22	7:P:96:CYS:H	1.64	0.46
5:M:273:PHE:CZ	6:N:269:LEU:HD12	2.51	0.46
8:Q:20:THR:HG22	8:Q:74:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m:264:LEU:HA	5:m:267:LEU:HD12	1.97	0.46
7:P:18:MET:SD	7:P:19:LYS:N	2.87	0.46
7:P:48:MET:HG2	7:P:64:PHE:CG	2.51	0.46
8:O:63:SER:OG	8:O:74:THR:OG1	2.32	0.46
8:O:54:LEU:HD11	8:O:60:SER:HA	1.98	0.45
4:G:109:GLU:HB2	6:N:257:LEU:HD12	1.98	0.45
7:R:180:LYS:HE3	8:Q:181:THR:HG21	1.98	0.45
8:Q:140:PHE:CD1	8:Q:145:ILE:HD13	2.50	0.45
2:D:109:VAL:HA	2:D:112:VAL:HG22	1.98	0.45
7:R:6:GLN:HE22	7:R:96:CYS:H	1.64	0.45
1:b:31:LEU:O	1:b:35:LEU:HG	2.17	0.45
4:g:107:CYS:O	6:n:257:LEU:HD13	2.16	0.45
8:O:18:ARG:HG2	8:O:76:SER:HA	1.99	0.45
7:R:48:MET:HG2	7:R:64:PHE:CG	2.51	0.45
7:R:218:LYS:HG2	7:R:220:VAL:HG23	1.98	0.45
2:d:30:GLU:OE1	2:d:31:ASP:HB2	2.16	0.45
2:d:110:THR:C	5:m:272:LEU:HD11	2.42	0.45
7:P:180:LYS:HE3	8:O:181:THR:HG21	1.98	0.45
5:M:271:MET:O	5:M:275:LYS:HG2	2.16	0.45
8:O:20:THR:HG22	8:O:74:THR:HG22	1.97	0.45
7:R:18:MET:SD	7:R:19:LYS:N	2.87	0.45
1:b:48:ALA:HA	1:b:51:LEU:HD23	1.99	0.45
1:b:41:ILE:O	1:b:45:ILE:HG12	2.17	0.45
7:P:94:TYR:CE2	7:P:118:LEU:HD12	2.51	0.45
1:B:30:LYS:HA	1:B:33:TYR:CD1	2.52	0.45
2:d:32:ARG:HH21	2:d:33:VAL:HG22	1.82	0.45
4:g:109:GLU:N	6:n:257:LEU:HD12	2.32	0.45
8:O:126:LEU:O	8:O:184:LYS:NZ	2.34	0.45
1:B:41:ILE:O	1:B:45:ILE:HG12	2.17	0.44
8:Q:54:LEU:HD11	8:Q:60:SER:HA	1.98	0.44
7:R:6:GLN:NE2	7:R:96:CYS:H	2.15	0.44
5:m:276:THR:O	5:m:280:ASN:ND2	2.50	0.44
1:B:31:LEU:O	1:B:35:LEU:HG	2.17	0.44
3:F:110:PHE:CE2	4:G:84:MET:HE1	2.53	0.44
1:a:28:ASP:OD1	1:a:29:PRO:HD2	2.17	0.44
2:d:96:CYS:HB3	3:e:122:CYS:SG	2.58	0.44
2:d:109:VAL:HA	2:d:112:VAL:HG22	1.99	0.44
8:O:3:GLN:CD	7:R:41:HIS:HD1	2.26	0.44
2:D:50:THR:OG1	2:D:59:ASP:OD1	2.32	0.44
7:R:8:GLY:H	7:R:116:THR:HG22	1.82	0.44
8:Q:18:ARG:HG2	8:Q:76:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:110:PHE:CE2	4:g:84:MET:HE1	2.53	0.44
5:m:261:MET:CA	5:m:264:LEU:HB2	2.46	0.44
4:G:109:GLU:N	6:N:257:LEU:HD12	2.33	0.44
2:D:110:THR:C	5:M:272:LEU:HD11	2.42	0.44
3:E:136:VAL:O	3:E:140:ILE:HG23	2.18	0.44
6:N:282:CYS:SG	6:N:283:CYS:N	2.90	0.44
2:d:91:ARG:HB3	3:e:116:ALA:HB1	2.00	0.44
1:A:28:ASP:OD1	1:A:29:PRO:HD2	2.18	0.44
3:E:107:ASP:OD1	3:E:107:ASP:N	2.51	0.44
1:B:48:ALA:HA	1:B:51:LEU:HD23	1.99	0.43
2:D:62:LYS:HB2	2:D:62:LYS:HE3	1.86	0.43
3:F:87:PHE:HB3	3:F:118:VAL:HG21	2.00	0.43
8:Q:19:VAL:HG21	8:Q:104:LEU:HD21	2.00	0.43
2:d:97:VAL:O	3:e:122:CYS:HA	2.19	0.43
6:n:282:CYS:SG	6:n:283:CYS:N	2.92	0.43
2:D:32:ARG:HH21	2:D:33:VAL:HG22	1.83	0.43
7:P:6:GLN:NE2	7:P:96:CYS:H	2.15	0.43
7:P:8:GLY:H	7:P:116:THR:HG22	1.82	0.43
8:O:167:GLN:NE2	8:O:172:SER:OG	2.48	0.43
5:M:260:ASN:O	5:M:264:LEU:HD13	2.18	0.43
1:a:30:LYS:HA	1:a:30:LYS:HD3	1.84	0.43
1:b:30:LYS:HA	1:b:33:TYR:CD1	2.54	0.43
4:g:129:LEU:HD13	6:n:272:LYS:HZ1	1.84	0.43
1:a:27:LEU:HD13	1:a:31:LEU:HD13	2.01	0.43
3:f:87:PHE:HB3	3:f:118:VAL:HG21	2.00	0.43
8:O:33:LEU:HB3	8:O:51:THR:HB	2.00	0.43
2:D:72:ARG:HG2	2:D:85:THR:HG22	2.00	0.43
2:d:78:ILE:H	2:d:78:ILE:HG13	1.70	0.43
5:m:261:MET:CB	5:m:264:LEU:HB2	2.49	0.43
2:D:90:TYR:HE1	3:E:113:TYR:CE2	2.36	0.43
3:F:66:ILE:HD13	3:F:66:ILE:HA	1.80	0.43
7:P:6:GLN:NE2	7:P:96:CYS:SG	2.92	0.43
1:a:35:LEU:HD22	5:m:270:ARG:HG2	1.99	0.42
7:P:36:TRP:CE3	7:P:81:MET:HE2	2.54	0.42
5:M:276:THR:O	5:M:280:ASN:ND2	2.52	0.42
7:P:62:GLN:O	7:P:65:LYS:HG2	2.19	0.42
8:O:132:SER:HA	8:O:180:LEU:O	2.19	0.42
2:D:97:VAL:HG12	5:M:260:ASN:HB2	2.00	0.42
7:R:62:GLN:HA	7:R:65:LYS:NZ	2.34	0.42
7:R:62:GLN:O	7:R:65:LYS:HG2	2.19	0.42
7:R:104:ASP:O	7:R:107:TRP:NE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:33:LEU:HB3	8:Q:51:THR:HB	2.00	0.42
7:P:66:ASP:OD2	7:P:66:ASP:N	2.52	0.42
7:P:154:TYR:O	7:P:184:TYR:HB2	2.19	0.42
5:M:271:MET:HE2	5:M:271:MET:N	2.34	0.42
7:R:66:ASP:OD2	7:R:66:ASP:N	2.52	0.42
2:d:37:CYS:O	2:d:56:THR:HG22	2.20	0.42
2:d:50:THR:OG1	2:d:59:ASP:OD1	2.32	0.42
5:m:271:MET:HE2	5:m:271:MET:N	2.35	0.42
6:n:269:LEU:HD13	6:n:272:LYS:HD3	2.00	0.42
4:G:80:ASP:HB3	4:G:82:ARG:NH1	2.35	0.42
8:Q:132:SER:HA	8:Q:180:LEU:O	2.19	0.42
8:O:145:ILE:HD12	8:O:199:HIS:HA	2.01	0.42
5:M:283:LEU:HD11	6:N:280:ILE:CG2	2.49	0.42
2:d:72:ARG:HG2	2:d:85:THR:HG22	2.01	0.42
3:f:126:ASP:N	3:f:129:SER:OG	2.52	0.42
4:G:55:TRP:C	4:G:56:PHE:HD1	2.28	0.42
4:G:125:SER:HB2	6:N:272:LYS:NZ	2.35	0.42
8:Q:33:LEU:HD22	8:Q:71:TYR:CG	2.54	0.42
3:E:37:LYS:HB3	3:E:37:LYS:HE3	1.86	0.42
3:E:84:LEU:HD22	3:E:87:PHE:HD1	1.84	0.42
7:R:36:TRP:CE3	7:R:81:MET:HE2	2.54	0.42
7:P:163:TRP:CD1	7:P:190:VAL:HB	2.55	0.42
3:F:52:TYR:HB2	3:F:57:ILE:HD11	2.01	0.42
4:G:46:CYS:HB2	4:G:55:TRP:CZ2	2.55	0.42
7:R:154:TYR:O	7:R:184:TYR:HB2	2.19	0.42
6:n:279:ILE:HG22	6:n:280:ILE:HD13	2.02	0.41
7:P:62:GLN:HA	7:P:65:LYS:NZ	2.34	0.41
8:O:46:LEU:HD23	8:O:55:HIS:CD2	2.56	0.41
2:D:37:CYS:O	2:D:56:THR:HG22	2.20	0.41
7:R:61:ASN:OD1	7:R:62:GLN:N	2.54	0.41
8:Q:46:LEU:HD23	8:Q:55:HIS:CD2	2.56	0.41
8:Q:139:ASN:HA	8:Q:173:THR:HB	2.01	0.41
3:f:52:TYR:HB2	3:f:57:ILE:HD11	2.01	0.41
7:P:87:THR:HG23	7:P:89:GLU:H	1.86	0.41
8:O:19:VAL:HG21	8:O:104:LEU:HD21	2.01	0.41
3:E:44:THR:HG22	3:E:85:LYS:HG2	2.02	0.41
8:Q:190:HIS:O	8:Q:212:ARG:NH2	2.43	0.41
7:R:6:GLN:NE2	7:R:96:CYS:SG	2.92	0.41
4:g:80:ASP:HB3	4:g:82:ARG:NH1	2.35	0.41
7:P:109:PHE:HB2	7:P:112:TRP:HE1	1.85	0.41
7:P:155:PHE:HB3	7:P:156:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:33:LEU:HD22	8:O:71:TYR:CG	2.55	0.41
7:R:163:TRP:CD1	7:R:190:VAL:HB	2.55	0.41
8:O:139:ASN:HA	8:O:173:THR:HB	2.02	0.41
6:N:269:LEU:HD13	6:N:272:LYS:HD3	2.02	0.41
7:R:87:THR:HG23	7:R:89:GLU:H	1.86	0.41
8:Q:145:ILE:HD12	8:Q:199:HIS:HA	2.02	0.41
2:d:90:TYR:HE1	3:e:113:TYR:CE2	2.38	0.41
4:g:31:VAL:HG22	4:g:97:LEU:HD23	2.03	0.41
4:g:55:TRP:C	4:g:56:PHE:HD1	2.28	0.41
7:R:109:PHE:HB2	7:R:112:TRP:HE1	1.85	0.41
3:F:126:ASP:N	3:F:129:SER:OG	2.53	0.41
2:d:62:LYS:HE3	2:d:62:LYS:HB2	1.87	0.41
4:g:46:CYS:HB2	4:g:55:TRP:CZ2	2.55	0.41
4:g:65:LEU:HD23	4:g:65:LEU:HA	1.89	0.41
7:P:47:TRP:HZ2	7:P:50:LEU:HD23	1.86	0.41
7:P:60:TYR:OH	7:P:70:LEU:N	2.50	0.41
7:R:60:TYR:OH	7:R:70:LEU:N	2.50	0.41
2:D:97:VAL:HG21	3:E:125:MET:SD	2.60	0.41
8:Q:35:TRP:CD1	8:Q:48:ILE:HD11	2.56	0.41
3:f:107:ASP:OD1	3:f:107:ASP:N	2.54	0.40
3:F:34:THR:HA	3:F:35:PRO:HD3	1.96	0.40
8:Q:38:GLN:O	8:Q:84:ALA:HB1	2.20	0.40
4:g:48:ALA:HB3	4:g:53:ILE:HD13	2.03	0.40
7:P:61:ASN:OD1	7:P:62:GLN:N	2.54	0.40
8:O:35:TRP:CD1	8:O:48:ILE:HD11	2.57	0.40
7:R:155:PHE:HB3	7:R:156:PRO:HD3	2.02	0.40
1:a:31:LEU:O	1:a:34:LEU:HG	2.22	0.40
4:g:80:ASP:OD2	4:g:80:ASP:N	2.55	0.40
4:g:87:CYS:HB3	4:g:94:SER:HB3	2.04	0.40
4:g:125:SER:HB2	6:n:272:LYS:NZ	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	29/166 (18%)	27 (93%)	1 (3%)	1 (3%)	3	18
1	B	27/166 (16%)	26 (96%)	1 (4%)	0	100	100
1	a	29/166 (18%)	27 (93%)	1 (3%)	1 (3%)	3	18
1	b	27/166 (16%)	26 (96%)	1 (4%)	0	100	100
2	D	103/171 (60%)	98 (95%)	5 (5%)	0	100	100
2	d	103/171 (60%)	98 (95%)	5 (5%)	0	100	100
3	E	119/207 (58%)	117 (98%)	2 (2%)	0	100	100
3	F	120/207 (58%)	107 (89%)	13 (11%)	0	100	100
3	e	119/207 (58%)	117 (98%)	2 (2%)	0	100	100
3	f	120/207 (58%)	109 (91%)	11 (9%)	0	100	100
4	G	113/182 (62%)	106 (94%)	7 (6%)	0	100	100
4	g	113/182 (62%)	106 (94%)	7 (6%)	0	100	100
5	M	34/292 (12%)	34 (100%)	0	0	100	100
5	m	34/292 (12%)	34 (100%)	0	0	100	100
6	N	36/315 (11%)	36 (100%)	0	0	100	100
6	n	36/315 (11%)	36 (100%)	0	0	100	100
7	P	187/222 (84%)	180 (96%)	7 (4%)	0	100	100
7	R	187/222 (84%)	179 (96%)	8 (4%)	0	100	100
8	O	205/212 (97%)	194 (95%)	11 (5%)	0	100	100
8	Q	205/212 (97%)	195 (95%)	10 (5%)	0	100	100
All	All	1946/4280 (46%)	1852 (95%)	92 (5%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	28	ASP
1	A	28	ASP

### 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	28/136 (21%)	26 (93%)	2 (7%)	13	40
1	B	26/136 (19%)	24 (92%)	2 (8%)	12	37
1	a	28/136 (21%)	25 (89%)	3 (11%)	6	24
1	b	26/136 (19%)	24 (92%)	2 (8%)	12	37
2	D	93/147 (63%)	93 (100%)	0	100	100
2	d	93/147 (63%)	93 (100%)	0	100	100
3	E	109/177 (62%)	109 (100%)	0	100	100
3	F	110/177 (62%)	105 (96%)	5 (4%)	24	53
3	e	109/177 (62%)	109 (100%)	0	100	100
3	f	110/177 (62%)	105 (96%)	5 (4%)	24	53
4	G	97/155 (63%)	93 (96%)	4 (4%)	27	55
4	g	97/155 (63%)	93 (96%)	4 (4%)	27	55
5	M	32/259 (12%)	31 (97%)	1 (3%)	35	60
5	m	32/259 (12%)	32 (100%)	0	100	100
6	N	36/284 (13%)	35 (97%)	1 (3%)	38	62
6	n	36/284 (13%)	36 (100%)	0	100	100
7	P	171/193 (89%)	167 (98%)	4 (2%)	44	66
7	R	171/193 (89%)	167 (98%)	4 (2%)	44	66
8	O	175/189 (93%)	173 (99%)	2 (1%)	65	76
8	Q	175/189 (93%)	171 (98%)	4 (2%)	44	66
All	All	1754/3706 (47%)	1711 (98%)	43 (2%)	42	64

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	31	LEU
1	a	39	LEU
1	a	49	LEU
1	b	47	THR
1	b	51	LEU
3	f	34	THR
3	f	38	VAL
3	f	66	ILE

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Mol	Chain	Res	Type
3	f	107	ASP
3	f	119	CYS
4	g	31	VAL
4	g	62	ILE
4	g	106	ASN
4	g	115	ILE
7	P	2	VAL
7	P	46	GLU
7	P	117	THR
7	P	119	THR
8	O	8	THR
8	O	166	ASP
1	A	31	LEU
1	A	49	LEU
1	B	47	THR
1	B	51	LEU
3	F	33	GLN
3	F	38	VAL
3	F	66	ILE
3	F	107	ASP
3	F	119	CYS
4	G	31	VAL
4	G	62	ILE
4	G	106	ASN
4	G	115	ILE
5	M	283	LEU
6	N	268	LEU
7	R	2	VAL
7	R	46	GLU
7	R	117	THR
7	R	119	THR
8	Q	3	GLN
8	Q	8	THR
8	Q	166	ASP
8	Q	167	GLN

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

Mol	Chain	Res	Type
2	d	36	ASN
3	e	92	GLN
3	f	33	GLN

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Mol	Chain	Res	Type
4	g	86	GLN
7	P	35	ASN
3	E	92	GLN
4	G	86	GLN
5	M	260	ASN
7	R	35	ASN
8	Q	167	GLN

### 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](#)

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.



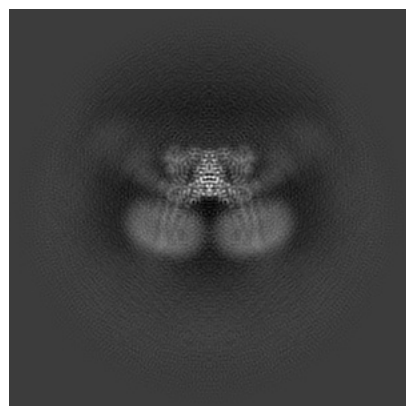
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61887. These allow visual inspection of the internal detail of the map and identification of artifacts.

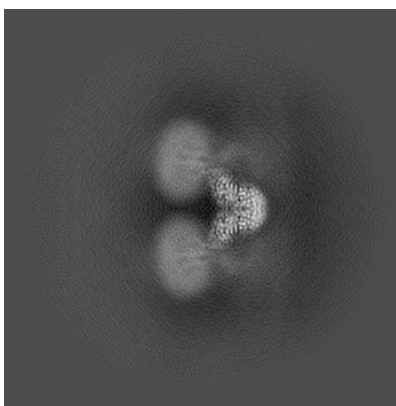
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

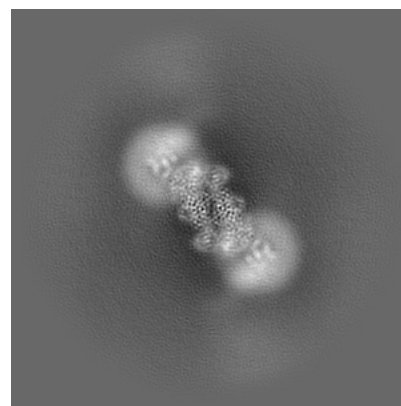
#### 6.1.1 Primary map



X

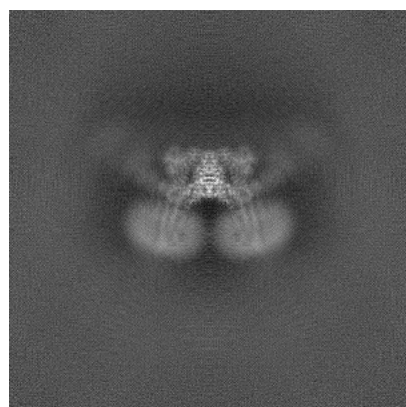


Y

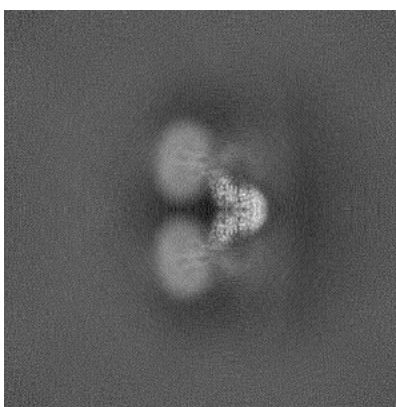


Z

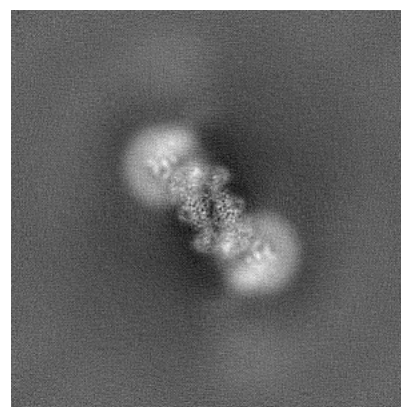
#### 6.1.2 Raw map



X



Y



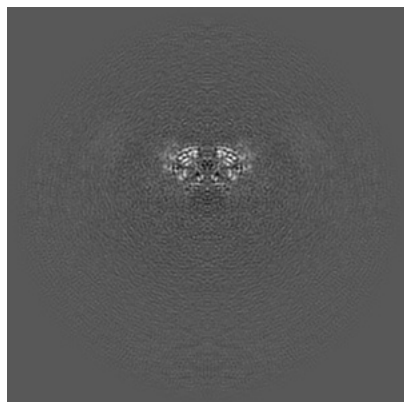
Z

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

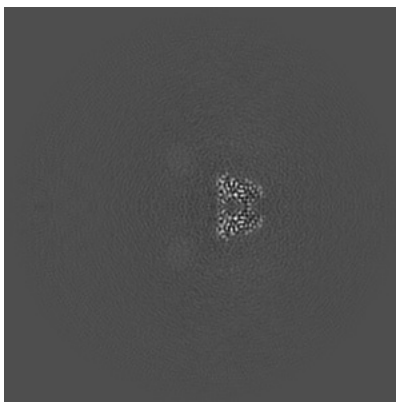


## 6.2 Central slices [i](#)

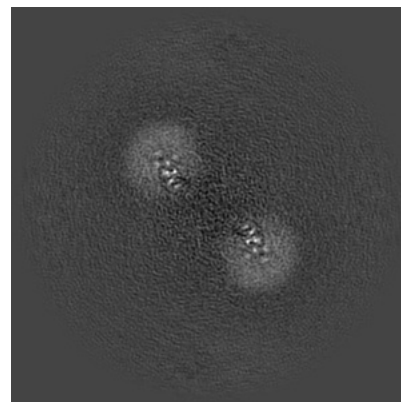
### 6.2.1 Primary map



X Index: 256

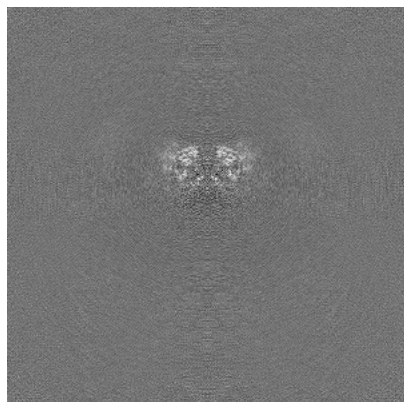


Y Index: 256

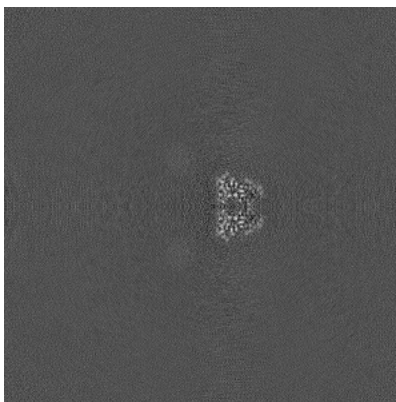


Z Index: 256

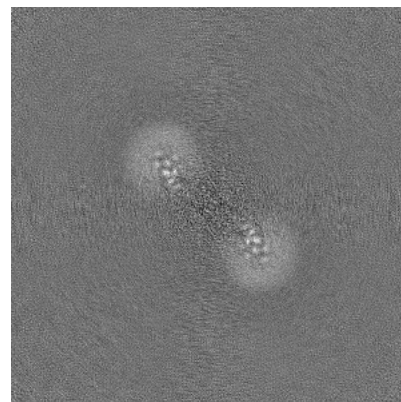
### 6.2.2 Raw map



X Index: 256



Y Index: 256



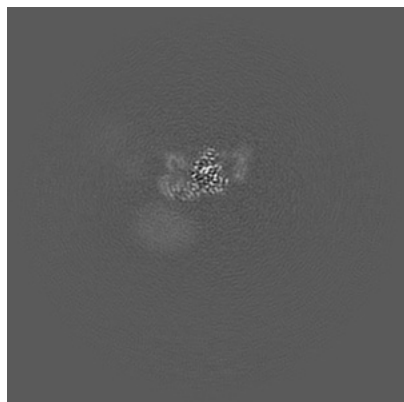
Z Index: 256

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

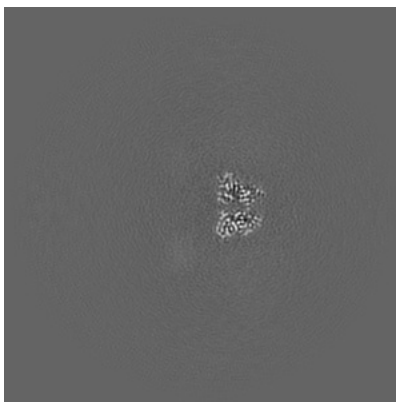


## 6.3 Largest variance slices [i](#)

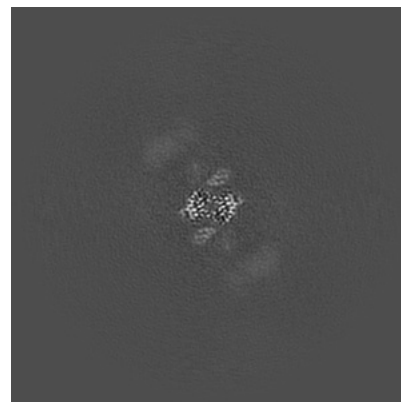
### 6.3.1 Primary map



X Index: 276

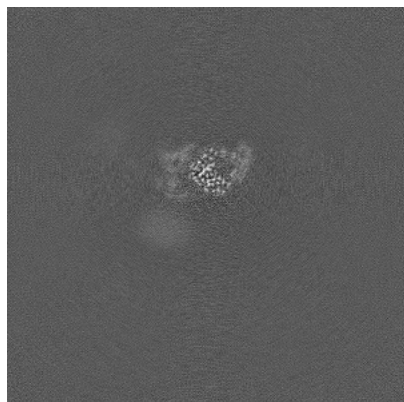


Y Index: 258



Z Index: 296

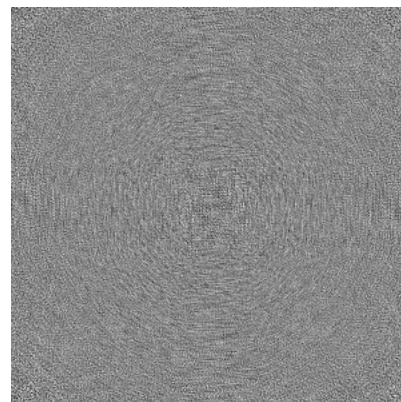
### 6.3.2 Raw map



X Index: 270



Y Index: 258



Z Index: 0

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

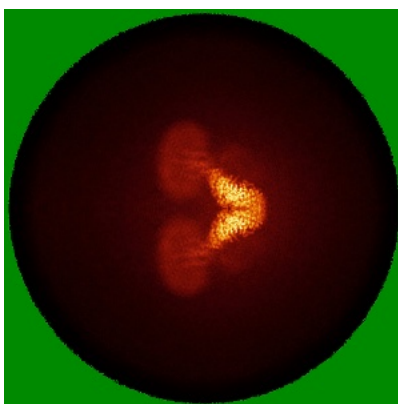


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

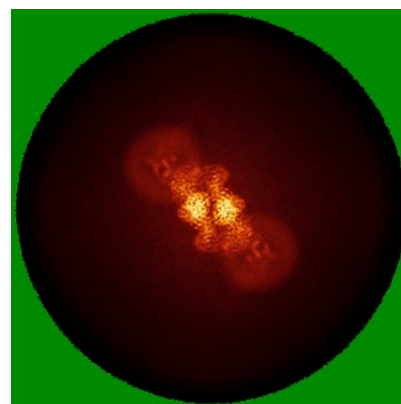
### 6.4.1 Primary map



X

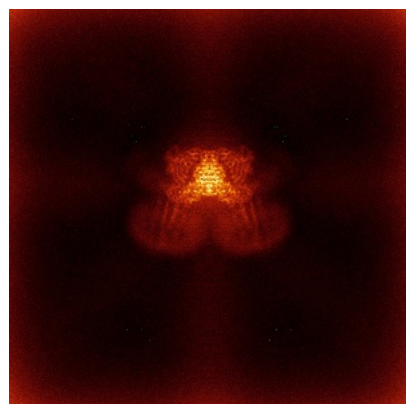


Y

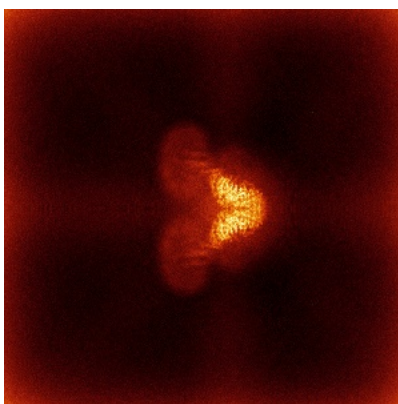


Z

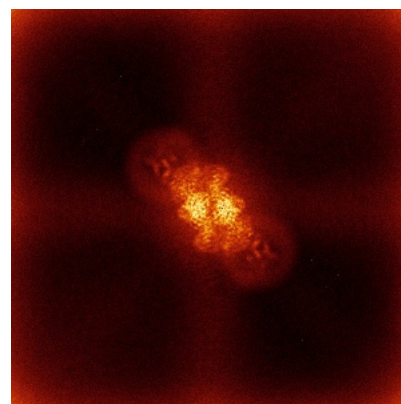
### 6.4.2 Raw map



X



Y



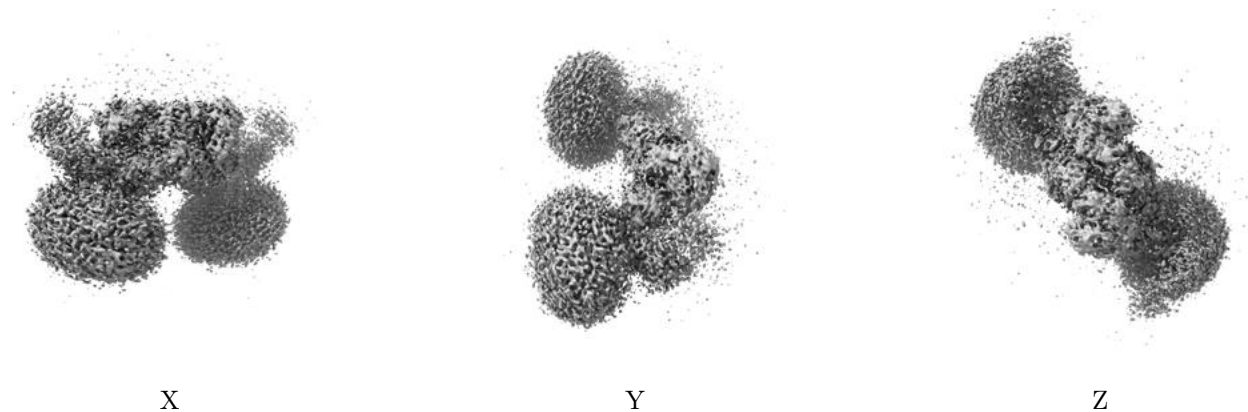
Z

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.



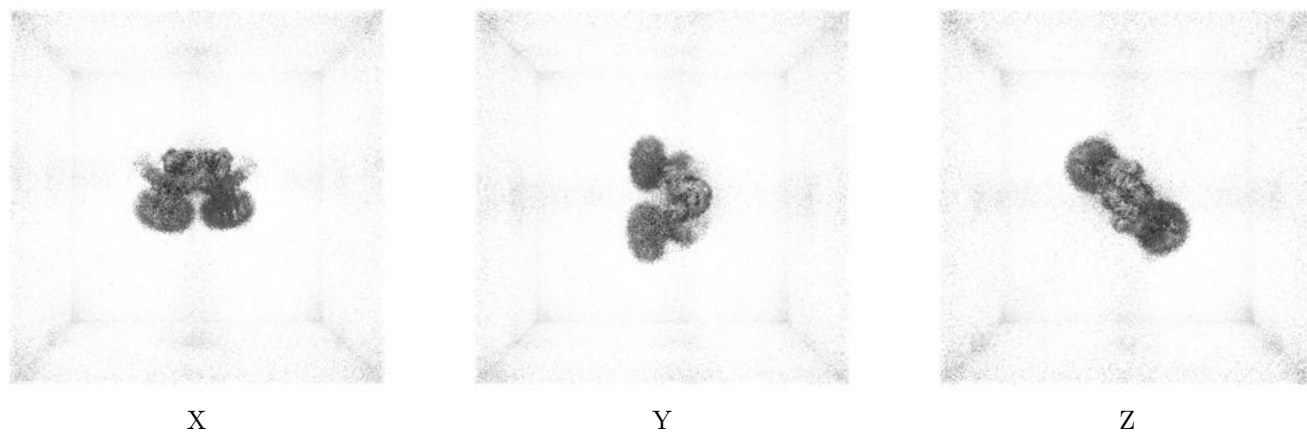
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.074. 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](#)

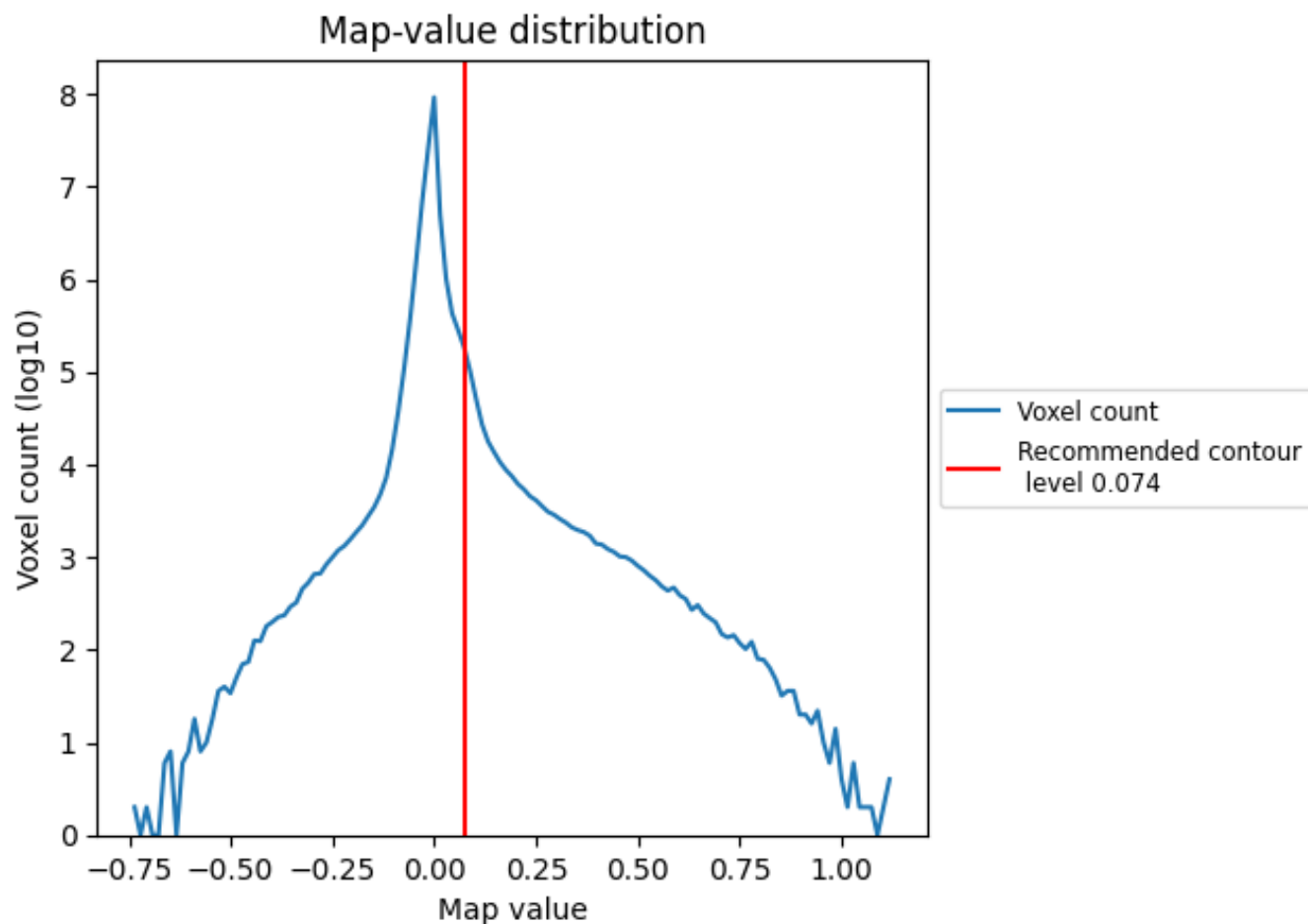
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

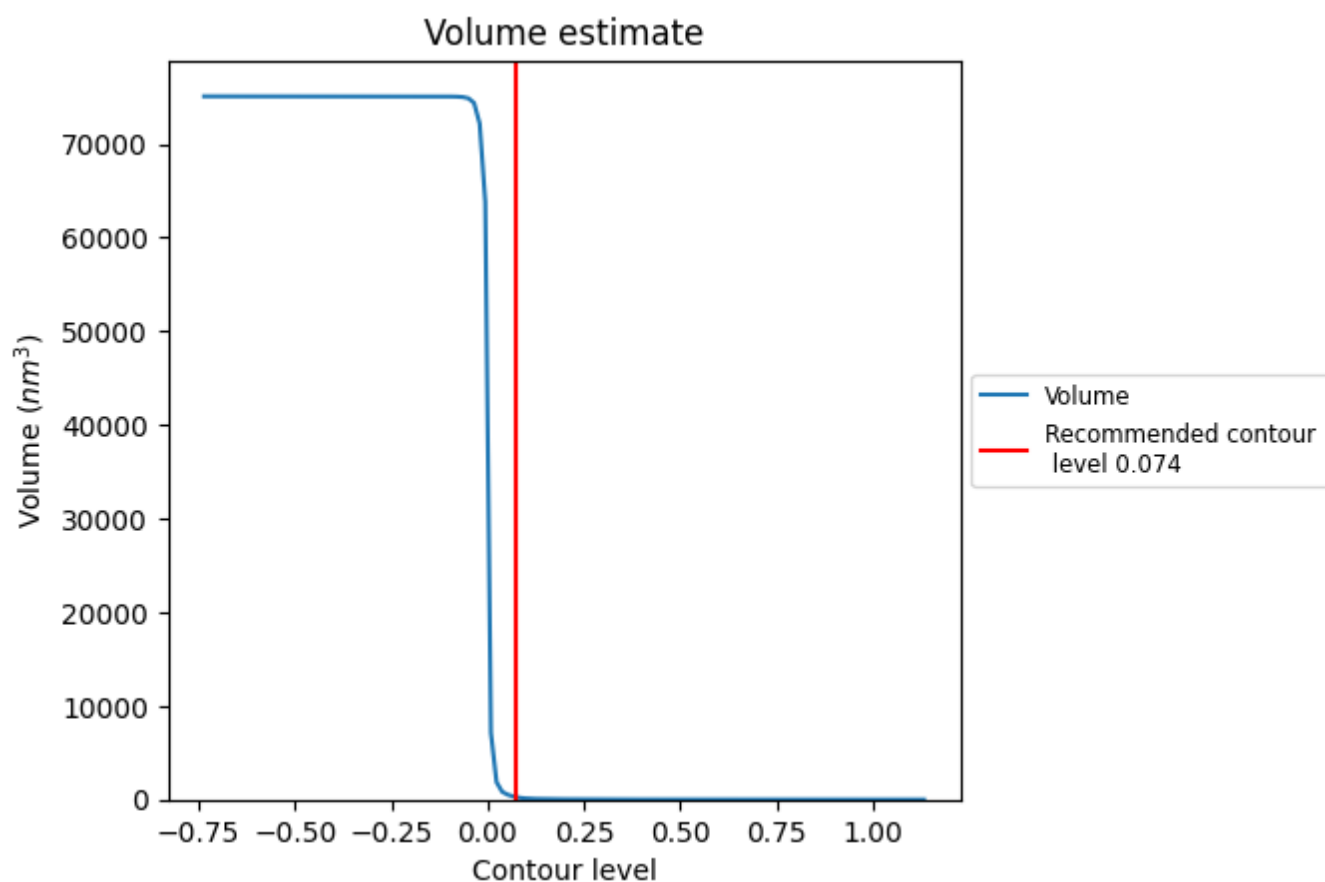
### 7.1 Map-value distribution [i](#)



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](#)

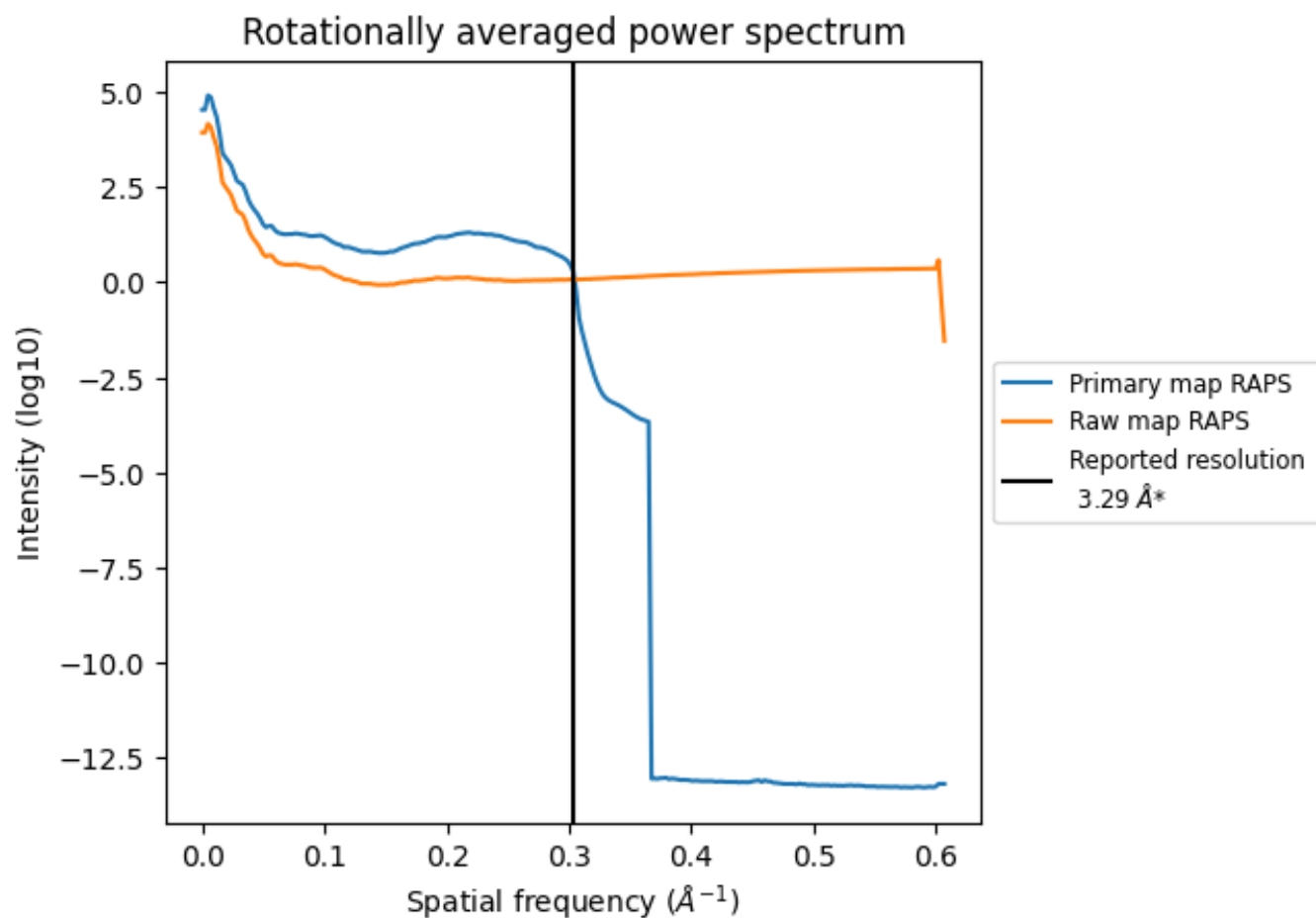


The volume at the recommended contour level is 270 nm<sup>3</sup>; this corresponds to an approximate mass of 244 kDa.

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 ⓘ



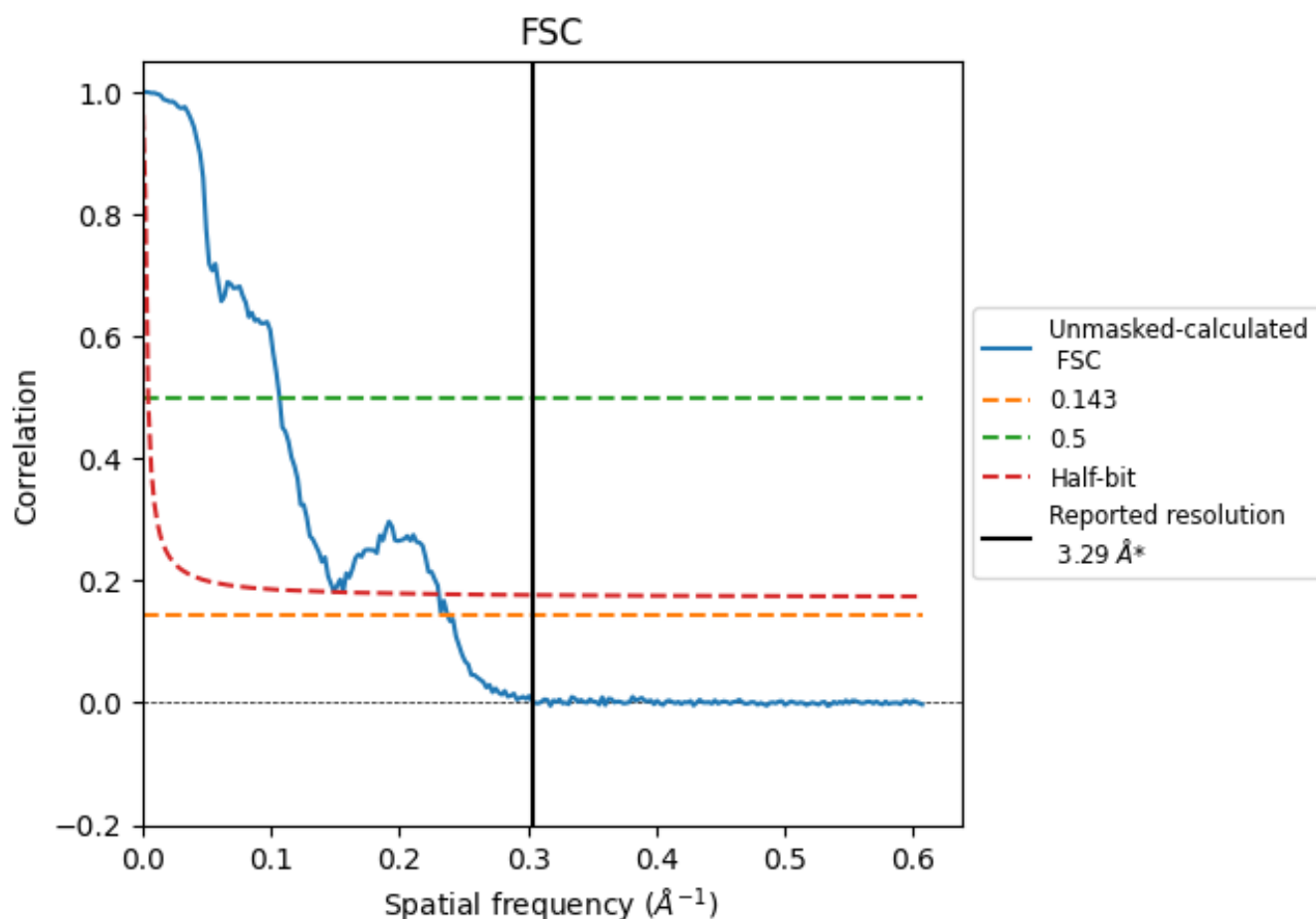
\*Reported resolution corresponds to spatial frequency of 0.304  $\text{\AA}^{-1}$



## 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 0.304 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	9.36	4.33

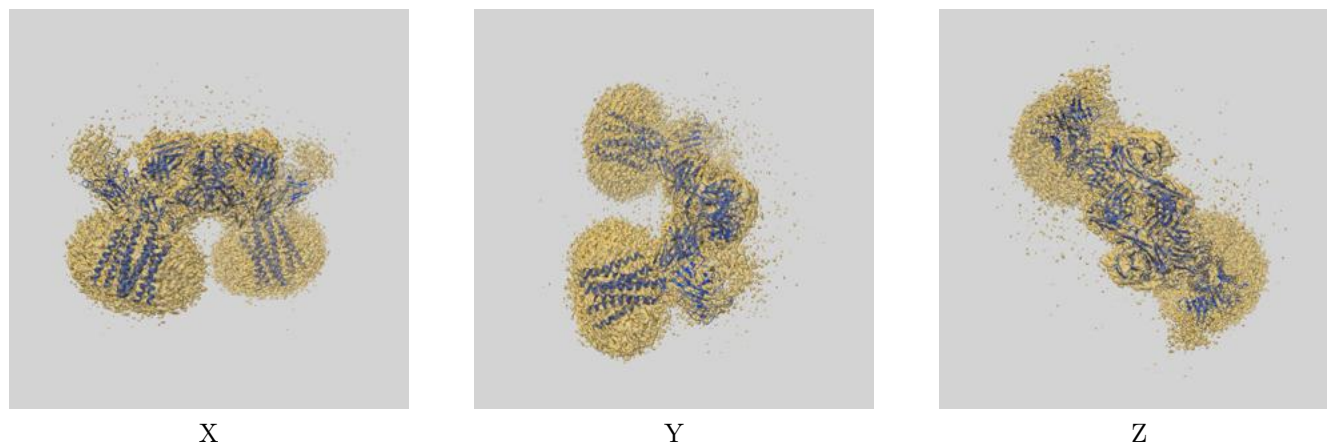
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.29 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61887 and PDB model 9JY4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

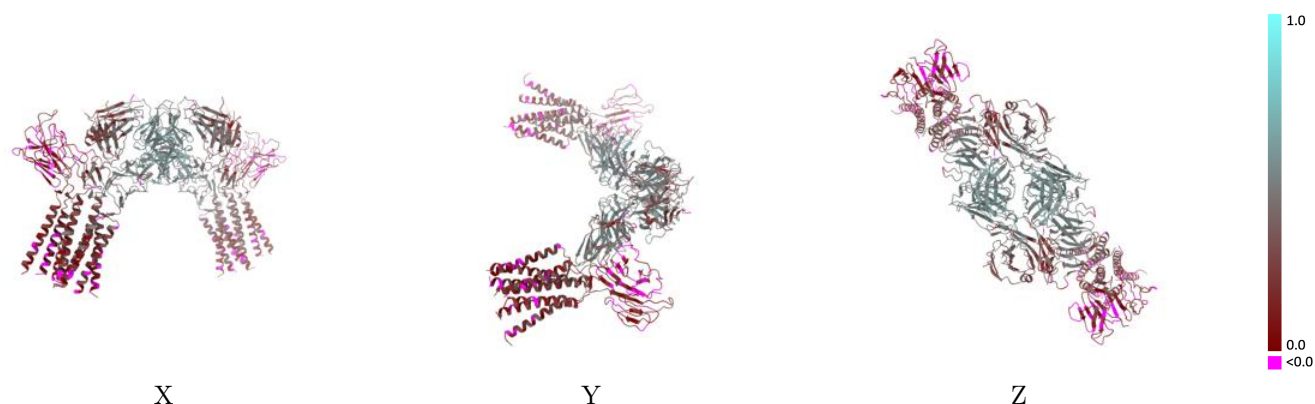
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.074 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.

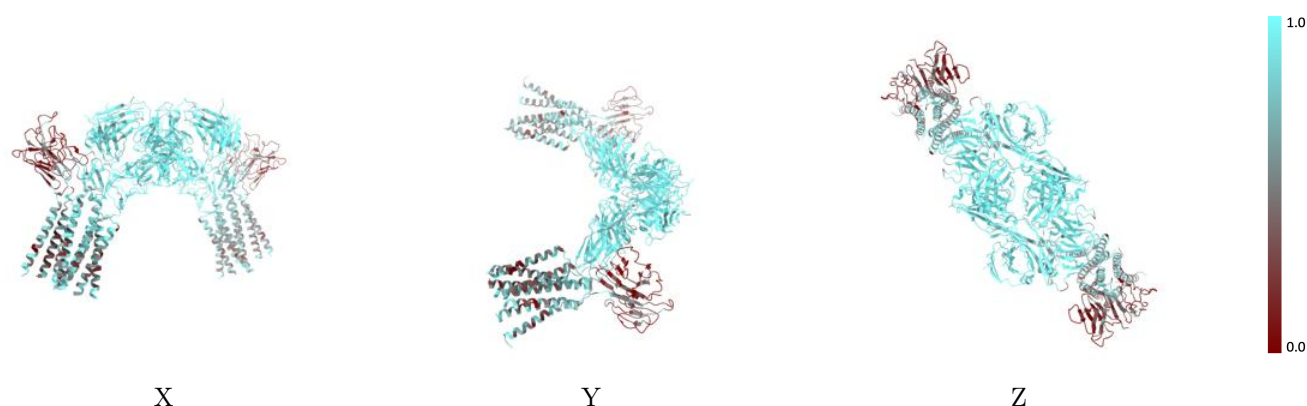


## 9.2 Q-score mapped to coordinate model [i](#)



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.

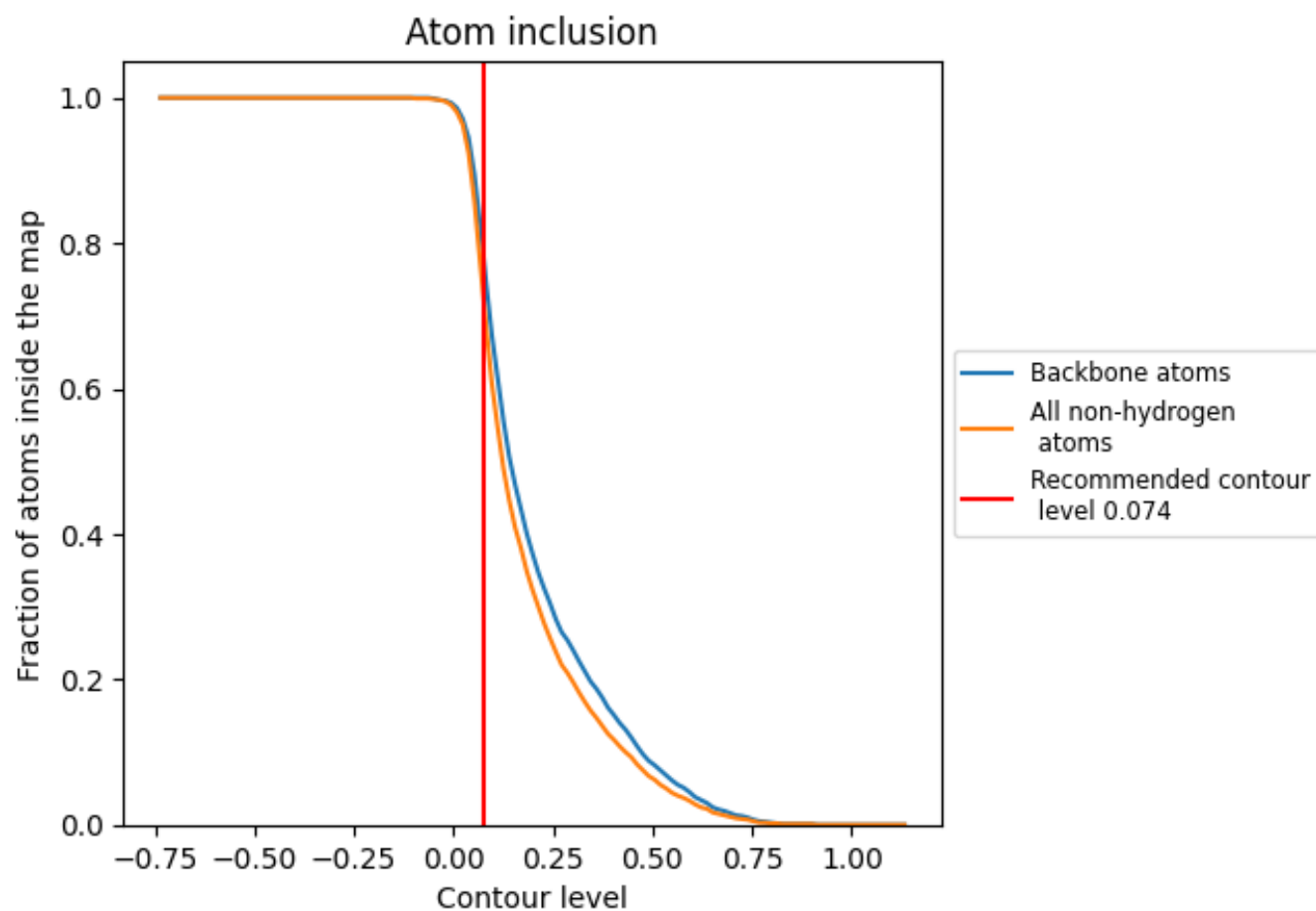
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.074).



## 9.4 Atom inclusion [i](#)













































At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.074) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.3230
A	 0.6600	 0.2040
B	 0.6390	 0.1750
D	 0.3510	 0.1230
E	 0.3220	 0.1020
F	 0.8470	 0.3920
G	 0.7610	 0.3040
M	 0.6610	 0.2440
N	 0.6690	 0.2330
O	 0.9250	 0.4580
P	 0.9380	 0.4720
Q	 0.9240	 0.4560
R	 0.9380	 0.4730
a	 0.6600	 0.2040
b	 0.6570	 0.1740
d	 0.3460	 0.1210
e	 0.3240	 0.1060
f	 0.8450	 0.3880
g	 0.7630	 0.3050
m	 0.6640	 0.2410
n	 0.6690	 0.2400

