



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:27 PM UTC

PDB ID : 7LUC / pdb_00007luc
EMDB ID : EMD-23520
Title : Cryo-EM structure of RSV preF bound by Fabs 32.4K and 01.4B
Authors : Wrapp, D.; McLellan, J.S.
Deposited on : 2021-02-22
Resolution : 3.21 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:

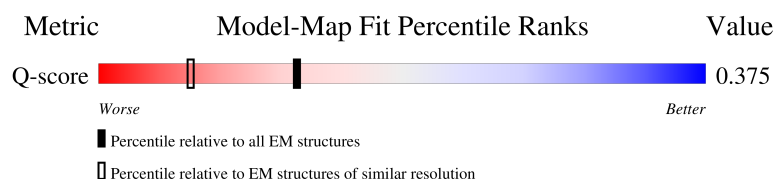
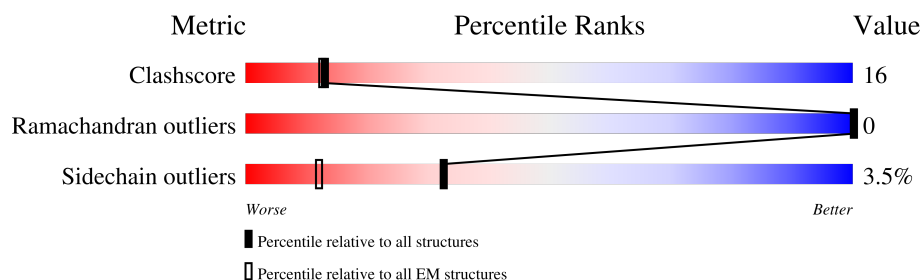
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.21 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	14613 (2.71 - 3.71)

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	527	
1	B	527	
1	C	527	
2	D	121	

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Mol	Chain	Length	Quality of chain
2	F	121	9% 78% 20% .
2	H	121	13% 75% 22% .
3	E	112	10% 65% 34% .
3	G	112	9% 66% 33% .
3	I	112	13% 62% 37% .
4	J	129	12% 68% 31% .
4	L	129	14% 70% 29% .
4	N	129	15% 70% 29% .
5	K	107	10% 68% 32% .
5	M	107	10% 68% 32% .
5	O	107	10% 61% 38% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21288 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3477	2199	572	685	21		
1	B	449	Total	C	N	O	S	0	0
			3477	2199	572	685	21		
1	C	449	Total	C	N	O	S	0	0
			3477	2199	572	685	21		

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	LYS	conflict	UNP C3UPB8
A	67	ILE	ASN	engineered mutation	UNP C3UPB8
A	76	VAL	ILE	conflict	UNP C3UPB8
A	215	PRO	SER	engineered mutation	UNP C3UPB8
A	514	SER	-	expression tag	UNP C3UPB8
A	515	ALA	-	expression tag	UNP C3UPB8
A	516	ILE	-	expression tag	UNP C3UPB8
A	517	GLY	-	expression tag	UNP C3UPB8
A	518	GLY	-	expression tag	UNP C3UPB8
A	519	TYR	-	expression tag	UNP C3UPB8
A	520	ILE	-	expression tag	UNP C3UPB8
A	521	PRO	-	expression tag	UNP C3UPB8
A	522	GLU	-	expression tag	UNP C3UPB8
A	523	ALA	-	expression tag	UNP C3UPB8
A	524	PRO	-	expression tag	UNP C3UPB8
A	525	ARG	-	expression tag	UNP C3UPB8
A	526	ASP	-	expression tag	UNP C3UPB8
A	527	GLY	-	expression tag	UNP C3UPB8
A	528	GLN	-	expression tag	UNP C3UPB8
A	529	ALA	-	expression tag	UNP C3UPB8
A	530	TYR	-	expression tag	UNP C3UPB8
A	531	VAL	-	expression tag	UNP C3UPB8
A	532	ARG	-	expression tag	UNP C3UPB8
A	533	LYS	-	expression tag	UNP C3UPB8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	534	ASP	-	expression tag	UNP C3UPB8
A	535	GLY	-	expression tag	UNP C3UPB8
A	536	GLU	-	expression tag	UNP C3UPB8
A	537	TRP	-	expression tag	UNP C3UPB8
A	538	VAL	-	expression tag	UNP C3UPB8
A	539	LEU	-	expression tag	UNP C3UPB8
A	540	LEU	-	expression tag	UNP C3UPB8
A	541	SER	-	expression tag	UNP C3UPB8
A	542	THR	-	expression tag	UNP C3UPB8
A	543	PHE	-	expression tag	UNP C3UPB8
A	544	LEU	-	expression tag	UNP C3UPB8
A	545	GLY	-	expression tag	UNP C3UPB8
A	546	SER	-	expression tag	UNP C3UPB8
A	547	LEU	-	expression tag	UNP C3UPB8
A	548	GLU	-	expression tag	UNP C3UPB8
A	549	VAL	-	expression tag	UNP C3UPB8
A	550	LEU	-	expression tag	UNP C3UPB8
A	551	PHE	-	expression tag	UNP C3UPB8
A	552	GLN	-	expression tag	UNP C3UPB8
B	66	GLU	LYS	conflict	UNP C3UPB8
B	67	ILE	ASN	engineered mutation	UNP C3UPB8
B	76	VAL	ILE	conflict	UNP C3UPB8
B	215	PRO	SER	engineered mutation	UNP C3UPB8
B	514	SER	-	expression tag	UNP C3UPB8
B	515	ALA	-	expression tag	UNP C3UPB8
B	516	ILE	-	expression tag	UNP C3UPB8
B	517	GLY	-	expression tag	UNP C3UPB8
B	518	GLY	-	expression tag	UNP C3UPB8
B	519	TYR	-	expression tag	UNP C3UPB8
B	520	ILE	-	expression tag	UNP C3UPB8
B	521	PRO	-	expression tag	UNP C3UPB8
B	522	GLU	-	expression tag	UNP C3UPB8
B	523	ALA	-	expression tag	UNP C3UPB8
B	524	PRO	-	expression tag	UNP C3UPB8
B	525	ARG	-	expression tag	UNP C3UPB8
B	526	ASP	-	expression tag	UNP C3UPB8
B	527	GLY	-	expression tag	UNP C3UPB8
B	528	GLN	-	expression tag	UNP C3UPB8
B	529	ALA	-	expression tag	UNP C3UPB8
B	530	TYR	-	expression tag	UNP C3UPB8
B	531	VAL	-	expression tag	UNP C3UPB8
B	532	ARG	-	expression tag	UNP C3UPB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	533	LYS	-	expression tag	UNP C3UPB8
B	534	ASP	-	expression tag	UNP C3UPB8
B	535	GLY	-	expression tag	UNP C3UPB8
B	536	GLU	-	expression tag	UNP C3UPB8
B	537	TRP	-	expression tag	UNP C3UPB8
B	538	VAL	-	expression tag	UNP C3UPB8
B	539	LEU	-	expression tag	UNP C3UPB8
B	540	LEU	-	expression tag	UNP C3UPB8
B	541	SER	-	expression tag	UNP C3UPB8
B	542	THR	-	expression tag	UNP C3UPB8
B	543	PHE	-	expression tag	UNP C3UPB8
B	544	LEU	-	expression tag	UNP C3UPB8
B	545	GLY	-	expression tag	UNP C3UPB8
B	546	SER	-	expression tag	UNP C3UPB8
B	547	LEU	-	expression tag	UNP C3UPB8
B	548	GLU	-	expression tag	UNP C3UPB8
B	549	VAL	-	expression tag	UNP C3UPB8
B	550	LEU	-	expression tag	UNP C3UPB8
B	551	PHE	-	expression tag	UNP C3UPB8
B	552	GLN	-	expression tag	UNP C3UPB8
C	66	GLU	LYS	conflict	UNP C3UPB8
C	67	ILE	ASN	engineered mutation	UNP C3UPB8
C	76	VAL	ILE	conflict	UNP C3UPB8
C	215	PRO	SER	engineered mutation	UNP C3UPB8
C	514	SER	-	expression tag	UNP C3UPB8
C	515	ALA	-	expression tag	UNP C3UPB8
C	516	ILE	-	expression tag	UNP C3UPB8
C	517	GLY	-	expression tag	UNP C3UPB8
C	518	GLY	-	expression tag	UNP C3UPB8
C	519	TYR	-	expression tag	UNP C3UPB8
C	520	ILE	-	expression tag	UNP C3UPB8
C	521	PRO	-	expression tag	UNP C3UPB8
C	522	GLU	-	expression tag	UNP C3UPB8
C	523	ALA	-	expression tag	UNP C3UPB8
C	524	PRO	-	expression tag	UNP C3UPB8
C	525	ARG	-	expression tag	UNP C3UPB8
C	526	ASP	-	expression tag	UNP C3UPB8
C	527	GLY	-	expression tag	UNP C3UPB8
C	528	GLN	-	expression tag	UNP C3UPB8
C	529	ALA	-	expression tag	UNP C3UPB8
C	530	TYR	-	expression tag	UNP C3UPB8
C	531	VAL	-	expression tag	UNP C3UPB8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	532	ARG	-	expression tag	UNP C3UPB8
C	533	LYS	-	expression tag	UNP C3UPB8
C	534	ASP	-	expression tag	UNP C3UPB8
C	535	GLY	-	expression tag	UNP C3UPB8
C	536	GLU	-	expression tag	UNP C3UPB8
C	537	TRP	-	expression tag	UNP C3UPB8
C	538	VAL	-	expression tag	UNP C3UPB8
C	539	LEU	-	expression tag	UNP C3UPB8
C	540	LEU	-	expression tag	UNP C3UPB8
C	541	SER	-	expression tag	UNP C3UPB8
C	542	THR	-	expression tag	UNP C3UPB8
C	543	PHE	-	expression tag	UNP C3UPB8
C	544	LEU	-	expression tag	UNP C3UPB8
C	545	GLY	-	expression tag	UNP C3UPB8
C	546	SER	-	expression tag	UNP C3UPB8
C	547	LEU	-	expression tag	UNP C3UPB8
C	548	GLU	-	expression tag	UNP C3UPB8
C	549	VAL	-	expression tag	UNP C3UPB8
C	550	LEU	-	expression tag	UNP C3UPB8
C	551	PHE	-	expression tag	UNP C3UPB8
C	552	GLN	-	expression tag	UNP C3UPB8

- Molecule 2 is a protein called 01.4B Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	121	Total	C	N	O	S	0	0
			925	588	157	175	5		
2	F	121	Total	C	N	O	S	0	0
			925	588	157	175	5		
2	H	121	Total	C	N	O	S	0	0
			925	588	157	175	5		

- Molecule 3 is a protein called 01.4B Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	112	Total	C	N	O	S	0	0
			879	550	159	167	3		
3	G	112	Total	C	N	O	S	0	0
			879	550	159	167	3		
3	I	112	Total	C	N	O	S	0	0
			879	550	159	167	3		

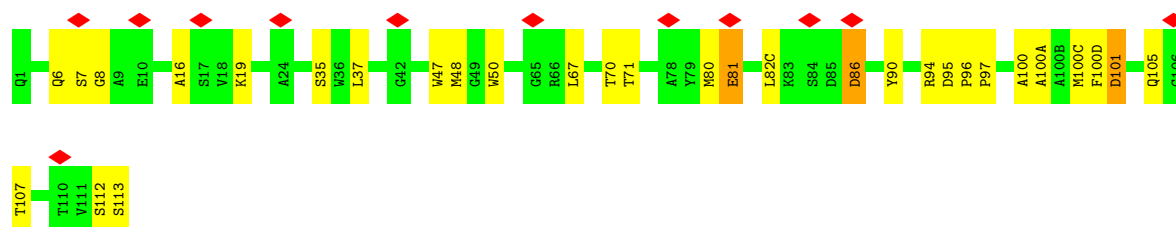
- Molecule 4 is a protein called 32.4K Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	129	Total	C	N	O	S	0	0
			995	634	162	194	5		
4	L	129	Total	C	N	O	S	0	0
			995	634	162	194	5		
4	N	129	Total	C	N	O	S	0	0
			995	634	162	194	5		

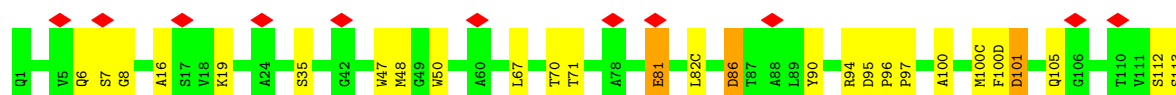
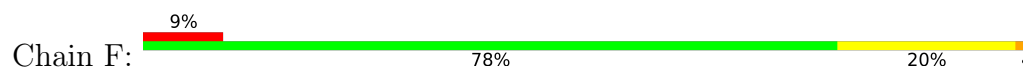
- Molecule 5 is a protein called 32.4K Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	107	Total	C	N	O	S	2	0
			820	520	137	160	3		
5	M	107	Total	C	N	O	S	2	0
			820	520	137	160	3		
5	O	107	Total	C	N	O	S	2	0
			820	520	137	160	3		

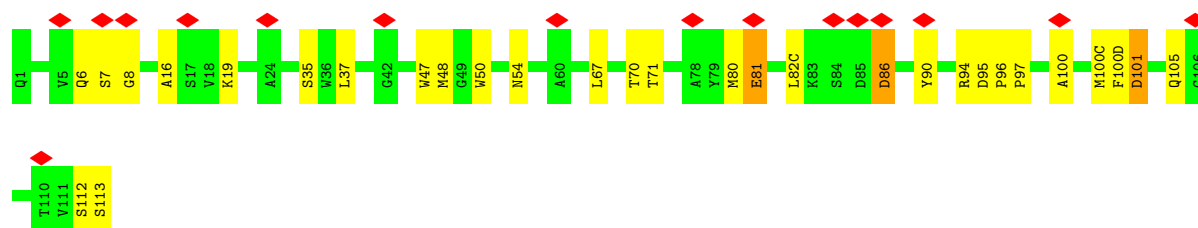
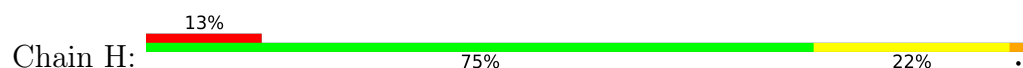




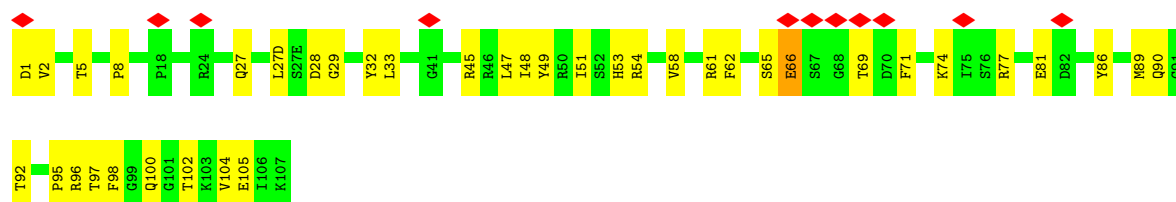
• Molecule 2: 01.4B Fab Heavy chain



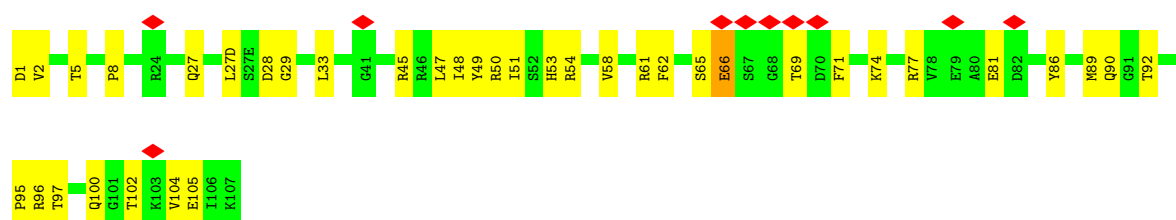
• Molecule 2: 01.4B Fab Heavy chain



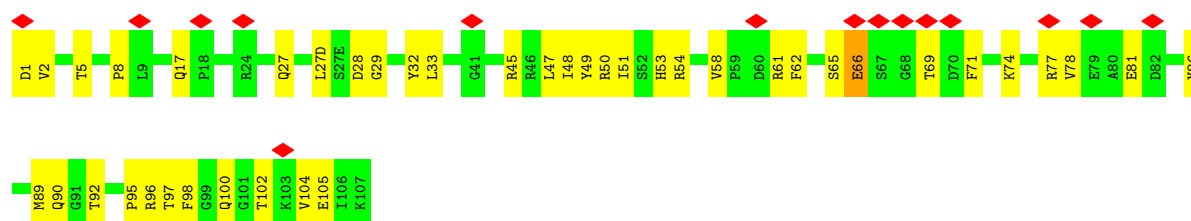
• Molecule 3: 01.4B Fab Light chain



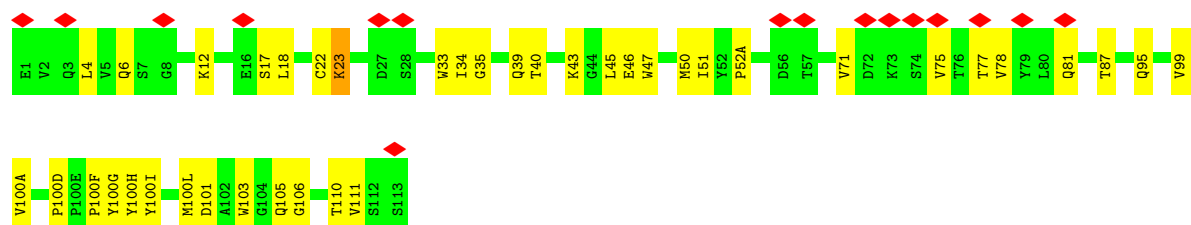
• Molecule 3: 01.4B Fab Light chain



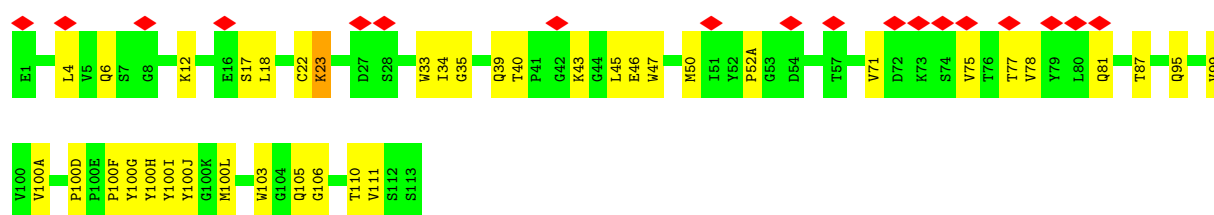
• Molecule 3: 01.4B Fab Light chain



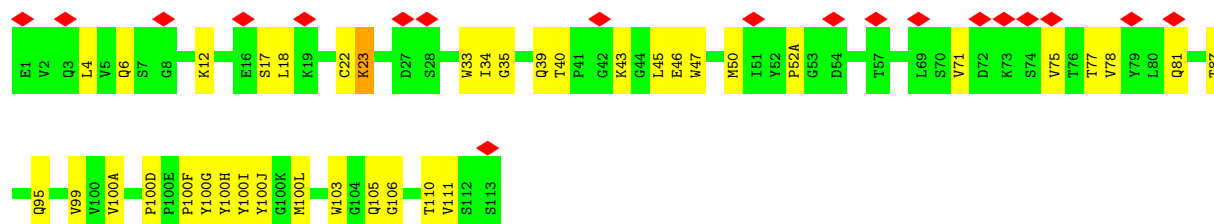
- Molecule 4: 32.4K Fab Heavy chain



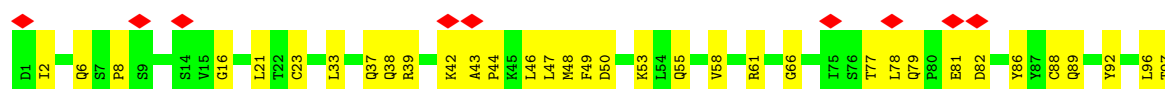
- Molecule 4: 32.4K Fab Heavy chain



- Molecule 4: 32.4K Fab Heavy chain

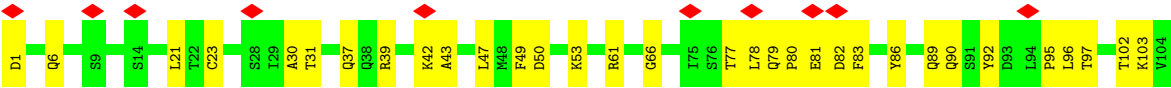


- Molecule 5: 32.4K Fab Light chain

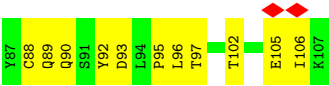
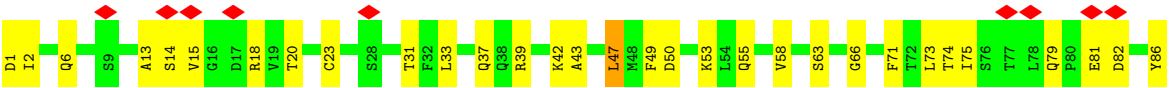




• Molecule 5: 32.4K Fab Light chain



• Molecule 5: 32.4K Fab Light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	526804	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 ($e^-/\text{\AA}^2$)	37.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.366	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.127	Depositor
Map size ($\text{\AA}$)	360.52798, 360.52798, 360.52798	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.073, 1.073, 1.073	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	2/3527 (0.1%)	0.44	3/4779 (0.1%)
1	B	0.20	1/3527 (0.0%)	0.44	5/4779 (0.1%)
1	C	0.43	7/3527 (0.2%)	0.49	4/4779 (0.1%)
2	D	0.12	0/948	0.29	0/1287
2	F	0.12	0/948	0.29	0/1287
2	H	0.12	0/948	0.29	0/1287
3	E	0.14	0/901	0.43	1/1222 (0.1%)
3	G	0.14	0/901	0.43	1/1222 (0.1%)
3	I	0.14	0/901	0.43	1/1222 (0.1%)
4	J	0.14	0/1023	0.34	0/1395
4	L	0.14	0/1023	0.34	0/1395
4	N	0.14	0/1023	0.34	0/1395
5	K	0.12	0/839	0.45	0/1139
5	M	0.11	0/839	0.39	0/1139
5	O	0.12	0/839	0.41	0/1139
All	All	0.23	10/21714 (0.0%)	0.42	15/29466 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	ASN	C-O	-9.83	1.12	1.24
1	A	350	SER	CA-C	8.14	1.64	1.53
1	C	346	ALA	C-O	-8.01	1.16	1.24
1	C	350	SER	CA-C	7.86	1.63	1.53
1	A	350	SER	CA-CB	-6.67	1.42	1.53
1	C	349	VAL	CA-C	-6.61	1.45	1.52
1	C	349	VAL	N-CA	-6.61	1.38	1.46
1	B	350	SER	CA-C	5.96	1.60	1.52
1	C	350	SER	CA-CB	-5.91	1.43	1.53
1	C	349	VAL	C-O	-5.70	1.17	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	ALA	N-CA-C	9.11	122.16	108.31
1	B	215	PRO	CA-N-CD	-9.04	99.34	112.00
1	C	215	PRO	CA-N-CD	-9.04	99.34	112.00
1	A	215	PRO	CA-N-CD	-9.02	99.37	112.00
1	C	347	GLY	N-CA-C	7.22	122.70	113.24
1	A	347	GLY	N-CA-C	6.73	120.80	112.73
3	G	81	GLU	CA-CB-CG	6.33	126.75	114.10
3	E	81	GLU	CA-CB-CG	6.31	126.72	114.10
3	I	81	GLU	CA-CB-CG	6.30	126.71	114.10
1	C	81	GLN	CA-CB-CG	6.15	126.40	114.10
1	B	81	GLN	CA-CB-CG	6.14	126.39	114.10
1	A	81	GLN	CA-CB-CG	6.13	126.36	114.10
1	B	347	GLY	N-CA-C	5.52	119.83	112.77
1	B	349	VAL	N-CA-C	5.31	117.28	109.63
1	B	346	ALA	CB-CA-C	-5.08	110.69	116.54

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	3477	0	3529	136	0
1	B	3477	0	3529	136	0
1	C	3477	0	3529	132	0
2	D	925	0	901	20	0
2	F	925	0	901	16	0
2	H	925	0	901	19	0
3	E	879	0	859	24	0
3	G	879	0	859	23	0
3	I	879	0	859	28	0
4	J	995	0	955	41	0
4	L	995	0	955	39	0
4	N	995	0	955	40	0
5	K	820	0	811	25	0
5	M	820	0	811	26	0
5	O	820	0	811	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21288	0	21165	694	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 16.

All (694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:HB3	1:A:375:LEU:O	1.22	1.32
1:C:348:SER:HB3	1:C:375:LEU:O	1.43	1.17
1:C:46:SER:OG	1:C:311:THR:HG22	1.45	1.16
1:B:348:SER:HB3	1:B:375:LEU:O	0.99	1.15
1:B:46:SER:OG	1:B:311:THR:HG22	1.45	1.15
1:B:348:SER:CB	1:B:375:LEU:O	1.94	1.15
1:A:46:SER:OG	1:A:311:THR:HG22	1.45	1.13
1:B:146:SER:OG	1:B:149:ALA:HB2	1.50	1.12
1:C:146:SER:OG	1:C:149:ALA:HB2	1.50	1.12
1:A:146:SER:OG	1:A:149:ALA:HB2	1.50	1.11
1:A:348:SER:CB	1:A:375:LEU:O	2.00	1.09
1:A:215:PRO:HD2	1:A:216:ASN:H	1.12	1.09
1:C:348:SER:CB	1:C:375:LEU:O	2.01	1.08
1:B:215:PRO:HD2	1:B:216:ASN:H	1.12	1.07
1:C:215:PRO:HD2	1:C:216:ASN:H	1.12	1.07
4:L:87:THR:HG22	4:L:111:VAL:H	1.22	1.04
4:N:87:THR:HG22	4:N:111:VAL:H	1.22	1.02
4:J:87:THR:HG22	4:J:111:VAL:H	1.22	1.01
1:A:505:PHE:HD1	1:A:508:LYS:HE2	1.24	1.00
1:B:209:LYS:NZ	5:M:50:ASP:OD2	1.94	0.99
1:B:505:PHE:HD1	1:B:508:LYS:HE2	1.24	0.99
1:B:67:ILE:CD1	1:B:83:LEU:HB3	1.92	0.99
1:C:67:ILE:CD1	1:C:83:LEU:HB3	1.92	0.98
1:A:67:ILE:CD1	1:A:83:LEU:HB3	1.93	0.98
1:B:348:SER:HB3	1:B:375:LEU:C	1.90	0.96
1:C:505:PHE:HD1	1:C:508:LYS:HE2	1.24	0.96
1:C:67:ILE:HD13	1:C:83:LEU:HB3	1.49	0.95
1:C:209:LYS:NZ	5:O:50:ASP:OD2	2.01	0.93
1:B:67:ILE:HD13	1:B:83:LEU:HB3	1.49	0.93
4:L:87:THR:CG2	4:L:111:VAL:H	1.82	0.93
4:N:87:THR:CG2	4:N:111:VAL:H	1.82	0.92
1:A:67:ILE:HD13	1:A:83:LEU:HB3	1.49	0.92
4:J:87:THR:CG2	4:J:111:VAL:H	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:OG	1:B:352:PHE:CE1	2.23	0.91
1:B:215:PRO:HD2	1:B:216:ASN:N	1.90	0.86
1:C:342:TYR:HB3	1:C:349:VAL:HG11	1.59	0.84
1:B:429:ARG:NH1	1:B:432:ILE:HD12	1.93	0.84
5:O:37:GLN:HE21	5:O:39:ARG:HE	1.26	0.84
1:C:505:PHE:CD1	1:C:508:LYS:HE2	2.12	0.84
1:A:429:ARG:NH1	1:A:432:ILE:HD12	1.93	0.83
1:A:505:PHE:CD1	1:A:508:LYS:HE2	2.12	0.83
1:C:205:PRO:O	1:C:209:LYS:HG3	1.79	0.83
1:C:429:ARG:NH1	1:C:432:ILE:HD12	1.93	0.83
1:A:205:PRO:O	1:A:209:LYS:HG3	1.79	0.83
1:B:205:PRO:O	1:B:209:LYS:HG3	1.79	0.82
1:C:311:THR:OG1	1:C:344:ASP:O	1.96	0.82
1:A:215:PRO:HD2	1:A:216:ASN:N	1.90	0.82
1:C:215:PRO:HD2	1:C:216:ASN:N	1.90	0.82
4:L:87:THR:HG22	4:L:111:VAL:N	1.95	0.82
4:J:87:THR:HG22	4:J:111:VAL:N	1.95	0.81
1:B:146:SER:HG	1:B:149:ALA:HB2	1.42	0.81
4:J:33:TRP:CE3	4:J:50:MET:HE2	2.16	0.81
4:N:87:THR:HG22	4:N:111:VAL:N	1.95	0.81
4:L:33:TRP:CE3	4:L:50:MET:HE2	2.16	0.81
1:B:505:PHE:CD1	1:B:508:LYS:HE2	2.12	0.80
4:N:33:TRP:CE3	4:N:50:MET:HE2	2.16	0.80
1:C:314:TRP:HH2	1:C:349:VAL:HG21	1.46	0.80
1:B:178:VAL:HG23	2:H:97:PRO:HG3	1.63	0.80
4:L:33:TRP:CE3	4:L:50:MET:CE	2.65	0.80
4:J:33:TRP:CZ3	4:J:50:MET:HE2	2.18	0.79
4:J:33:TRP:CE3	4:J:50:MET:CE	2.65	0.79
4:N:33:TRP:CE3	4:N:50:MET:CE	2.65	0.79
4:N:33:TRP:CZ3	4:N:50:MET:HE2	2.18	0.78
4:L:33:TRP:CZ3	4:L:50:MET:HE2	2.18	0.78
1:A:146:SER:HG	1:A:149:ALA:HB2	1.46	0.77
1:A:62:SER:OG	1:A:199:ILE:HG21	1.86	0.76
1:C:215:PRO:CD	1:C:216:ASN:H	1.96	0.76
1:C:146:SER:HG	1:C:149:ALA:HB2	1.48	0.76
1:C:348:SER:HB2	1:C:375:LEU:O	1.84	0.76
1:C:209:LYS:NZ	4:N:100(J):TYR:CE1	2.52	0.76
1:C:46:SER:CB	1:C:311:THR:HG22	2.17	0.75
1:B:62:SER:OG	1:B:199:ILE:HG21	1.86	0.75
1:C:308:VAL:HG11	1:C:345:ASN:OD1	1.86	0.75
4:J:75:VAL:HG12	4:J:75:VAL:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:SER:OG	1:C:199:ILE:HG21	1.86	0.75
2:H:6:GLN:H	2:H:105:GLN:HE22	1.34	0.75
4:L:75:VAL:HG12	4:L:75:VAL:O	1.87	0.75
1:A:46:SER:CB	1:A:311:THR:HG22	2.17	0.74
1:A:215:PRO:CD	1:A:216:ASN:H	1.96	0.74
4:J:50:MET:HE1	4:J:100(I):TYR:OH	1.87	0.74
4:N:75:VAL:O	4:N:75:VAL:HG12	1.87	0.74
4:N:50:MET:HE1	4:N:100(I):TYR:OH	1.87	0.74
1:B:151:GLY:HA3	1:B:288:ILE:HD13	1.70	0.74
4:L:50:MET:HE1	4:L:100(I):TYR:OH	1.87	0.74
1:C:314:TRP:CH2	1:C:349:VAL:HG21	2.23	0.74
2:F:6:GLN:H	2:F:105:GLN:HE22	1.34	0.74
1:B:46:SER:CB	1:B:311:THR:HG22	2.17	0.73
1:A:151:GLY:HA3	1:A:288:ILE:HD13	1.70	0.73
1:B:215:PRO:CD	1:B:216:ASN:H	1.96	0.73
1:C:151:GLY:HA3	1:C:288:ILE:HD13	1.70	0.73
1:A:67:ILE:HD13	1:A:83:LEU:CB	2.19	0.72
1:A:178:VAL:HG23	2:F:97:PRO:HG3	1.71	0.72
1:C:67:ILE:HD13	1:C:83:LEU:CB	2.19	0.72
1:C:212:CYS:SG	4:N:99:VAL:HG11	2.30	0.72
2:D:6:GLN:H	2:D:105:GLN:HE22	1.34	0.72
1:B:67:ILE:HD13	1:B:83:LEU:CB	2.19	0.72
1:A:67:ILE:HD11	1:A:83:LEU:HB3	1.72	0.71
1:B:67:ILE:HD11	1:B:83:LEU:HB3	1.72	0.71
1:C:67:ILE:HD11	1:C:83:LEU:HB3	1.72	0.71
1:C:349:VAL:HG12	1:C:350:SER:O	1.90	0.70
5:K:6:GLN:HG3	5:K:23:CYS:SG	2.31	0.70
5:K:89:GLN:HE22	5:K:96:LEU:HB3	1.57	0.69
5:O:20:THR:HG22	5:O:74:THR:HG22	1.74	0.69
5:O:79:GLN:HG3	5:O:82:ASP:HB2	1.74	0.69
1:B:209:LYS:HZ1	5:M:50:ASP:CG	1.96	0.69
2:H:100:ALA:O	3:I:96:ARG:NH2	2.26	0.68
1:B:175:ASN:OD1	3:I:32:TYR:OH	2.08	0.68
5:M:39:ARG:NH2	5:M:81:GLU:OE1	2.28	0.67
2:D:100:ALA:O	3:E:96:ARG:NH2	2.28	0.67
2:H:94:ARG:NH2	2:H:101:ASP:OD2	2.28	0.67
5:O:63:SER:OG	5:O:74:THR:OG1	2.13	0.66
1:A:81:GLN:HE22	1:B:225:GLN:HB3	1.60	0.66
2:D:94:ARG:NH2	2:D:101:ASP:OD2	2.28	0.66
1:C:178:VAL:HG23	2:D:97:PRO:HG3	1.78	0.66
2:F:94:ARG:NH2	2:F:101:ASP:OD2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:HB3	1:A:375:LEU:C	2.16	0.65
2:F:101:ASP:O	3:G:45:ARG:NH2	2.30	0.65
1:B:482:VAL:CG2	1:B:502:SER:OG	2.45	0.65
1:A:482:VAL:CG2	1:A:502:SER:OG	2.45	0.65
1:C:308:VAL:CB	1:C:345:ASN:OD1	2.45	0.65
5:K:42:LYS:HD2	5:K:43:ALA:H	1.62	0.65
1:B:350:SER:OG	1:B:352:PHE:CZ	2.43	0.65
1:C:482:VAL:CG2	1:C:502:SER:OG	2.45	0.65
3:E:47:LEU:HD23	3:E:48:ILE:HG12	1.79	0.65
5:K:61:ARG:NH1	5:K:77:THR:O	2.31	0.65
1:B:46:SER:HG	1:B:311:THR:HG22	1.58	0.64
3:E:74:LYS:HE3	5:O:66:GLY:HA2	1.79	0.64
1:B:505:PHE:HD1	1:B:508:LYS:CE	2.07	0.64
4:L:23:LYS:HD2	4:L:77:THR:HG22	1.79	0.64
3:I:47:LEU:HD23	3:I:48:ILE:HG12	1.79	0.64
1:B:308:VAL:HG11	1:B:345:ASN:OD1	1.98	0.64
1:C:308:VAL:CG1	1:C:345:ASN:OD1	2.46	0.64
4:J:23:LYS:HD2	4:J:77:THR:HG22	1.79	0.64
3:G:47:LEU:HD23	3:G:48:ILE:HG12	1.79	0.63
5:M:21:LEU:HD21	5:M:102:THR:HG21	1.80	0.63
4:N:23:LYS:HD2	4:N:77:THR:HG22	1.79	0.63
1:C:215:PRO:CD	1:C:216:ASN:N	2.58	0.63
1:A:215:PRO:CD	1:A:216:ASN:N	2.58	0.63
2:F:100:ALA:O	3:G:96:ARG:NH2	2.32	0.63
1:B:344:ASP:HA	1:B:349:VAL:HG13	1.80	0.63
1:C:229:ARG:NE	1:C:250:TYR:O	2.33	0.62
2:H:86:ASP:OD1	2:H:90:TYR:OH	2.17	0.62
1:C:325:ASN:ND2	1:C:330:SER:OG	2.33	0.62
1:A:229:ARG:NE	1:A:250:TYR:O	2.33	0.62
2:F:86:ASP:OD1	2:F:90:TYR:OH	2.17	0.62
4:N:6:GLN:H	4:N:105:GLN:HE22	1.48	0.62
3:G:5:THR:HA	3:G:100:GLN:HE22	1.64	0.62
2:D:86:ASP:OD1	2:D:90:TYR:OH	2.17	0.62
2:H:48:MET:HB3	2:H:67:LEU:HD11	1.82	0.62
1:B:215:PRO:CD	1:B:216:ASN:N	2.58	0.62
5:K:42:LYS:HD2	5:K:43:ALA:N	2.15	0.62
1:B:325:ASN:ND2	1:B:330:SER:OG	2.33	0.62
5:O:6:GLN:HE21	5:O:102:THR:HG23	1.65	0.61
1:A:325:ASN:ND2	1:A:330:SER:OG	2.33	0.61
1:B:388:ASN:OD1	1:B:391:TYR:N	2.33	0.61
1:B:229:ARG:NE	1:B:250:TYR:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:5:THR:HA	3:I:100:GLN:HE22	1.64	0.61
2:H:101:ASP:O	3:I:45:ARG:NH2	2.33	0.61
2:D:48:MET:HB3	2:D:67:LEU:HD11	1.82	0.61
2:F:48:MET:HB3	2:F:67:LEU:HD11	1.82	0.61
1:C:336:ARG:NH2	1:C:382:CYS:SG	2.74	0.61
4:J:23:LYS:HZ3	4:J:75:VAL:HG12	1.66	0.61
2:D:101:ASP:OD1	2:D:101:ASP:N	2.29	0.61
1:B:175:ASN:ND2	3:I:28:ASP:OD2	2.34	0.61
1:A:172:LEU:O	3:G:50:ARG:NH1	2.34	0.60
5:M:78:LEU:HB3	5:M:83:PHE:HE1	1.65	0.60
1:A:336:ARG:NH2	1:A:382:CYS:SG	2.74	0.60
3:E:5:THR:HA	3:E:100:GLN:HE22	1.64	0.60
1:B:336:ARG:NH2	1:B:382:CYS:SG	2.74	0.60
4:L:6:GLN:H	4:L:105:GLN:HE22	1.47	0.60
4:L:43:LYS:NZ	4:L:46:GLU:OE1	2.35	0.60
5:M:82:ASP:OD1	5:M:86:TYR:OH	2.18	0.60
5:O:6:GLN:HG2	5:O:23:CYS:HB3	1.83	0.60
4:J:6:GLN:H	4:J:105:GLN:HE22	1.48	0.60
4:N:43:LYS:NZ	4:N:46:GLU:OE1	2.35	0.59
4:N:23:LYS:HZ2	4:N:75:VAL:HG12	1.67	0.59
4:J:43:LYS:NZ	4:J:46:GLU:OE1	2.35	0.59
1:A:505:PHE:HD1	1:A:508:LYS:CE	2.08	0.59
5:M:37:GLN:HB2	5:M:47:LEU:HD11	1.85	0.58
1:B:172:LEU:O	3:I:50:ARG:NH1	2.37	0.58
3:E:49:TYR:CZ	3:E:53:HIS:HB3	2.39	0.58
2:F:105:GLN:OE1	2:F:105:GLN:N	2.36	0.58
5:M:89:GLN:HE22	5:M:96:LEU:HB3	1.69	0.58
1:C:319:SER:OG	1:C:406:VAL:HG22	2.04	0.58
3:E:105:GLU:N	3:E:105:GLU:OE2	2.37	0.58
3:G:49:TYR:CZ	3:G:53:HIS:HB3	2.39	0.58
4:J:100(A):VAL:HG12	4:J:100(H):TYR:HD2	1.69	0.58
1:C:505:PHE:HD1	1:C:508:LYS:CE	2.08	0.57
5:M:79:GLN:HG3	5:M:81:GLU:H	1.68	0.57
1:C:388:ASN:OD1	1:C:391:TYR:N	2.33	0.57
3:I:49:TYR:CZ	3:I:53:HIS:HB3	2.39	0.57
3:I:105:GLU:OE2	3:I:105:GLU:N	2.37	0.57
1:A:185:VAL:HA	1:B:427:LYS:NZ	2.20	0.57
1:A:319:SER:OG	1:A:406:VAL:HG22	2.04	0.57
5:K:39:ARG:NH2	5:K:81:GLU:O	2.37	0.57
3:G:105:GLU:OE2	3:G:105:GLU:N	2.37	0.57
4:J:75:VAL:O	4:J:75:VAL:CG1	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:ASP:O	3:E:45:ARG:NH2	2.38	0.57
4:L:100(A):VAL:HG12	4:L:100(H):TYR:HD2	1.69	0.57
1:A:311:THR:HG21	1:A:344:ASP:O	2.05	0.56
1:A:388:ASN:OD1	1:A:391:TYR:N	2.33	0.56
1:B:319:SER:OG	1:B:406:VAL:HG22	2.04	0.56
1:B:348:SER:OG	1:B:376:PRO:HA	2.05	0.56
3:G:90:GLN:HE21	3:G:97:THR:H	1.52	0.56
2:H:105:GLN:OE1	2:H:105:GLN:N	2.36	0.56
3:E:90:GLN:HE21	3:E:97:THR:H	1.52	0.56
4:N:100(A):VAL:HG12	4:N:100(H):TYR:HD2	1.69	0.56
1:A:93:LEU:HD22	1:A:297:LEU:HD11	1.88	0.56
1:C:308:VAL:HB	1:C:345:ASN:OD1	2.04	0.56
2:F:101:ASP:OD1	2:F:101:ASP:N	2.29	0.56
3:I:66:GLU:HB3	3:I:71:PHE:HA	1.87	0.56
1:C:93:LEU:HD22	1:C:297:LEU:HD11	1.88	0.56
3:E:66:GLU:HB3	3:E:71:PHE:HA	1.87	0.56
1:A:348:SER:OG	1:A:376:PRO:HA	2.06	0.56
1:A:236:GLU:O	1:A:240:ASN:HB2	2.06	0.56
4:L:23:LYS:HZ3	4:L:75:VAL:HG12	1.70	0.56
1:C:175:ASN:OD1	3:E:32:TYR:OH	2.13	0.56
2:D:105:GLN:OE1	2:D:105:GLN:N	2.36	0.56
1:A:46:SER:HG	1:A:311:THR:HG22	1.67	0.56
1:B:323:THR:HG23	1:B:325:ASN:H	1.72	0.55
4:L:75:VAL:O	4:L:75:VAL:CG1	2.53	0.55
4:N:75:VAL:O	4:N:75:VAL:CG1	2.53	0.55
5:K:46:LEU:HD11	5:K:49:PHE:HB3	1.88	0.55
1:A:308:VAL:HG11	1:A:345:ASN:OD1	2.06	0.55
1:B:316:LEU:HD22	1:B:383:ASN:HD21	1.71	0.55
1:A:323:THR:HG22	1:A:331:ASN:HB2	1.89	0.55
1:C:316:LEU:HD22	1:C:383:ASN:HD21	1.71	0.55
1:B:93:LEU:HD22	1:B:297:LEU:HD11	1.88	0.55
4:J:52(A):PRO:HA	4:J:71:VAL:HG21	1.88	0.55
2:H:101:ASP:OD1	2:H:101:ASP:N	2.29	0.55
3:I:90:GLN:HE21	3:I:97:THR:H	1.52	0.55
5:M:61:ARG:NH1	5:M:77:THR:O	2.38	0.55
1:B:197:ASN:OD1	1:B:201:LYS:HE2	2.07	0.55
1:C:197:ASN:OD1	1:C:201:LYS:HE2	2.07	0.55
1:C:236:GLU:O	1:C:240:ASN:HB2	2.06	0.55
1:B:236:GLU:O	1:B:240:ASN:HB2	2.06	0.54
1:C:273:LEU:HD13	1:C:309:ILE:HD12	1.89	0.54
1:A:225:GLN:HB3	1:C:81:GLN:HE22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:74:LYS:HE3	5:M:66:GLY:HA2	1.89	0.54
3:G:66:GLU:HB3	3:G:71:PHE:HA	1.87	0.54
5:K:82:ASP:OD1	5:K:86:TYR:OH	2.25	0.54
4:L:52(A):PRO:HA	4:L:71:VAL:HG21	1.89	0.54
1:A:197:ASN:OD1	1:A:201:LYS:HE2	2.07	0.54
1:A:323:THR:HG23	1:A:325:ASN:H	1.72	0.54
1:C:323:THR:HG23	1:C:325:ASN:H	1.72	0.54
1:C:495:VAL:O	1:C:499:ILE:HG12	2.08	0.54
4:N:52(A):PRO:HA	4:N:71:VAL:HG21	1.88	0.54
4:J:33:TRP:HB2	4:J:95:GLN:HG3	1.89	0.54
1:B:273:LEU:HD13	1:B:309:ILE:HD12	1.89	0.54
1:C:323:THR:HG22	1:C:331:ASN:HB2	1.89	0.54
1:A:47:ALA:HB2	1:A:273:LEU:HD11	1.90	0.53
1:A:495:VAL:O	1:A:499:ILE:HG12	2.08	0.53
4:L:33:TRP:HB2	4:L:95:GLN:HG3	1.89	0.53
1:A:273:LEU:HD13	1:A:309:ILE:HD12	1.89	0.53
1:C:49:ARG:HH21	1:C:370:MET:HB2	1.74	0.53
1:C:482:VAL:HG13	1:C:499:ILE:HD12	1.89	0.53
4:N:33:TRP:CE3	4:N:50:MET:HE3	2.44	0.53
1:A:49:ARG:HH21	1:A:370:MET:HB2	1.73	0.53
1:B:49:ARG:HH21	1:B:370:MET:HB2	1.73	0.53
1:B:323:THR:HG22	1:B:331:ASN:HB2	1.89	0.53
1:A:316:LEU:HD22	1:A:383:ASN:HD21	1.71	0.53
1:B:482:VAL:HG13	1:B:499:ILE:HD12	1.89	0.53
4:N:33:TRP:HB2	4:N:95:GLN:HG3	1.89	0.53
1:A:482:VAL:HG13	1:A:499:ILE:HD12	1.89	0.53
1:C:47:ALA:HB2	1:C:273:LEU:HD11	1.90	0.53
5:O:47:LEU:HB3	5:O:58:VAL:HG11	1.89	0.53
1:C:447:VAL:O	1:C:461:LYS:NZ	2.42	0.53
1:A:60:GLU:O	1:A:196:LYS:N	2.40	0.53
1:B:47:ALA:HB2	1:B:273:LEU:HD11	1.90	0.53
5:O:37:GLN:NE2	5:O:39:ARG:HE	2.01	0.53
1:C:48:LEU:HD21	1:C:352:PHE:HZ	1.74	0.52
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.91	0.52
1:B:495:VAL:O	1:B:499:ILE:HG12	2.08	0.52
1:C:348:SER:OG	1:C:376:PRO:HA	2.10	0.52
1:A:308:VAL:CB	1:A:345:ASN:OD1	2.58	0.52
4:L:33:TRP:CE3	4:L:50:MET:HE3	2.44	0.52
5:M:49:PHE:HE1	5:M:53:LYS:HD2	1.73	0.52
4:N:23:LYS:NZ	4:N:75:VAL:HG12	2.25	0.52
5:O:37:GLN:HB2	5:O:47:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD21	1:A:352:PHE:HZ	1.74	0.52
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.91	0.52
2:D:19:LYS:HD2	2:D:81:GLU:HG3	1.92	0.52
4:J:33:TRP:CE3	4:J:50:MET:HE3	2.44	0.52
5:M:6:GLN:HG2	5:M:23:CYS:HB3	1.91	0.52
5:O:18:ARG:HA	5:O:75:ILE:O	2.10	0.52
1:A:185:VAL:HA	1:B:427:LYS:HZ1	1.75	0.52
1:A:219:THR:HA	1:A:222:GLU:HG2	1.91	0.52
1:B:447:VAL:O	1:B:461:LYS:NZ	2.42	0.52
1:A:69:CYS:HB2	1:A:80:LYS:HD3	1.92	0.52
1:B:369:THR:HA	1:B:372:SER:OG	2.10	0.52
4:L:23:LYS:NZ	4:L:75:VAL:HG12	2.25	0.52
1:A:429:ARG:HH12	1:A:432:ILE:HD12	1.74	0.52
1:A:447:VAL:O	1:A:461:LYS:NZ	2.42	0.52
1:B:207:VAL:HG22	1:B:214:ILE:HD11	1.92	0.52
1:C:219:THR:HA	1:C:222:GLU:HG2	1.91	0.52
1:C:369:THR:HA	1:C:372:SER:OG	2.10	0.52
5:O:14:SER:HA	5:O:106:ILE:HG13	1.91	0.52
1:B:48:LEU:HD21	1:B:352:PHE:HZ	1.74	0.51
2:F:19:LYS:HD2	2:F:81:GLU:HG3	1.92	0.51
1:B:219:THR:HA	1:B:222:GLU:HG2	1.91	0.51
1:C:207:VAL:HG22	1:C:214:ILE:HD11	1.92	0.51
3:I:66:GLU:OE1	3:I:66:GLU:HA	2.11	0.51
4:J:23:LYS:NZ	4:J:75:VAL:HG12	2.25	0.51
5:O:42:LYS:NZ	5:O:43:ALA:O	2.24	0.51
1:A:207:VAL:HG22	1:A:214:ILE:HD11	1.92	0.51
1:C:348:SER:HB3	1:C:376:PRO:CA	2.41	0.51
3:G:33:LEU:HD22	3:G:71:PHE:CD2	2.45	0.51
3:G:66:GLU:HA	3:G:66:GLU:OE1	2.11	0.51
5:O:39:ARG:HB2	5:O:42:LYS:HB3	1.92	0.51
1:C:69:CYS:HB2	1:C:80:LYS:HD3	1.92	0.51
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.91	0.51
1:C:397:THR:OG1	1:C:484:PRO:O	2.17	0.51
1:C:46:SER:HG	1:C:311:THR:HG22	1.69	0.51
3:G:1:ASP:HB3	3:G:95:PRO:HD2	1.93	0.51
1:A:369:THR:HA	1:A:372:SER:OG	2.10	0.51
3:E:33:LEU:HD22	3:E:71:PHE:CD2	2.45	0.51
3:I:33:LEU:HD22	3:I:71:PHE:CD2	2.45	0.51
4:J:100(L):MET:O	4:J:103:TRP:NE1	2.36	0.51
1:A:392:ASP:OD2	1:A:491:SER:OG	2.25	0.51
1:B:212:CYS:SG	4:L:99:VAL:HG11	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:CYS:HB2	1:B:435:PHE:HB2	1.94	0.50
2:H:19:LYS:HD2	2:H:81:GLU:HG3	1.92	0.50
1:B:66:GLU:N	1:B:66:GLU:OE2	2.45	0.50
5:K:47:LEU:HD12	5:K:48:MET:HB2	1.92	0.50
4:L:23:LYS:HD2	4:L:77:THR:CG2	2.42	0.50
5:O:79:GLN:HE22	5:O:81:GLU:HB3	1.77	0.50
1:C:422:CYS:HB2	1:C:435:PHE:HB2	1.94	0.50
4:J:23:LYS:HD2	4:J:77:THR:CG2	2.42	0.50
4:N:100(L):MET:O	4:N:103:TRP:NE1	2.36	0.50
1:A:422:CYS:HB2	1:A:435:PHE:HB2	1.94	0.50
1:C:66:GLU:OE2	1:C:66:GLU:N	2.45	0.50
3:G:47:LEU:HD13	3:G:86:TYR:HE2	1.77	0.50
4:N:23:LYS:HD2	4:N:77:THR:CG2	2.42	0.50
1:B:53:TYR:HE2	1:B:260:LEU:HD11	1.77	0.50
3:E:47:LEU:HD13	3:E:86:TYR:HE2	1.77	0.50
3:E:66:GLU:HA	3:E:66:GLU:OE1	2.11	0.50
3:I:47:LEU:HD13	3:I:86:TYR:HE2	1.77	0.50
1:A:66:GLU:OE2	1:A:66:GLU:N	2.45	0.50
1:B:429:ARG:HH12	1:B:432:ILE:HD12	1.74	0.50
1:A:53:TYR:HE2	1:A:260:LEU:HD11	1.77	0.49
1:B:69:CYS:HB2	1:B:80:LYS:HD3	1.92	0.49
1:B:336:ARG:HA	1:B:395:ILE:HG22	1.93	0.49
1:C:46:SER:CB	1:C:311:THR:CG2	2.89	0.49
1:A:273:LEU:HD13	1:A:309:ILE:HG23	1.94	0.49
1:C:336:ARG:HA	1:C:395:ILE:HG22	1.93	0.49
1:C:348:SER:CB	1:C:376:PRO:HA	2.42	0.49
4:L:47:TRP:HZ2	4:L:50:MET:HB3	1.77	0.49
4:N:6:GLN:H	4:N:105:GLN:NE2	2.11	0.49
1:A:336:ARG:HA	1:A:395:ILE:HG22	1.93	0.49
1:B:60:GLU:O	1:B:196:LYS:N	2.40	0.49
1:C:60:GLU:O	1:C:196:LYS:N	2.40	0.49
5:K:37:GLN:HB2	5:K:47:LEU:HD23	1.94	0.49
1:C:53:TYR:HE2	1:C:260:LEU:HD11	1.77	0.49
2:H:37:LEU:HD21	3:I:98:PHE:CE1	2.47	0.49
3:I:1:ASP:HB3	3:I:95:PRO:HD2	1.93	0.49
4:L:34:ILE:HG21	4:L:78:VAL:HG11	1.94	0.49
1:B:490:ALA:HA	1:B:494:GLN:HE21	1.78	0.49
3:E:1:ASP:HB3	3:E:95:PRO:HD2	1.93	0.49
3:E:8:PRO:O	3:E:102:THR:OG1	2.23	0.49
1:B:273:LEU:HD13	1:B:309:ILE:HG23	1.94	0.49
4:J:6:GLN:H	4:J:105:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:90:GLN:HE21	5:M:96:LEU:HA	1.78	0.49
4:N:47:TRP:HZ2	4:N:50:MET:HB3	1.77	0.49
5:O:37:GLN:HE22	5:O:39:ARG:HH21	1.59	0.49
1:A:292:ILE:HD12	1:A:297:LEU:HD12	1.95	0.49
2:H:96:PRO:HD3	2:H:100(C):MET:HG2	1.95	0.49
5:K:55:GLN:O	5:K:58:VAL:HG12	2.13	0.49
5:O:13:ALA:O	5:O:106:ILE:HG13	2.12	0.49
1:C:273:LEU:HD13	1:C:309:ILE:HG23	1.94	0.48
2:F:96:PRO:HD3	2:F:100(C):MET:HG2	1.95	0.48
4:J:34:ILE:HG21	4:J:78:VAL:HG11	1.94	0.48
5:M:95:PRO:O	5:M:97:THR:HG23	2.13	0.48
4:J:47:TRP:HZ2	4:J:50:MET:HB3	1.77	0.48
4:L:100(L):MET:O	4:L:103:TRP:NE1	2.36	0.48
1:A:185:VAL:HG23	1:B:427:LYS:HE3	1.95	0.48
1:A:314:TRP:HH2	1:A:349:VAL:HG21	1.77	0.48
1:B:199:ILE:HG23	1:B:204:LEU:HD13	1.96	0.48
1:B:343:CYS:C	1:B:349:VAL:HG13	2.38	0.48
3:G:8:PRO:O	3:G:102:THR:OG1	2.23	0.48
1:A:215:PRO:HD2	1:A:216:ASN:OD1	2.13	0.48
1:A:348:SER:HB2	1:A:375:LEU:O	2.07	0.48
1:B:292:ILE:HD12	1:B:297:LEU:HD12	1.95	0.48
1:C:350:SER:OG	1:C:352:PHE:CE1	2.66	0.48
5:O:1:ASP:HB2	5:O:95:PRO:HD2	1.95	0.48
1:A:46:SER:CB	1:A:311:THR:CG2	2.89	0.48
1:A:199:ILE:HG23	1:A:204:LEU:HD13	1.96	0.48
1:A:490:ALA:HA	1:A:494:GLN:HE21	1.78	0.48
1:C:441:TYR:HB3	1:C:468:TYR:CE2	2.49	0.48
1:C:199:ILE:HG23	1:C:204:LEU:HD13	1.96	0.48
1:B:215:PRO:HD2	1:B:216:ASN:OD1	2.13	0.48
1:B:232:GLU:HG3	1:B:250:TYR:CZ	2.49	0.48
1:B:397:THR:OG1	1:B:484:PRO:O	2.17	0.48
1:C:429:ARG:HH12	1:C:432:ILE:HD12	1.73	0.48
2:D:96:PRO:HD3	2:D:100(C):MET:HG2	1.95	0.48
1:B:46:SER:CB	1:B:311:THR:CG2	2.90	0.48
1:C:215:PRO:HD2	1:C:216:ASN:OD1	2.13	0.48
1:C:490:ALA:HA	1:C:494:GLN:HE21	1.78	0.48
5:K:61:ARG:NH1	5:K:79:GLN:HG2	2.29	0.48
1:B:76:VAL:HA	1:B:79:ILE:HG22	1.96	0.48
5:M:42:LYS:HD2	5:M:43:ALA:H	1.78	0.48
5:O:2:ILE:O	5:O:97:THR:HG21	2.13	0.48
4:J:39:GLN:HB2	4:J:45:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:HG3	1:A:250:TYR:CZ	2.49	0.47
1:B:199:ILE:HA	1:B:203:LEU:HB3	1.96	0.47
3:G:28:ASP:OD1	3:G:29:GLY:N	2.47	0.47
4:L:6:GLN:H	4:L:105:GLN:NE2	2.10	0.47
4:L:87:THR:HG22	4:L:110:THR:HA	1.96	0.47
1:C:76:VAL:HA	1:C:79:ILE:HG22	1.96	0.47
3:I:28:ASP:OD1	3:I:29:GLY:N	2.47	0.47
5:K:6:GLN:HG2	5:K:23:CYS:HB2	1.96	0.47
5:K:6:GLN:CG	5:K:23:CYS:SG	3.00	0.47
4:N:34:ILE:HG21	4:N:78:VAL:HG11	1.94	0.47
1:B:168:LYS:NZ	1:B:294:GLU:O	2.38	0.47
3:E:28:ASP:OD1	3:E:29:GLY:N	2.47	0.47
1:B:441:TYR:HB3	1:B:468:TYR:CE2	2.49	0.47
1:C:292:ILE:HD12	1:C:297:LEU:HD12	1.95	0.47
1:A:199:ILE:HA	1:A:203:LEU:HB3	1.96	0.47
1:C:232:GLU:HG3	1:C:250:TYR:CZ	2.49	0.47
4:J:87:THR:HG22	4:J:110:THR:HA	1.96	0.47
4:L:39:GLN:HB2	4:L:45:LEU:HG	1.96	0.47
4:N:6:GLN:HE21	4:N:106:GLY:H	1.62	0.47
5:O:82:ASP:OD1	5:O:86:TYR:OH	2.32	0.47
1:A:348:SER:CB	1:A:376:PRO:HA	2.44	0.47
1:A:441:TYR:HB3	1:A:468:TYR:CE2	2.49	0.47
1:B:258:LEU:HG	1:B:278:VAL:HG11	1.97	0.47
1:B:392:ASP:OD2	1:B:491:SER:OG	2.25	0.47
1:C:199:ILE:HA	1:C:203:LEU:HB3	1.96	0.47
1:C:213:SER:O	1:C:213:SER:OG	2.32	0.47
3:E:54:ARG:NH2	3:E:58:VAL:O	2.47	0.47
4:N:17:SER:HB3	4:N:81:GLN:HE22	1.79	0.47
4:N:23:LYS:NZ	4:N:75:VAL:CG1	2.78	0.47
1:B:167:ILE:HD13	1:B:179:VAL:HG21	1.97	0.47
1:B:332:ILE:HG13	1:B:475:ILE:HD11	1.97	0.47
1:C:312:PRO:O	1:C:344:ASP:HB2	2.15	0.47
3:G:54:ARG:NH2	3:G:58:VAL:O	2.47	0.47
4:J:17:SER:HB3	4:J:81:GLN:HE22	1.79	0.47
5:K:33:LEU:HD21	5:K:88:CYS:HB2	1.96	0.47
4:N:39:GLN:HB2	4:N:45:LEU:HG	1.96	0.47
1:A:63:ASN:OD1	1:A:63:ASN:N	2.48	0.47
1:C:332:ILE:HG13	1:C:475:ILE:HD11	1.97	0.47
4:L:6:GLN:HE21	4:L:106:GLY:H	1.62	0.47
4:J:6:GLN:HE21	4:J:106:GLY:H	1.62	0.47
4:L:23:LYS:NZ	4:L:75:VAL:CG1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HA	1:A:79:ILE:HG22	1.96	0.46
3:G:51:ILE:HG22	3:G:65:SER:HA	1.96	0.46
3:I:54:ARG:NH2	3:I:58:VAL:O	2.47	0.46
5:O:73:LEU:HD21	5:O:75:ILE:HD11	1.97	0.46
1:A:209:LYS:NZ	5:K:50:ASP:OD2	2.46	0.46
1:C:167:ILE:HD13	1:C:179:VAL:HG21	1.97	0.46
1:C:204:LEU:HD23	4:N:100(H):TYR:CE2	2.50	0.46
5:O:90:GLN:NE2	5:O:93:ASP:O	2.40	0.46
1:B:81:GLN:HE22	1:C:225:GLN:HB3	1.79	0.46
3:I:51:ILE:HG22	3:I:65:SER:HA	1.96	0.46
4:J:23:LYS:NZ	4:J:75:VAL:CG1	2.78	0.46
4:N:87:THR:HG22	4:N:110:THR:HA	1.96	0.46
1:B:397:THR:HB	1:B:483:PHE:CE2	2.51	0.46
4:J:100(F):PRO:HB3	5:K:92:TYR:CE1	2.50	0.46
1:A:213:SER:O	1:A:213:SER:OG	2.32	0.46
1:A:332:ILE:HG13	1:A:475:ILE:HD11	1.97	0.46
3:G:47:LEU:HD21	3:G:62:PHE:HB3	1.97	0.46
1:A:397:THR:HB	1:A:483:PHE:CE2	2.51	0.46
1:B:378:GLU:OE2	1:B:390:LYS:HD3	2.16	0.46
4:L:17:SER:HB3	4:L:81:GLN:HE22	1.79	0.46
1:A:444:ASN:ND2	1:A:462:GLN:O	2.49	0.46
1:C:258:LEU:HG	1:C:278:VAL:HG11	1.97	0.46
3:E:51:ILE:HG22	3:E:65:SER:HA	1.96	0.46
4:L:35:GLY:HA2	4:L:50:MET:HA	1.98	0.46
1:A:308:VAL:HB	1:A:345:ASN:OD1	2.16	0.46
1:C:354:GLN:O	1:C:357:THR:OG1	2.34	0.46
3:E:47:LEU:HD21	3:E:62:PHE:HB3	1.97	0.46
3:I:47:LEU:HD21	3:I:62:PHE:HB3	1.97	0.46
1:B:385:ASP:HB2	1:B:388:ASN:HB3	1.98	0.45
1:A:258:LEU:HG	1:A:278:VAL:HG11	1.97	0.45
1:B:213:SER:O	1:B:213:SER:OG	2.32	0.45
1:B:393:CYS:O	1:B:492:ILE:HG12	2.16	0.45
1:C:378:GLU:OE2	1:C:390:LYS:HD3	2.16	0.45
5:O:37:GLN:NE2	5:O:39:ARG:HH21	2.14	0.45
1:A:385:ASP:HB2	1:A:388:ASN:HB3	1.98	0.45
4:J:35:GLY:HA2	4:J:50:MET:HA	1.98	0.45
1:A:167:ILE:HD13	1:A:179:VAL:HG21	1.97	0.45
1:B:175:ASN:ND2	3:I:27(D):LEU:HD23	2.32	0.45
2:H:112:SER:OG	2:H:113:SER:N	2.50	0.45
4:N:71:VAL:HG23	4:N:78:VAL:HG12	1.98	0.45
5:O:33:LEU:HD21	5:O:88:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:63:SER:O	5:O:74:THR:OG1	2.28	0.45
1:A:393:CYS:O	1:A:492:ILE:HG12	2.16	0.45
1:C:209:LYS:HZ3	4:N:100(J):TYR:HE1	1.44	0.45
3:I:2:VAL:HB	3:I:27:GLN:HG2	1.98	0.45
4:L:23:LYS:HZ1	4:L:75:VAL:CG1	2.29	0.45
1:A:378:GLU:OE2	1:A:390:LYS:HD3	2.16	0.45
1:C:348:SER:HB3	1:C:376:PRO:HA	1.96	0.45
1:C:444:ASN:ND2	1:C:462:GLN:O	2.49	0.45
5:K:16:GLY:H	5:K:78:LEU:HB2	1.82	0.45
5:O:49:PHE:HE1	5:O:55:GLN:HA	1.81	0.45
1:A:205:PRO:O	1:A:209:LYS:CG	2.59	0.45
1:C:205:PRO:O	1:C:209:LYS:CG	2.59	0.45
2:F:112:SER:OG	2:F:113:SER:N	2.50	0.45
3:G:74:LYS:HE3	5:K:66:GLY:HA2	1.99	0.45
1:B:354:GLN:O	1:B:357:THR:OG1	2.34	0.45
1:B:444:ASN:ND2	1:B:462:GLN:O	2.49	0.45
1:C:397:THR:HB	1:C:483:PHE:CE2	2.51	0.45
2:D:112:SER:OG	2:D:113:SER:N	2.50	0.45
5:O:13:ALA:O	5:O:106:ILE:HA	2.17	0.45
5:O:42:LYS:HD2	5:O:43:ALA:N	2.32	0.45
3:G:2:VAL:HB	3:G:27:GLN:HG2	1.98	0.45
1:C:385:ASP:HB2	1:C:388:ASN:HB3	1.98	0.44
4:J:71:VAL:HG23	4:J:78:VAL:HG12	1.98	0.44
5:M:89:GLN:NE2	5:M:96:LEU:HB3	2.32	0.44
1:A:498:LYS:HA	1:A:501:GLN:HE21	1.82	0.44
1:B:505:PHE:HA	1:B:508:LYS:HG2	2.00	0.44
1:C:505:PHE:CD1	1:C:508:LYS:CE	2.92	0.44
3:E:2:VAL:HB	3:E:27:GLN:HG2	1.98	0.44
1:A:369:THR:HG23	1:B:455:THR:OG1	2.17	0.44
1:C:393:CYS:O	1:C:492:ILE:HG12	2.16	0.44
4:N:35:GLY:HA2	4:N:50:MET:HA	1.98	0.44
1:A:46:SER:HA	1:A:365:VAL:HG23	2.00	0.44
1:A:505:PHE:HA	1:A:508:LYS:HG2	2.00	0.44
3:I:8:PRO:O	3:I:102:THR:OG1	2.23	0.44
1:B:209:LYS:NZ	5:M:50:ASP:CG	2.68	0.44
2:D:37:LEU:HD21	3:E:98:PHE:CE1	2.52	0.44
3:E:27(D):LEU:HD22	3:E:92:THR:HG22	2.00	0.44
4:L:71:VAL:HG23	4:L:78:VAL:HG12	1.98	0.44
1:B:46:SER:HA	1:B:365:VAL:HG23	2.00	0.44
1:B:308:VAL:HG21	1:B:345:ASN:OD1	2.18	0.44
1:C:505:PHE:HA	1:C:508:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:89:GLN:HE22	5:O:96:LEU:HB3	1.83	0.44
5:O:105:GLU:OE1	5:O:106:ILE:N	2.50	0.44
1:C:392:ASP:OD2	1:C:491:SER:OG	2.25	0.44
3:I:27(D):LEU:HD22	3:I:92:THR:HG22	2.00	0.44
4:J:12:LYS:HD2	4:J:18:LEU:HD12	2.00	0.44
1:A:512:LEU:HD13	1:B:513:LEU:HB2	2.00	0.44
1:C:498:LYS:HA	1:C:501:GLN:HE21	1.82	0.44
4:L:12:LYS:HD2	4:L:18:LEU:HD12	2.00	0.44
1:B:220:VAL:O	1:B:224:GLN:HG3	2.18	0.44
1:B:331:ASN:HD21	1:B:401:ASP:HB2	1.83	0.44
1:C:228:ASN:O	1:C:232:GLU:HG2	2.18	0.44
2:D:47:TRP:HZ2	2:D:50:TRP:HB3	1.83	0.44
4:J:103:TRP:CE3	5:K:44:PRO:HD2	2.52	0.44
1:A:228:ASN:O	1:A:232:GLU:HG2	2.18	0.43
1:C:331:ASN:HD21	1:C:401:ASP:HB2	1.83	0.43
2:F:47:TRP:HZ2	2:F:50:TRP:HB3	1.83	0.43
4:J:100(D):PRO:HB2	4:J:100(G):TYR:CE1	2.53	0.43
1:A:373:LEU:HD23	1:B:402:VAL:HG21	1.99	0.43
2:H:47:TRP:HZ2	2:H:50:TRP:HB3	1.83	0.43
1:A:378:GLU:HG3	1:A:391:TYR:HB2	2.00	0.43
1:B:228:ASN:O	1:B:232:GLU:HG2	2.18	0.43
1:B:314:TRP:CZ3	1:B:344:ASP:OD1	2.71	0.43
5:K:2:ILE:O	5:K:97:THR:HG21	2.18	0.43
4:L:50:MET:HE1	4:L:100(I):TYR:CZ	2.53	0.43
5:M:79:GLN:CD	5:M:80:PRO:HD2	2.44	0.43
1:A:197:ASN:CG	1:A:201:LYS:HE2	2.43	0.43
1:A:354:GLN:O	1:A:357:THR:OG1	2.34	0.43
1:B:325:ASN:HD21	1:B:327:LYS:HE2	1.83	0.43
1:C:46:SER:HA	1:C:365:VAL:HG23	2.00	0.43
3:G:27(D):LEU:HD22	3:G:92:THR:HG22	2.00	0.43
4:L:100(D):PRO:HB2	4:L:100(G):TYR:CE1	2.53	0.43
5:M:105:GLU:OE1	5:M:106:ILE:N	2.51	0.43
5:O:53:LYS:HB2	5:O:53:LYS:HE2	1.65	0.43
1:A:308:VAL:CG1	1:A:345:ASN:OD1	2.66	0.43
1:A:314:TRP:CH2	1:A:349:VAL:HG11	2.54	0.43
1:A:331:ASN:HD21	1:A:401:ASP:HB2	1.83	0.43
4:N:12:LYS:HD2	4:N:18:LEU:HD12	2.00	0.43
1:B:197:ASN:CG	1:B:201:LYS:HE2	2.43	0.43
1:A:378:GLU:CG	1:A:391:TYR:HB2	2.49	0.43
1:B:344:ASP:CA	1:B:349:VAL:HG13	2.47	0.43
1:B:482:VAL:HG22	1:B:502:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:ILE:H	3:E:51:ILE:HG13	1.65	0.43
3:I:27(D):LEU:HD12	3:I:27(D):LEU:HA	1.80	0.43
1:B:498:LYS:HA	1:B:501:GLN:HE21	1.82	0.43
1:C:75:LYS:H	1:C:75:LYS:HG2	1.59	0.43
1:C:251:MET:SD	1:C:287:SER:OG	2.70	0.43
1:C:325:ASN:HD21	1:C:327:LYS:HE2	1.83	0.43
4:N:100(D):PRO:HB2	4:N:100(G):TYR:CE1	2.53	0.43
5:O:89:GLN:NE2	5:O:96:LEU:HB3	2.33	0.43
1:A:482:VAL:HG22	1:A:502:SER:OG	2.19	0.43
1:C:378:GLU:HG3	1:C:391:TYR:HB2	2.01	0.43
4:N:50:MET:HE1	4:N:100(I):TYR:CZ	2.53	0.43
5:O:37:GLN:CB	5:O:47:LEU:HD11	2.48	0.43
1:A:314:TRP:HZ3	1:A:344:ASP:OD1	2.02	0.43
1:A:322:CYS:HA	1:A:333:CYS:HA	2.01	0.43
1:A:348:SER:HB3	1:A:376:PRO:CA	2.48	0.43
1:C:220:VAL:O	1:C:224:GLN:HG3	2.18	0.43
1:C:378:GLU:CG	1:C:391:TYR:HB2	2.49	0.43
5:M:1:ASP:HB2	5:M:95:PRO:HD2	1.99	0.43
4:N:23:LYS:HZ3	4:N:75:VAL:CG1	2.32	0.43
1:A:325:ASN:HD21	1:A:327:LYS:HE2	1.83	0.42
1:B:63:ASN:OD1	1:B:63:ASN:N	2.49	0.42
1:C:197:ASN:CG	1:C:201:LYS:HE2	2.43	0.42
1:B:378:GLU:CG	1:B:391:TYR:HB2	2.49	0.42
1:B:378:GLU:HG3	1:B:391:TYR:HB2	2.00	0.42
1:B:424:ALA:HB2	1:B:435:PHE:CE2	2.55	0.42
5:M:6:GLN:CG	5:M:23:CYS:HB3	2.49	0.42
1:B:308:VAL:CG1	1:B:345:ASN:OD1	2.67	0.42
5:K:49:PHE:CZ	5:K:53:LYS:HD2	2.54	0.42
1:A:67:ILE:HA	4:J:100:VAL:HG22	2.01	0.42
1:A:220:VAL:O	1:A:224:GLN:HG3	2.18	0.42
1:B:322:CYS:HA	1:B:333:CYS:HA	2.01	0.42
5:K:8:PRO:HD2	5:K:21:LEU:HD23	2.00	0.42
1:A:158:LEU:HD21	1:A:167:ILE:HG13	2.01	0.42
1:A:427:LYS:NZ	1:C:185:VAL:HA	2.34	0.42
1:B:311:THR:HG21	1:B:344:ASP:O	2.19	0.42
1:C:482:VAL:HG22	1:C:502:SER:OG	2.19	0.42
2:F:16:ALA:O	2:F:82(C):LEU:HD13	2.19	0.42
4:J:50:MET:HE1	4:J:100(I):TYR:CZ	2.53	0.42
1:A:264:MET:HA	1:A:265:PRO:HD3	1.90	0.42
1:A:308:VAL:HG21	1:A:345:ASN:OD1	2.20	0.42
1:A:348:SER:HB3	1:A:376:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ALA:HB2	1:A:435:PHE:CE2	2.55	0.42
2:D:35:SER:HB2	2:D:100(D):PHE:CE1	2.55	0.42
2:H:16:ALA:O	2:H:82(C):LEU:HD13	2.19	0.42
1:B:392:ASP:CG	1:B:493:SER:H	2.28	0.42
2:F:35:SER:HB2	2:F:100(D):PHE:CE1	2.55	0.42
5:O:31:THR:HA	5:O:71:PHE:HE2	1.85	0.42
1:A:31:GLU:HB2	1:A:40:VAL:HG23	2.02	0.42
1:C:31:GLU:HB2	1:C:40:VAL:HG23	2.01	0.42
2:D:16:ALA:O	2:D:82(C):LEU:HD13	2.19	0.42
1:A:156:LYS:HE3	1:B:462:GLN:HA	2.02	0.42
1:B:421:LYS:O	1:B:453:GLY:N	2.53	0.42
1:C:322:CYS:HA	1:C:333:CYS:HA	2.01	0.42
2:H:35:SER:HB2	2:H:100(D):PHE:CE1	2.55	0.41
5:O:47:LEU:HA	5:O:58:VAL:HG21	2.01	0.41
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.55	0.41
1:A:421:LYS:O	1:A:453:GLY:N	2.53	0.41
1:B:209:LYS:NZ	4:L:100(J):TYR:CE1	2.76	0.41
1:C:392:ASP:CG	1:C:493:SER:H	2.28	0.41
4:N:4:LEU:HD23	4:N:22:CYS:SG	2.61	0.41
1:A:392:ASP:CG	1:A:493:SER:H	2.28	0.41
1:B:31:GLU:HB2	1:B:40:VAL:HG23	2.02	0.41
4:L:100(F):PRO:HB3	5:M:92:TYR:CE1	2.55	0.41
2:D:80:MET:HB3	2:D:80:MET:HE3	1.77	0.41
4:L:50:MET:CE	4:L:100(I):TYR:OH	2.65	0.41
5:O:15:VAL:HG13	5:O:106:ILE:HD12	2.02	0.41
1:A:325:ASN:ND2	1:A:327:LYS:H	2.18	0.41
1:C:325:ASN:ND2	1:C:327:LYS:H	2.19	0.41
1:C:424:ALA:HB2	1:C:435:PHE:CE2	2.55	0.41
3:I:17:GLN:O	3:I:78:VAL:HG22	2.20	0.41
4:L:4:LEU:HD23	4:L:22:CYS:SG	2.61	0.41
1:A:397:THR:OG1	1:A:484:PRO:O	2.17	0.41
1:B:75:LYS:H	1:B:75:LYS:HG2	1.59	0.41
1:B:414:VAL:HG21	1:B:450:VAL:HG21	2.02	0.41
1:B:265:PRO:HB3	2:H:54:ASN:HA	2.03	0.41
1:B:325:ASN:ND2	1:B:327:LYS:H	2.19	0.41
2:H:80:MET:HB3	2:H:80:MET:HE3	1.77	0.41
4:J:23:LYS:HZ1	4:J:75:VAL:CG1	2.33	0.41
1:A:168:LYS:NZ	1:A:294:GLU:O	2.38	0.41
1:A:455:THR:OG1	1:C:369:THR:HG23	2.21	0.41
1:B:158:LEU:HD21	1:B:167:ILE:HG13	2.01	0.41
3:E:61:ARG:HD2	3:E:77:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:SER:OG	2:H:8:GLY:N	2.54	0.41
5:M:103:LYS:HE3	5:M:103:LYS:HB2	1.82	0.41
1:A:212:CYS:SG	4:J:99:VAL:HG11	2.61	0.41
1:B:77:LYS:NZ	1:B:81:GLN:OE1	2.53	0.41
1:B:205:PRO:O	1:B:209:LYS:CG	2.59	0.41
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.55	0.41
1:C:40:VAL:HA	1:C:315:LYS:O	2.21	0.41
1:C:158:LEU:HD21	1:C:167:ILE:HG13	2.01	0.41
3:G:27(D):LEU:HD12	3:G:27(D):LEU:HA	1.80	0.41
5:M:6:GLN:NE2	5:M:102:THR:HG23	2.35	0.41
5:M:30:ALA:O	5:M:31:THR:HG22	2.21	0.41
1:A:40:VAL:HA	1:A:315:LYS:O	2.21	0.41
1:A:452:VAL:O	1:A:455:THR:HG22	2.21	0.41
1:B:336:ARG:HD2	1:B:395:ILE:HG22	2.03	0.41
1:C:414:VAL:HG21	1:C:450:VAL:HG21	2.02	0.41
2:D:7:SER:OG	2:D:8:GLY:N	2.54	0.41
4:N:100(F):PRO:HB3	5:O:92:TYR:CE1	2.56	0.41
1:A:77:LYS:NZ	1:A:81:GLN:OE1	2.54	0.40
1:B:39:ALA:HB2	1:B:413:ILE:HD11	2.03	0.40
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.55	0.40
1:C:394:LYS:HB3	1:C:394:LYS:HE3	1.87	0.40
2:D:6:GLN:HB3	2:D:107:THR:OG1	2.21	0.40
4:J:4:LEU:HD23	4:J:22:CYS:SG	2.61	0.40
1:A:197:ASN:OD1	1:A:201:LYS:CE	2.69	0.40
1:A:349:VAL:HG23	1:A:377:SER:HA	2.03	0.40
1:B:452:VAL:O	1:B:455:THR:HG22	2.21	0.40
1:C:39:ALA:HB2	1:C:413:ILE:HD11	2.04	0.40
1:C:336:ARG:HD2	1:C:395:ILE:HG22	2.04	0.40
2:F:7:SER:OG	2:F:8:GLY:N	2.54	0.40
3:G:61:ARG:HD2	3:G:77:ARG:O	2.21	0.40
3:I:61:ARG:HD2	3:I:77:ARG:O	2.21	0.40
1:A:414:VAL:HG21	1:A:450:VAL:HG21	2.02	0.40
1:B:251:MET:SD	1:B:287:SER:OG	2.70	0.40
1:C:168:LYS:NZ	1:C:294:GLU:O	2.38	0.40
4:J:51:ILE:HD12	4:J:71:VAL:HB	2.04	0.40
1:A:314:TRP:CZ3	1:A:344:ASP:OD1	2.75	0.40
1:B:314:TRP:HZ3	1:B:344:ASP:OD1	2.03	0.40
1:C:197:ASN:OD1	1:C:201:LYS:CE	2.69	0.40
4:J:101:ASP:OD1	4:J:101:ASP:N	2.53	0.40
1:A:274:MET:HE2	1:A:306:TYR:HD2	1.87	0.40
1:C:159:HIS:CD2	1:C:291:ILE:HG22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:TRP:HZ3	1:C:344:ASP:OD2	2.05	0.40
2:D:96:PRO:HG2	2:D:100(A):ALA:O	2.22	0.40
5:K:38:GLN:HG3	5:K:42:LYS:O	2.22	0.40
5:K:42:LYS:HE3	5:K:43:ALA:O	2.21	0.40
5:O:42:LYS:HD2	5:O:43:ALA:H	1.86	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	445/527 (84%)	432 (97%)	13 (3%)	0	100	100
1	B	445/527 (84%)	430 (97%)	15 (3%)	0	100	100
1	C	445/527 (84%)	430 (97%)	15 (3%)	0	100	100
2	D	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
2	F	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
2	H	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
3	E	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
3	G	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
3	I	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
4	J	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
4	L	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
4	N	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
5	K	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
5	M	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
5	O	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	2718/2988 (91%)	2622 (96%)	96 (4%)	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	410/477 (86%)	394 (96%)	16 (4%)	28	60
1	B	410/477 (86%)	394 (96%)	16 (4%)	28	60
1	C	410/477 (86%)	394 (96%)	16 (4%)	28	60
2	D	96/96 (100%)	90 (94%)	6 (6%)	16	46
2	F	96/96 (100%)	90 (94%)	6 (6%)	16	46
2	H	96/96 (100%)	90 (94%)	6 (6%)	16	46
3	E	100/100 (100%)	96 (96%)	4 (4%)	28	59
3	G	100/100 (100%)	96 (96%)	4 (4%)	28	59
3	I	100/100 (100%)	96 (96%)	4 (4%)	28	59
4	J	108/108 (100%)	106 (98%)	2 (2%)	50	71
4	L	108/108 (100%)	106 (98%)	2 (2%)	50	71
4	N	108/108 (100%)	106 (98%)	2 (2%)	50	71
5	K	93/93 (100%)	93 (100%)	0	100	100
5	M	93/93 (100%)	93 (100%)	0	100	100
5	O	93/93 (100%)	92 (99%)	1 (1%)	65	77
All	All	2421/2622 (92%)	2336 (96%)	85 (4%)	32	61

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	37	CYS
1	A	50	THR
1	A	163	GLU
1	A	174	THR
1	A	218	GLU
1	A	245	THR

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	292	ILE
1	A	323	THR
1	A	337	THR
1	A	344	ASP
1	A	350	SER
1	A	369	THR
1	A	384	VAL
1	A	402	VAL
1	B	29	THR
1	B	37	CYS
1	B	50	THR
1	B	163	GLU
1	B	174	THR
1	B	218	GLU
1	B	245	THR
1	B	273	LEU
1	B	292	ILE
1	B	323	THR
1	B	337	THR
1	B	344	ASP
1	B	350	SER
1	B	369	THR
1	B	384	VAL
1	B	402	VAL
1	C	29	THR
1	C	37	CYS
1	C	50	THR
1	C	163	GLU
1	C	174	THR
1	C	218	GLU
1	C	245	THR
1	C	273	LEU
1	C	292	ILE
1	C	323	THR
1	C	337	THR
1	C	344	ASP
1	C	350	SER
1	C	369	THR
1	C	384	VAL
1	C	402	VAL
2	D	70	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	71	THR
2	D	81	GLU
2	D	86	ASP
2	D	95	ASP
2	D	101	ASP
3	E	66	GLU
3	E	69	THR
3	E	89	MET
3	E	104	VAL
2	F	70	THR
2	F	71	THR
2	F	81	GLU
2	F	86	ASP
2	F	95	ASP
2	F	101	ASP
3	G	66	GLU
3	G	69	THR
3	G	89	MET
3	G	104	VAL
2	H	70	THR
2	H	71	THR
2	H	81	GLU
2	H	86	ASP
2	H	95	ASP
2	H	101	ASP
3	I	66	GLU
3	I	69	THR
3	I	89	MET
3	I	104	VAL
4	J	23	LYS
4	J	40	THR
4	L	23	LYS
4	L	40	THR
4	N	23	LYS
4	N	40	THR
5	O	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	270	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	ASN
1	A	331	ASN
1	A	383	ASN
1	A	460	ASN
1	A	501	GLN
1	B	262	ASN
1	B	270	GLN
1	B	325	ASN
1	B	331	ASN
1	B	383	ASN
1	B	454	ASN
1	B	460	ASN
1	B	501	GLN
1	C	270	GLN
1	C	325	ASN
1	C	331	ASN
1	C	383	ASN
1	C	428	ASN
1	C	460	ASN
1	C	501	GLN
2	D	30	ASN
2	D	39	GLN
3	E	27	GLN
2	F	30	ASN
2	F	39	GLN
2	F	108	GLN
3	G	27	GLN
2	H	30	ASN
2	H	39	GLN
2	H	108	GLN
3	I	27	GLN
4	J	81	GLN
4	J	95	GLN
5	K	89	GLN
4	L	81	GLN
4	L	95	GLN
5	M	89	GLN
4	N	95	GLN
5	O	37	GLN
5	O	89	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-23520. These allow visual inspection of the internal detail of the map and identification of artifacts.

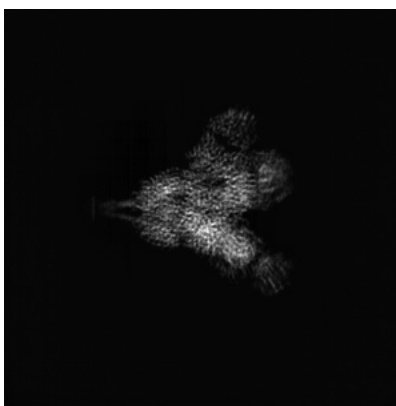
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

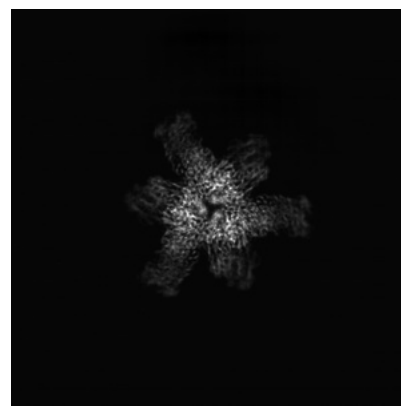
6.1.1 Primary map



X

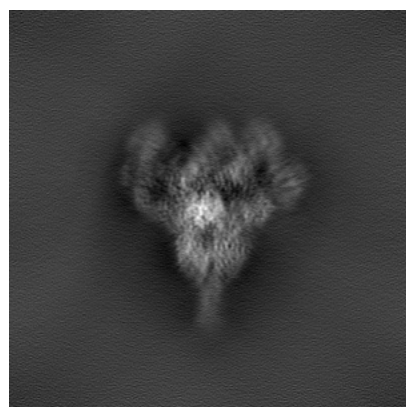


Y

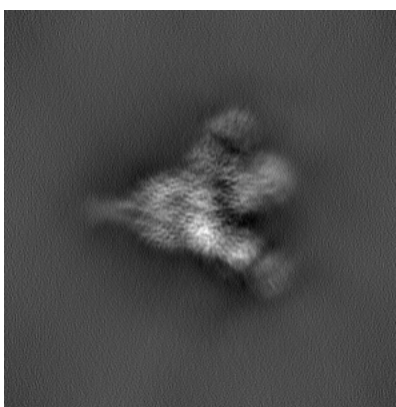


Z

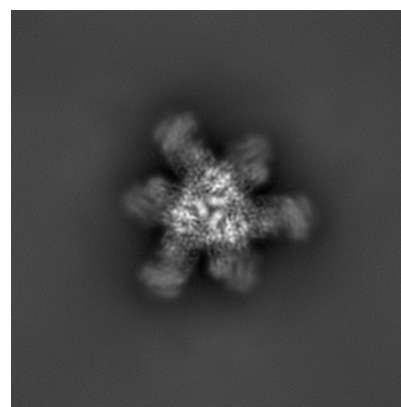
6.1.2 Raw map



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: 168

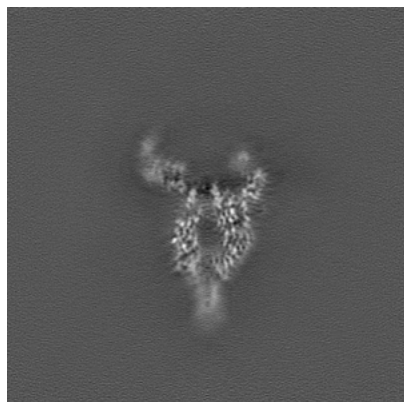


Y Index: 168

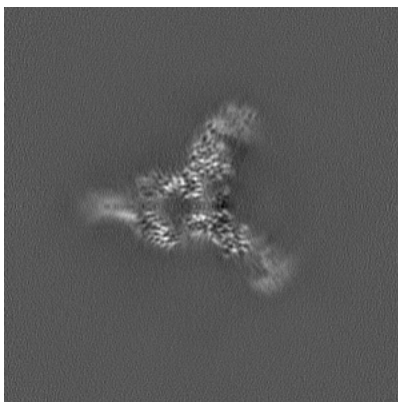


Z Index: 168

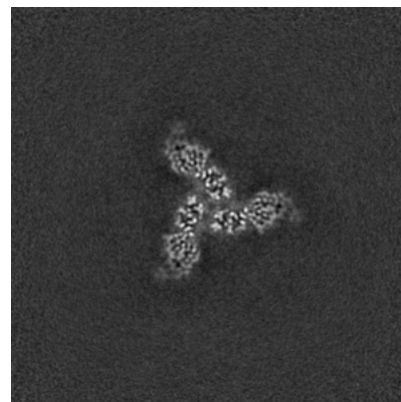
6.2.2 Raw map



X Index: 168



Y Index: 168



Z Index: 168

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: 182

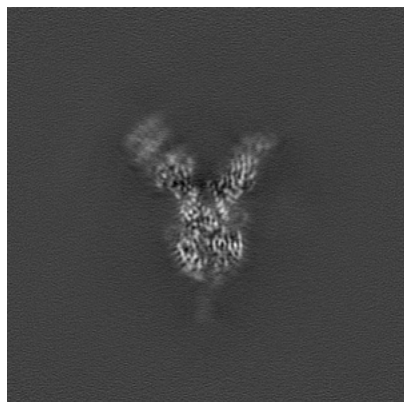


Y Index: 161

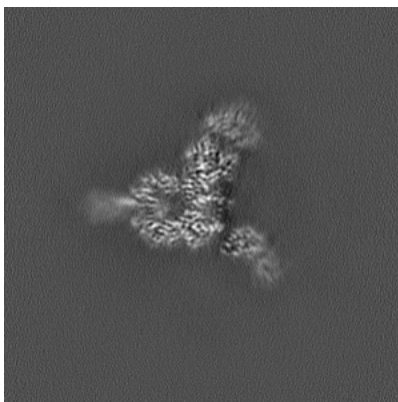


Z Index: 171

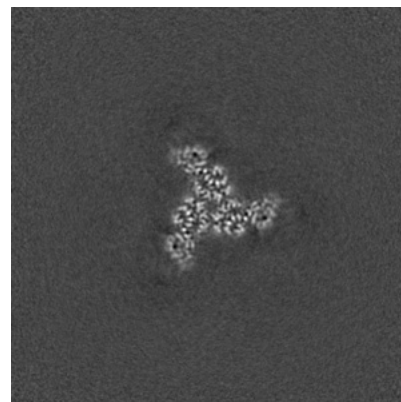
6.3.2 Raw map



X Index: 182



Y Index: 161

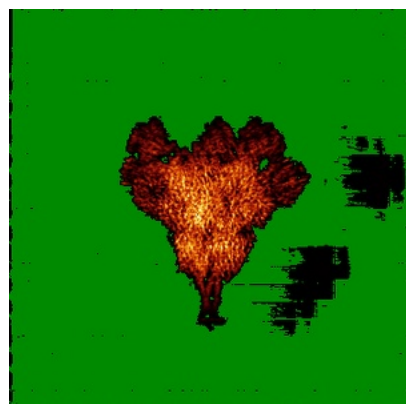


Z Index: 163

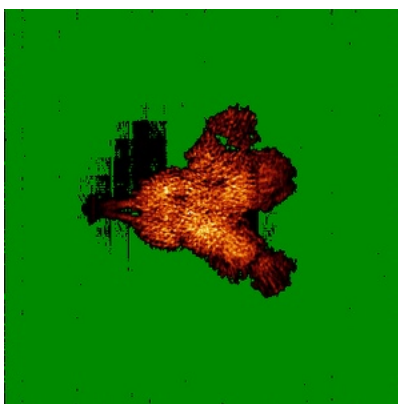
The images above show the largest variance slices of the map in three orthogonal directions.

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

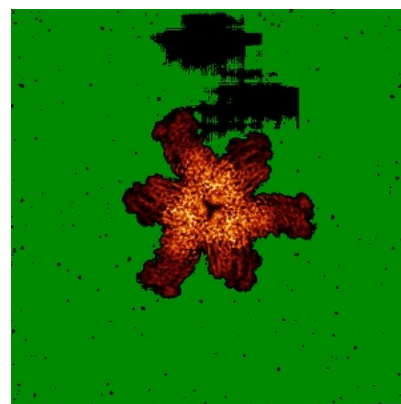
6.4.1 Primary map



X

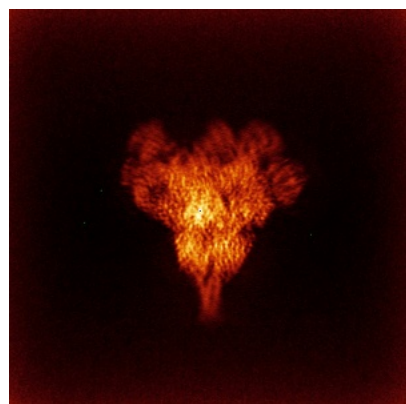


Y

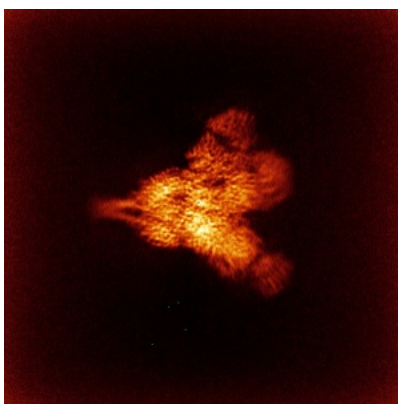


Z

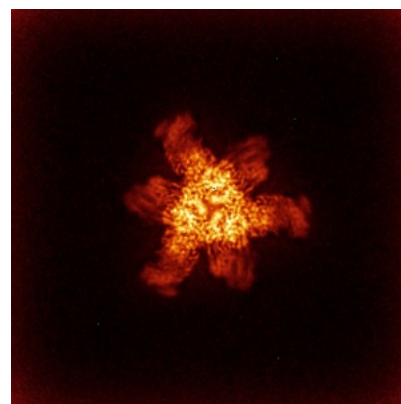
6.4.2 Raw map



X



Y

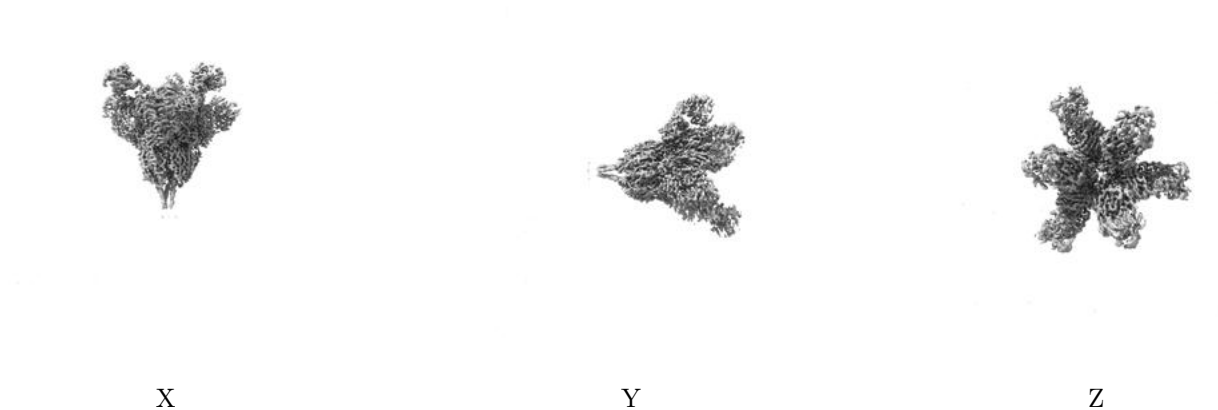


Z

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 0.127. 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.

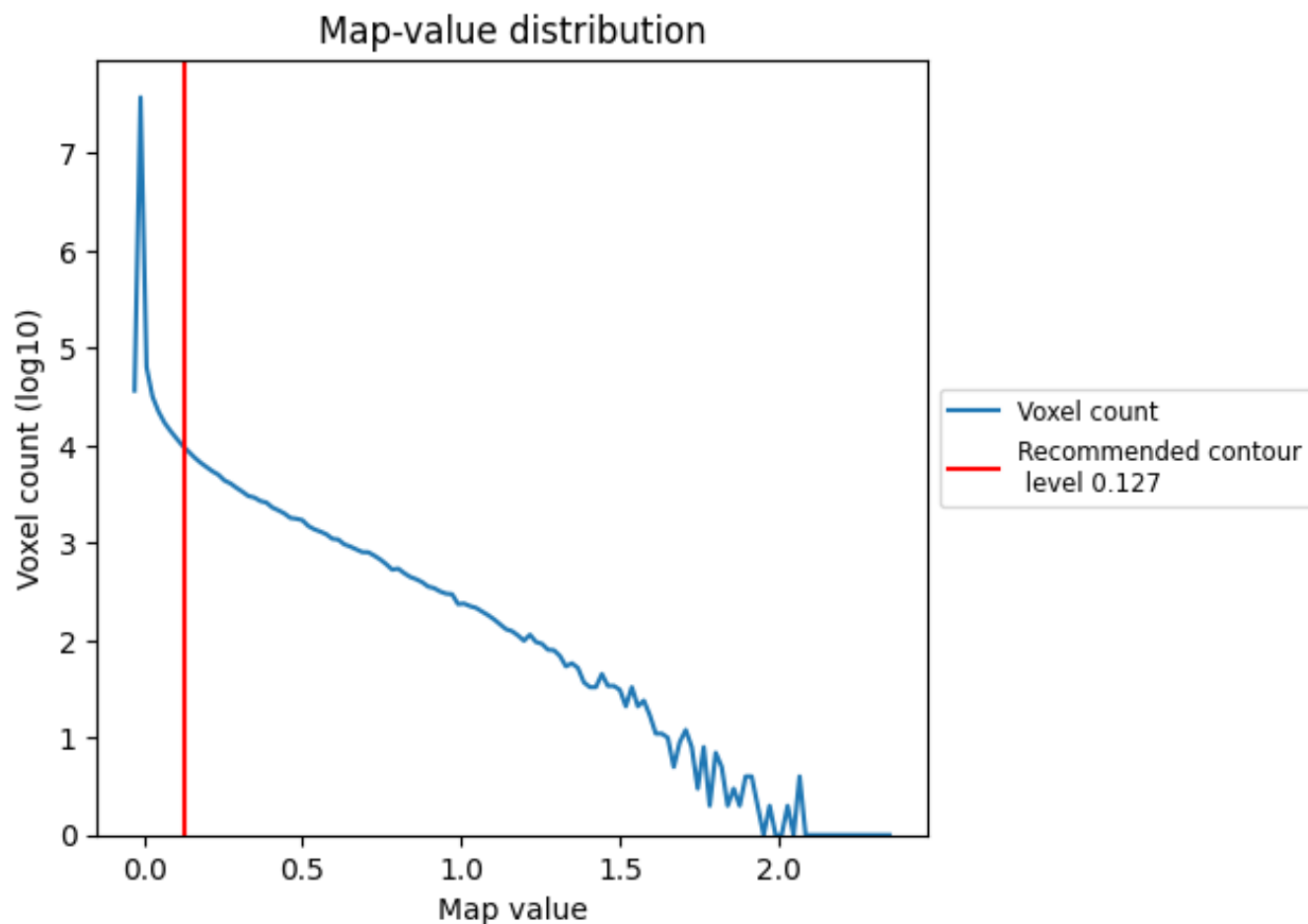
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

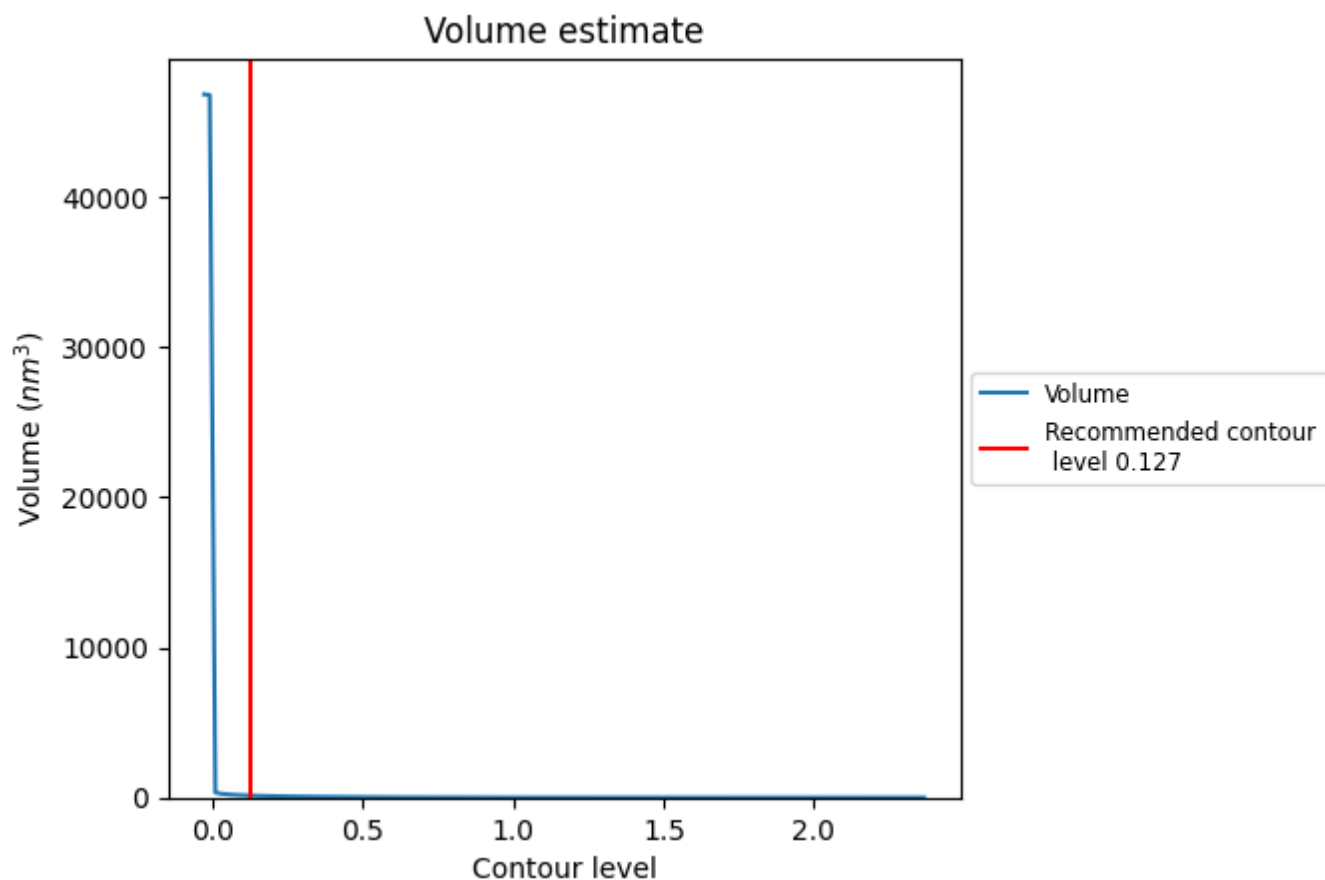
This section contains the results of statistical analysis of the map.

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.

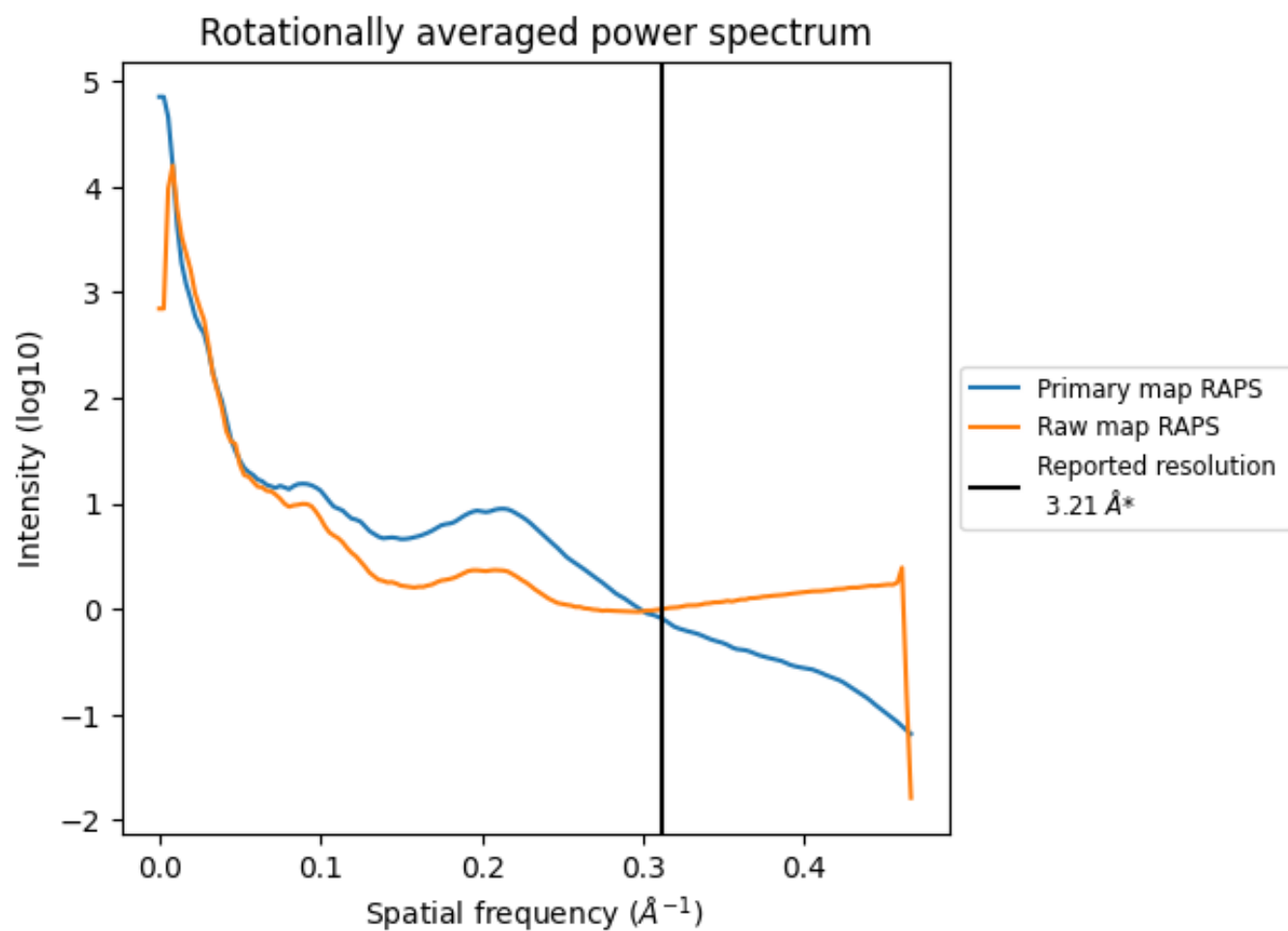
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 ⓘ

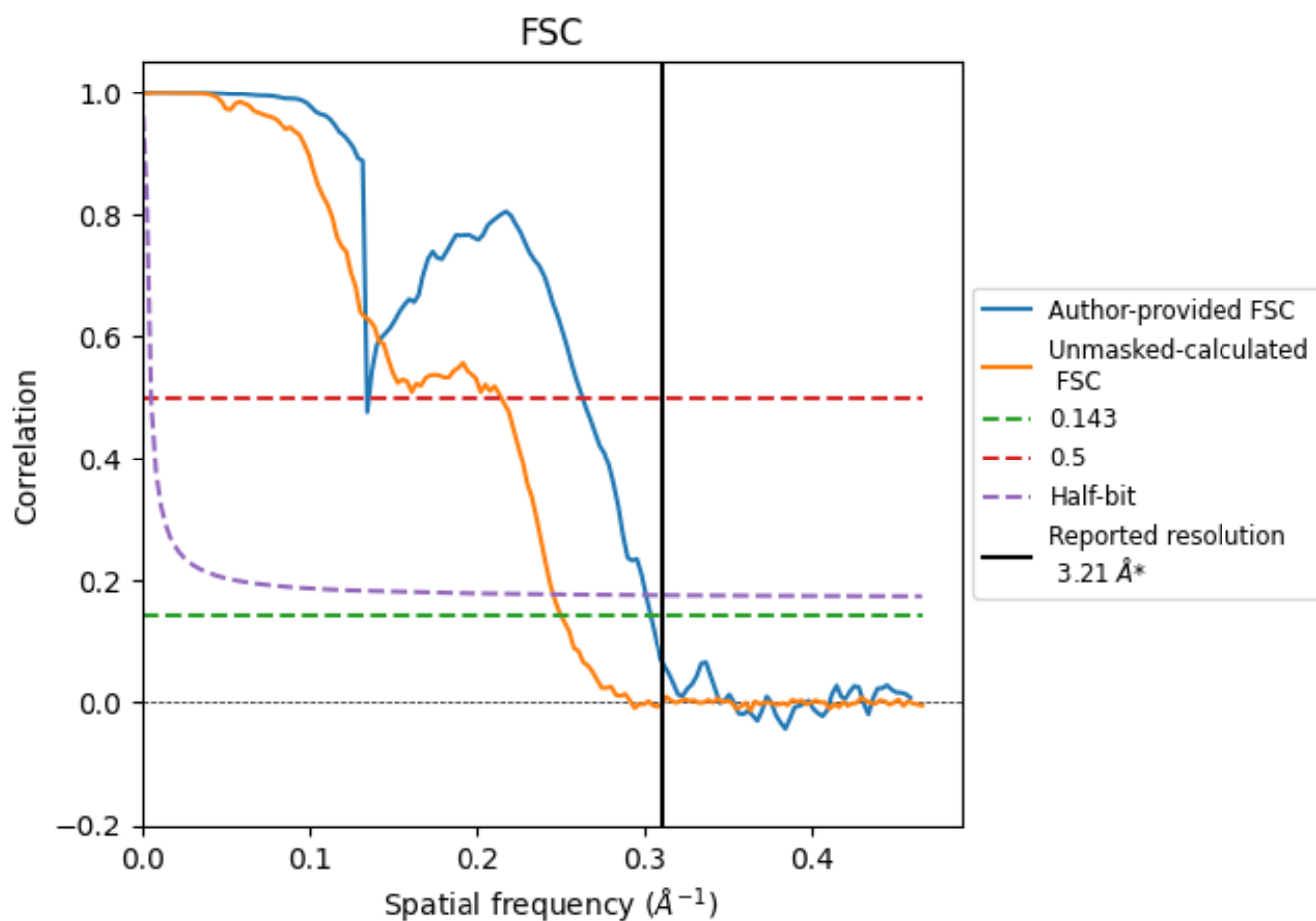


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

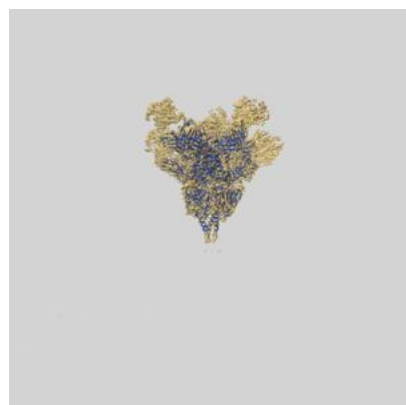
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.29	7.44	3.32
Unmasked-calculated*	3.99	4.66	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.21 by more than 10 %

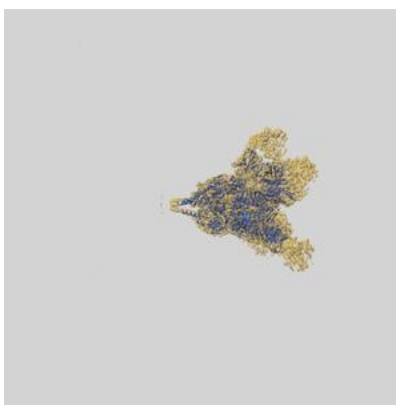
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23520 and PDB model 7LUC. Per-residue inclusion information can be found in section 3 on page 9.

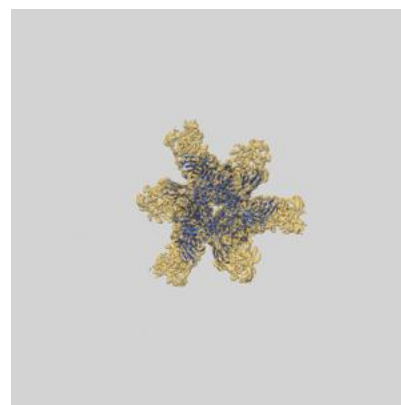
9.1 Map-model overlay [i](#)



X



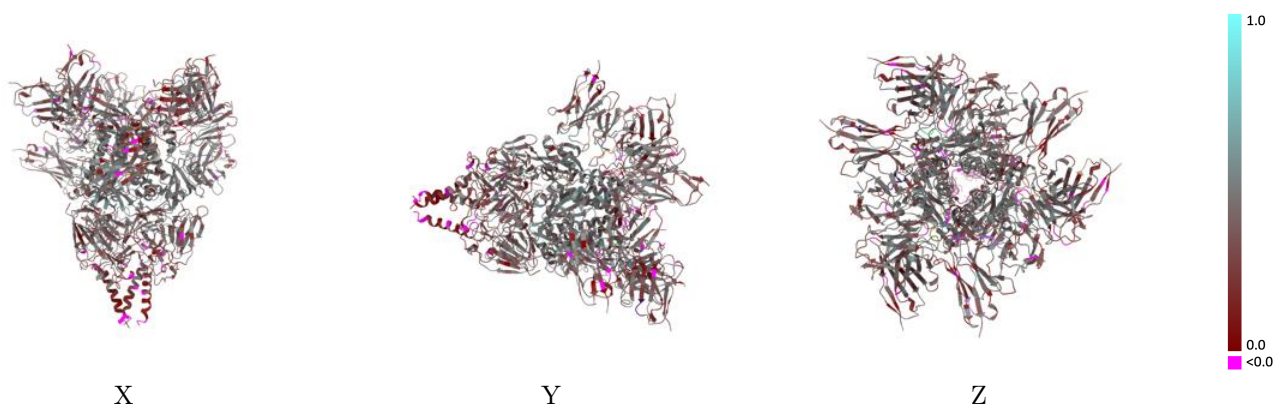
Y



Z

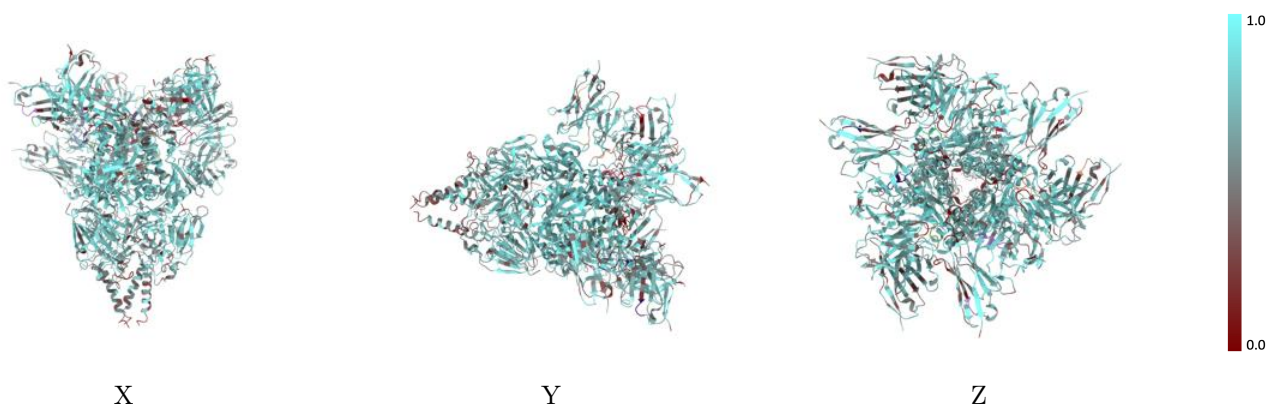
The images above show the 3D surface view of the map at the recommended contour level 0.127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



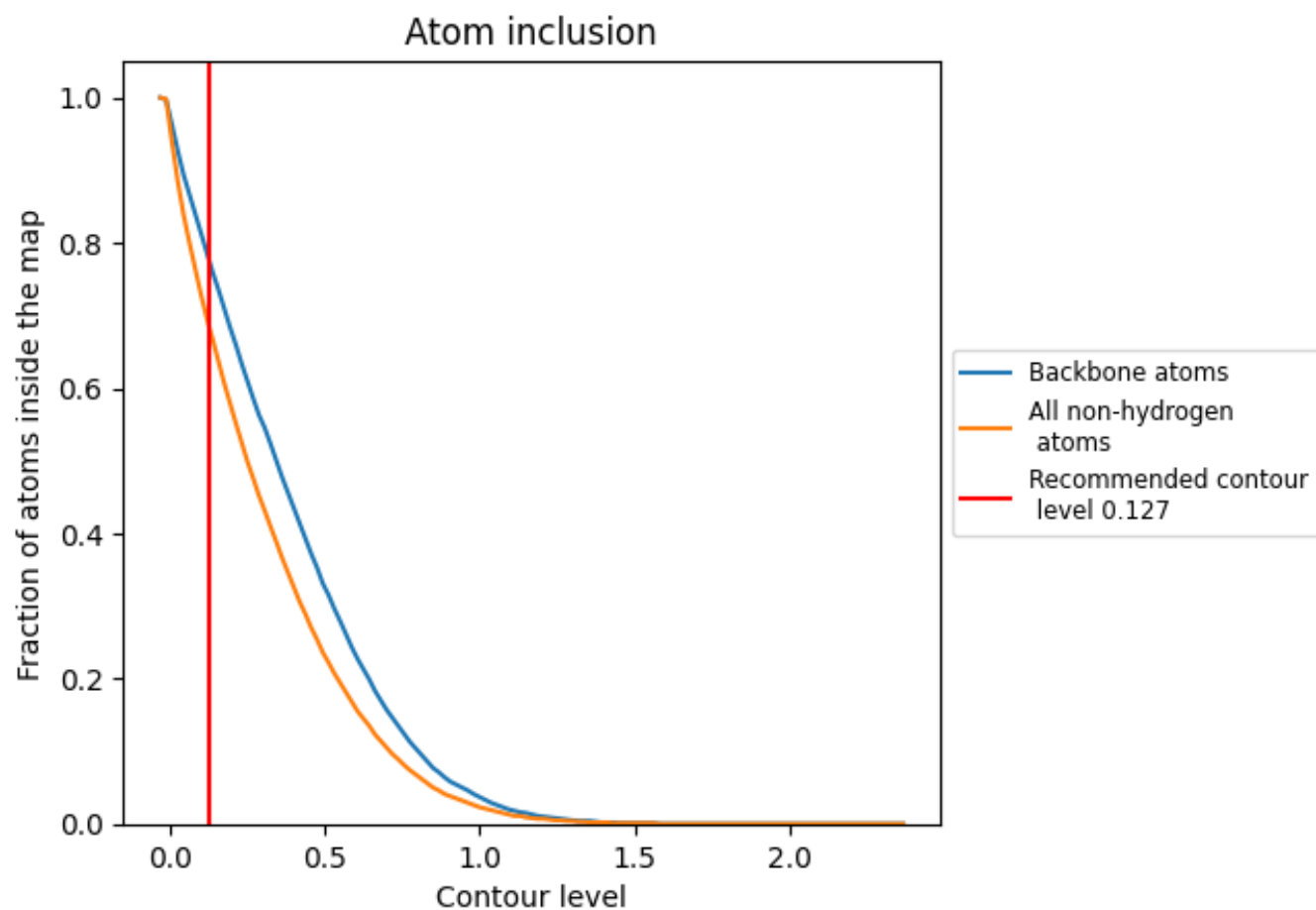
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.127).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.3750
A	0.7010	0.3810
B	0.6960	0.3790
C	0.6920	0.3790
D	0.6900	0.3660
E	0.6920	0.3800
F	0.6880	0.3740
G	0.7020	0.3780
H	0.6660	0.3660
I	0.6850	0.3850
J	0.6480	0.3430
K	0.7020	0.3880
L	0.6530	0.3460
M	0.6950	0.3850
N	0.6340	0.3490
O	0.6860	0.3860

1.0

0.0

<0.0