



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 7XST / pdb_00007xst
EMDB ID : EMD-33434
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike glycoprotein in complex with three F61 Fab and three D2 Fab
Authors : Wang, X.; Li, X.
Deposited on : 2022-05-15
Resolution : 3.04 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

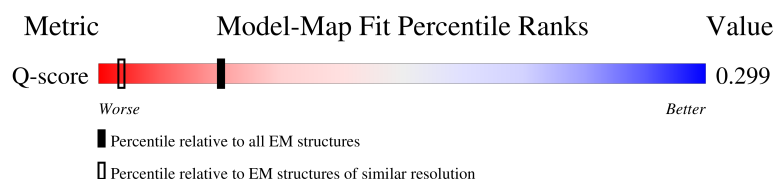
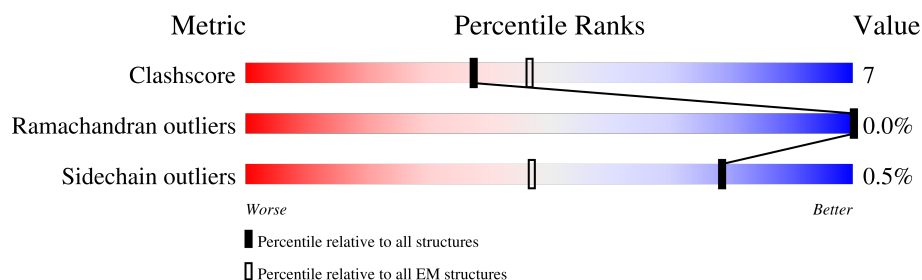
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

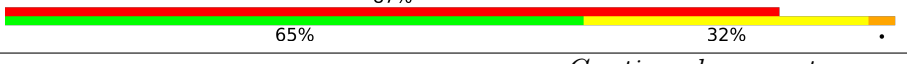
The reported resolution of this entry is 3.04 Å.

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	13952 (2.54 - 3.54)

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	1210	
1	B	1210	
1	C	1210	
2	D	117	

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Mol	Chain	Length	Quality of chain
2	H	117	100% 70% 27% .
2	L	117	100% 68% 31% .
3	E	110	83% 83% 15% .
3	I	110	100% 85% 14% .
3	M	110	100% 81% 18% .
4	F	123	37% 87% 13%
4	J	123	89% 84% 16%
4	N	123	99% 87% 13%
5	G	110	37% 86% 13% .
5	K	110	98% 86% 13% .
5	O	110	100% 89% 10% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33532 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total	C	N	O	S	0	0
			7633	4881	1273	1445	34		
1	B	1009	Total	C	N	O	S	0	0
			7611	4869	1271	1437	34		
1	C	1008	Total	C	N	O	S	0	0
			7638	4894	1275	1435	34		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	conflict	UNP P0DTC2
A	210D	GLU	LEU	conflict	UNP P0DTC2
A	210E	PRO	VAL	conflict	UNP P0DTC2
A	210F	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	conflict	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	conflict	UNP P0DTC2
B	210D	GLU	LEU	conflict	UNP P0DTC2
B	210E	PRO	VAL	conflict	UNP P0DTC2
B	210F	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	conflict	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	210C	ARG	ASN	conflict	UNP P0DTC2
C	210D	GLU	LEU	conflict	UNP P0DTC2
C	210E	PRO	VAL	conflict	UNP P0DTC2
C	210F	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	981	PHE	LEU	conflict	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called F61 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	117	Total	C	N	O	S	0	0
			874	545	151	174	4		
2	H	117	Total	C	N	O	S	0	0
			872	543	151	174	4		
2	D	117	Total	C	N	O	S	0	0
			874	545	151	174	4		

- Molecule 3 is a protein called F61 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	110	Total	C	N	O	S	0	0
			803	500	135	166	2		
3	I	110	Total	C	N	O	S	0	0
			803	500	135	166	2		
3	E	110	Total	C	N	O	S	0	0
			803	500	135	166	2		

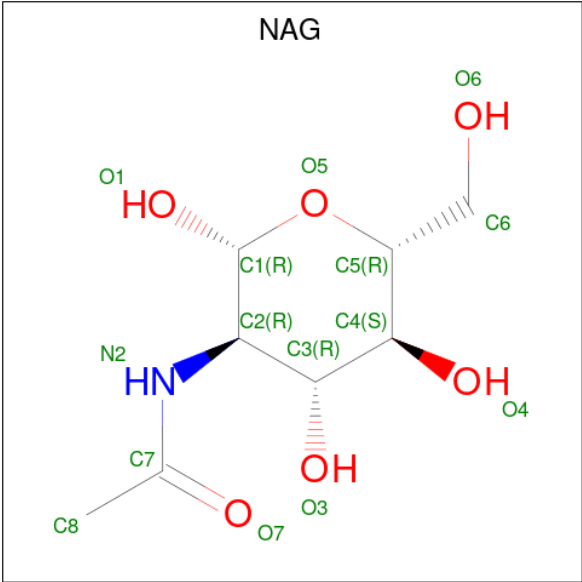
- Molecule 4 is a protein called D2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	123	Total	C	N	O	S	0	0
			943	594	157	188	4		
4	J	123	Total	C	N	O	S	0	0
			943	594	157	188	4		
4	F	123	Total	C	N	O	S	0	0
			943	594	157	188	4		

- Molecule 5 is a protein called D2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	110	Total	C	N	O	S	0	0
			786	490	131	163	2		
5	K	110	Total	C	N	O	S	0	0
			786	490	131	163	2		
5	G	110	Total	C	N	O	S	0	0
			786	490	131	163	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

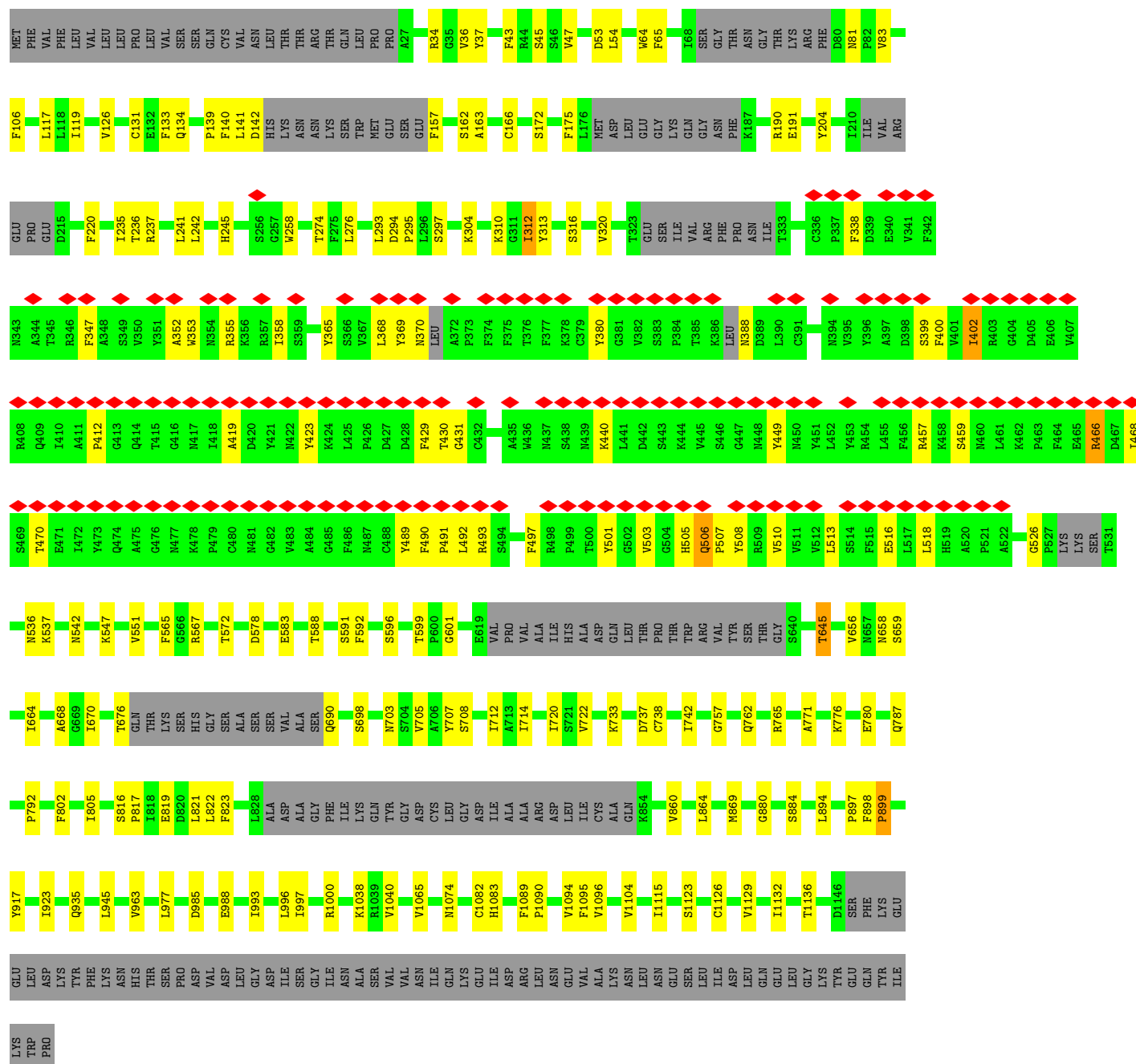
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

GLN
GLU
LEU
GLY
LEU
LYS
TYR
GLU
GLN
TYR
ILE
LYS
TRP
PRO

• Molecule 1: Spike glycoprotein

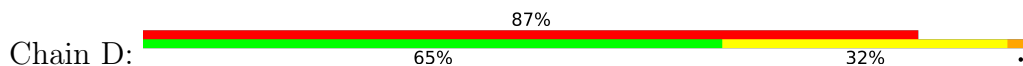


• Molecule 1: Spike glycoprotein

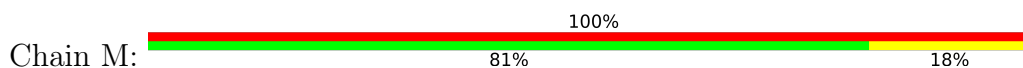




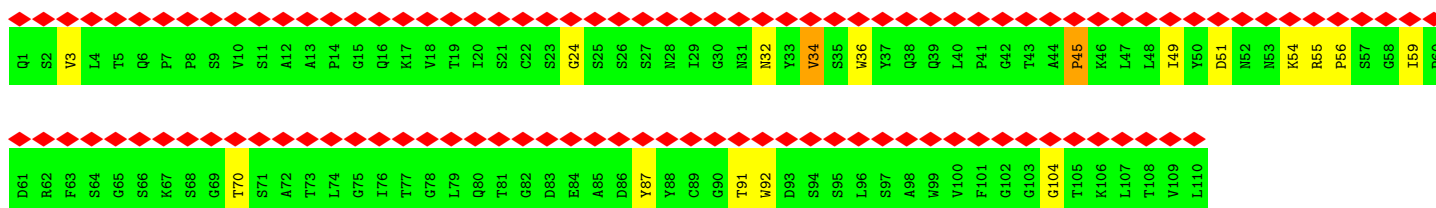
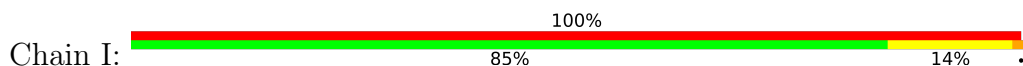
• Molecule 2: F61 heavy chain



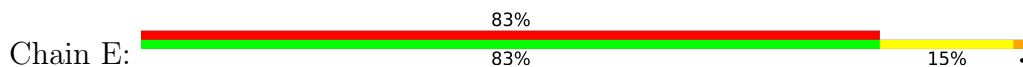
• Molecule 3: F61 light chain

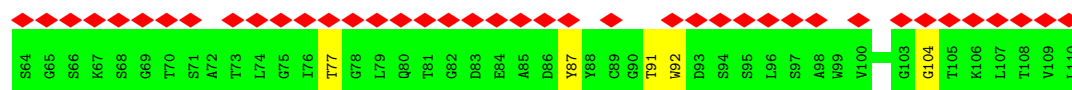


• Molecule 3: F61 light chain

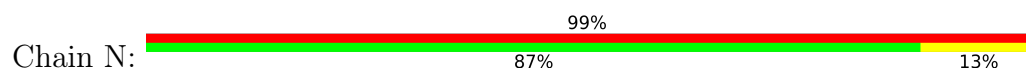


• Molecule 3: F61 light chain

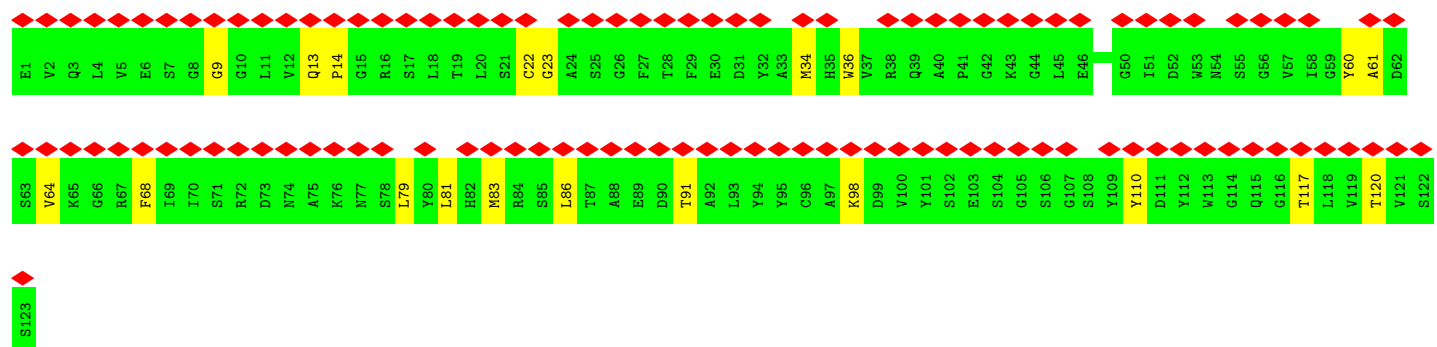
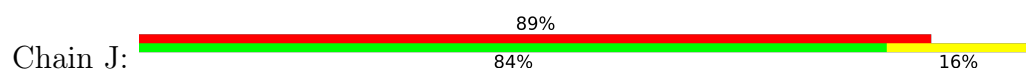




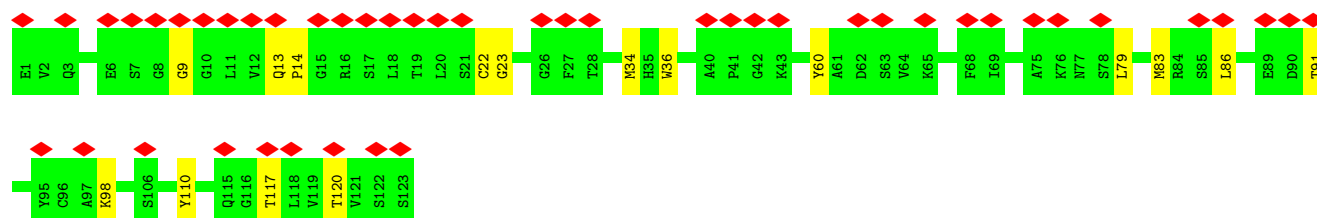
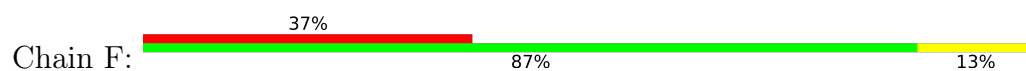
• Molecule 4: D2 heavy chain



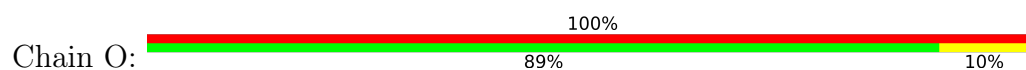
• Molecule 4: D2 heavy chain

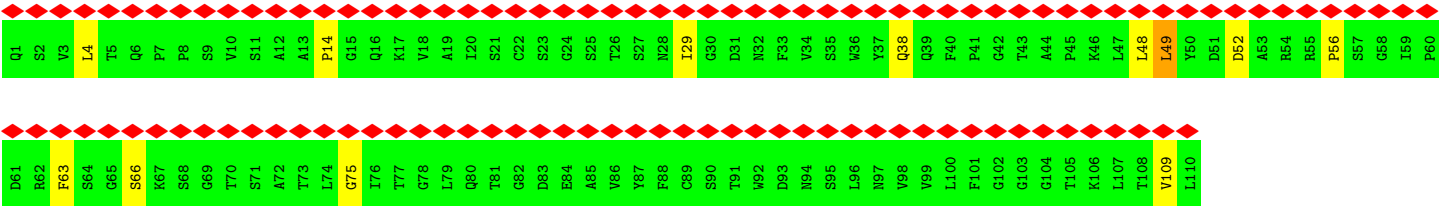


• Molecule 4: D2 heavy chain

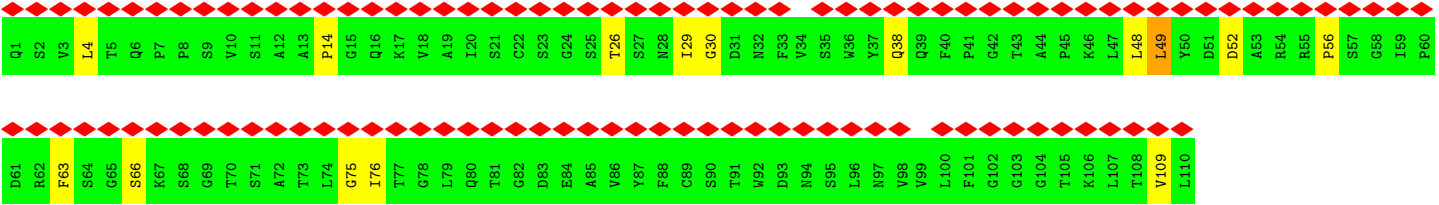
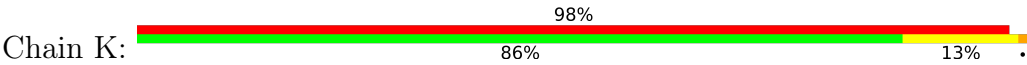


• Molecule 5: D2 light chain

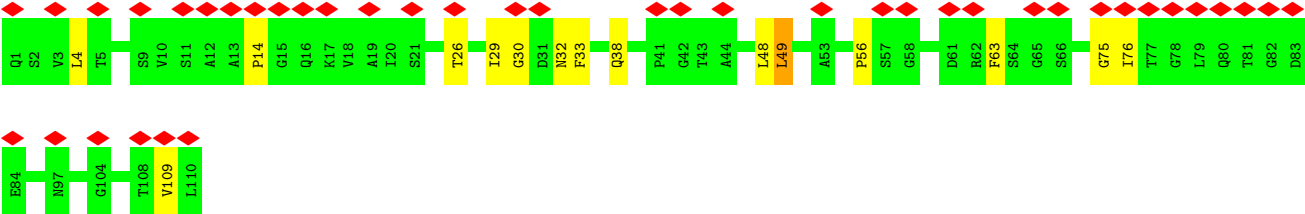
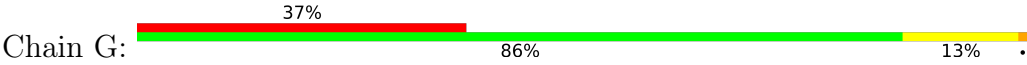




● Molecule 5: D2 light chain



● Molecule 5: D2 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	670525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.291	Depositor
Minimum map value	-2.646	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.173	Depositor
Map size ($\text{\AA}$)	329.80002, 329.80002, 329.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.97, 0.97, 0.97	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	10/7812 (0.1%)	0.73	14/10664 (0.1%)
1	B	0.52	9/7789 (0.1%)	0.77	22/10633 (0.2%)
1	C	0.56	7/7817 (0.1%)	0.74	14/10665 (0.1%)
2	D	0.75	1/891 (0.1%)	1.27	12/1208 (1.0%)
2	H	0.75	1/889 (0.1%)	1.27	12/1205 (1.0%)
2	L	0.75	1/891 (0.1%)	1.27	12/1208 (1.0%)
3	E	0.45	0/822	0.70	1/1120 (0.1%)
3	I	0.45	0/822	0.69	1/1120 (0.1%)
3	M	0.84	1/822 (0.1%)	0.71	2/1120 (0.2%)
4	F	0.46	0/966	0.67	0/1308
4	J	0.46	0/966	0.67	0/1308
4	N	0.45	0/966	0.67	0/1308
5	G	0.56	0/803	0.90	5/1097 (0.5%)
5	K	0.56	0/803	0.89	5/1097 (0.5%)
5	O	0.56	0/803	0.89	5/1097 (0.5%)
All	All	0.56	30/33862 (0.1%)	0.80	105/46158 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	H	0	1
2	L	0	1
All	All	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	45	PRO	N-CD	-20.40	1.19	1.47
1	C	897	PRO	N-CD	-12.80	1.29	1.47
1	C	899	PRO	N-CD	-12.25	1.30	1.47
1	B	897	PRO	C-O	-10.05	1.12	1.23
1	C	897	PRO	C-O	-9.14	1.13	1.23
1	A	897	PRO	C-O	-8.86	1.12	1.23
1	C	295	PRO	N-CD	-8.25	1.36	1.47
1	A	816	SER	CA-CB	-7.94	1.42	1.53
1	B	899	PRO	C-O	-6.49	1.15	1.24
1	B	316	SER	CA-CB	-6.48	1.46	1.54
1	A	1123	SER	CA-CB	-6.01	1.43	1.53
1	B	816	SER	CA-CB	-5.91	1.44	1.53
1	B	295	PRO	C-O	-5.80	1.17	1.24
1	A	878	LEU	C-O	-5.74	1.16	1.24
1	A	295	PRO	C-O	-5.69	1.17	1.24
1	B	817	PRO	C-O	-5.68	1.16	1.24
1	A	899	PRO	C-O	-5.62	1.16	1.24
1	C	295	PRO	C-O	-5.61	1.17	1.24
1	B	313	TYR	C-O	-5.48	1.17	1.24
1	B	297	SER	CA-CB	-5.39	1.44	1.53
1	B	402	ILE	C-O	-5.30	1.18	1.24
1	A	402	ILE	C-O	-5.28	1.18	1.24
1	C	402	ILE	C-O	-5.26	1.18	1.24
1	A	884	SER	CA-CB	-5.23	1.44	1.53
2	L	49	SER	CA-CB	-5.16	1.45	1.53
2	D	49	SER	CA-CB	-5.13	1.45	1.53
2	H	49	SER	CA-CB	-5.10	1.45	1.53
1	A	1089	PHE	C-O	-5.08	1.17	1.24
1	A	1121	PHE	C-O	-5.05	1.18	1.24
1	C	894	LEU	C-O	-5.02	1.18	1.24

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1121	PHE	CA-CB-CG	10.38	124.18	113.80
1	C	599	THR	CB-CA-C	-9.20	97.01	109.42
1	A	322	PRO	CB-CA-C	-8.53	101.13	111.11
1	B	503	VAL	N-CA-C	-7.88	104.89	112.29
1	C	503	VAL	N-CA-C	-7.87	104.89	112.29
1	A	503	VAL	N-CA-C	-7.85	104.91	112.29
1	B	897	PRO	N-CA-CB	-7.85	96.33	103.31
5	O	56	PRO	CB-CA-C	-7.69	100.88	110.95
5	G	56	PRO	CB-CA-C	-7.63	100.95	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	56	PRO	CB-CA-C	-7.62	100.96	110.95
1	C	897	PRO	N-CA-CB	-7.60	96.55	103.31
1	C	234	ASN	CB-CA-C	-6.84	99.52	110.81
1	A	569	ILE	CA-C-O	-6.62	113.45	121.13
1	B	899	PRO	N-CA-CB	-6.58	97.27	103.52
1	B	708	SER	N-CA-C	-6.57	98.68	108.99
3	I	45	PRO	N-CA-CB	-6.54	97.49	103.25
3	E	45	PRO	N-CA-CB	-6.54	97.50	103.25
3	M	45	PRO	N-CA-CB	-6.53	97.51	103.25
1	A	41	LYS	CB-CA-C	-6.48	102.53	111.73
1	B	817	PRO	CA-C-N	6.34	130.69	120.55
1	B	817	PRO	C-N-CA	6.34	130.69	120.55
1	B	703	ASN	N-CA-C	-6.25	99.62	109.50
1	B	312	ILE	N-CA-C	-6.21	99.64	108.58
1	B	737	ASP	CB-CA-C	-6.19	100.43	110.77
2	L	33	TYR	CB-CA-C	-6.15	101.33	110.67
2	H	33	TYR	CB-CA-C	-6.14	101.33	110.67
2	D	33	TYR	CB-CA-C	-6.13	101.35	110.67
1	C	899	PRO	N-CA-CB	-6.12	97.71	103.52
2	D	37	VAL	CA-C-O	-5.74	115.64	121.67
2	L	37	VAL	CA-C-O	-5.73	115.65	121.67
2	L	103	TYR	O-C-N	-5.72	117.07	123.48
2	D	103	TYR	O-C-N	-5.72	117.07	123.48
3	M	45	PRO	CA-N-CD	5.72	120.00	112.00
2	H	37	VAL	CA-C-O	-5.68	115.70	121.67
1	A	569	ILE	N-CA-C	-5.67	101.71	109.37
1	B	313	TYR	CB-CA-C	-5.66	99.46	109.70
2	H	103	TYR	O-C-N	-5.64	117.16	123.48
2	H	33	TYR	CA-C-O	-5.58	113.98	120.62
5	G	38	GLN	CB-CA-C	-5.58	99.51	109.71
1	C	466	ARG	CA-C-N	-5.57	115.15	123.00
1	C	466	ARG	C-N-CA	-5.57	115.15	123.00
2	L	33	TYR	CA-C-O	-5.57	114.00	120.62
2	D	33	TYR	CA-C-O	-5.56	114.00	120.62
5	O	38	GLN	CB-CA-C	-5.55	99.56	109.71
1	B	1074	ASN	CA-C-O	-5.54	114.83	120.71
1	B	466	ARG	CA-C-N	-5.54	115.19	123.00
1	B	466	ARG	C-N-CA	-5.54	115.19	123.00
5	K	38	GLN	CB-CA-C	-5.53	99.59	109.71
5	K	49	LEU	CA-C-N	5.53	132.10	121.54
5	K	49	LEU	C-N-CA	5.53	132.10	121.54
1	A	466	ARG	CA-C-N	-5.52	115.22	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	ARG	C-N-CA	-5.52	115.22	123.00
1	A	901	GLN	CA-C-O	-5.52	113.14	119.60
1	C	506	GLN	CB-CA-C	5.52	117.13	108.63
5	G	49	LEU	CA-C-N	5.52	132.07	121.54
5	G	49	LEU	C-N-CA	5.52	132.07	121.54
1	A	506	GLN	CB-CA-C	5.51	117.12	108.63
5	O	49	LEU	CA-C-N	5.50	132.05	121.54
5	O	49	LEU	C-N-CA	5.50	132.05	121.54
1	B	860	VAL	CA-C-N	5.50	131.38	120.94
1	B	860	VAL	C-N-CA	5.50	131.38	120.94
1	C	310	LYS	CB-CA-C	-5.47	102.45	110.06
1	B	506	GLN	CB-CA-C	5.47	117.06	108.63
1	C	897	PRO	CA-N-CD	5.47	119.66	112.00
1	B	738	CYS	N-CA-CB	-5.44	102.12	110.01
2	H	49	SER	N-CA-C	5.44	117.35	108.76
2	D	49	SER	N-CA-C	5.43	117.34	108.76
2	L	105	ASP	N-CA-C	5.41	116.98	111.14
2	L	49	SER	N-CA-C	5.40	117.30	108.76
2	D	105	ASP	N-CA-C	5.39	116.96	111.14
1	B	468	ILE	N-CA-C	-5.38	105.48	113.39
1	A	468	ILE	N-CA-C	-5.37	105.49	113.39
2	H	105	ASP	N-CA-C	5.36	116.93	111.14
2	L	38	ARG	CB-CA-C	-5.35	98.31	110.07
2	D	38	ARG	CB-CA-C	-5.34	98.31	110.07
2	H	38	ARG	CB-CA-C	-5.34	98.32	110.07
1	C	468	ILE	N-CA-C	-5.34	105.54	113.39
1	C	296	LEU	N-CA-C	-5.33	105.39	111.14
1	C	796	TYR	CB-CA-C	-5.28	102.24	110.74
1	B	645	THR	N-CA-CB	-5.19	102.96	110.70
2	H	91	ALA	N-CA-C	5.14	116.11	108.60
1	C	897	PRO	CA-C-O	-5.13	115.49	121.34
1	A	1089	PHE	CA-CB-CG	5.12	118.92	113.80
2	L	91	ALA	N-CA-C	5.12	116.07	108.60
2	D	91	ALA	N-CA-C	5.11	116.06	108.60
1	A	40	ASP	N-CA-C	5.09	121.24	113.19
2	D	97	ARG	CA-C-N	-5.09	115.63	122.86
2	D	97	ARG	C-N-CA	-5.09	115.63	122.86
2	D	20	LEU	CA-C-N	-5.07	114.72	122.62
2	D	20	LEU	C-N-CA	-5.07	114.72	122.62
2	H	97	ARG	CA-C-N	-5.06	115.67	122.86
2	H	97	ARG	C-N-CA	-5.06	115.67	122.86
5	G	49	LEU	CA-C-O	-5.05	115.69	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	897	PRO	CA-C-O	-5.05	115.58	121.34
1	B	565	PHE	CB-CA-C	-5.05	101.92	113.33
2	L	20	LEU	CA-C-N	-5.04	114.76	122.62
2	L	20	LEU	C-N-CA	-5.04	114.76	122.62
2	L	97	ARG	CA-C-N	-5.04	115.70	122.86
2	L	97	ARG	C-N-CA	-5.04	115.70	122.86
5	K	49	LEU	CA-C-O	-5.03	115.71	120.94
5	O	49	LEU	CA-C-O	-5.03	115.71	120.94
1	B	757	GLY	N-CA-C	5.02	116.29	111.67
2	H	20	LEU	CA-C-N	-5.01	114.80	122.62
2	H	20	LEU	C-N-CA	-5.01	114.80	122.62
1	A	33	THR	N-CA-C	-5.00	105.24	113.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	103	TYR	Mainchain
2	H	103	TYR	Mainchain
2	L	103	TYR	Mainchain

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	7633	0	7162	124	0
1	B	7611	0	7143	124	0
1	C	7638	0	7218	116	0
2	D	874	0	810	30	0
2	H	872	0	803	25	0
2	L	874	0	810	29	0
3	E	803	0	766	10	0
3	I	803	0	766	9	0
3	M	803	0	766	13	0
4	F	943	0	882	9	0
4	J	943	0	882	11	0
4	N	943	0	882	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	786	0	742	6	0
5	K	786	0	742	6	0
5	O	786	0	742	5	0
6	A	140	0	130	0	0
6	B	140	0	130	0	0
6	C	154	0	143	1	0
All	All	33532	0	31519	486	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 7.

All (486) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ARG:HG2	2:H:106:PHE:H	1.46	0.81
2:L:97:ARG:HG2	2:L:106:PHE:H	1.46	0.80
2:D:97:ARG:HG2	2:D:106:PHE:H	1.46	0.79
1:B:353:TRP:HZ3	1:B:355:ARG:HE	1.34	0.74
2:H:97:ARG:O	2:H:97:ARG:HG3	1.89	0.73
3:M:34:VAL:HG12	3:M:52:ASN:OD1	1.88	0.73
2:D:97:ARG:HG3	2:D:97:ARG:O	1.89	0.72
2:L:97:ARG:O	2:L:97:ARG:HG3	1.89	0.72
1:C:898:PHE:N	1:C:899:PRO:HD2	2.10	0.66
1:A:898:PHE:CD2	1:A:901:GLN:NE2	2.64	0.66
1:A:898:PHE:CE2	1:A:901:GLN:NE2	2.64	0.65
1:A:798:GLY:HA3	1:A:899:PRO:HG3	1.79	0.64
1:C:716:THR:HG21	1:C:1073:LYS:HE2	1.80	0.64
1:A:900:MET:HG2	1:A:900:MET:O	1.97	0.64
2:D:97:ARG:HG2	2:D:106:PHE:N	2.13	0.63
2:H:97:ARG:HG2	2:H:106:PHE:N	2.13	0.62
1:B:712:ILE:HG13	1:C:896:ILE:HG22	1.82	0.62
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.83	0.61
2:L:97:ARG:HG2	2:L:106:PHE:N	2.13	0.60
2:H:97:ARG:O	2:H:97:ARG:CG	2.49	0.60
2:L:97:ARG:O	2:L:97:ARG:CG	2.49	0.60
1:B:1089:PHE:HB3	1:C:913:GLN:HE21	1.67	0.60
1:A:742:ILE:O	1:A:1000:ARG:NH2	2.35	0.60
1:A:566:GLY:HA2	1:B:43:PHE:O	2.01	0.60
1:B:742:ILE:HG22	1:B:997:ILE:HD12	1.85	0.59
1:B:1090:PRO:HD2	1:C:913:GLN:NE2	2.17	0.59
1:B:312:ILE:O	1:B:312:ILE:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:97:ARG:CG	2:L:106:PHE:H	2.16	0.59
2:D:97:ARG:O	2:D:97:ARG:CG	2.49	0.59
1:C:930:ALA:O	1:C:934:ILE:HG12	2.03	0.59
1:B:707:TYR:HB2	1:C:883:THR:HG23	1.85	0.59
1:B:1090:PRO:HD2	1:C:913:GLN:HE22	1.67	0.59
4:N:13:GLN:HB3	4:N:14:PRO:HD2	1.85	0.58
2:H:97:ARG:CG	2:H:106:PHE:H	2.15	0.58
1:A:894:LEU:CD2	1:C:1072:GLU:HB3	2.34	0.58
1:A:894:LEU:HD21	1:C:1072:GLU:HB3	1.85	0.58
1:B:320:VAL:CG2	1:B:591:SER:OG	2.51	0.58
1:B:592:PHE:HZ	1:C:855:PHE:HB2	1.69	0.58
1:A:369:TYR:O	1:A:370:ASN:C	2.46	0.58
2:D:97:ARG:CG	2:D:106:PHE:H	2.16	0.58
4:F:13:GLN:HB3	4:F:14:PRO:HD2	1.85	0.57
1:A:543:PHE:HD2	1:A:576:VAL:HG11	1.68	0.57
1:B:369:TYR:O	1:B:370:ASN:C	2.46	0.57
2:D:43:LYS:HG3	2:D:44:GLY:H	1.69	0.57
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.85	0.57
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.86	0.57
1:C:352:ALA:HB1	1:C:466:ARG:HH21	1.70	0.57
1:A:317:ASN:ND2	1:A:319:ARG:HD3	2.20	0.57
1:C:276:LEU:HD11	1:C:304:LYS:HA	1.86	0.57
2:L:75:LYS:HE2	2:D:15:GLY:HA3	1.86	0.57
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.85	0.57
1:C:106:PHE:HB3	1:C:235:ILE:CG2	2.35	0.57
1:C:369:TYR:O	1:C:370:ASN:C	2.46	0.57
1:B:1104:VAL:HG13	1:B:1115:ILE:HD13	1.87	0.56
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.86	0.56
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.88	0.56
2:L:43:LYS:HG3	2:L:44:GLY:H	1.69	0.56
2:H:43:LYS:HG3	2:H:44:GLY:H	1.69	0.56
4:J:13:GLN:HB3	4:J:14:PRO:HD2	1.85	0.56
1:A:352:ALA:HB1	1:A:466:ARG:HH21	1.70	0.56
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.87	0.56
1:B:352:ALA:HB1	1:B:466:ARG:HH21	1.70	0.56
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.88	0.56
1:B:320:VAL:HG23	1:B:591:SER:OG	2.06	0.55
1:B:131:CYS:HB3	1:B:166:CYS:HA	1.88	0.55
1:B:542:ASN:HD22	1:B:547:LYS:HD3	1.71	0.55
1:C:599:THR:HG22	1:C:601:GLY:H	1.70	0.55
1:B:712:ILE:CG1	1:C:896:ILE:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.07	0.55
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.89	0.55
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.89	0.55
1:B:64:TRP:HD1	1:B:65:PHE:N	2.04	0.55
3:I:32:ASN:ND2	3:I:92:TRP:O	2.40	0.54
3:E:32:ASN:ND2	3:E:92:TRP:O	2.40	0.54
1:A:64:TRP:HD1	1:A:65:PHE:N	2.04	0.54
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.38	0.54
3:M:32:ASN:ND2	3:M:92:TRP:O	2.40	0.54
1:A:81:ASN:HD22	1:A:242:LEU:HD13	1.73	0.54
1:C:64:TRP:HD1	1:C:65:PHE:N	2.05	0.54
1:C:142:ASP:OD1	1:C:157:PHE:N	2.41	0.54
1:A:83:VAL:HG21	1:A:237:ARG:HH11	1.73	0.54
1:A:142:ASP:OD1	1:A:157:PHE:N	2.41	0.54
1:C:603:ASN:OD1	1:C:604:THR:N	2.41	0.54
1:C:83:VAL:HG21	1:C:237:ARG:HH11	1.73	0.53
1:A:953:ASN:O	1:A:957:GLN:HG2	2.09	0.53
1:C:81:ASN:HD22	1:C:242:LEU:HD13	1.73	0.53
1:C:298:GLU:O	1:C:302:THR:HG23	2.07	0.53
3:E:36:TRP:HB2	3:E:49:ILE:HB	1.90	0.53
3:M:36:TRP:HB2	3:M:49:ILE:HB	1.91	0.53
1:B:81:ASN:HD22	1:B:242:LEU:HD13	1.73	0.53
1:B:142:ASP:OD1	1:B:157:PHE:N	2.41	0.53
1:A:900:MET:O	1:A:900:MET:CG	2.55	0.53
1:B:338:PHE:CD2	1:B:368:LEU:HD11	2.43	0.53
1:C:134:GLN:HB2	1:C:162:SER:HB3	1.91	0.53
1:A:134:GLN:HB2	1:A:162:SER:HB3	1.91	0.53
1:B:83:VAL:HG21	1:B:237:ARG:HH11	1.73	0.53
2:L:75:LYS:HE2	2:D:15:GLY:CA	2.39	0.52
1:B:312:ILE:O	1:B:312:ILE:CG2	2.57	0.52
1:B:659:SER:HB3	1:B:698:SER:HB3	1.91	0.52
1:C:338:PHE:CD2	1:C:368:LEU:HD11	2.43	0.52
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.92	0.52
1:A:535:LYS:HE3	1:A:554:GLU:HG3	1.90	0.52
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.24	0.52
1:B:134:GLN:HB2	1:B:162:SER:HB3	1.91	0.52
2:L:47:TRP:HH2	2:L:58:PHE:HB3	1.74	0.52
1:A:338:PHE:CD2	1:A:368:LEU:HD11	2.43	0.52
1:B:347:PHE:CE2	1:B:399:SER:HB2	2.44	0.52
1:B:489:TYR:OH	2:H:97:ARG:NH2	2.43	0.52
2:H:47:TRP:HH2	2:H:58:PHE:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.44	0.52
1:A:489:TYR:OH	2:D:97:ARG:NH2	2.43	0.52
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.44	0.52
1:C:905:ARG:NH2	1:C:1049:LEU:O	2.41	0.52
1:B:599:THR:HG22	1:B:601:GLY:H	1.74	0.52
1:C:457:ARG:HD3	1:C:459:SER:O	2.10	0.52
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.92	0.52
1:C:489:TYR:OH	2:L:97:ARG:NH2	2.43	0.52
4:F:98:LYS:O	4:F:110:TYR:HA	2.10	0.52
1:B:645:THR:HG23	1:B:670:ILE:HD13	1.92	0.51
4:N:98:LYS:O	4:N:110:TYR:HA	2.10	0.51
3:I:36:TRP:HB2	3:I:49:ILE:HB	1.90	0.51
2:D:47:TRP:HH2	2:D:58:PHE:HB3	1.74	0.51
3:E:56:PRO:O	3:E:59:ILE:HG12	2.10	0.51
1:C:543:PHE:HD2	1:C:579:PRO:HD2	1.74	0.51
3:M:56:PRO:O	3:M:59:ILE:HG12	2.10	0.51
1:A:457:ARG:HD3	1:A:459:SER:O	2.10	0.51
5:O:52:ASP:O	5:O:66:SER:OG	2.21	0.51
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.93	0.51
1:A:821:LEU:HD11	1:A:939:SER:HB2	1.91	0.51
1:C:106:PHE:HB3	1:C:235:ILE:HG23	1.92	0.51
3:I:56:PRO:O	3:I:59:ILE:HG12	2.10	0.51
1:C:53:ASP:OD1	1:C:54:LEU:N	2.42	0.51
1:C:131:CYS:CB	1:C:166:CYS:HA	2.41	0.51
1:A:759:PHE:O	1:A:763:LEU:HD23	2.10	0.51
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.75	0.51
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.93	0.51
1:C:598:ILE:HD12	1:C:650:LEU:HD11	1.93	0.51
2:H:98:SER:O	2:H:99:TYR:C	2.54	0.51
1:B:985:ASP:N	1:B:988:GLU:OE2	2.41	0.51
1:B:457:ARG:HD3	1:B:459:SER:O	2.10	0.50
1:A:290:ASP:O	1:A:297:SER:HB3	2.11	0.50
4:J:98:LYS:O	4:J:110:TYR:HA	2.10	0.50
1:A:131:CYS:CB	1:A:166:CYS:HA	2.41	0.50
1:B:126:VAL:HG21	1:B:175:PHE:CZ	2.47	0.50
1:A:501:TYR:CD2	1:A:505:HIS:HD2	2.30	0.50
1:B:776:LYS:O	1:B:780:GLU:HG3	2.11	0.50
1:C:1103:PHE:HZ	6:C:1305:NAG:H61	1.76	0.50
1:C:126:VAL:HG21	1:C:175:PHE:CZ	2.47	0.50
1:A:735:SER:OG	1:A:859:THR:OG1	2.30	0.49
1:C:501:TYR:CD2	1:C:505:HIS:HD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:CYS:CB	1:B:166:CYS:HA	2.41	0.49
1:C:826:VAL:HG13	1:C:1057:PRO:HG2	1.94	0.49
1:A:53:ASP:OD1	1:A:54:LEU:N	2.42	0.49
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.48	0.49
1:B:501:TYR:CD2	1:B:505:HIS:HD2	2.30	0.49
4:F:83:MET:SD	4:F:86:LEU:HD21	2.53	0.49
1:A:126:VAL:HG21	1:A:175:PHE:CZ	2.47	0.49
1:C:567:ARG:HH21	1:C:567:ARG:HG3	1.77	0.49
1:A:659:SER:HB3	1:A:698:SER:HB3	1.94	0.49
1:A:922:LEU:HD11	1:A:926:GLN:HE21	1.78	0.49
1:B:380:TYR:O	1:B:430:THR:HA	2.13	0.49
4:N:83:MET:SD	4:N:86:LEU:HD21	2.53	0.49
4:J:83:MET:SD	4:J:86:LEU:HD21	2.53	0.49
1:A:431:GLY:HA3	1:A:513:LEU:O	2.13	0.48
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.95	0.48
2:H:39:GLN:HB3	2:H:45:LEU:HD13	1.94	0.48
1:A:493:ARG:NH2	3:E:51:ASP:OD2	2.47	0.48
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.48	0.48
2:L:2:VAL:HA	2:L:26:GLU:HB3	1.95	0.48
2:H:2:VAL:HA	2:H:26:GLU:HB3	1.96	0.48
2:D:48:VAL:HG13	2:D:63:VAL:HG11	1.95	0.48
1:B:236:THR:O	1:B:237:ARG:HG3	2.13	0.48
2:H:48:VAL:HG13	2:H:63:VAL:HG11	1.95	0.48
2:D:25:SER:C	2:D:27:ILE:H	2.21	0.48
1:A:669:GLY:N	1:B:864:LEU:O	2.46	0.48
1:C:493:ARG:NH2	3:M:51:ASP:OD2	2.47	0.48
2:D:39:GLN:HB3	2:D:45:LEU:HD13	1.94	0.48
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.49	0.48
1:B:117:LEU:HD21	1:B:119:ILE:HG13	1.96	0.48
1:B:493:ARG:NH2	3:I:51:ASP:OD2	2.46	0.48
1:C:139:PRO:HB2	1:C:241:LEU:HD22	1.96	0.48
1:C:312:ILE:HG13	1:C:596:SER:HB3	1.95	0.48
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.48	0.48
1:A:380:TYR:O	1:A:430:THR:HA	2.13	0.48
1:C:490:PHE:CD1	1:C:491:PRO:HD2	2.49	0.48
1:B:139:PRO:HB2	1:B:241:LEU:HD22	1.96	0.48
1:C:993:ILE:O	1:C:997:ILE:HG12	2.14	0.48
2:L:25:SER:C	2:L:27:ILE:H	2.21	0.48
2:L:48:VAL:HG13	2:L:63:VAL:HG11	1.95	0.48
3:M:51:ASP:HB3	3:M:54:LYS:HD3	1.96	0.48
2:D:98:SER:O	2:D:99:TYR:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:VAL:HG22	1:A:1095:PHE:N	2.29	0.48
1:C:431:GLY:HA3	1:C:513:LEU:O	2.14	0.47
4:F:34:MET:HB3	4:F:79:LEU:HD22	1.96	0.47
1:C:380:TYR:O	1:C:430:THR:HA	2.13	0.47
1:B:431:GLY:HA3	1:B:513:LEU:O	2.13	0.47
2:L:98:SER:O	2:L:99:TYR:C	2.54	0.47
1:B:567:ARG:HA	1:B:572:THR:O	2.14	0.47
1:C:117:LEU:HD21	1:C:119:ILE:HG13	1.96	0.47
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.97	0.47
2:H:24:ALA:HB1	2:H:27:ILE:HG13	1.97	0.47
2:H:39:GLN:HG3	2:H:39:GLN:O	2.15	0.47
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.96	0.47
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.96	0.47
1:B:578:ASP:HB3	1:B:583:GLU:H	1.79	0.47
2:H:25:SER:C	2:H:27:ILE:H	2.21	0.47
1:A:139:PRO:HB2	1:A:241:LEU:HD22	1.96	0.47
1:A:402:ILE:CD1	1:A:510:VAL:HG21	2.45	0.47
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.96	0.47
1:B:190:ARG:O	1:B:191:GLU:HG3	2.15	0.47
1:B:819:GLU:O	1:B:823:PHE:HD1	1.98	0.47
1:C:748:GLU:O	1:C:751:ASN:HB2	2.15	0.47
1:C:1139:ASP:OD1	1:C:1139:ASP:N	2.43	0.47
2:D:2:VAL:HA	2:D:26:GLU:HB3	1.95	0.47
2:D:24:ALA:HB1	2:D:27:ILE:HG13	1.97	0.47
2:D:32:ASN:HD21	2:D:97:ARG:HH21	1.63	0.47
5:G:48:LEU:O	5:G:49:LEU:HG	2.15	0.47
1:A:117:LEU:HD21	1:A:119:ILE:HG13	1.96	0.47
4:J:34:MET:HB3	4:J:79:LEU:HD22	1.96	0.47
1:A:190:ARG:O	1:A:191:GLU:HG3	2.15	0.47
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.49	0.47
1:B:656:VAL:HG12	1:B:658:ASN:H	1.79	0.47
1:C:190:ARG:O	1:C:191:GLU:HG3	2.15	0.47
1:C:402:ILE:CD1	1:C:510:VAL:HG21	2.45	0.47
1:C:546:LEU:HD22	1:C:565:PHE:HE1	1.79	0.47
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.48	0.47
4:N:34:MET:HB3	4:N:79:LEU:HD22	1.96	0.47
4:J:91:THR:OG1	4:J:120:THR:HA	2.15	0.47
5:K:48:LEU:O	5:K:49:LEU:HG	2.15	0.47
1:B:402:ILE:CD1	1:B:510:VAL:HG21	2.45	0.46
2:L:39:GLN:O	2:L:39:GLN:HG3	2.15	0.46
4:N:91:THR:OG1	4:N:120:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.80	0.46
3:E:51:ASP:HB3	3:E:54:LYS:HD3	1.96	0.46
4:F:91:THR:OG1	4:F:120:THR:HA	2.15	0.46
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.37	0.46
1:B:821:LEU:HD13	1:B:935:GLN:HG3	1.97	0.46
1:C:315:THR:HG23	1:C:316:SER:N	2.30	0.46
1:C:746:SER:HB2	1:C:749:CYS:SG	2.55	0.46
2:L:24:ALA:HB1	2:L:27:ILE:HG13	1.97	0.46
5:O:48:LEU:O	5:O:49:LEU:HG	2.15	0.46
1:A:578:ASP:OD1	1:A:583:GLU:N	2.45	0.46
1:B:53:ASP:OD1	1:B:54:LEU:N	2.42	0.46
5:O:63:PHE:HA	5:O:75:GLY:O	2.16	0.46
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.98	0.46
1:C:353:TRP:CD1	1:C:353:TRP:H	2.33	0.46
1:B:353:TRP:H	1:B:353:TRP:CD1	2.33	0.46
1:C:1086:LYS:HD3	1:C:1122:VAL:HG11	1.98	0.46
5:O:14:PRO:HG3	5:O:109:VAL:HG13	1.98	0.46
3:I:51:ASP:HB3	3:I:54:LYS:HD3	1.96	0.46
2:D:28:ILE:HG21	2:D:31:ARG:HH11	1.81	0.46
1:C:309:GLU:O	1:C:313:TYR:OH	2.29	0.46
2:L:28:ILE:HG21	2:L:31:ARG:HH11	1.81	0.46
2:D:39:GLN:O	2:D:39:GLN:HG3	2.15	0.46
1:A:599:THR:HG22	1:A:601:GLY:H	1.80	0.46
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.98	0.46
2:L:32:ASN:HD21	2:L:97:ARG:HH21	1.63	0.46
1:C:449:TYR:HD2	4:N:60:TYR:HE2	1.64	0.45
2:H:28:ILE:HG21	2:H:31:ARG:HH11	1.81	0.45
3:I:34:VAL:HA	3:I:91:THR:HG22	1.99	0.45
5:K:63:PHE:HA	5:K:75:GLY:O	2.16	0.45
1:A:388:ASN:ND2	1:A:526:GLY:O	2.48	0.45
1:B:440:LYS:H	1:B:440:LYS:HD2	1.81	0.45
1:B:536:ASN:C	1:B:537:LYS:HD3	2.41	0.45
1:B:449:TYR:HD2	4:J:60:TYR:HE2	1.64	0.45
1:C:440:LYS:H	1:C:440:LYS:HD2	1.81	0.45
5:K:14:PRO:HG3	5:K:109:VAL:HG13	1.98	0.45
5:G:63:PHE:HA	5:G:75:GLY:O	2.16	0.45
1:C:1104:VAL:HG11	1:C:1119:ASN:ND2	2.31	0.45
1:A:578:ASP:OD1	1:A:578:ASP:N	2.48	0.45
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.16	0.45
2:L:85:LEU:C	2:L:86:ARG:HD3	2.42	0.45
2:H:32:ASN:HD21	2:H:97:ARG:HH21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:VAL:HG12	2:H:63:VAL:O	2.17	0.45
5:G:14:PRO:HG3	5:G:109:VAL:HG13	1.98	0.45
1:A:353:TRP:CD1	1:A:353:TRP:H	2.33	0.45
1:C:388:ASN:ND2	1:C:526:GLY:O	2.48	0.45
2:L:63:VAL:HG12	2:L:63:VAL:O	2.17	0.45
3:M:34:VAL:HA	3:M:91:THR:HG22	1.98	0.45
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.41	0.45
1:B:400:PHE:HD1	1:B:402:ILE:HG23	1.82	0.45
1:A:126:VAL:HG13	1:A:126:VAL:O	2.17	0.45
1:B:293:LEU:HD23	1:B:294:ASP:CG	2.42	0.45
1:C:126:VAL:O	1:C:126:VAL:HG13	2.17	0.45
1:A:400:PHE:HD1	1:A:402:ILE:HG23	1.82	0.45
1:A:449:TYR:HD2	4:F:60:TYR:HE2	1.64	0.45
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.98	0.45
1:C:400:PHE:HD1	1:C:402:ILE:HG23	1.82	0.45
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.51	0.44
1:B:126:VAL:HG13	1:B:126:VAL:O	2.17	0.44
1:C:298:GLU:HG2	1:C:315:THR:OG1	2.18	0.44
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.98	0.44
1:A:612:TYR:HE2	1:A:651:ILE:HD12	1.81	0.44
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.99	0.44
1:C:1094:VAL:HG22	1:C:1095:PHE:N	2.33	0.44
3:E:34:VAL:HA	3:E:91:THR:HG22	1.98	0.44
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.40	0.44
1:A:763:LEU:HD12	1:A:1008:VAL:HG21	1.98	0.44
1:B:388:ASN:ND2	1:B:526:GLY:O	2.48	0.44
5:K:52:ASP:O	5:K:66:SER:OG	2.21	0.44
3:E:55:ARG:HG2	3:E:59:ILE:HB	2.00	0.44
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.52	0.44
1:A:440:LYS:H	1:A:440:LYS:HD2	1.81	0.44
1:A:752:LEU:HD12	1:A:993:ILE:HG21	2.00	0.44
1:B:1038:LYS:HA	1:B:1038:LYS:HD2	1.85	0.44
1:A:973:ILE:HD11	1:A:980:ILE:HG12	1.98	0.44
1:C:315:THR:HG22	1:C:595:VAL:O	2.18	0.44
1:B:712:ILE:HD11	1:C:896:ILE:HG22	2.00	0.44
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.52	0.44
1:C:236:THR:O	1:C:237:ARG:HG3	2.17	0.44
1:C:338:PHE:CE1	1:C:358:ILE:HD13	2.53	0.44
3:M:34:VAL:HG22	3:M:35:SER:N	2.33	0.44
1:A:37:TYR:CD1	1:A:204:TYR:HE2	2.36	0.44
1:A:460:ASN:ND2	2:D:54:GLY:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:CD1	1:B:204:TYR:HE2	2.36	0.44
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.89	0.44
2:L:44:GLY:O	2:L:45:LEU:C	2.60	0.44
5:G:4:LEU:HD22	5:G:29:ILE:HD11	2.00	0.44
1:B:36:VAL:HG11	1:B:220:PHE:CZ	2.52	0.44
3:M:55:ARG:HG2	3:M:59:ILE:HB	2.00	0.44
5:K:4:LEU:HD22	5:K:29:ILE:HD11	2.00	0.44
2:D:63:VAL:HG12	2:D:63:VAL:O	2.17	0.44
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.99	0.44
1:A:898:PHE:HA	1:A:901:GLN:HG2	2.00	0.44
2:H:85:LEU:C	2:H:86:ARG:HD3	2.42	0.44
1:A:233:ILE:HG22	1:A:234:ASN:N	2.33	0.43
1:B:551:VAL:HG12	1:B:588:THR:O	2.18	0.43
2:D:85:LEU:C	2:D:86:ARG:HD3	2.42	0.43
1:A:338:PHE:CE1	1:A:358:ILE:HD13	2.53	0.43
2:H:96:ALA:HB1	2:H:104:VAL:HG13	2.00	0.43
1:A:707:TYR:HB3	1:B:792:PRO:HG3	2.00	0.43
3:I:55:ARG:HG2	3:I:59:ILE:HB	2.00	0.43
1:A:1089:PHE:CE2	1:B:917:TYR:HD2	2.37	0.43
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.87	0.43
2:D:96:ALA:HB1	2:D:104:VAL:HG13	2.00	0.43
1:B:338:PHE:CE1	1:B:358:ILE:HD13	2.53	0.43
5:O:4:LEU:HD22	5:O:29:ILE:HD11	2.00	0.43
2:D:28:ILE:HG21	2:D:31:ARG:NH1	2.34	0.43
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.53	0.43
1:C:338:PHE:HE1	1:C:358:ILE:HD13	1.84	0.43
1:C:560:LEU:N	1:C:563:GLN:OE1	2.48	0.43
1:A:950:ASP:OD1	1:A:951:VAL:N	2.52	0.43
1:B:312:ILE:CG1	1:B:596:SER:HB3	2.49	0.43
2:L:96:ALA:HB1	2:L:104:VAL:HG13	2.00	0.43
2:D:44:GLY:O	2:D:45:LEU:C	2.60	0.43
1:C:37:TYR:CD1	1:C:204:TYR:HE2	2.36	0.43
1:C:460:ASN:ND2	2:L:54:GLY:O	2.47	0.43
2:L:12:VAL:HG21	2:L:18:LEU:HD11	2.01	0.43
1:B:106:PHE:HB3	1:B:235:ILE:CG2	2.49	0.42
1:B:822:LEU:HD22	1:B:945:LEU:HD21	2.00	0.42
3:M:87:TYR:O	3:M:104:GLY:HA2	2.19	0.42
2:H:44:GLY:O	2:H:45:LEU:C	2.60	0.42
1:A:338:PHE:HE1	1:A:358:ILE:HD13	1.84	0.42
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	2.01	0.42
1:A:1072:GLU:HB3	1:B:894:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ILE:CD1	1:C:896:ILE:HG22	2.49	0.42
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	2.01	0.42
1:B:762:GLN:HA	1:B:765:ARG:HE	1.84	0.42
1:B:140:PHE:CD1	1:B:141:LEU:N	2.87	0.42
1:C:236:THR:C	1:C:237:ARG:HG3	2.44	0.42
1:C:977:LEU:HD21	1:C:1000:ARG:HH22	1.85	0.42
4:N:9:GLY:HA3	4:N:117:THR:OG1	2.19	0.42
5:G:32:ASN:OD1	5:G:33:PHE:N	2.44	0.42
1:A:140:PHE:CD1	1:A:141:LEU:N	2.87	0.42
1:A:232:GLY:O	1:A:233:ILE:HD13	2.18	0.42
1:A:412:PRO:HG3	1:A:429:PHE:HB3	2.01	0.42
1:C:402:ILE:HD11	1:C:510:VAL:HG21	2.02	0.42
1:C:617:CYS:C	1:C:619:GLU:H	2.27	0.42
1:A:53:ASP:CG	1:A:54:LEU:H	2.26	0.42
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.01	0.42
1:B:320:VAL:HG21	1:B:591:SER:OG	2.18	0.42
1:B:742:ILE:O	1:B:1000:ARG:NH2	2.49	0.42
1:B:898:PHE:N	1:B:899:PRO:HD2	2.34	0.42
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.93	0.42
4:N:22:CYS:SG	4:N:23:GLY:N	2.93	0.42
4:J:22:CYS:SG	4:J:23:GLY:N	2.93	0.42
1:A:458:LYS:HB3	1:A:458:LYS:HE3	1.85	0.42
1:C:140:PHE:CD1	1:C:141:LEU:N	2.87	0.42
2:L:28:ILE:HG21	2:L:31:ARG:NH1	2.34	0.42
2:H:28:ILE:HG21	2:H:31:ARG:NH1	2.34	0.42
4:J:9:GLY:HA3	4:J:117:THR:OG1	2.19	0.42
3:E:87:TYR:O	3:E:104:GLY:HA2	2.19	0.42
4:F:22:CYS:SG	4:F:23:GLY:N	2.93	0.42
1:B:245:HIS:H	1:B:258:TRP:CD1	2.38	0.42
1:B:880:GLY:O	1:B:884:SER:OG	2.33	0.42
1:C:53:ASP:CG	1:C:54:LEU:H	2.26	0.42
1:C:412:PRO:HG3	1:C:429:PHE:HB3	2.01	0.42
1:C:419:ALA:HA	1:C:423:TYR:O	2.20	0.42
4:F:9:GLY:HA3	4:F:117:THR:OG1	2.19	0.42
1:A:470:THR:HG22	1:A:492:LEU:HD11	2.02	0.42
1:B:705:VAL:HB	1:C:883:THR:HG21	2.02	0.42
1:C:1083:HIS:O	1:C:1086:LYS:HG2	2.20	0.42
1:A:697:MET:CG	1:B:869:MET:HE1	2.50	0.41
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.02	0.41
1:B:236:THR:C	1:B:237:ARG:HG3	2.45	0.41
1:B:402:ILE:HD11	1:B:510:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ALA:HA	1:B:423:TYR:O	2.20	0.41
1:B:720:ILE:CD1	1:B:923:ILE:HG23	2.50	0.41
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.41
4:F:36:TRP:HE1	4:F:79:LEU:HG	1.86	0.41
1:B:45:SER:O	1:B:47:VAL:HG23	2.21	0.41
1:B:1123:SER:CB	1:C:914:ASN:ND2	2.83	0.41
1:C:126:VAL:HG21	1:C:175:PHE:CE1	2.56	0.41
1:C:245:HIS:H	1:C:258:TRP:CD1	2.38	0.41
1:C:458:LYS:HE3	1:C:458:LYS:HB3	1.85	0.41
1:A:245:HIS:H	1:A:258:TRP:CD1	2.38	0.41
1:B:126:VAL:HG21	1:B:175:PHE:CE1	2.55	0.41
1:B:412:PRO:HG3	1:B:429:PHE:HB3	2.01	0.41
1:B:470:THR:HG22	1:B:492:LEU:HD11	2.02	0.41
4:J:36:TRP:HE1	4:J:79:LEU:HG	1.86	0.41
2:D:12:VAL:HG21	2:D:18:LEU:HD11	2.01	0.41
1:A:318:PHE:CE1	1:A:620:VAL:HG23	2.55	0.41
1:B:338:PHE:HE1	1:B:358:ILE:HD13	1.84	0.41
1:B:676:THR:HA	1:B:690:GLN:N	2.35	0.41
1:C:816:SER:HB2	1:C:817:PRO:HD2	2.01	0.41
2:H:47:TRP:HH2	2:H:58:PHE:CB	2.34	0.41
3:I:87:TYR:O	3:I:104:GLY:HA2	2.19	0.41
1:A:365:TYR:HD2	1:A:388:ASN:HB2	1.85	0.41
1:B:1089:PHE:HE2	1:C:917:TYR:CD2	2.38	0.41
1:C:45:SER:O	1:C:47:VAL:HG23	2.21	0.41
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.21	0.41
1:B:668:ALA:O	1:B:670:ILE:HD12	2.20	0.41
1:C:976:VAL:O	1:C:980:ILE:HG12	2.21	0.41
3:M:24:GLY:O	3:M:70:THR:OG1	2.38	0.41
2:D:47:TRP:HH2	2:D:58:PHE:CB	2.34	0.41
1:A:419:ALA:HA	1:A:423:TYR:O	2.20	0.41
1:B:53:ASP:CG	1:B:54:LEU:H	2.26	0.41
1:B:365:TYR:HD2	1:B:388:ASN:HB2	1.85	0.41
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.54	0.41
2:H:12:VAL:HG21	2:H:18:LEU:HD11	2.01	0.41
1:B:516:GLU:OE2	1:B:518:LEU:HD21	2.21	0.41
1:C:567:ARG:HG3	1:C:567:ARG:NH2	2.35	0.41
2:L:24:ALA:O	2:L:76:ASN:ND2	2.54	0.41
2:H:97:ARG:CG	2:H:106:PHE:N	2.81	0.41
3:I:24:GLY:O	3:I:70:THR:OG1	2.38	0.41
2:D:24:ALA:O	2:D:76:ASN:ND2	2.54	0.41
1:A:64:TRP:CD1	1:A:65:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:O	1:B:274:THR:HG23	2.21	0.41
1:C:506:GLN:O	1:C:508:TYR:HD1	2.03	0.41
3:M:17:LYS:HG3	3:M:77:THR:HA	2.03	0.41
4:N:36:TRP:HE1	4:N:79:LEU:HG	1.86	0.41
2:D:68:THR:O	2:D:80:LEU:HD12	2.21	0.41
1:A:908:GLY:O	1:A:1038:LYS:HE3	2.21	0.41
1:B:133:PHE:HA	1:B:163:ALA:O	2.21	0.41
3:E:37:TYR:HD1	3:E:47:LEU:HA	1.86	0.41
1:A:133:PHE:HA	1:A:163:ALA:O	2.21	0.40
1:A:733:LYS:HE3	1:A:771:ALA:HB1	2.03	0.40
1:A:759:PHE:O	1:A:762:GLN:HG2	2.21	0.40
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.57	0.40
1:C:126:VAL:HG12	1:C:172:SER:C	2.46	0.40
1:C:241:LEU:C	1:C:242:LEU:HD12	2.47	0.40
1:C:516:GLU:OE2	1:C:518:LEU:HD21	2.21	0.40
5:K:26:THR:HA	5:K:30:GLY:HA3	2.03	0.40
3:E:17:LYS:HG3	3:E:77:THR:HA	2.03	0.40
1:A:126:VAL:HG12	1:A:172:SER:C	2.46	0.40
1:A:318:PHE:CD2	1:A:615:VAL:HG21	2.56	0.40
1:A:506:GLN:O	1:A:508:TYR:HD1	2.03	0.40
1:A:572:THR:O	1:A:573:THR:C	2.64	0.40
1:C:140:PHE:O	1:C:159:VAL:HB	2.22	0.40
3:M:44:ALA:HA	3:M:45:PRO:HD3	1.77	0.40
4:J:68:PHE:CD2	4:J:81:LEU:HD21	2.56	0.40
2:D:32:ASN:HD21	2:D:97:ARG:NH2	2.18	0.40
1:A:126:VAL:HG21	1:A:175:PHE:CE1	2.55	0.40
1:A:126:VAL:O	1:A:171:VAL:HA	2.22	0.40
1:A:516:GLU:OE2	1:A:518:LEU:HD21	2.21	0.40
1:A:898:PHE:O	1:A:899:PRO:C	2.63	0.40
1:B:126:VAL:HG12	1:B:172:SER:C	2.46	0.40
1:B:241:LEU:C	1:B:242:LEU:HD12	2.46	0.40
1:B:402:ILE:HD13	1:B:402:ILE:HG21	1.88	0.40
1:B:506:GLN:O	1:B:508:TYR:HD1	2.03	0.40
1:C:48:LEU:HD23	1:C:276:LEU:HD21	2.04	0.40
2:L:47:TRP:HH2	2:L:58:PHE:CB	2.34	0.40
4:J:61:ALA:HB3	4:J:64:VAL:HG22	2.03	0.40
1:A:45:SER:O	1:A:47:VAL:HG23	2.21	0.40
1:A:140:PHE:O	1:A:159:VAL:HB	2.22	0.40
1:A:299:THR:O	1:A:303:LEU:HG	2.22	0.40
1:A:880:GLY:O	1:A:884:SER:HB2	2.22	0.40
1:B:1094:VAL:HG22	1:B:1095:PHE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:VAL:HG13	1:C:917:TYR:HB3	2.03	0.40
1:C:365:TYR:HD2	1:C:388:ASN:HB2	1.85	0.40
5:G:26:THR:HA	5:G:30:GLY:HA3	2.03	0.40
1:B:977:LEU:HD22	1:B:993:ILE:HD12	2.04	0.40
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.03	0.40
1:C:804:GLN:HA	1:C:817:PRO:HG2	2.03	0.40
2:L:32:ASN:HD21	2:L:97:ARG:NH2	2.19	0.40
2:L:99:TYR:O	2:L:100:GLY:C	2.64	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	986/1210 (82%)	928 (94%)	57 (6%)	1 (0%)	48	78
1	B	985/1210 (81%)	930 (94%)	55 (6%)	0	100	100
1	C	984/1210 (81%)	925 (94%)	59 (6%)	0	100	100
2	D	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
2	H	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
2	L	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
3	E	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
3	I	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
3	M	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
4	F	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
4	J	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
4	N	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
5	G	108/110 (98%)	102 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
5	O	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
All	All	4311/5010 (86%)	4048 (94%)	262 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	806/1061 (76%)	805 (100%)	1 (0%)	88	91
1	B	801/1061 (76%)	801 (100%)	0	100	100
1	C	808/1061 (76%)	807 (100%)	1 (0%)	88	91
2	D	89/98 (91%)	85 (96%)	4 (4%)	24	56
2	H	88/98 (90%)	86 (98%)	2 (2%)	44	70
2	L	89/98 (91%)	89 (100%)	0	100	100
3	E	88/90 (98%)	85 (97%)	3 (3%)	32	63
3	I	88/90 (98%)	85 (97%)	3 (3%)	32	63
3	M	88/90 (98%)	88 (100%)	0	100	100
4	F	98/99 (99%)	98 (100%)	0	100	100
4	J	98/99 (99%)	98 (100%)	0	100	100
4	N	98/99 (99%)	98 (100%)	0	100	100
5	G	85/90 (94%)	84 (99%)	1 (1%)	63	79
5	K	85/90 (94%)	84 (99%)	1 (1%)	63	79
5	O	85/90 (94%)	85 (100%)	0	100	100
All	All	3494/4314 (81%)	3478 (100%)	16 (0%)	78	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
1	C	355	ARG
2	H	45	LEU
2	H	111	THR
3	I	3	VAL
3	I	34	VAL
3	I	45	PRO
5	K	76	ILE
2	D	2	VAL
2	D	23	GLU
2	D	45	LEU
2	D	111	THR
3	E	3	VAL
3	E	34	VAL
3	E	45	PRO
5	G	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	87	ASN
1	A	125	ASN
1	A	505	HIS
1	A	536	ASN
1	A	907	ASN
1	A	954	HIS
1	A	992	GLN
1	A	1088	HIS
1	B	66	HIS
1	B	87	ASN
1	B	125	ASN
1	B	505	HIS
1	B	536	ASN
1	B	564	GLN
1	B	606	ASN
1	B	641	ASN
1	B	751	ASN
1	B	895	GLN
1	B	954	HIS
1	B	1010	GLN

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Mol	Chain	Res	Type
1	B	1071	GLN
1	B	1083	HIS
1	C	66	HIS
1	C	87	ASN
1	C	125	ASN
1	C	505	HIS
1	C	913	GLN
1	C	1005	GLN
1	C	1106	GLN
2	L	3	GLN
2	L	81	GLN
2	L	83	ASN
2	L	109	GLN
3	M	1	GLN
4	N	39	GLN
5	O	39	GLN
5	O	94	ASN
2	H	3	GLN
2	H	81	GLN
2	H	83	ASN
2	H	109	GLN
3	I	1	GLN
4	J	39	GLN
5	K	39	GLN
5	K	94	ASN
2	D	3	GLN
2	D	81	GLN
2	D	83	ASN
2	D	109	GLN
3	E	1	GLN
4	F	39	GLN
5	G	39	GLN
5	G	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	1304	1	14,14,15	0.35	0	17,19,21	1.50	2 (11%)
6	NAG	B	1306	1	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
6	NAG	C	1311	1	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	B	1308	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
6	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.38	0
6	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	C	1306	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
6	NAG	B	1302	1	14,14,15	0.58	0	17,19,21	0.71	0
6	NAG	C	1310	1	14,14,15	0.41	0	17,19,21	0.76	0
6	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.66	0
6	NAG	A	1308	1	14,14,15	0.42	0	17,19,21	0.75	0
6	NAG	C	1309	1	14,14,15	0.41	0	17,19,21	0.76	0
6	NAG	B	1309	1	14,14,15	0.33	0	17,19,21	0.63	0
6	NAG	C	1303	1	14,14,15	0.18	0	17,19,21	0.49	0
6	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	B	1310	1	14,14,15	0.42	0	17,19,21	1.09	2 (11%)
6	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	A	1301	1	14,14,15	0.17	0	17,19,21	0.63	1 (5%)
6	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	B	1303	1	14,14,15	0.69	0	17,19,21	1.11	2 (11%)
6	NAG	C	1308	1	14,14,15	0.28	0	17,19,21	0.57	0
6	NAG	A	1303	1	14,14,15	0.39	0	17,19,21	0.54	0
6	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.49	0
6	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	A	1304	1	14,14,15	0.18	0	17,19,21	0.44	0
6	NAG	B	1307	1	14,14,15	0.39	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1307	1	14,14,15	0.36	0	17,19,21	0.64	0
6	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	A	1309	1	14,14,15	0.40	0	17,19,21	0.76	0
6	NAG	B	1301	1	14,14,15	0.56	0	17,19,21	1.33	2 (11%)
6	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1304	NAG	C2-N2-C7	4.57	129.02	122.90
6	B	1301	NAG	C1-O5-C5	3.28	116.58	112.19
6	B	1310	NAG	C2-N2-C7	-2.97	118.92	122.90
6	B	1306	NAG	C1-C2-N2	-2.81	106.01	110.43
6	B	1304	NAG	C1-O5-C5	2.70	115.81	112.19
6	B	1303	NAG	C1-C2-N2	-2.64	106.27	110.43
6	B	1310	NAG	C4-C3-C2	-2.59	107.22	111.02
6	B	1301	NAG	C1-C2-N2	-2.23	106.92	110.43
6	B	1308	NAG	C1-O5-C5	2.22	115.17	112.19
6	B	1303	NAG	C1-O5-C5	2.16	115.08	112.19
6	A	1301	NAG	C1-O5-C5	2.05	114.94	112.19
6	C	1306	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1310	NAG	C8-C7-N2-C2
6	A	1310	NAG	O7-C7-N2-C2
6	B	1306	NAG	C8-C7-N2-C2
6	B	1306	NAG	O7-C7-N2-C2
6	B	1308	NAG	C8-C7-N2-C2
6	B	1308	NAG	O7-C7-N2-C2
6	B	1310	NAG	C8-C7-N2-C2
6	B	1310	NAG	O7-C7-N2-C2
6	C	1311	NAG	C8-C7-N2-C2
6	C	1311	NAG	O7-C7-N2-C2
6	B	1304	NAG	C8-C7-N2-C2
6	B	1304	NAG	O7-C7-N2-C2
6	C	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	1306	NAG	O5-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	C8-C7-N2-C2
6	B	1301	NAG	O7-C7-N2-C2
6	A	1303	NAG	O5-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	C	1307	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	C	1306	NAG	C3-C2-N2-C7
6	C	1307	NAG	C3-C2-N2-C7
6	A	1308	NAG	C1-C2-N2-C7
6	B	1310	NAG	C1-C2-N2-C7
6	C	1306	NAG	C1-C2-N2-C7
6	C	1307	NAG	C1-C2-N2-C7
6	C	1309	NAG	C1-C2-N2-C7
6	B	1309	NAG	C8-C7-N2-C2
6	B	1309	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

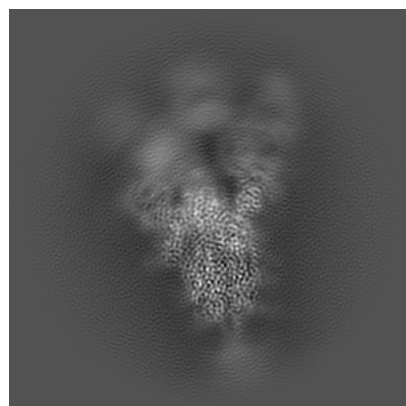
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33434. These allow visual inspection of the internal detail of the map and identification of artifacts.

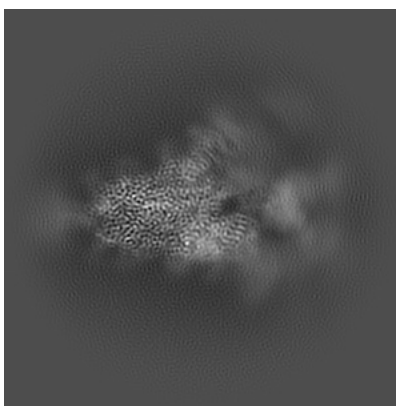
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

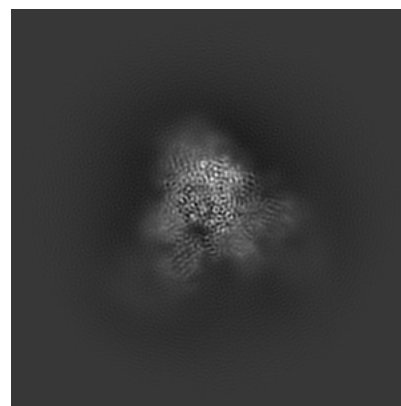
6.1.1 Primary map



X

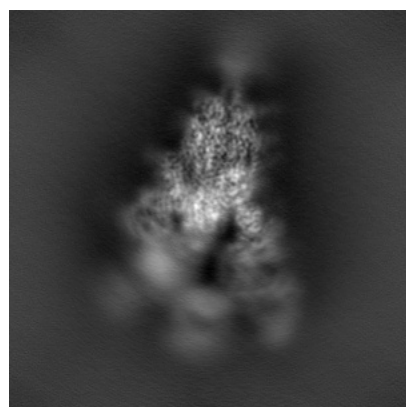


Y

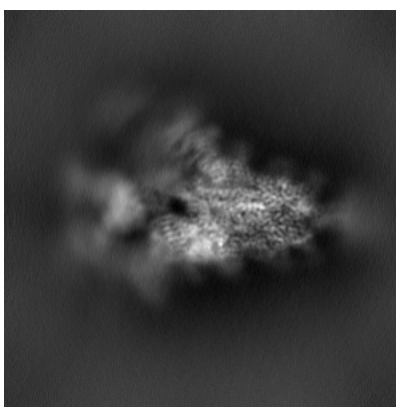


Z

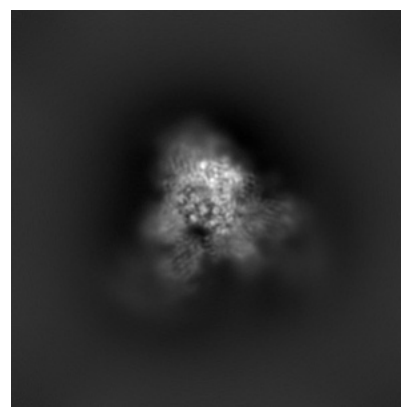
6.1.2 Raw map



X



Y

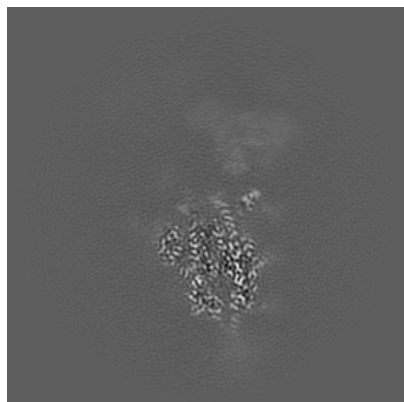


Z

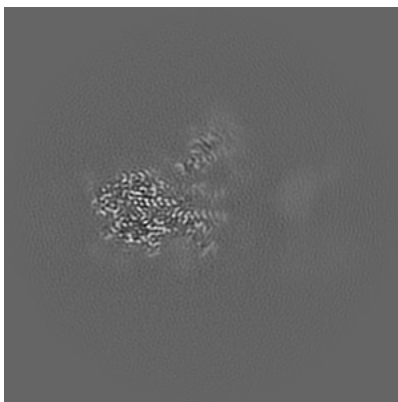
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

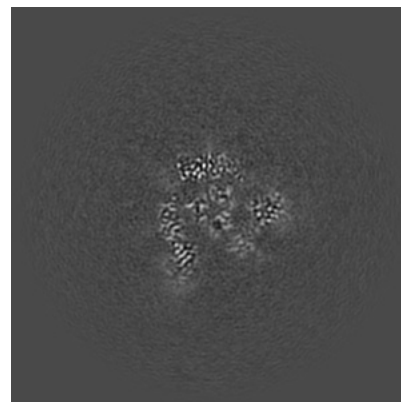
6.2.1 Primary map



X Index: 170

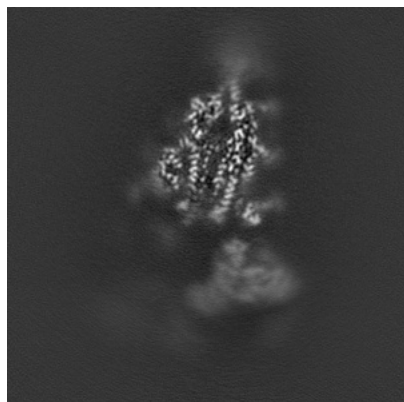


Y Index: 170

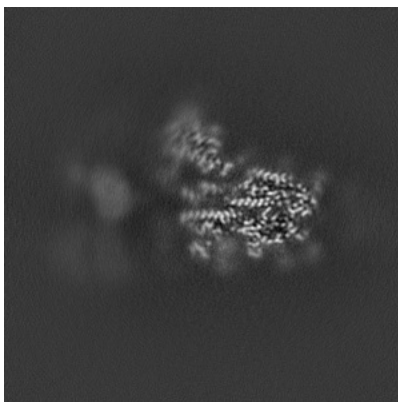


Z Index: 170

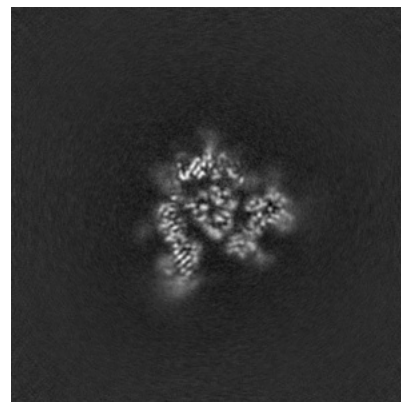
6.2.2 Raw map



X Index: 170



Y Index: 170

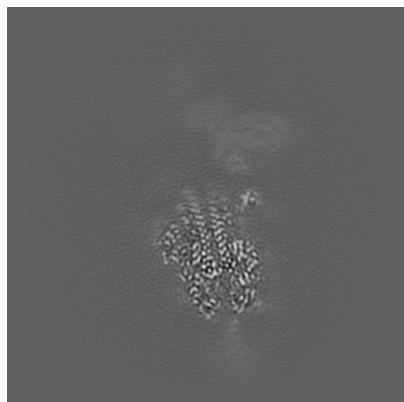


Z Index: 170

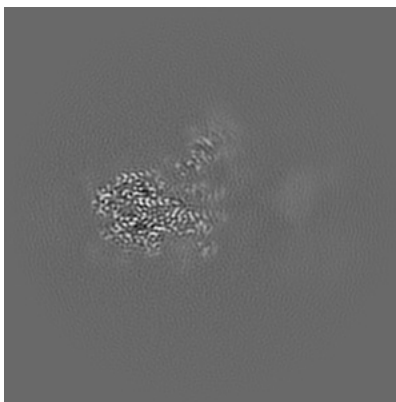
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

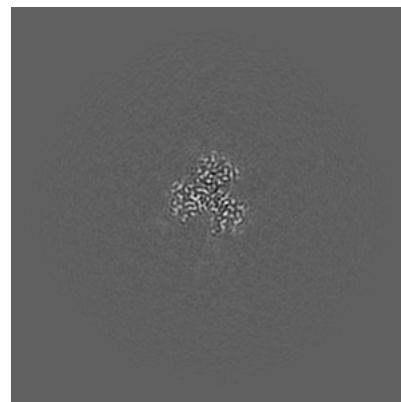
6.3.1 Primary map



X Index: 174

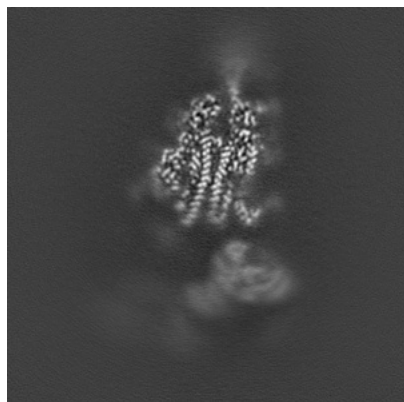


Y Index: 171

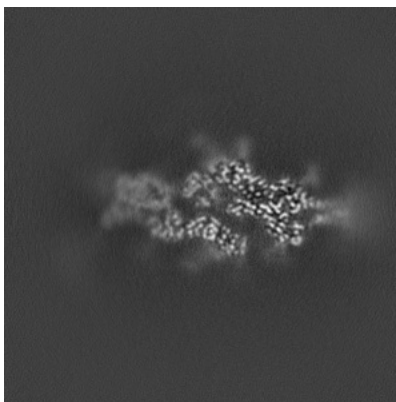


Z Index: 118

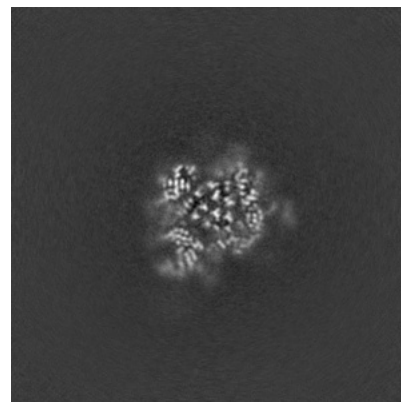
6.3.2 Raw map



X Index: 173



Y Index: 195

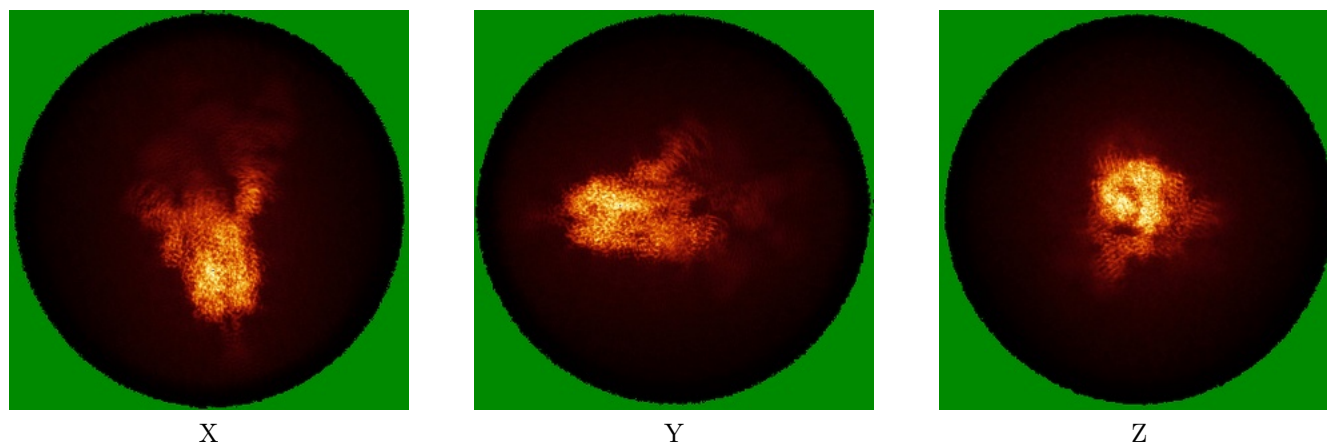


Z Index: 183

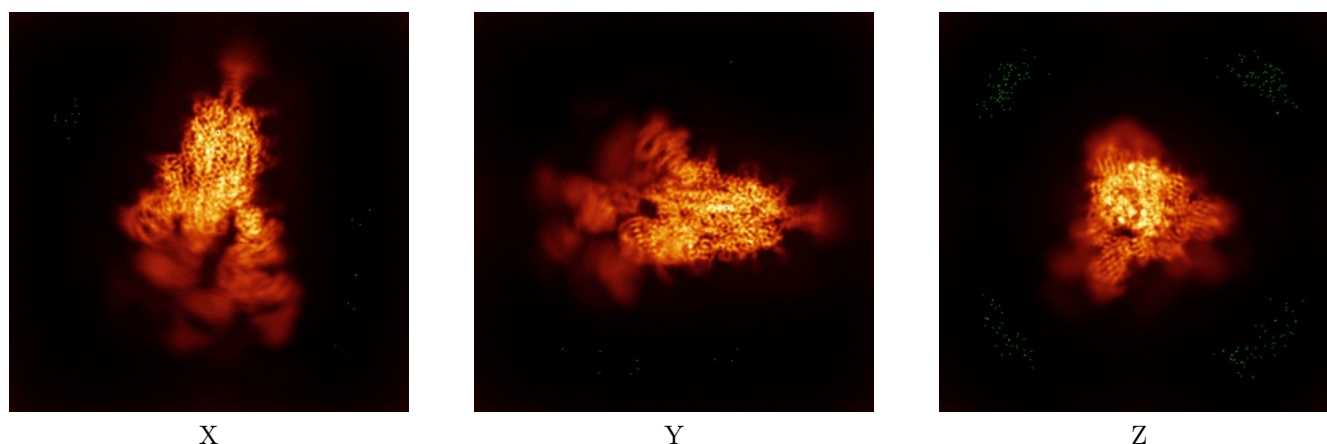
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

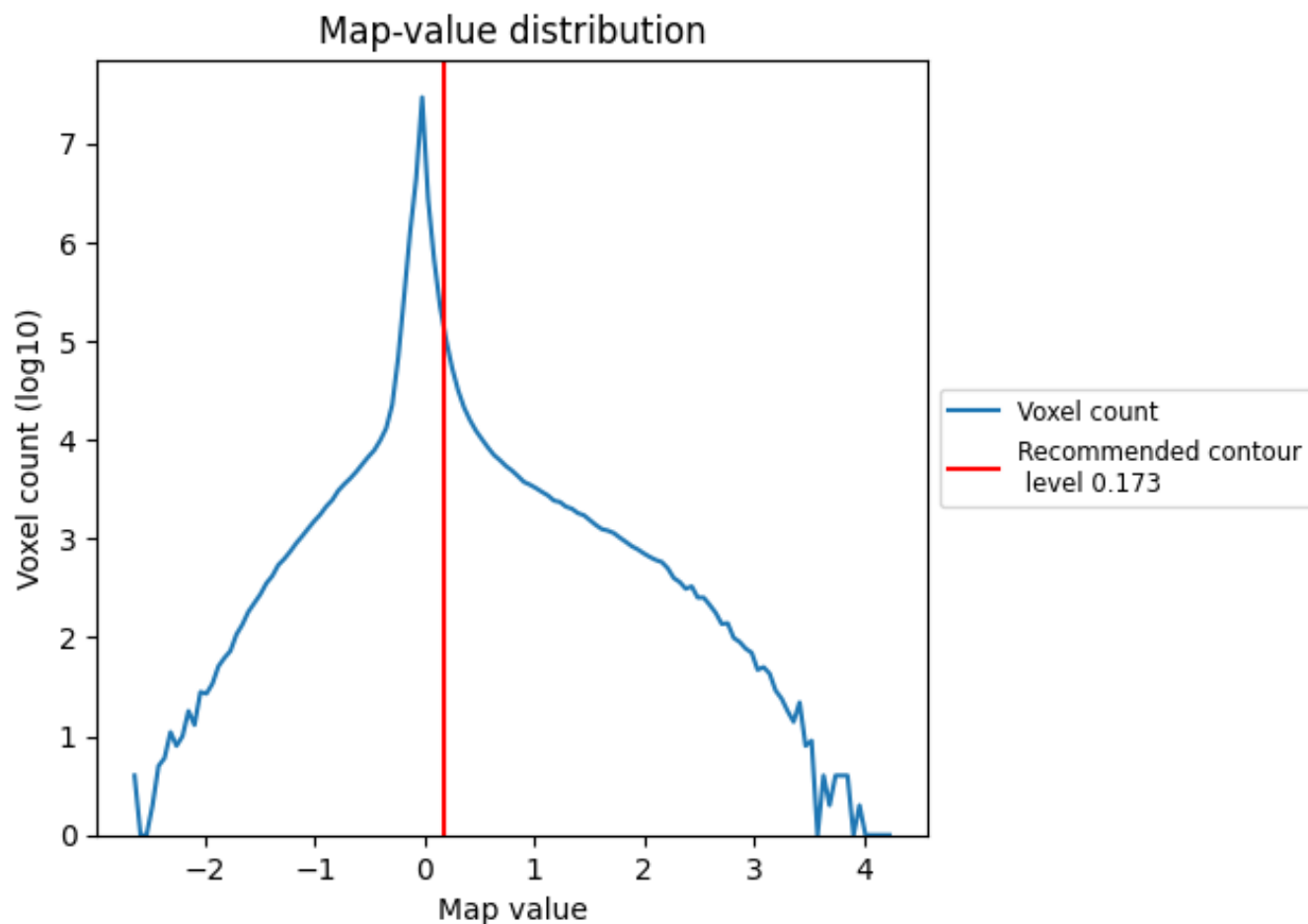
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

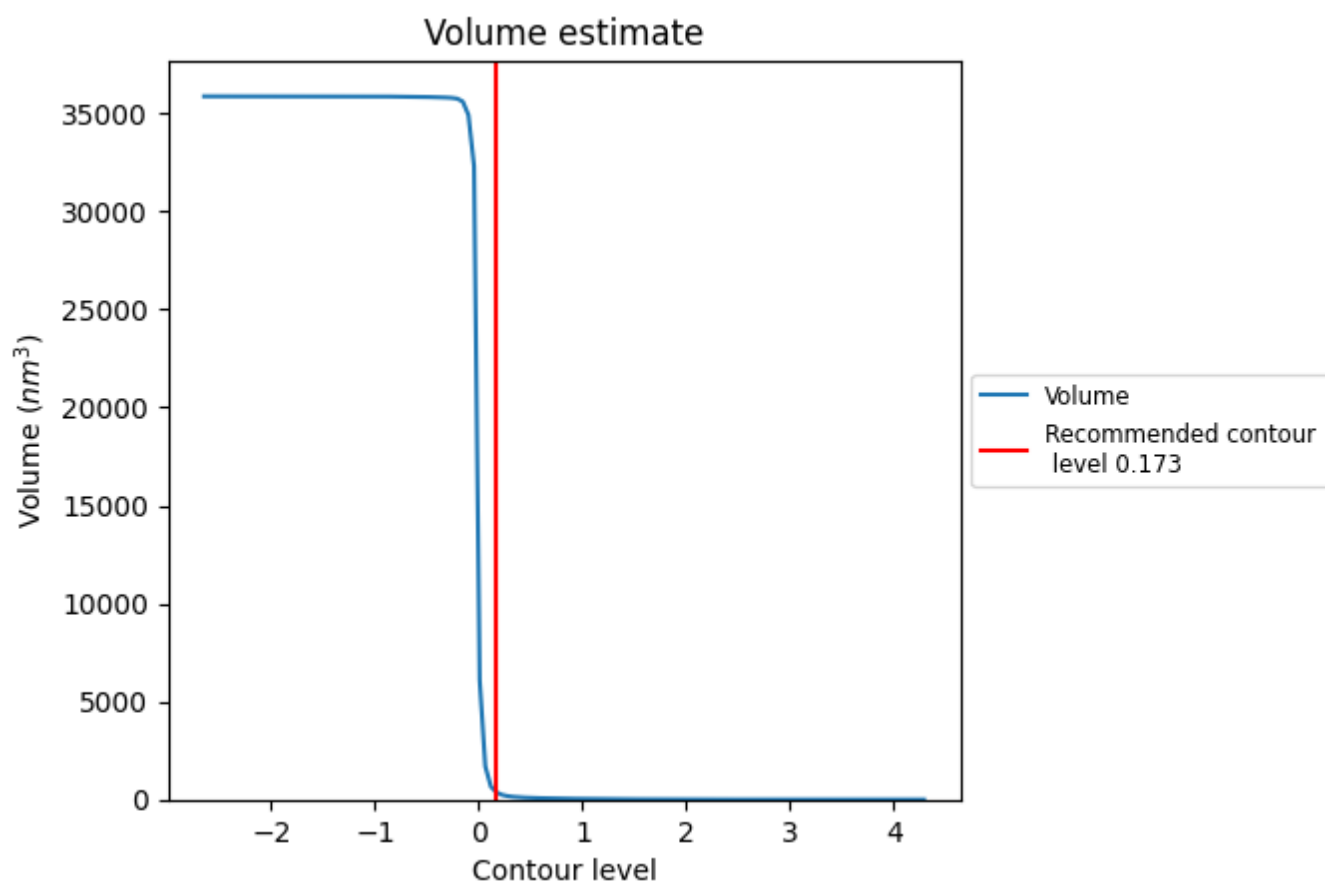
This section contains the results of statistical analysis of the map.

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.

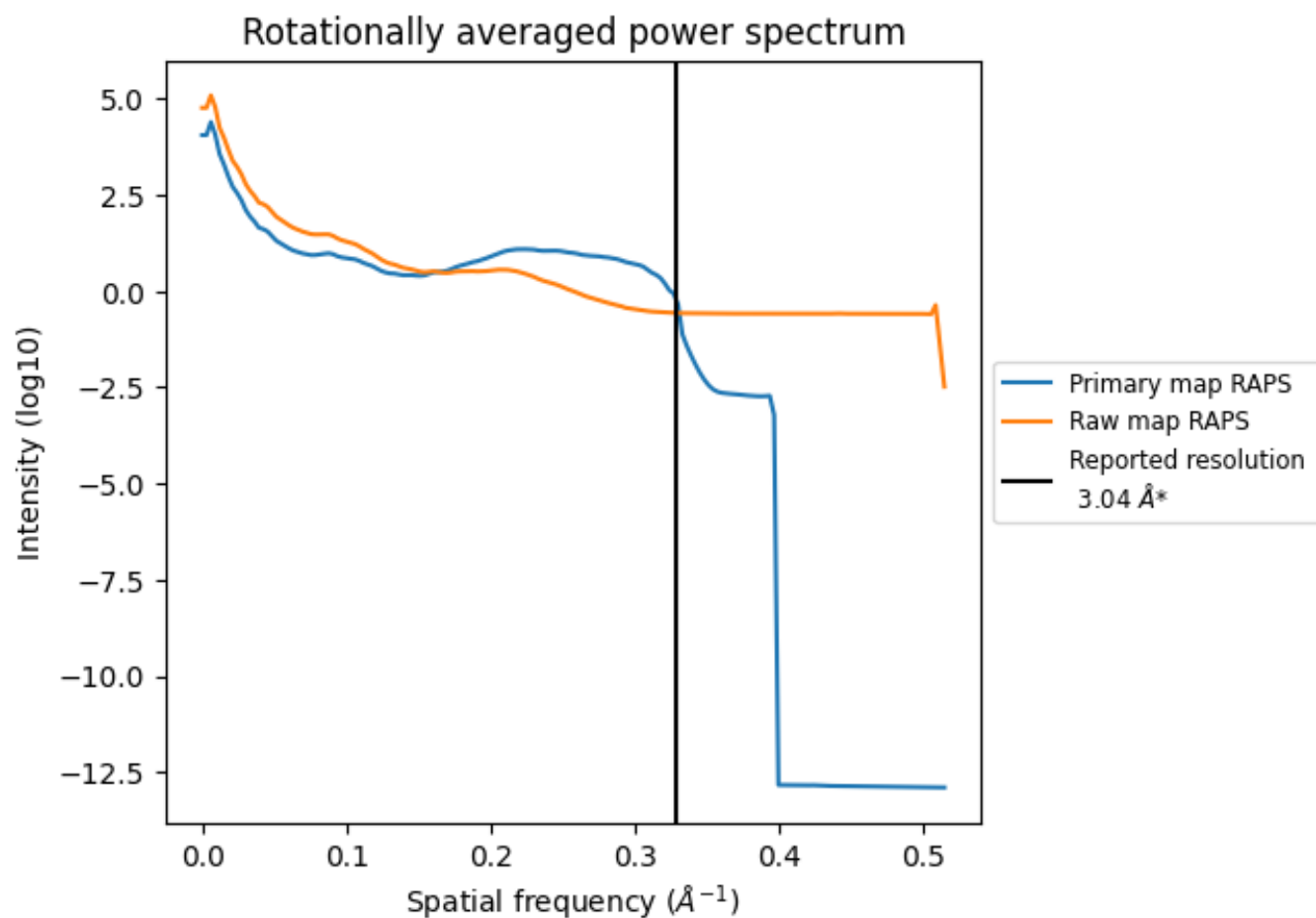
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm³; this corresponds to an approximate mass of 325 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 ⓘ

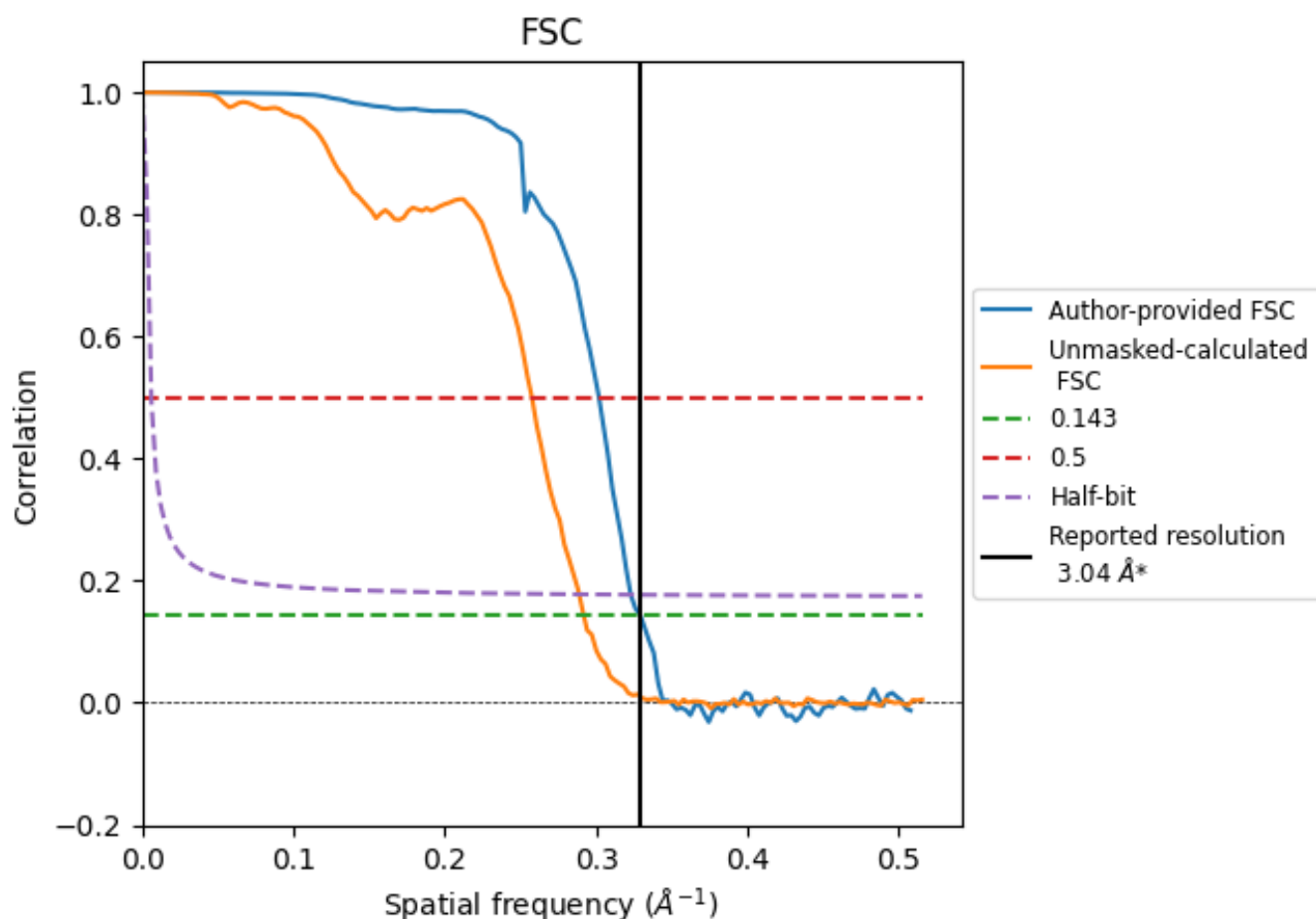


*Reported resolution corresponds to spatial frequency of $0.329 \text{ \AA}^{-1}$

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 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

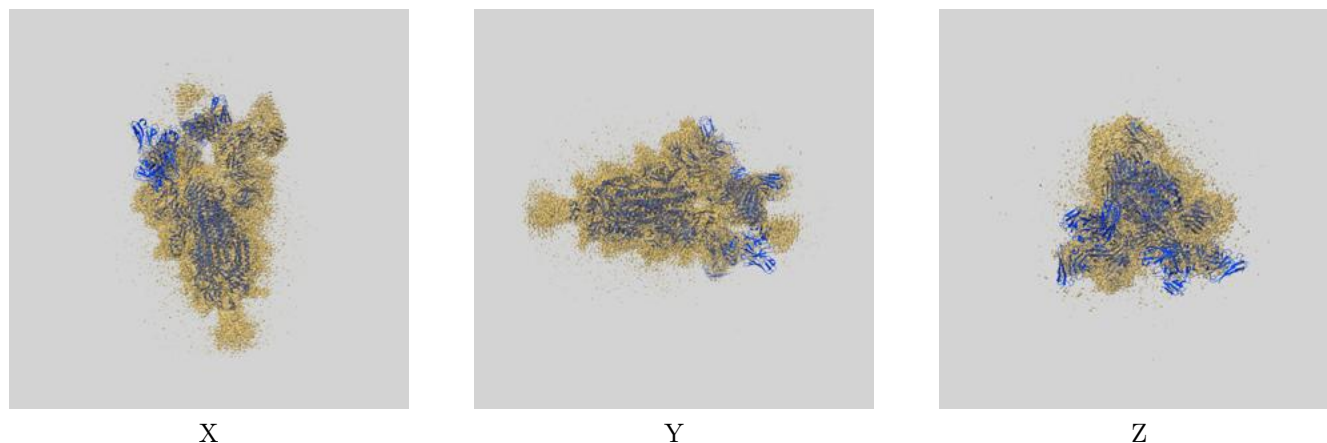
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.31	3.10
Unmasked-calculated*	3.43	3.88	3.46

*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 3.43 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

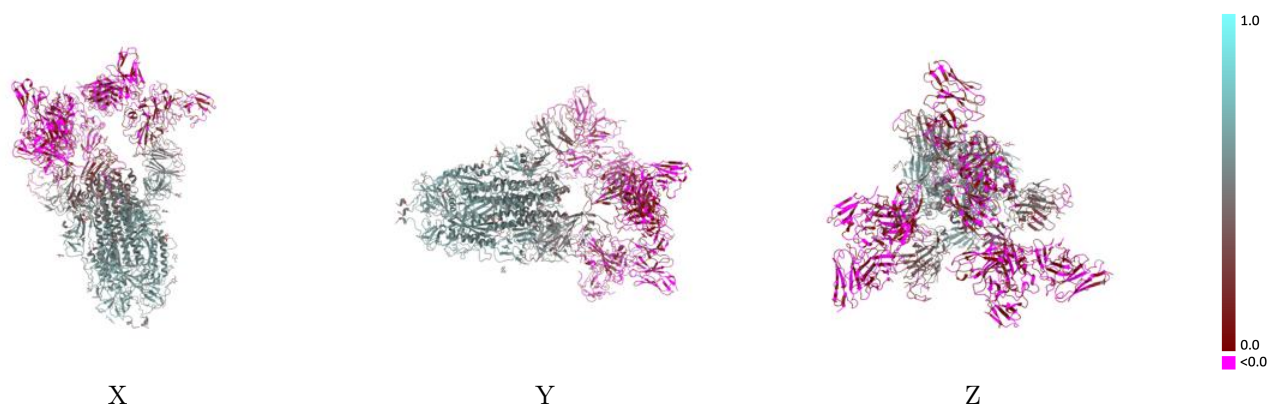
This section contains information regarding the fit between EMDB map EMD-33434 and PDB model 7XST. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



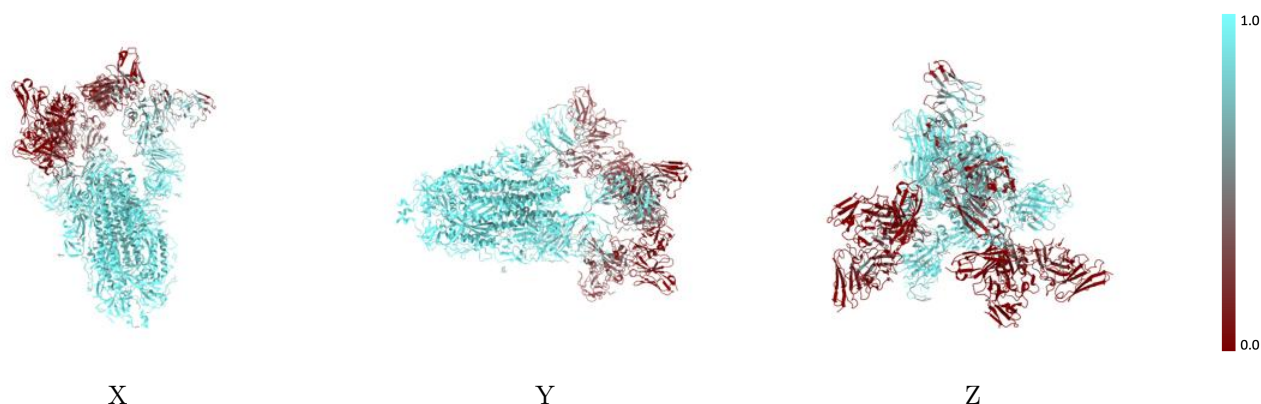
The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



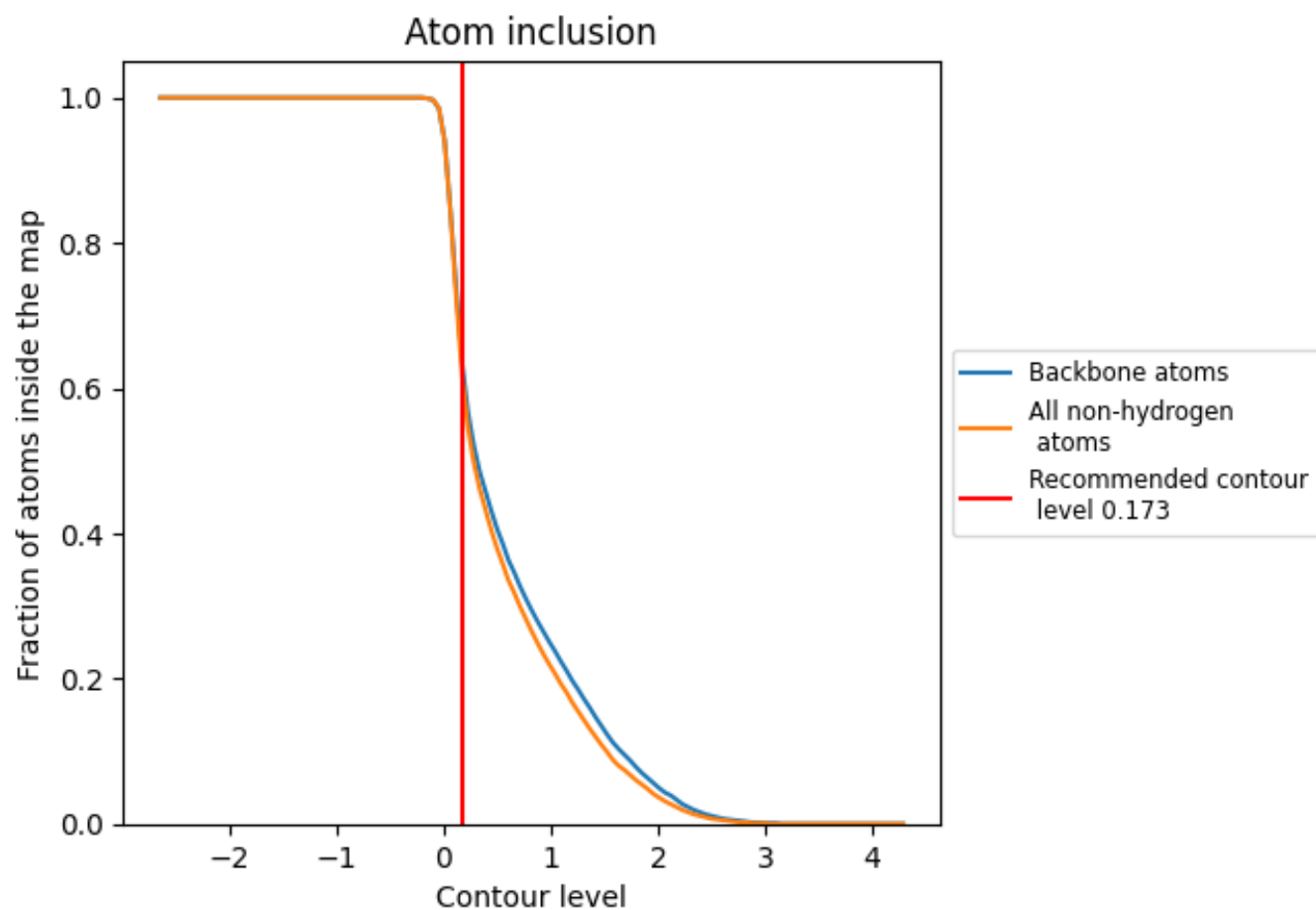
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.173).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 62% 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 (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.2990
A	0.8660	0.4230
B	0.8100	0.4230
C	0.7800	0.4020
D	0.2200	0.0310
E	0.1970	0.0170
F	0.5210	0.0900
G	0.5080	0.0780
H	0.0180	0.0410
I	0.0110	-0.0130
J	0.1620	0.0200
K	0.0600	0.0100
L	0.0130	0.0370
M	0.0050	0.0080
N	0.0740	0.0360
O	0.0120	0.0100

1.0

0.0

<0.0