



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:28 AM UTC

PDB ID : 8U1S / pdb_00008u1s
EMDB ID : EMD-41826
Title : A mechanistic understanding of protective influenza B neuraminidase mAbs at the airway interface
Authors : Ferguson, J.A.; Raghavan, S.S.R.; Ward, A.B.
Deposited on : 2023-09-02
Resolution : 3.21 Å(reported)
Based on initial model : .

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

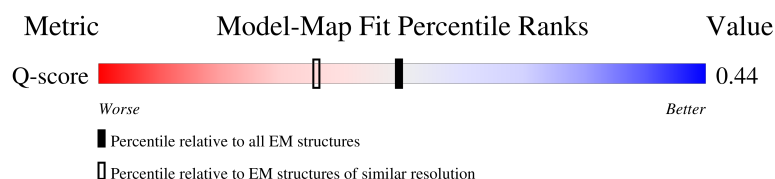
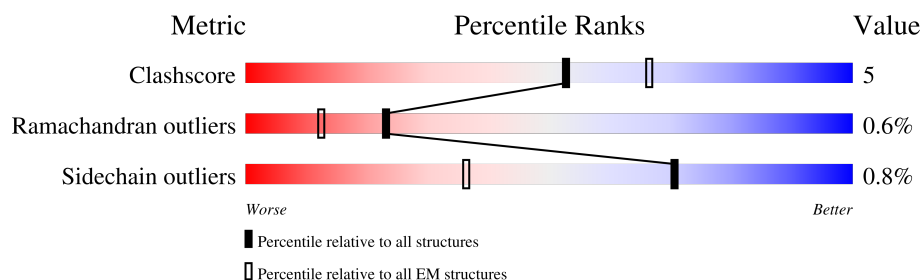
1 Overall quality at a glance

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.



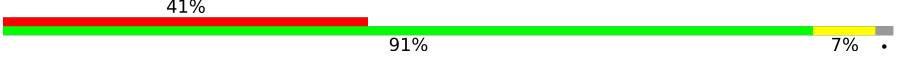
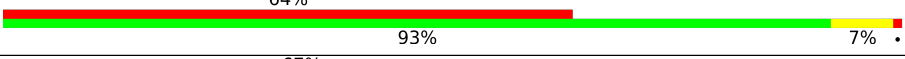
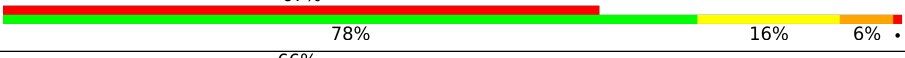
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

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	466	
1	B	466	
1	C	466	
1	D	466	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	123	
2	G	123	
2	H	123	
2	J	123	
3	F	107	
3	I	107	
3	K	107	
3	L	107	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17465 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 Neuraminidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	337	Total	C	N	O	S	0	0
			2613	1647	453	485	28		
1	B	331	Total	C	N	O	S	0	0
			2559	1610	442	479	28		
1	C	329	Total	C	N	O	S	0	0
			2548	1604	440	476	28		
1	D	332	Total	C	N	O	S	0	0
			2569	1619	443	479	28		

- Molecule 2 is a protein called mAb-393 heavy chain.

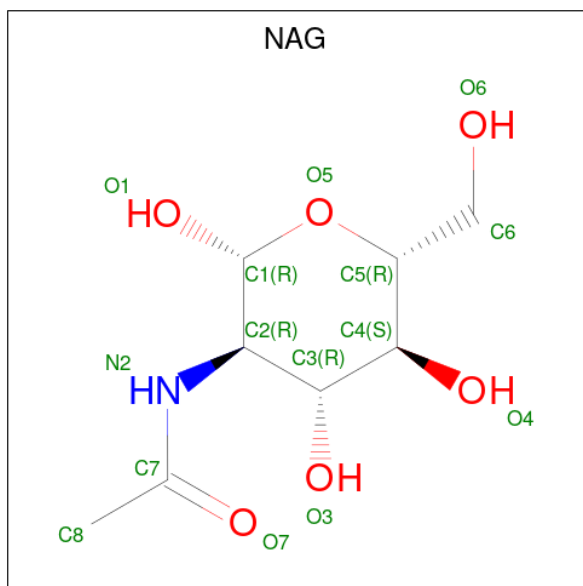
Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	121	Total	C	N	O	S	0	0
			949	607	161	179	2		
2	G	121	Total	C	N	O	S	0	0
			949	607	161	179	2		
2	E	121	Total	C	N	O	S	0	0
			949	607	161	179	2		
2	H	121	Total	C	N	O	S	0	0
			949	607	161	179	2		

- Molecule 3 is a protein called mAb-393 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	107	Total	C	N	O	S	0	0
			831	526	135	167	3		
3	I	107	Total	C	N	O	S	0	0
			831	526	135	167	3		
3	F	107	Total	C	N	O	S	0	0
			831	526	135	167	3		
3	L	107	Total	C	N	O	S	0	0
			831	526	135	167	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

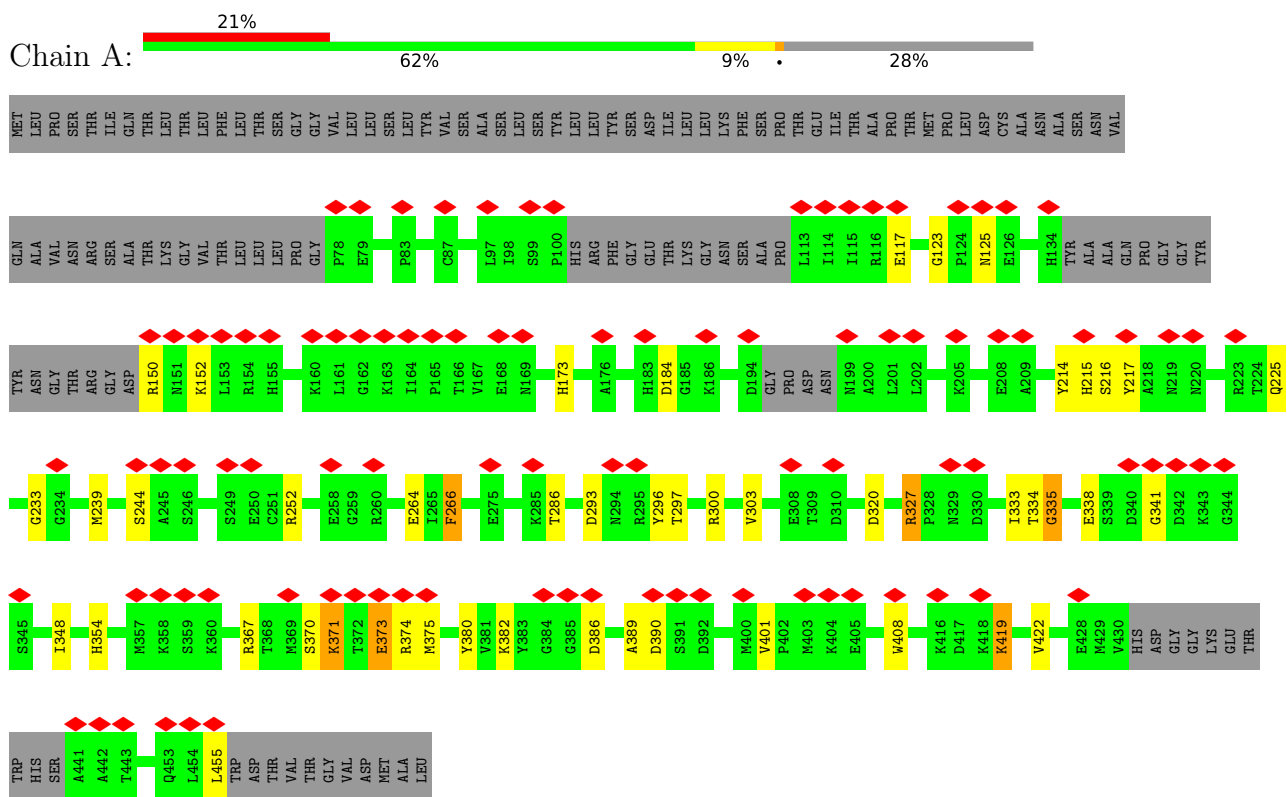


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

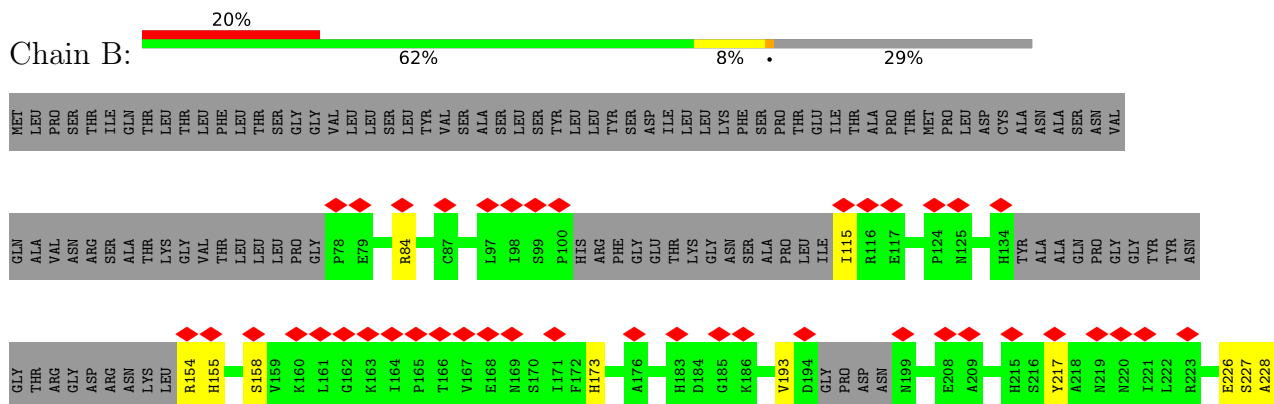
3 Residue-property plots

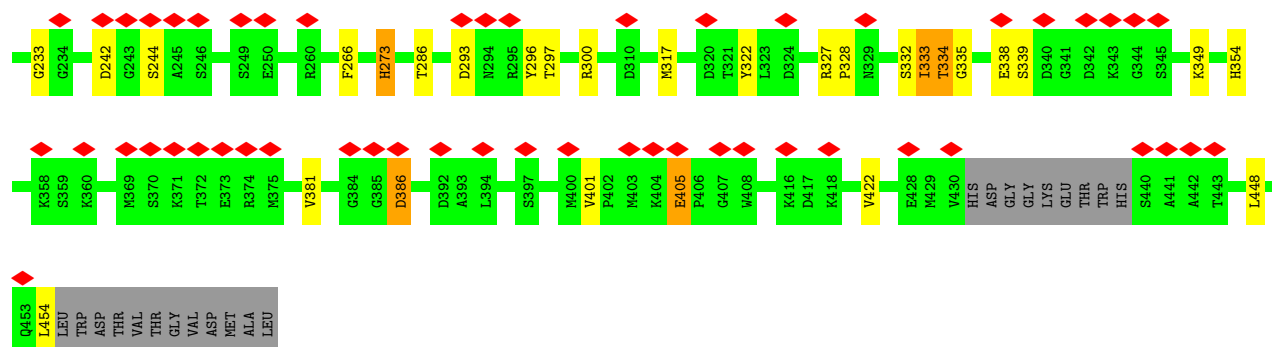
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Neuraminidase

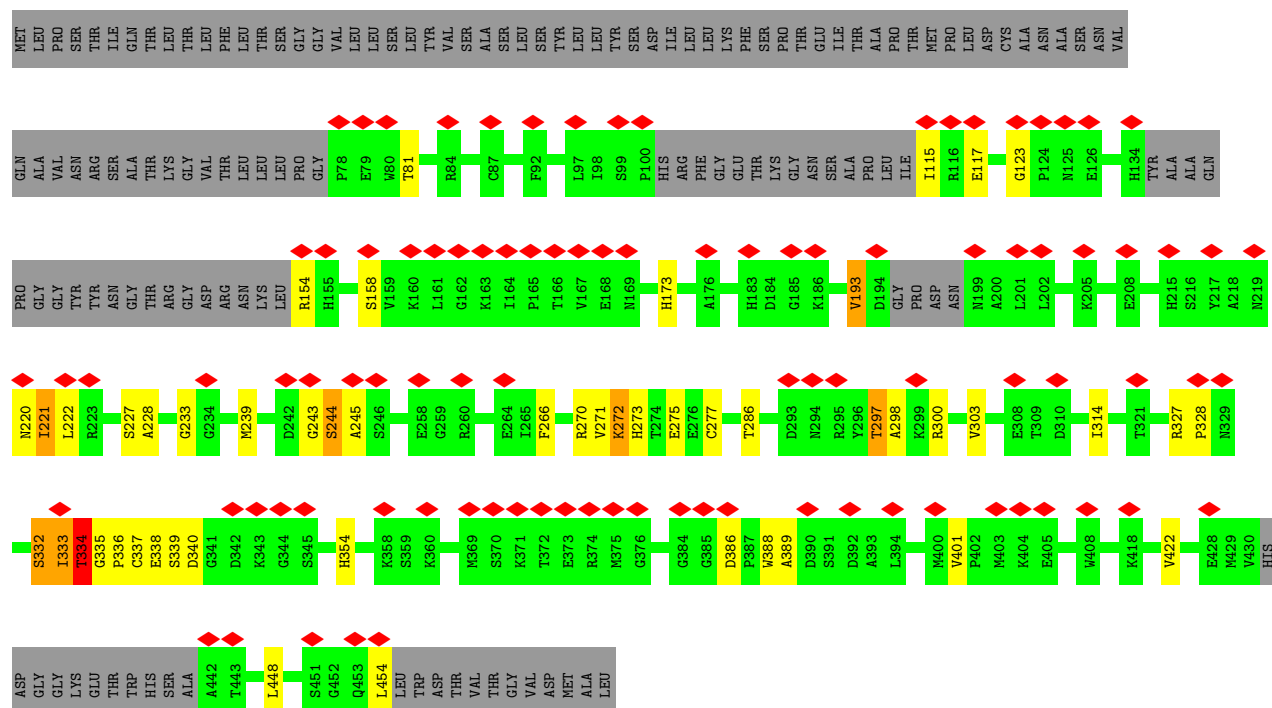


• Molecule 1: Neuraminidase

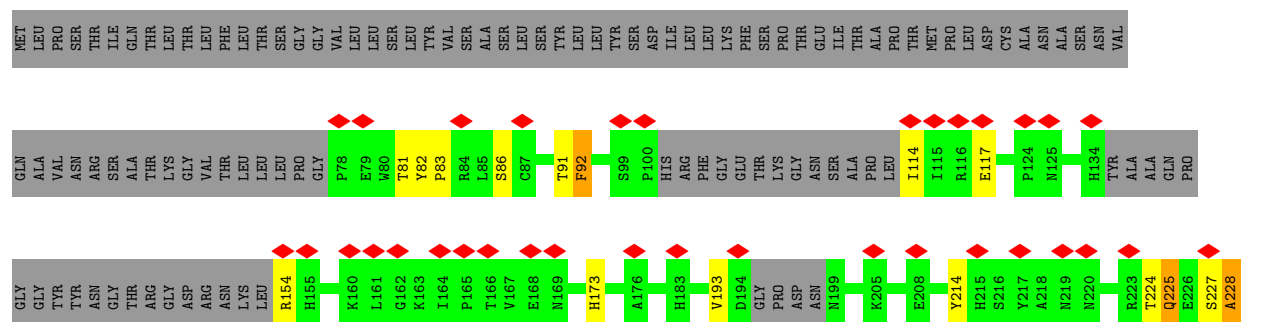


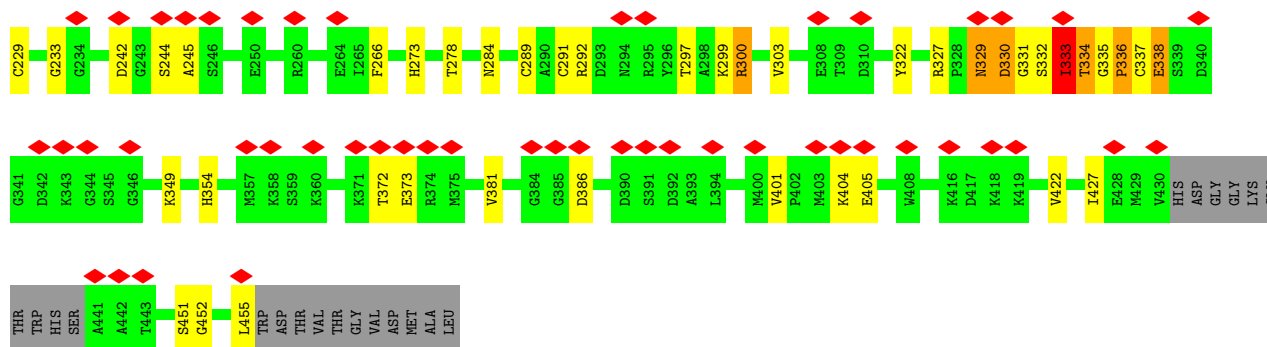


• Molecule 1: Neuraminidase



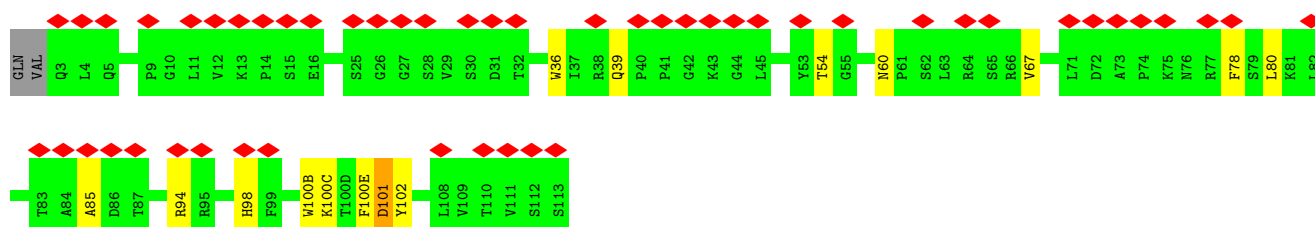
• Molecule 1: Neuraminidase





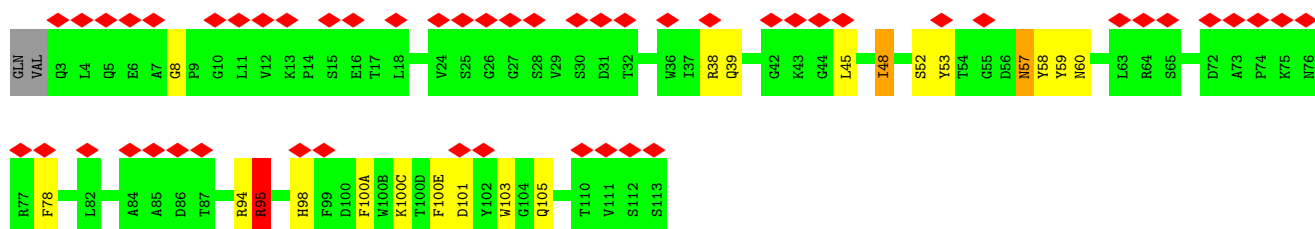
• Molecule 2: mAb-393 heavy chain

Chain J: 41% 86% 11% ..



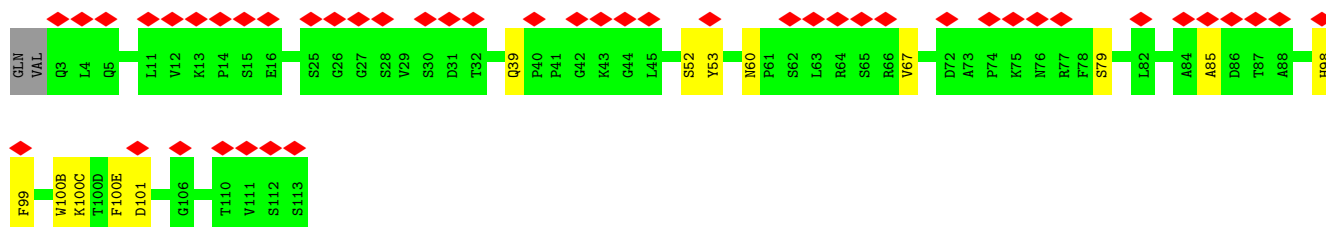
• Molecule 2: mAb-393 heavy chain

Chain G: 41% 81% 15% ...



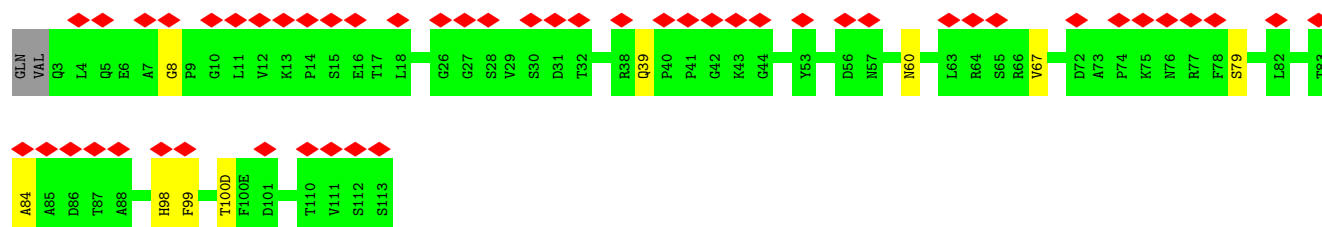
• Molecule 2: mAb-393 heavy chain

Chain E: 37% 88% 11% .

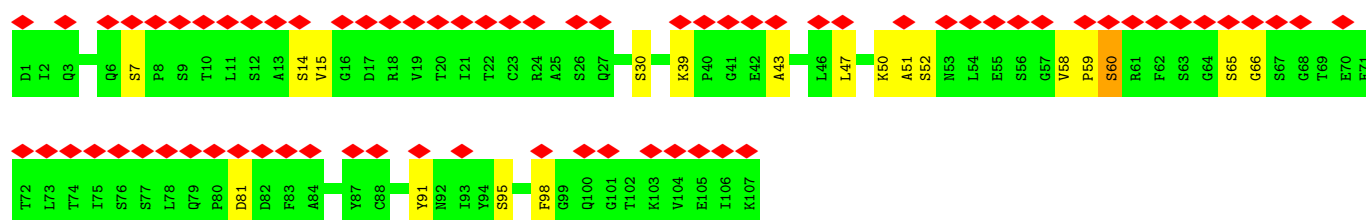
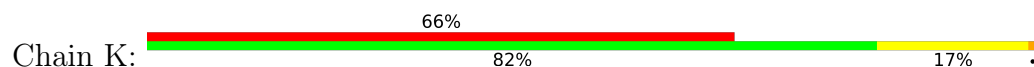


• Molecule 2: mAb-393 heavy chain

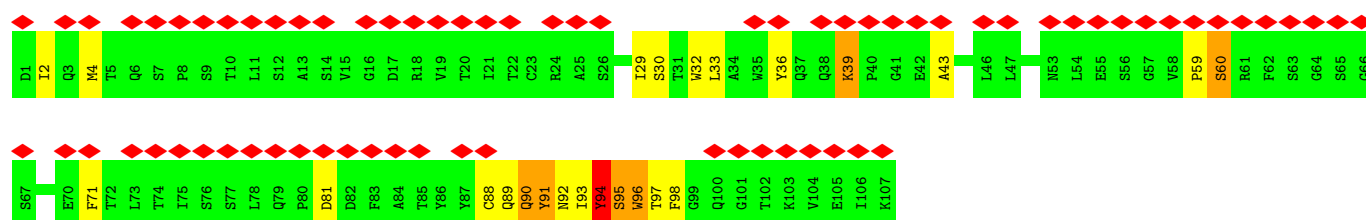
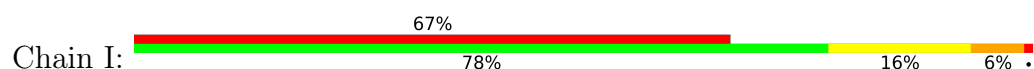
Chain H: 41% 91% 7% .



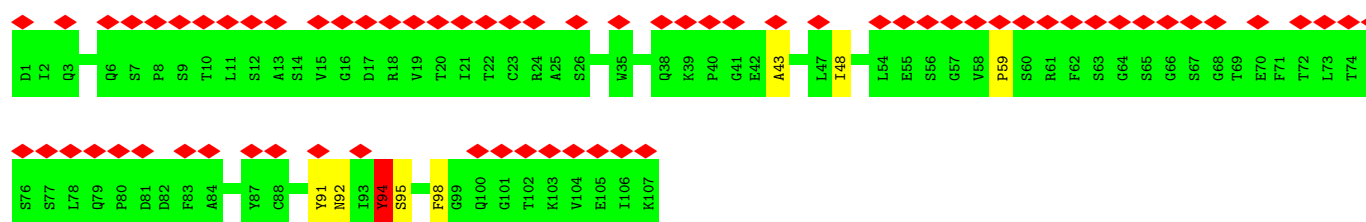
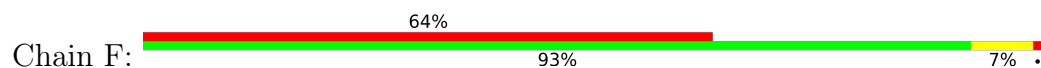
• Molecule 3: mAb-393 light chain



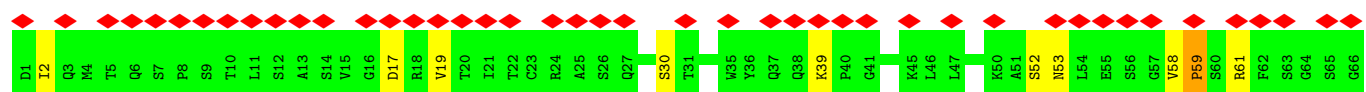
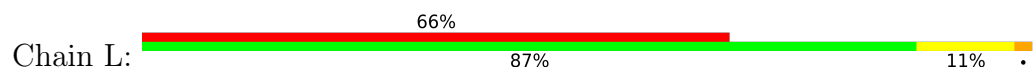
• Molecule 3: mAb-393 light chain

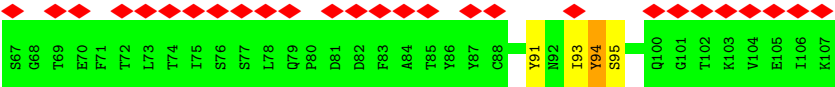


• Molecule 3: mAb-393 light chain



• Molecule 3: mAb-393 light chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.87	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	261.0, 261.0, 261.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

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	1.21	5/2670 (0.2%)	1.34	27/3596 (0.8%)
1	B	1.24	6/2616 (0.2%)	1.37	27/3524 (0.8%)
1	C	1.23	6/2605 (0.2%)	1.36	26/3509 (0.7%)
1	D	1.25	7/2626 (0.3%)	1.40	35/3538 (1.0%)
2	E	1.19	0/978	1.33	9/1334 (0.7%)
2	G	1.23	4/978 (0.4%)	1.42	11/1334 (0.8%)
2	H	1.13	0/978	1.33	9/1334 (0.7%)
2	J	1.23	1/978 (0.1%)	1.38	10/1334 (0.7%)
3	F	1.19	0/851	1.41	10/1157 (0.9%)
3	I	1.13	1/851 (0.1%)	1.32	6/1157 (0.5%)
3	K	1.22	1/851 (0.1%)	1.36	9/1157 (0.8%)
3	L	1.17	1/851 (0.1%)	1.34	10/1157 (0.9%)
All	All	1.21	32/17833 (0.2%)	1.36	189/24131 (0.8%)

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
1	D	0	1
2	G	0	1
All	All	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	HIS	CB-CG	-9.17	1.37	1.50
1	C	354	HIS	CB-CG	-9.07	1.37	1.50
1	A	354	HIS	CB-CG	-9.01	1.37	1.50
1	B	354	HIS	CB-CG	-8.60	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	454	LEU	CB-CG	7.29	1.68	1.53
1	B	154	ARG	NE-CZ	7.24	1.41	1.33
1	C	154	ARG	NE-CZ	7.00	1.40	1.33
1	C	115	ILE	CB-CG1	6.98	1.67	1.53
1	B	454	LEU	CB-CG	6.88	1.67	1.53
1	D	154	ARG	NE-CZ	6.46	1.40	1.33
1	A	150	ARG	NE-CZ	6.42	1.40	1.33
1	A	455	LEU	CB-CG	6.03	1.65	1.53
3	L	91	TYR	CB-CG	-6.00	1.38	1.51
1	D	455	LEU	CB-CG	6.00	1.65	1.53
2	G	103	TRP	NE1-CE2	-5.99	1.30	1.37
1	B	115	ILE	CB-CG1	5.96	1.65	1.53
1	D	273	HIS	CB-CG	-5.91	1.41	1.50
1	B	173	HIS	CB-CG	-5.69	1.42	1.50
1	A	173	HIS	CB-CG	-5.60	1.42	1.50
1	D	214	TYR	CB-CG	-5.47	1.39	1.51
1	D	114	ILE	CB-CG1	5.40	1.64	1.53
2	G	100(E)	PHE	CB-CG	-5.37	1.38	1.50
2	G	78	PHE	CB-CG	-5.25	1.38	1.50
3	K	47	LEU	CB-CG	-5.19	1.43	1.53
1	C	173	HIS	CB-CG	-5.19	1.42	1.50
2	J	78	PHE	CB-CG	-5.18	1.38	1.50
1	C	388	TRP	NE1-CE2	-5.12	1.31	1.37
1	A	214	TYR	CB-CG	-5.10	1.40	1.51
1	B	273	HIS	CB-CG	-5.04	1.43	1.50
3	I	32	TRP	NE1-CE2	-5.02	1.31	1.37
1	D	292	ARG	CD-NE	-5.02	1.39	1.46
2	G	78	PHE	CG-CD1	-5.01	1.28	1.38

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	59	PRO	CA-C-N	-11.49	99.32	122.31
3	F	59	PRO	C-N-CA	-11.49	99.32	122.31
3	F	94	TYR	N-CA-CB	10.99	125.19	110.25
3	K	95	SER	N-CA-C	-10.15	101.67	114.56
1	B	335	GLY	CA-C-N	8.23	128.12	120.21
1	B	335	GLY	C-N-CA	8.23	128.12	120.21
1	A	371	LYS	N-CA-C	-8.20	103.28	113.28
2	J	101	ASP	CA-CB-CG	8.07	120.67	112.60
2	J	54	THR	N-CA-C	-7.96	104.45	114.56
1	C	297	THR	N-CA-C	7.96	120.08	108.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	404	LYS	N-CA-C	-7.95	104.73	114.75
2	J	39	GLN	CA-C-N	7.86	125.39	119.66
2	J	39	GLN	C-N-CA	7.86	125.39	119.66
1	D	242	ASP	CA-CB-CG	7.63	120.23	112.60
1	C	275	GLU	N-CA-C	7.59	120.71	109.24
2	E	39	GLN	CA-C-N	7.46	125.11	119.66
2	E	39	GLN	C-N-CA	7.46	125.11	119.66
1	D	386	ASP	CA-C-N	7.44	127.15	119.56
1	D	386	ASP	C-N-CA	7.44	127.15	119.56
3	I	90	GLN	CB-CA-C	-7.38	100.11	112.00
1	A	401	VAL	CA-C-N	7.34	127.34	119.78
1	A	401	VAL	C-N-CA	7.34	127.34	119.78
1	C	401	VAL	CA-C-N	7.24	127.24	119.78
1	C	401	VAL	C-N-CA	7.24	127.24	119.78
3	I	94	TYR	N-CA-CB	7.23	120.72	110.24
3	L	58	VAL	CA-C-N	7.20	128.84	119.84
3	L	58	VAL	C-N-CA	7.20	128.84	119.84
2	H	39	GLN	CA-C-N	7.19	124.91	119.66
2	H	39	GLN	C-N-CA	7.19	124.91	119.66
1	B	300	ARG	CA-C-N	7.13	127.13	119.78
1	B	300	ARG	C-N-CA	7.13	127.13	119.78
1	A	335	GLY	CA-C-N	7.04	127.45	119.92
1	A	335	GLY	C-N-CA	7.04	127.45	119.92
2	G	57	ASN	CB-CA-C	-6.92	102.20	112.09
1	B	401	VAL	CA-C-N	6.86	127.26	119.92
1	B	401	VAL	C-N-CA	6.86	127.26	119.92
1	D	300	ARG	CA-C-N	6.85	126.83	119.78
1	D	300	ARG	C-N-CA	6.85	126.83	119.78
2	E	100(E)	PHE	N-CA-C	-6.83	97.21	108.07
1	D	336	PRO	N-CA-C	-6.83	101.67	111.22
2	G	39	GLN	CA-C-N	6.79	124.61	119.66
2	G	39	GLN	C-N-CA	6.79	124.61	119.66
1	D	81	THR	CB-CA-C	-6.75	101.13	112.00
2	G	48	ILE	N-CA-C	-6.74	105.15	111.48
1	C	233	GLY	N-CA-C	-6.66	99.64	112.02
1	A	327	ARG	CA-C-N	6.59	127.04	120.52
1	A	327	ARG	C-N-CA	6.59	127.04	120.52
1	C	81	THR	CB-CA-C	-6.46	101.59	112.00
1	A	296	TYR	N-CA-C	6.41	121.23	113.41
1	A	386	ASP	CA-C-N	6.39	126.08	119.56
1	A	386	ASP	C-N-CA	6.39	126.08	119.56
2	J	60	ASN	CA-C-N	6.38	126.07	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	60	ASN	C-N-CA	6.38	126.07	119.56
3	L	94	TYR	N-CA-CB	6.37	119.63	110.45
3	F	94	TYR	CA-CB-CG	-6.37	102.43	113.90
1	B	327	ARG	CA-C-N	6.37	126.82	120.52
1	B	327	ARG	C-N-CA	6.37	126.82	120.52
1	C	193	VAL	N-CA-C	6.36	117.93	108.46
1	B	233	GLY	N-CA-C	-6.32	100.59	111.47
1	D	327	ARG	CA-C-N	6.32	126.78	120.52
1	D	327	ARG	C-N-CA	6.32	126.78	120.52
1	D	233	GLY	N-CA-C	-6.30	100.29	112.02
2	H	60	ASN	CA-C-N	6.29	125.98	119.56
2	H	60	ASN	C-N-CA	6.29	125.98	119.56
1	D	225	GLN	CB-CA-C	-6.27	100.64	111.30
3	K	98	PHE	CA-CB-CG	6.25	120.05	113.80
2	J	98	HIS	CA-CB-CG	6.25	120.05	113.80
3	L	39	LYS	N-CA-C	-6.21	102.23	109.93
1	D	173	HIS	CA-CB-CG	-6.20	107.61	113.80
1	A	297	THR	N-CA-C	6.19	118.25	108.79
2	E	67	VAL	N-CA-C	6.16	117.63	108.46
3	I	39	LYS	N-CA-C	-6.14	102.31	109.93
1	B	193	VAL	N-CA-C	6.12	116.67	108.11
1	D	329	ASN	N-CA-C	-6.11	101.91	110.35
1	C	327	ARG	CA-C-N	6.09	127.50	120.98
1	C	327	ARG	C-N-CA	6.09	127.50	120.98
2	H	67	VAL	N-CA-C	6.08	117.52	108.46
3	F	43	ALA	CA-C-N	6.08	126.02	119.76
3	F	43	ALA	C-N-CA	6.08	126.02	119.76
1	B	293	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	300	ARG	CA-C-N	6.05	125.96	119.85
1	A	300	ARG	C-N-CA	6.05	125.96	119.85
1	A	117	GLU	CA-C-N	6.04	126.01	120.03
1	A	117	GLU	C-N-CA	6.04	126.01	120.03
3	L	17	ASP	CA-CB-CG	6.03	118.63	112.60
1	D	401	VAL	CA-C-N	6.03	125.99	119.78
1	D	401	VAL	C-N-CA	6.03	125.99	119.78
1	D	86	SER	CA-C-N	6.03	128.74	120.67
1	D	86	SER	C-N-CA	6.03	128.74	120.67
1	A	286	THR	N-CA-C	5.96	118.17	108.76
1	B	381	VAL	N-CA-C	5.94	117.25	108.45
1	C	340	ASP	CA-CB-CG	5.92	118.52	112.60
3	K	43	ALA	CA-C-N	5.91	125.82	119.85
3	K	43	ALA	C-N-CA	5.91	125.82	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	30	SER	CB-CA-C	-5.90	109.75	116.54
1	D	427	ILE	N-CA-C	5.84	115.53	108.06
1	A	266	PHE	CA-C-N	5.83	125.81	120.03
1	A	266	PHE	C-N-CA	5.83	125.81	120.03
2	E	101	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	286	THR	N-CA-C	5.83	117.38	108.52
1	C	123	GLY	CA-C-N	5.82	126.22	119.47
1	C	123	GLY	C-N-CA	5.82	126.22	119.47
2	J	67	VAL	N-CA-C	5.75	116.76	108.48
1	B	339	SER	N-CA-C	5.75	118.31	110.55
3	I	30	SER	CB-CA-C	-5.74	109.97	116.63
1	D	193	VAL	N-CA-C	5.73	117.00	108.46
1	B	266	PHE	CA-C-N	5.72	125.69	120.03
1	B	266	PHE	C-N-CA	5.72	125.69	120.03
2	E	60	ASN	CA-C-N	5.70	126.08	119.47
2	E	60	ASN	C-N-CA	5.70	126.08	119.47
3	I	43	ALA	CA-C-N	5.66	125.59	119.76
3	I	43	ALA	C-N-CA	5.66	125.59	119.76
3	K	51	ALA	CA-C-N	5.66	132.35	121.54
3	K	51	ALA	C-N-CA	5.66	132.35	121.54
2	H	8	GLY	CA-C-N	5.66	125.59	119.76
2	H	8	GLY	C-N-CA	5.66	125.59	119.76
3	K	58	VAL	N-CA-C	-5.65	103.77	108.63
1	B	405	GLU	CA-C-N	5.63	126.88	119.84
1	B	405	GLU	C-N-CA	5.63	126.88	119.84
1	C	300	ARG	CA-C-N	5.62	125.55	119.76
1	C	300	ARG	C-N-CA	5.62	125.55	119.76
2	J	100(E)	PHE	N-CA-C	-5.61	99.11	108.32
2	G	100(E)	PHE	N-CA-C	-5.61	98.85	110.80
1	A	233	GLY	N-CA-C	-5.61	101.83	111.47
2	G	8	GLY	CA-C-N	5.60	125.88	119.83
2	G	8	GLY	C-N-CA	5.60	125.88	119.83
1	D	297	THR	N-CA-C	5.60	117.61	108.76
1	D	266	PHE	CA-C-N	5.58	125.49	119.85
1	D	266	PHE	C-N-CA	5.58	125.49	119.85
1	D	117	GLU	CA-C-N	5.54	125.45	119.85
1	D	117	GLU	C-N-CA	5.54	125.45	119.85
1	A	422	VAL	CB-CA-C	-5.53	104.82	111.18
1	C	266	PHE	CA-C-N	5.51	125.41	119.85
1	C	266	PHE	C-N-CA	5.51	125.41	119.85
1	B	386	ASP	CA-C-N	5.50	126.71	119.84
1	B	386	ASP	C-N-CA	5.50	126.71	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	VAL	N-CA-C	5.49	113.47	107.60
2	E	79	SER	N-CA-C	5.47	117.50	109.24
2	H	100(D)	THR	CB-CA-C	-5.46	102.75	111.17
2	G	98	HIS	CA-CB-CG	5.46	119.26	113.80
1	C	286	THR	N-CA-C	5.45	117.38	108.76
3	K	7	SER	N-CA-C	5.44	112.91	108.07
3	L	59	PRO	N-CA-C	5.44	123.68	112.47
1	A	123	GLY	CA-C-N	5.44	125.78	119.47
1	A	123	GLY	C-N-CA	5.44	125.78	119.47
1	C	386	ASP	CA-C-N	5.42	126.62	119.84
1	C	386	ASP	C-N-CA	5.42	126.62	119.84
2	H	79	SER	N-CA-C	5.42	117.63	109.23
2	E	85	ALA	N-CA-C	-5.41	106.66	113.20
1	B	297	THR	N-CA-C	5.41	117.06	108.79
1	C	314	ILE	N-CA-C	5.41	115.68	108.11
1	D	381	VAL	N-CA-C	5.40	116.44	108.45
1	A	293	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	228	ALA	CA-C-N	5.38	129.77	122.19
1	D	228	ALA	C-N-CA	5.38	129.77	122.19
1	D	92	PHE	CA-CB-CG	5.36	119.16	113.80
1	B	422	VAL	N-CA-C	5.32	113.29	107.60
2	G	101	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	82	TYR	CA-C-N	5.30	125.20	119.85
1	D	82	TYR	C-N-CA	5.30	125.20	119.85
1	C	158	SER	N-CA-C	5.29	117.12	109.07
1	C	422	VAL	CB-CA-C	-5.28	105.10	111.18
3	F	94	TYR	CA-C-N	-5.26	114.98	122.93
3	F	94	TYR	C-N-CA	-5.26	114.98	122.93
3	F	98	PHE	CA-CB-CG	5.22	119.02	113.80
1	D	422	VAL	CB-CA-C	-5.22	105.18	111.18
1	C	117	GLU	CA-C-N	5.20	125.18	120.03
1	C	117	GLU	C-N-CA	5.20	125.18	120.03
1	B	317	MET	N-CA-C	-5.18	102.71	110.23
1	A	225	GLN	CB-CA-C	-5.18	102.07	109.84
1	D	229	CYS	CB-CA-C	5.17	118.28	109.80
3	L	94	TYR	CA-CB-CG	-5.17	104.59	113.90
2	J	85	ALA	N-CA-C	-5.16	106.96	113.20
1	A	239	MET	CG-SD-CE	5.13	112.19	100.90
2	G	60	ASN	CA-C-N	5.12	125.41	119.47
2	G	60	ASN	C-N-CA	5.12	125.41	119.47
1	B	296	TYR	N-CA-C	5.11	119.64	113.41
1	B	158	SER	N-CA-C	5.09	116.80	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	30	SER	CB-CA-C	-5.08	110.70	116.54
1	C	303	VAL	CB-CA-C	-5.05	103.97	110.84
3	F	48	ILE	N-CA-C	5.05	115.75	108.48
1	C	448	LEU	CB-CA-C	-5.03	103.78	111.83
1	B	155	HIS	N-CA-C	5.03	117.03	109.23
1	D	405	GLU	CA-C-N	5.02	124.92	119.85
1	D	405	GLU	C-N-CA	5.02	124.92	119.85
3	L	19	VAL	N-CA-C	5.02	115.19	108.17
1	A	303	VAL	CB-CA-C	-5.01	104.02	110.84
3	L	61	ARG	N-CA-C	-5.01	107.02	113.23
1	B	448	LEU	CB-CA-C	-5.00	103.94	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	330	ASP	Mainchain
2	G	95	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2613	0	2556	39	0
1	B	2559	0	2487	16	0
1	C	2548	0	2477	32	0
1	D	2569	0	2504	28	0
2	E	949	0	911	4	0
2	G	949	0	911	17	0
2	H	949	0	911	1	0
2	J	949	0	911	7	0
3	F	831	0	803	8	0
3	I	831	0	803	44	0
3	K	831	0	803	13	0
3	L	831	0	803	14	0
4	A	14	0	13	0	0
4	B	14	0	13	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	0	0
4	D	14	0	13	0	0
All	All	17465	0	16932	183	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 5.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:TYR:CE2	1:C:338:GLU:OE1	1.75	1.37
1:A:338:GLU:OE1	3:L:94:TYR:HE1	1.05	1.28
3:I:94:TYR:HE2	1:C:338:GLU:OE1	1.08	1.22
1:A:338:GLU:OE1	3:L:94:TYR:CE1	1.96	1.19
3:I:93:ILE:HD12	1:C:389:ALA:CB	1.71	1.18
1:A:348:ILE:CD1	1:A:374:ARG:HD3	1.78	1.13
1:A:252:ARG:HD3	1:A:266:PHE:CE2	1.84	1.12
1:A:348:ILE:HD12	1:A:374:ARG:HD3	1.27	1.12
3:I:93:ILE:HD12	1:C:389:ALA:HB2	1.30	1.10
2:J:101:ASP:OD1	2:J:102:TYR:CD2	2.08	1.06
1:A:348:ILE:HD12	1:A:374:ARG:CD	1.87	1.04
3:I:94:TYR:HE2	1:C:338:GLU:CD	1.65	1.04
1:B:84:ARG:HA	4:B:501:NAG:H62	1.36	1.03
3:I:93:ILE:CD1	1:C:389:ALA:HB2	1.90	1.00
3:I:89:GLN:OE1	3:I:98:PHE:CZ	2.17	0.96
3:I:94:TYR:CE2	1:C:338:GLU:CD	2.40	0.96
3:I:89:GLN:OE1	3:I:98:PHE:CE1	2.17	0.95
3:I:94:TYR:CD2	1:C:338:GLU:OE1	2.22	0.93
3:L:2:ILE:HG13	3:L:93:ILE:HD11	1.50	0.91
3:I:93:ILE:HD12	1:C:389:ALA:HB1	1.52	0.87
1:A:252:ARG:HD3	1:A:266:PHE:CZ	2.11	0.86
3:L:2:ILE:CD1	3:L:93:ILE:HD11	2.05	0.85
2:J:101:ASP:OD1	2:J:102:TYR:HD2	1.61	0.84
3:L:2:ILE:CG1	3:L:93:ILE:HD11	2.08	0.82
1:A:348:ILE:HD12	1:A:374:ARG:NE	1.95	0.80
1:C:220:ASN:HD22	1:C:243:GLY:C	1.90	0.79
2:G:100(C):LYS:HE2	3:I:89:GLN:HE21	1.49	0.78
2:G:100(C):LYS:CE	3:I:89:GLN:HE21	2.00	0.73
3:L:2:ILE:CD1	3:L:93:ILE:CD1	2.66	0.73
1:A:348:ILE:HD12	1:A:374:ARG:CZ	2.19	0.73
1:D:332:SER:O	1:D:333:ILE:C	2.32	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:VAL:HG21	1:C:222:LEU:HB3	1.71	0.71
1:B:328:PRO:HB2	1:B:332:SER:OG	1.91	0.70
3:K:91:TYR:CD2	1:D:336:PRO:HB3	2.27	0.70
1:C:220:ASN:ND2	1:C:243:GLY:O	2.24	0.69
1:A:217:TYR:HB2	1:A:252:ARG:HH22	1.57	0.69
3:I:4:MET:SD	3:I:90:GLN:NE2	2.66	0.68
2:G:57:ASN:HB3	2:G:59:TYR:HE1	1.60	0.67
2:G:100(C):LYS:HE2	3:I:89:GLN:NE2	2.08	0.67
1:A:252:ARG:CD	1:A:266:PHE:CZ	2.78	0.66
1:A:348:ILE:HD13	1:A:374:ARG:HD3	1.75	0.65
1:A:389:ALA:HB1	3:L:93:ILE:HG21	1.78	0.65
3:I:95:SER:O	3:I:97:THR:N	2.29	0.65
3:I:29:ILE:CD1	3:I:90:GLN:HB3	2.26	0.65
3:L:94:TYR:O	3:L:95:SER:OG	2.13	0.65
1:C:333:ILE:HD11	1:C:339:SER:OG	1.96	0.65
1:D:333:ILE:O	1:D:334:THR:C	2.39	0.65
3:I:94:TYR:CE2	1:C:338:GLU:OE2	2.49	0.65
1:A:374:ARG:HH11	1:A:408:TRP:HE3	1.40	0.65
3:I:29:ILE:HD11	3:I:90:GLN:HB3	1.79	0.64
1:B:217:TYR:OH	1:B:242:ASP:N	2.29	0.64
2:J:100(B):TRP:NE1	1:D:334:THR:O	2.30	0.64
1:C:271:VAL:O	1:C:272:LYS:C	2.40	0.63
1:A:217:TYR:CD2	1:A:252:ARG:NH1	2.66	0.63
1:C:333:ILE:HD13	1:C:335:GLY:H	1.61	0.63
1:A:374:ARG:HD2	1:A:408:TRP:CE3	2.34	0.62
3:L:2:ILE:HD11	3:L:93:ILE:CD1	2.29	0.62
3:F:94:TYR:HD1	3:F:95:SER:H	1.48	0.61
1:D:336:PRO:O	1:D:337:CYS:C	2.43	0.61
1:C:245:ALA:HA	1:C:273:HIS:NE2	2.15	0.61
3:K:91:TYR:HE2	1:D:336:PRO:HD3	1.66	0.61
1:D:332:SER:OG	1:D:333:ILE:N	2.34	0.60
3:I:93:ILE:CD1	1:C:389:ALA:CB	2.56	0.60
1:A:217:TYR:CG	1:A:252:ARG:NH1	2.70	0.59
1:A:374:ARG:NH1	1:A:408:TRP:CZ3	2.71	0.59
3:I:90:GLN:O	3:I:92:ASN:N	2.36	0.58
2:G:94:ARG:HG2	2:G:95:ARG:H	1.68	0.58
3:I:36:TYR:OH	3:I:89:GLN:NE2	2.36	0.58
1:D:278:THR:OG1	1:D:349:LYS:NZ	2.36	0.58
1:A:373:GLU:HB2	1:A:375:MET:HG2	1.85	0.57
1:A:419:LYS:HA	1:A:419:LYS:HE2	1.87	0.57
1:B:322:TYR:OH	1:B:333:ILE:HG12	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ARG:HD2	2:G:48:ILE:HD11	1.86	0.56
1:A:338:GLU:CD	3:L:94:TYR:HE1	2.02	0.56
1:A:252:ARG:CD	1:A:266:PHE:CE2	2.75	0.55
2:G:100(C):LYS:CE	3:I:89:GLN:NE2	2.67	0.55
1:C:221:ILE:HD12	1:C:244:SER:HA	1.89	0.55
3:I:4:MET:HE2	3:I:88:CYS:HB3	1.89	0.55
1:C:335:GLY:HA3	1:C:339:SER:HB3	1.88	0.55
3:L:2:ILE:HD11	3:L:93:ILE:HD13	1.88	0.55
3:I:89:GLN:HB3	3:I:98:PHE:CD1	2.42	0.54
3:I:95:SER:O	3:I:96:TRP:C	2.49	0.54
1:C:297:THR:OG1	1:C:298:ALA:N	2.38	0.54
1:A:382:LYS:NZ	1:A:390:ASP:OD2	2.38	0.54
3:F:94:TYR:HD1	3:F:95:SER:N	2.06	0.54
1:A:252:ARG:HD2	1:A:264:GLU:HG2	1.90	0.53
3:I:91:TYR:CZ	1:C:336:PRO:HG3	2.43	0.53
1:D:333:ILE:C	1:D:335:GLY:N	2.64	0.53
3:K:39:LYS:NZ	3:K:81:ASP:O	2.42	0.53
2:G:57:ASN:HB3	2:G:59:TYR:CE1	2.40	0.53
3:I:2:ILE:HB	3:I:90:GLN:HG3	1.91	0.52
2:J:94:ARG:NH2	2:J:102:TYR:CE2	2.78	0.51
3:K:91:TYR:CE2	1:D:336:PRO:HD3	2.45	0.51
2:G:100(A):PHE:O	3:I:91:TYR:OH	2.22	0.51
1:C:227:SER:OG	1:C:228:ALA:N	2.44	0.51
1:D:299:LYS:NZ	1:D:333:ILE:HG23	2.25	0.50
1:A:152:LYS:NZ	1:B:405:GLU:OE2	2.45	0.50
3:L:52:SER:OG	3:L:53:ASN:N	2.44	0.49
2:E:100(B):TRP:NE1	1:B:334:THR:O	2.44	0.49
3:I:36:TYR:CE1	3:I:98:PHE:HE1	2.30	0.49
3:F:92:ASN:OD1	3:F:92:ASN:N	2.44	0.49
2:E:98:HIS:O	2:E:99:PHE:C	2.56	0.49
1:B:226:GLU:O	1:B:349:LYS:NZ	2.45	0.49
3:K:59:PRO:O	3:K:60:SER:HB3	2.12	0.49
1:D:291:CYS:O	1:D:300:ARG:HG3	2.13	0.49
2:G:58:TYR:OH	1:C:270:ARG:HB2	2.12	0.48
1:D:227:SER:OG	1:D:228:ALA:N	2.46	0.48
1:D:322:TYR:CE2	1:D:332:SER:HB3	2.47	0.48
1:D:332:SER:C	1:D:333:ILE:HG13	2.37	0.48
3:K:50:LYS:C	3:K:52:SER:H	2.22	0.48
1:C:335:GLY:HA3	1:C:339:SER:CB	2.44	0.48
3:I:91:TYR:HE1	3:I:96:TRP:CZ2	2.31	0.47
1:A:333:ILE:HD13	1:A:341:GLY:HA3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:94:TYR:O	3:F:95:SER:HB2	2.15	0.47
3:K:14:SER:OG	3:K:15:VAL:N	2.47	0.46
3:I:59:PRO:O	3:I:60:SER:HB3	2.14	0.46
1:D:224:THR:OG1	1:D:225:GLN:N	2.48	0.46
1:A:374:ARG:HD2	1:A:408:TRP:CZ3	2.50	0.46
3:L:2:ILE:HD12	3:L:93:ILE:HD11	1.92	0.46
1:C:335:GLY:O	1:C:337:CYS:N	2.40	0.46
1:D:91:THR:OG1	1:D:92:PHE:N	2.48	0.45
3:F:94:TYR:HE2	1:B:338:GLU:OE2	2.00	0.45
3:K:91:TYR:CE2	1:D:336:PRO:HG3	2.52	0.44
1:D:333:ILE:HD12	1:D:334:THR:H	1.82	0.44
3:F:94:TYR:CD1	3:F:95:SER:N	2.82	0.44
2:G:105:GLN:H	2:G:105:GLN:CD	2.26	0.44
3:I:33:LEU:HD22	3:I:71:PHE:CD1	2.53	0.44
3:I:91:TYR:CE1	3:I:96:TRP:CZ2	3.06	0.44
3:I:91:TYR:CE2	1:C:336:PRO:HG3	2.53	0.44
1:D:451:SER:OG	1:D:452:GLY:N	2.50	0.44
1:A:333:ILE:O	1:A:335:GLY:N	2.49	0.43
1:A:367:ARG:NH2	1:A:380:TYR:OH	2.51	0.43
2:G:100(C):LYS:HD3	3:I:91:TYR:CG	2.53	0.43
2:G:52:SER:OG	2:G:53:TYR:N	2.48	0.43
2:E:100(C):LYS:HD3	3:F:91:TYR:CG	2.52	0.43
3:K:50:LYS:O	3:K:50:LYS:HG2	2.19	0.43
3:K:65:SER:OG	3:K:66:GLY:N	2.51	0.43
3:K:91:TYR:CE2	1:D:336:PRO:CG	3.01	0.43
2:G:105:GLN:CD	2:G:105:GLN:N	2.76	0.43
1:A:370:SER:HB3	1:A:373:GLU:O	2.19	0.43
2:G:100(C):LYS:HE3	3:I:89:GLN:HE21	1.79	0.43
1:D:289:CYS:HB2	1:D:303:VAL:CG1	2.49	0.43
1:D:330:ASP:OD1	1:D:330:ASP:N	2.42	0.43
3:F:94:TYR:CE2	1:B:338:GLU:CD	2.97	0.42
1:B:322:TYR:HH	1:B:333:ILE:HG12	1.84	0.42
3:I:29:ILE:HD13	3:I:90:GLN:HB3	2.00	0.42
3:I:90:GLN:C	3:I:92:ASN:H	2.28	0.42
1:B:227:SER:OG	1:B:228:ALA:N	2.51	0.42
2:G:45:LEU:O	3:I:98:PHE:HB2	2.20	0.42
2:G:95:ARG:HG3	3:I:96:TRP:HH2	1.83	0.42
1:A:320:ASP:OD1	1:A:320:ASP:C	2.61	0.42
1:B:273:HIS:CD2	1:B:273:HIS:C	2.98	0.42
1:A:252:ARG:HD2	1:A:264:GLU:CG	2.49	0.42
1:A:215:HIS:O	1:A:216:SER:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD12	1:A:374:ARG:NH1	2.35	0.42
2:H:98:HIS:CG	2:H:99:PHE:N	2.88	0.42
1:B:84:ARG:HA	4:B:501:NAG:C6	2.26	0.42
1:A:184:ASP:C	1:A:184:ASP:OD1	2.60	0.41
2:J:94:ARG:HH21	2:J:102:TYR:HE2	1.68	0.41
1:C:239:MET:HE2	1:C:277:CYS:H	1.84	0.41
1:C:328:PRO:HB2	1:C:332:SER:OG	2.20	0.41
3:I:39:LYS:NZ	3:I:81:ASP:O	2.54	0.41
1:A:370:SER:OG	1:A:373:GLU:N	2.54	0.41
1:B:338:GLU:O	1:B:338:GLU:HG2	2.20	0.41
1:A:125:ASN:N	1:A:125:ASN:OD1	2.53	0.41
1:C:333:ILE:HG12	1:C:334:THR:H	1.84	0.41
1:D:83:PRO:HG2	1:D:284:ASN:OD1	2.21	0.41
1:D:244:SER:OG	1:D:245:ALA:N	2.52	0.41
1:A:374:ARG:NH1	1:A:408:TRP:HZ3	2.17	0.41
1:B:333:ILE:O	1:B:333:ILE:HG13	2.20	0.41
2:J:36:TRP:CE2	2:J:80:LEU:HB2	2.56	0.41
3:L:2:ILE:HD12	3:L:93:ILE:CD1	2.48	0.41
1:A:327:ARG:CZ	1:A:371:LYS:HG2	2.51	0.41
3:K:59:PRO:O	3:K:60:SER:CB	2.68	0.41
3:I:59:PRO:O	3:I:60:SER:CB	2.68	0.41
1:C:243:GLY:O	1:C:244:SER:CB	2.69	0.41
1:D:329:ASN:C	1:D:331:GLY:H	2.29	0.40
3:K:91:TYR:CE2	1:D:336:PRO:HB3	2.55	0.40
2:E:52:SER:OG	2:E:53:TYR:N	2.54	0.40
1:B:386:ASP:OD1	1:B:386:ASP:C	2.65	0.40
1:D:372:THR:OG1	1:D:373:GLU:N	2.50	0.40
2:J:100(B):TRP:O	2:J:100(C):LYS:C	2.65	0.40
3:I:92:ASN:OD1	1:C:336:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	327/466 (70%)	314 (96%)	12 (4%)	1 (0%)	36	67
1	B	321/466 (69%)	311 (97%)	9 (3%)	1 (0%)	36	67
1	C	319/466 (68%)	299 (94%)	17 (5%)	3 (1%)	14	46
1	D	322/466 (69%)	295 (92%)	25 (8%)	2 (1%)	21	55
2	E	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
2	G	119/123 (97%)	108 (91%)	11 (9%)	0	100	100
2	H	119/123 (97%)	112 (94%)	6 (5%)	1 (1%)	16	48
2	J	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
3	F	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
3	I	105/107 (98%)	91 (87%)	10 (10%)	4 (4%)	2	17
3	K	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	12	44
3	L	105/107 (98%)	94 (90%)	10 (10%)	1 (1%)	12	44
All	All	2185/2784 (78%)	2039 (93%)	132 (6%)	14 (1%)	23	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	95	SER
3	I	96	TRP
3	K	60	SER
3	I	60	SER
3	I	91	TYR
2	H	84	ALA
3	L	59	PRO
1	C	244	SER
1	D	333	ILE
1	A	244	SER
1	B	244	SER
1	C	272	LYS
1	D	338	GLU
1	C	334	THR

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	283/388 (73%)	280 (99%)	3 (1%)	65	77
1	B	277/388 (71%)	275 (99%)	2 (1%)	76	81
1	C	276/388 (71%)	272 (99%)	4 (1%)	59	75
1	D	278/388 (72%)	275 (99%)	3 (1%)	65	77
2	E	103/105 (98%)	103 (100%)	0	100	100
2	G	103/105 (98%)	102 (99%)	1 (1%)	68	78
2	H	103/105 (98%)	103 (100%)	0	100	100
2	J	103/105 (98%)	103 (100%)	0	100	100
3	F	93/93 (100%)	92 (99%)	1 (1%)	65	77
3	I	93/93 (100%)	92 (99%)	1 (1%)	65	77
3	K	93/93 (100%)	93 (100%)	0	100	100
3	L	93/93 (100%)	93 (100%)	0	100	100
All	All	1898/2344 (81%)	1883 (99%)	15 (1%)	70	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	THR
1	A	373	GLU
1	A	419	LYS
2	G	95	ARG
3	I	94	TYR
3	F	94	TYR
1	B	333	ILE
1	B	334	THR
1	C	221	ILE
1	C	332	SER
1	C	333	ILE
1	C	334	THR
1	D	333	ILE
1	D	334	THR
1	D	338	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	98	HIS
3	I	37	GLN
3	I	89	GLN
3	F	37	GLN
3	F	79	GLN
2	H	5	GLN
1	C	199	ASN
1	C	220	ASN
1	D	199	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	NAG	B	501	1	14,14,15	0.40	0	17,19,21	0.42	0
4	NAG	A	501	1	14,14,15	2.20	5 (35%)	17,19,21	1.01	2 (11%)
4	NAG	D	501	1	14,14,15	0.40	0	17,19,21	0.67	1 (5%)
4	NAG	C	501	1	14,14,15	2.19	5 (35%)	17,19,21	0.97	1 (5%)

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
4	NAG	B	501	1	-	3/6/23/26	0/1/1/1
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	D	501	1	-	1/6/23/26	0/1/1/1
4	NAG	C	501	1	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	NAG	C1-C2	5.86	1.60	1.52
4	A	501	NAG	C1-C2	5.84	1.60	1.52
4	C	501	NAG	O5-C5	3.27	1.49	1.43
4	A	501	NAG	O5-C5	3.26	1.49	1.43
4	C	501	NAG	O5-C1	2.62	1.48	1.43
4	A	501	NAG	O5-C1	2.62	1.48	1.43
4	A	501	NAG	C3-C2	2.29	1.57	1.52
4	C	501	NAG	C3-C2	2.26	1.57	1.52
4	A	501	NAG	C4-C5	2.02	1.57	1.53
4	C	501	NAG	C4-C5	2.02	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C8-C7-N2	2.63	120.47	116.12
4	C	501	NAG	C8-C7-N2	2.35	120.01	116.12
4	D	501	NAG	C2-N2-C7	2.27	125.95	122.90
4	A	501	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

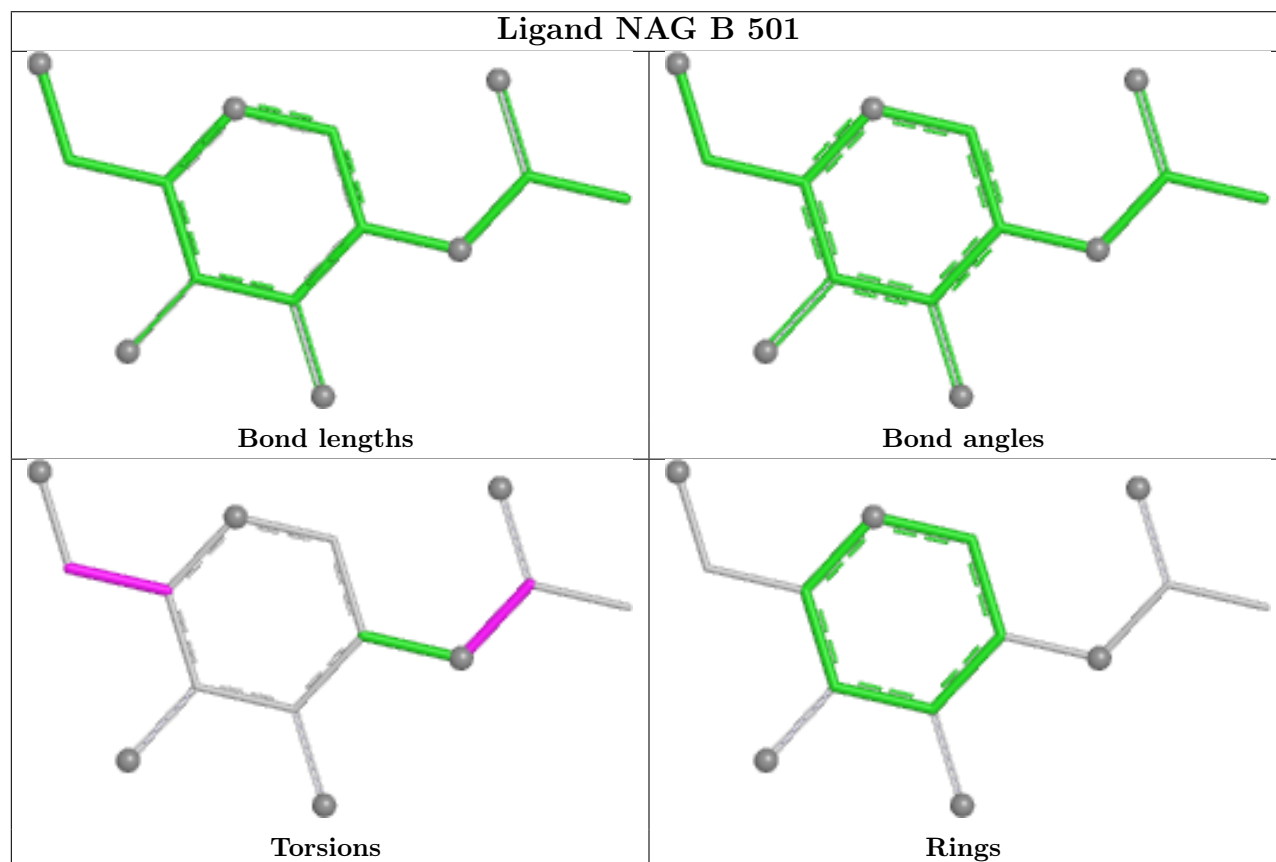
Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C8-C7-N2-C2
4	B	501	NAG	O7-C7-N2-C2
4	C	501	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	D	501	NAG	O5-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6

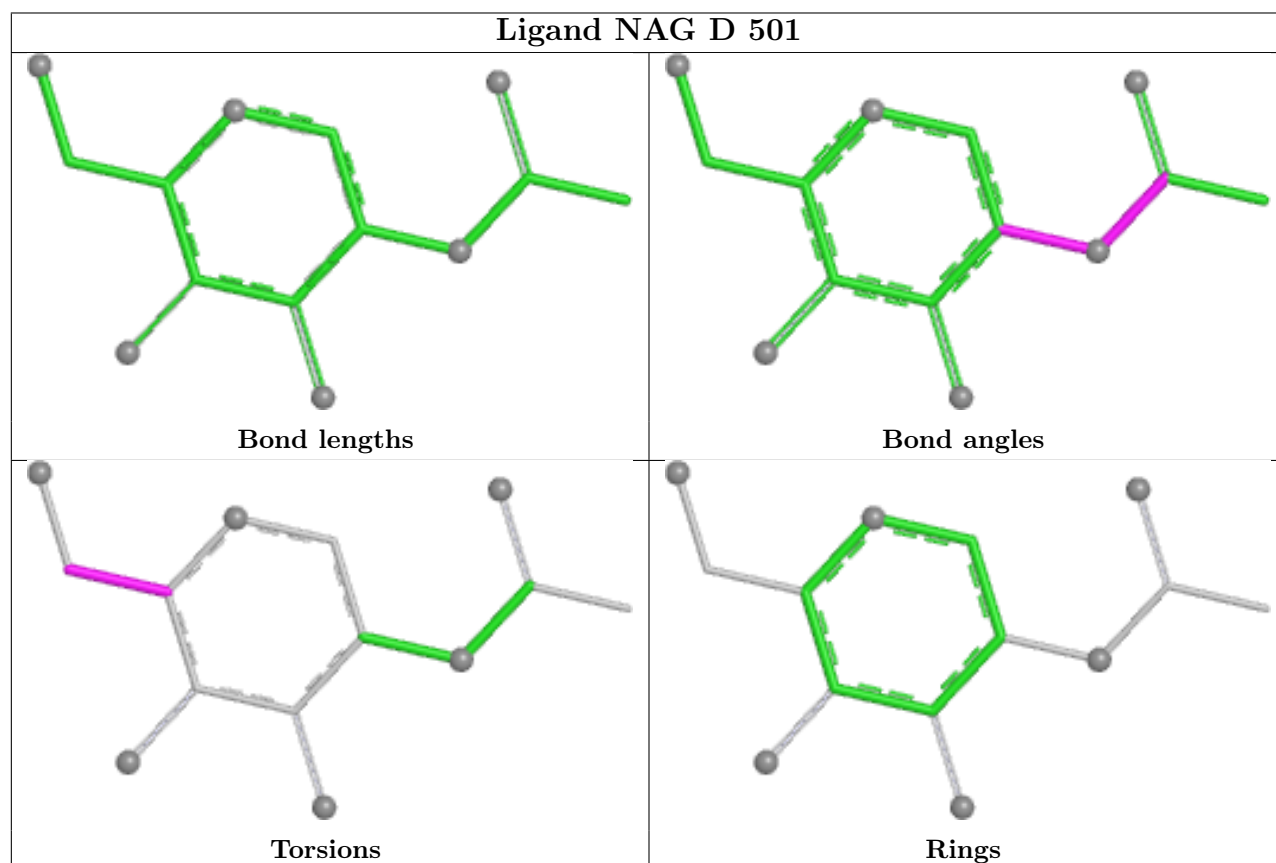
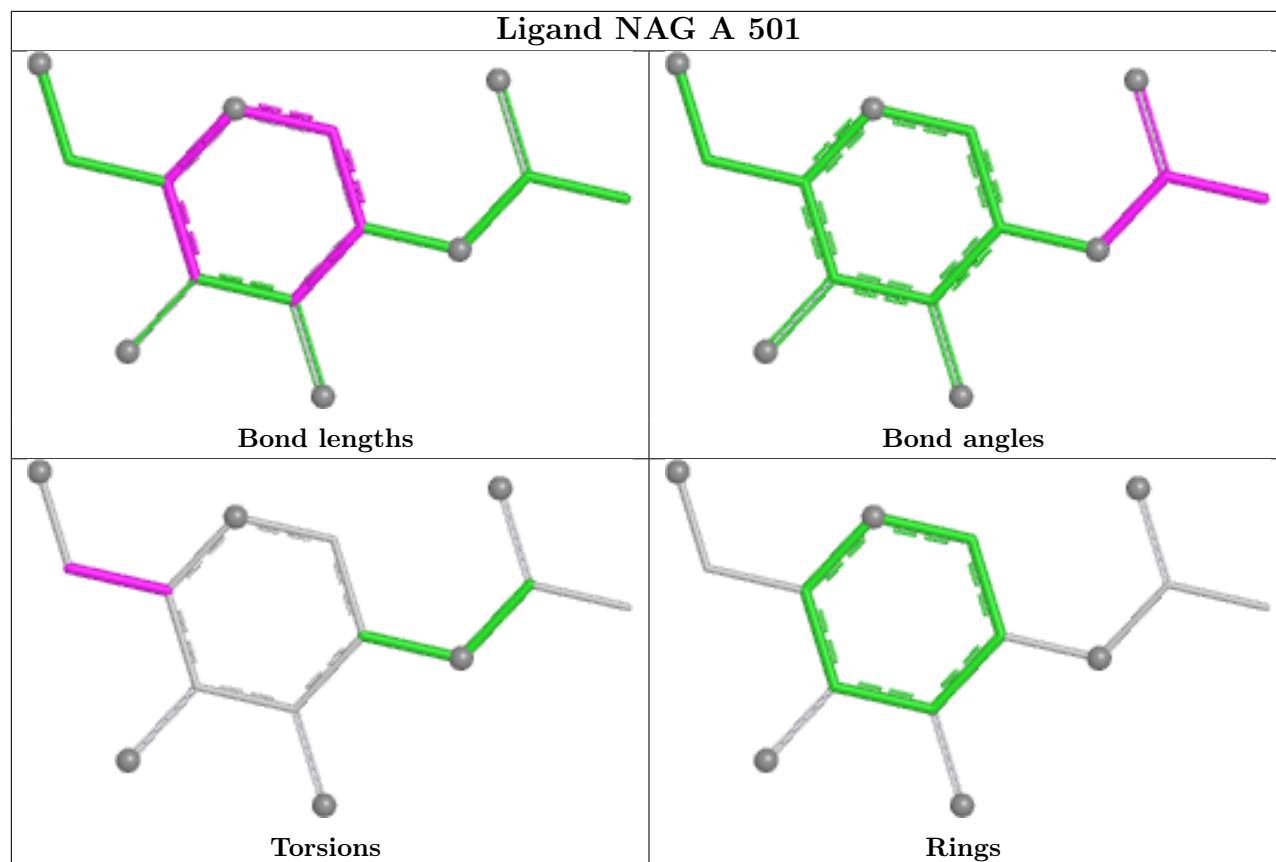
There are no ring outliers.

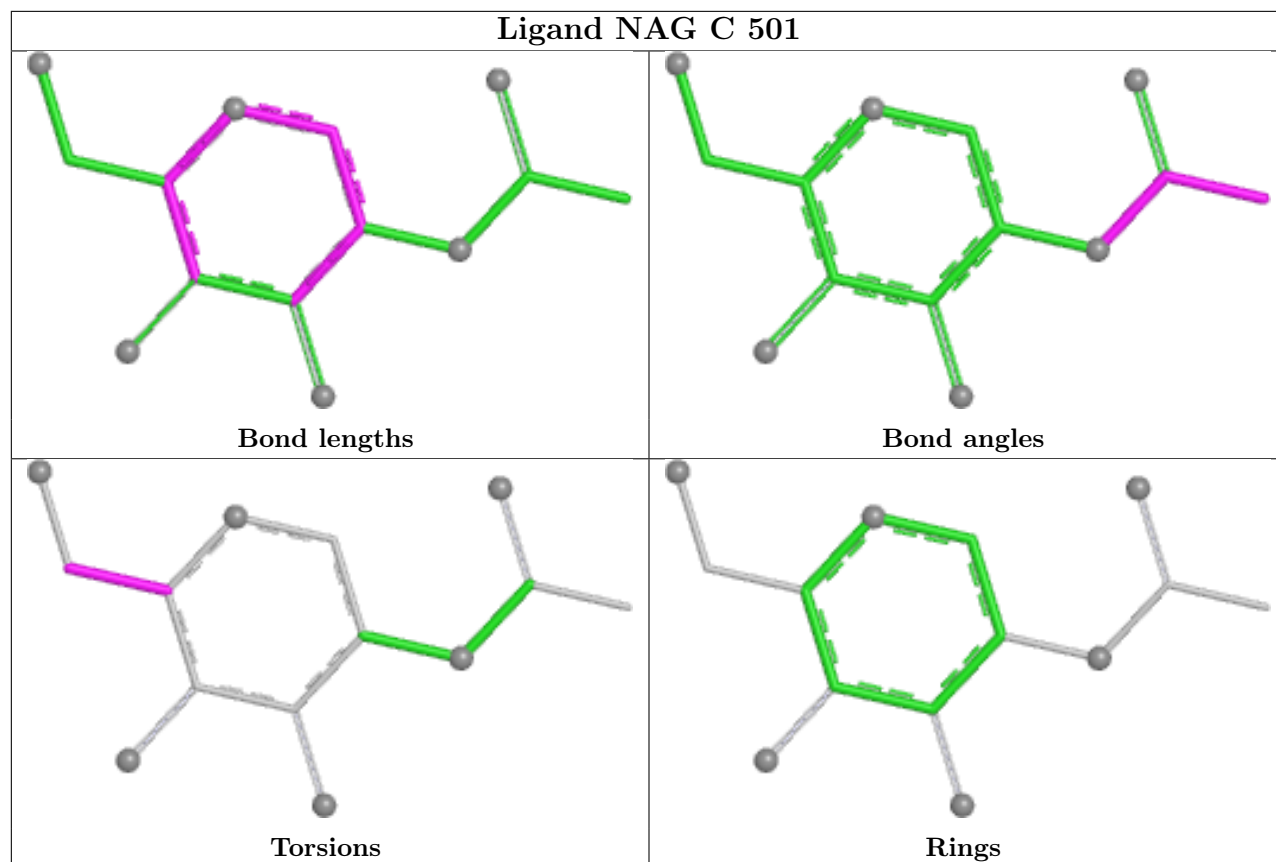
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

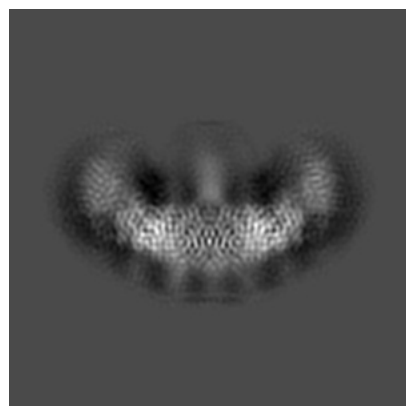
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41826. These allow visual inspection of the internal detail of the map and identification of artifacts.

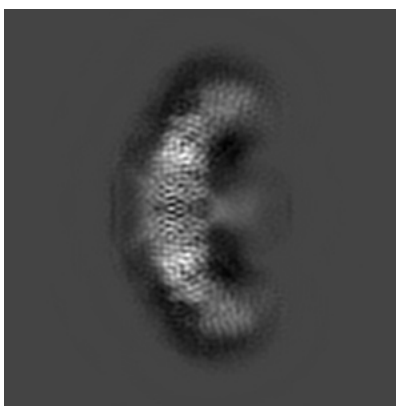
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

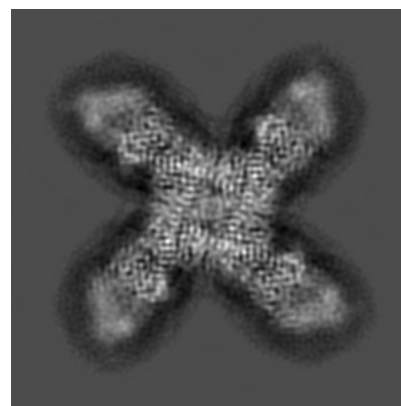
6.1.1 Primary map



X

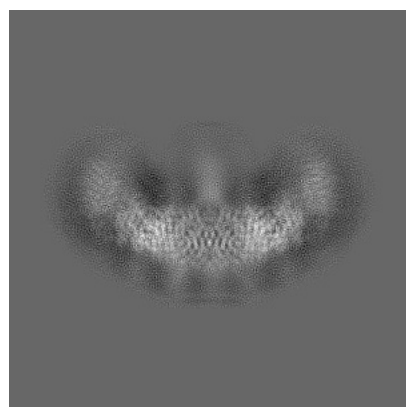


Y

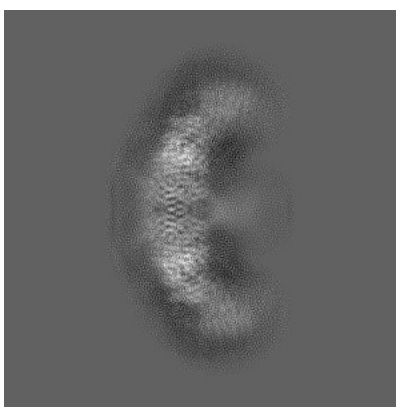


Z

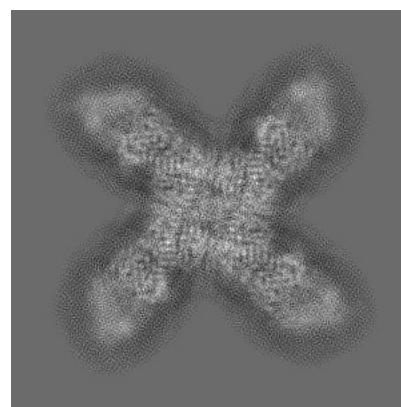
6.1.2 Raw map



X



Y

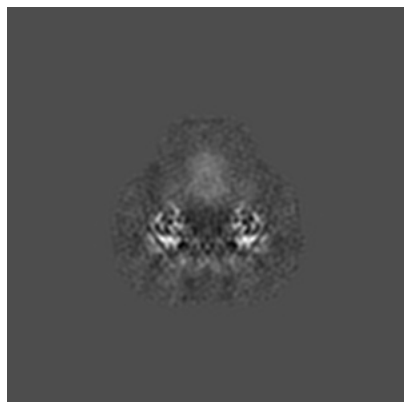


Z

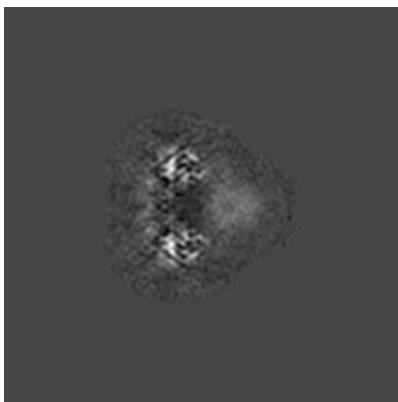
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

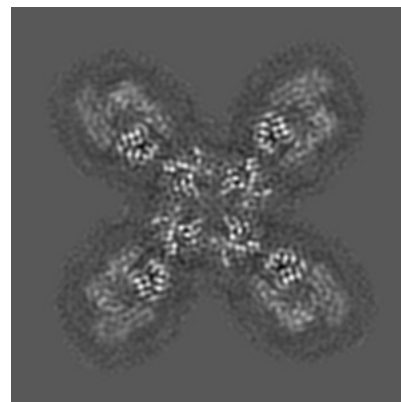
6.2.1 Primary map



X Index: 180

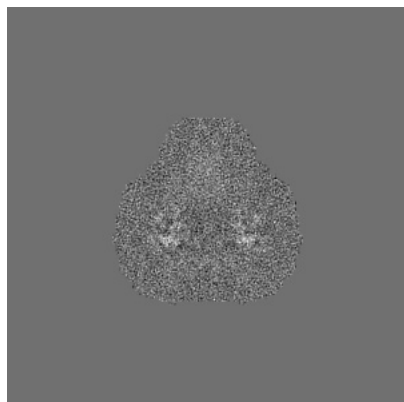


Y Index: 180

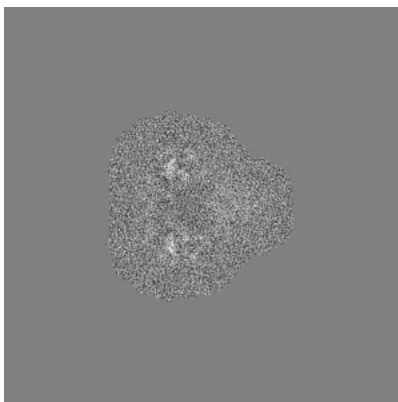


Z Index: 180

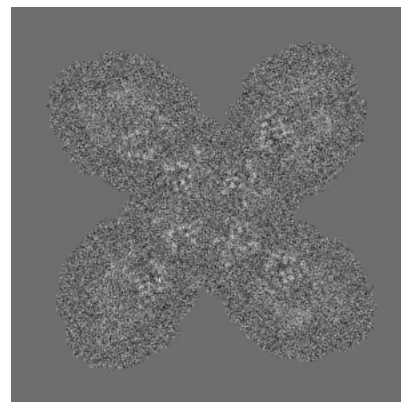
6.2.2 Raw map



X Index: 180



Y Index: 180

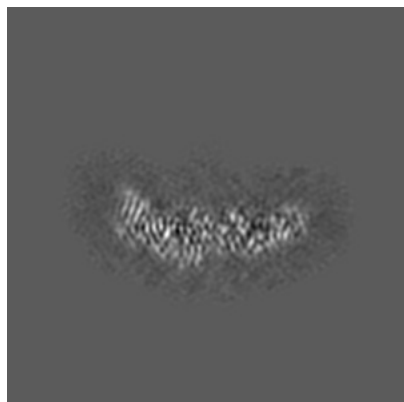


Z Index: 180

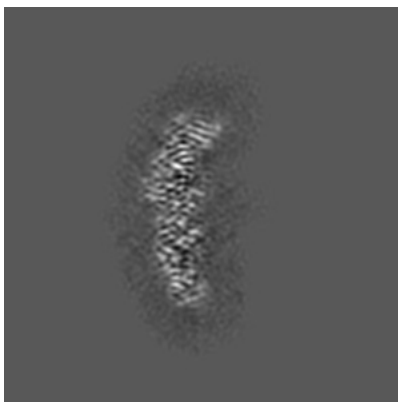
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

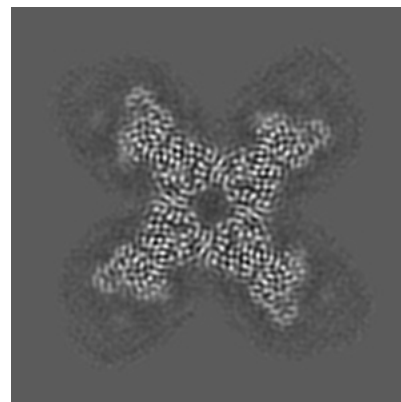
6.3.1 Primary map



X Index: 135

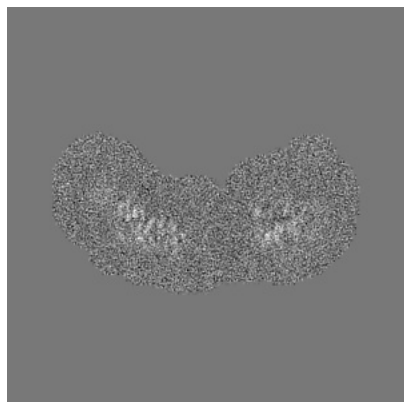


Y Index: 135

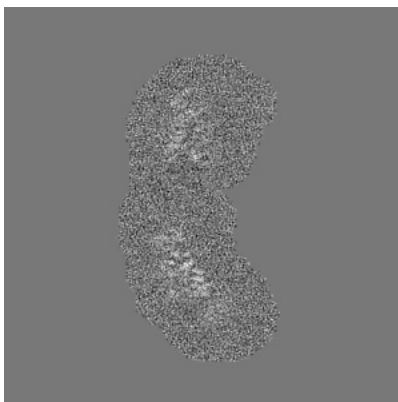


Z Index: 163

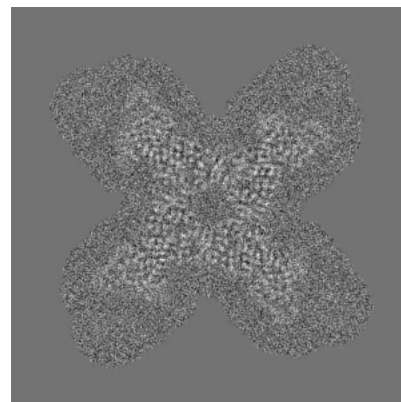
6.3.2 Raw map



X Index: 118



Y Index: 243

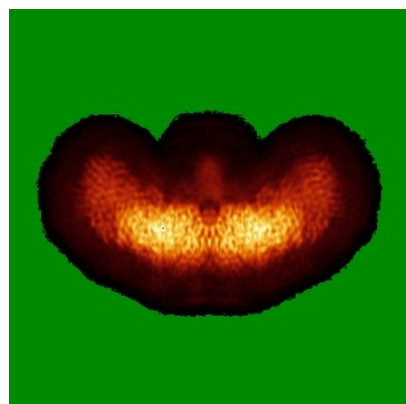


Z Index: 163

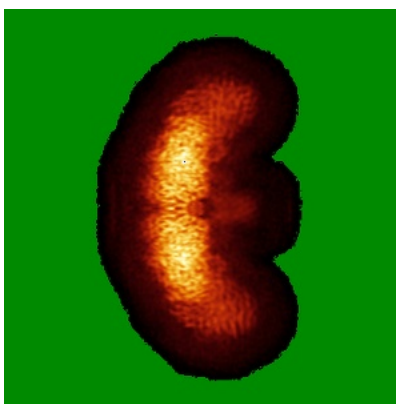
The images above show the largest variance slices of the map in three orthogonal directions.

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

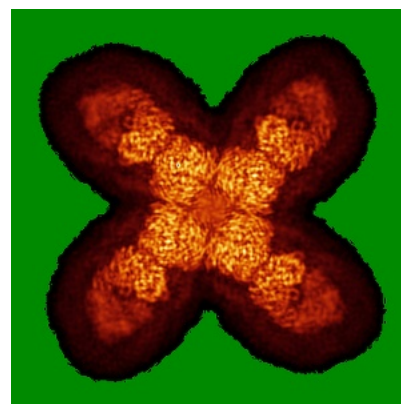
6.4.1 Primary map



X

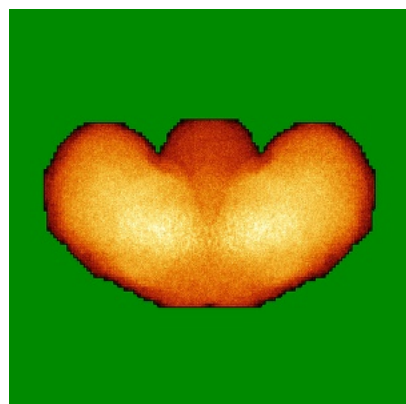


Y

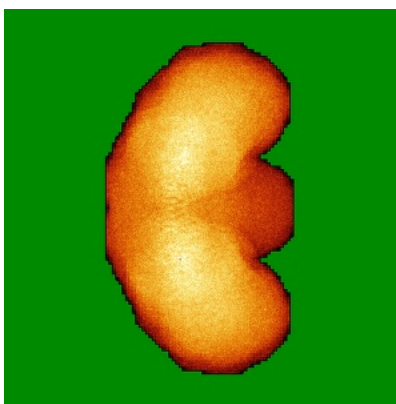


Z

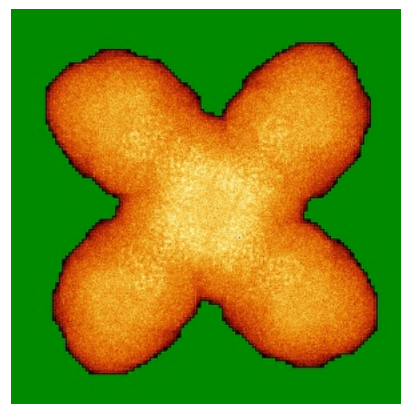
6.4.2 Raw map



X



Y

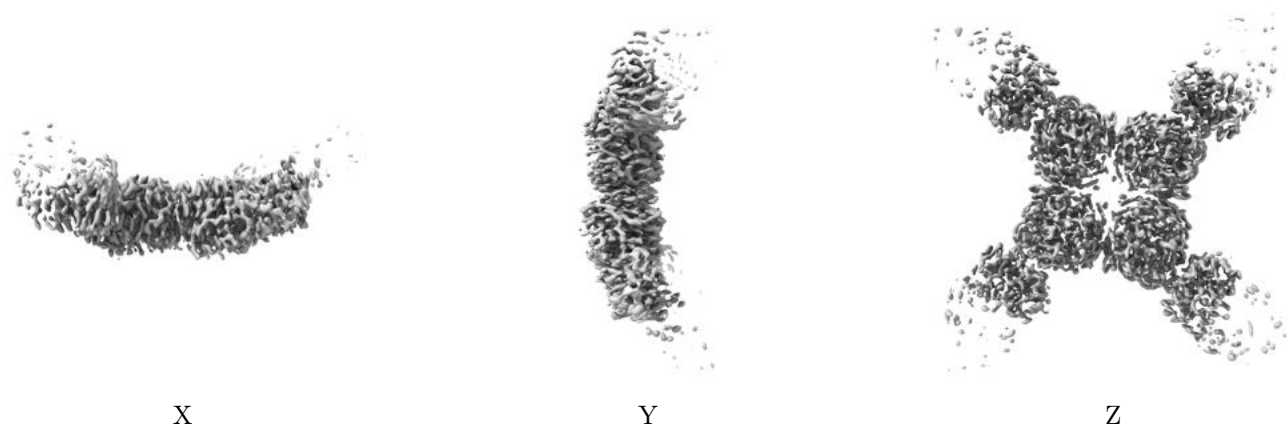


Z

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.

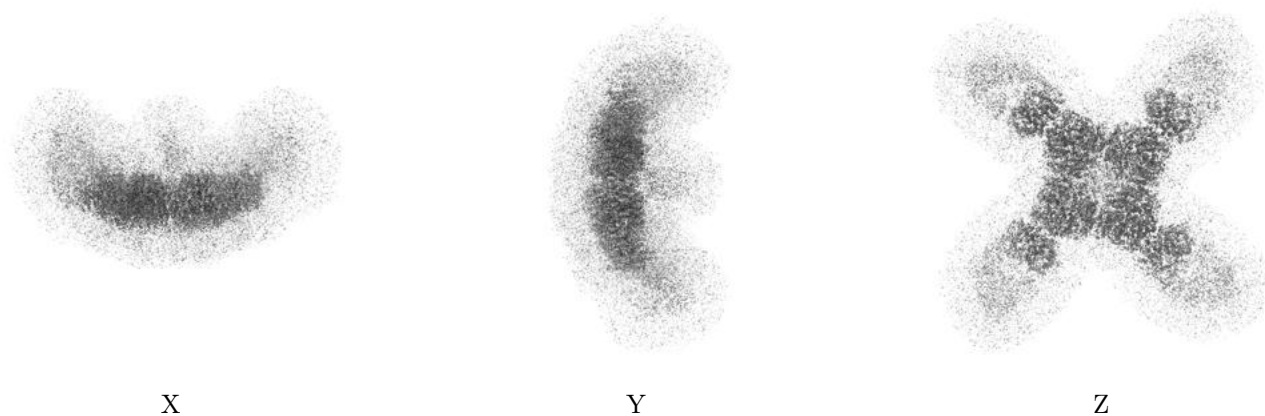
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

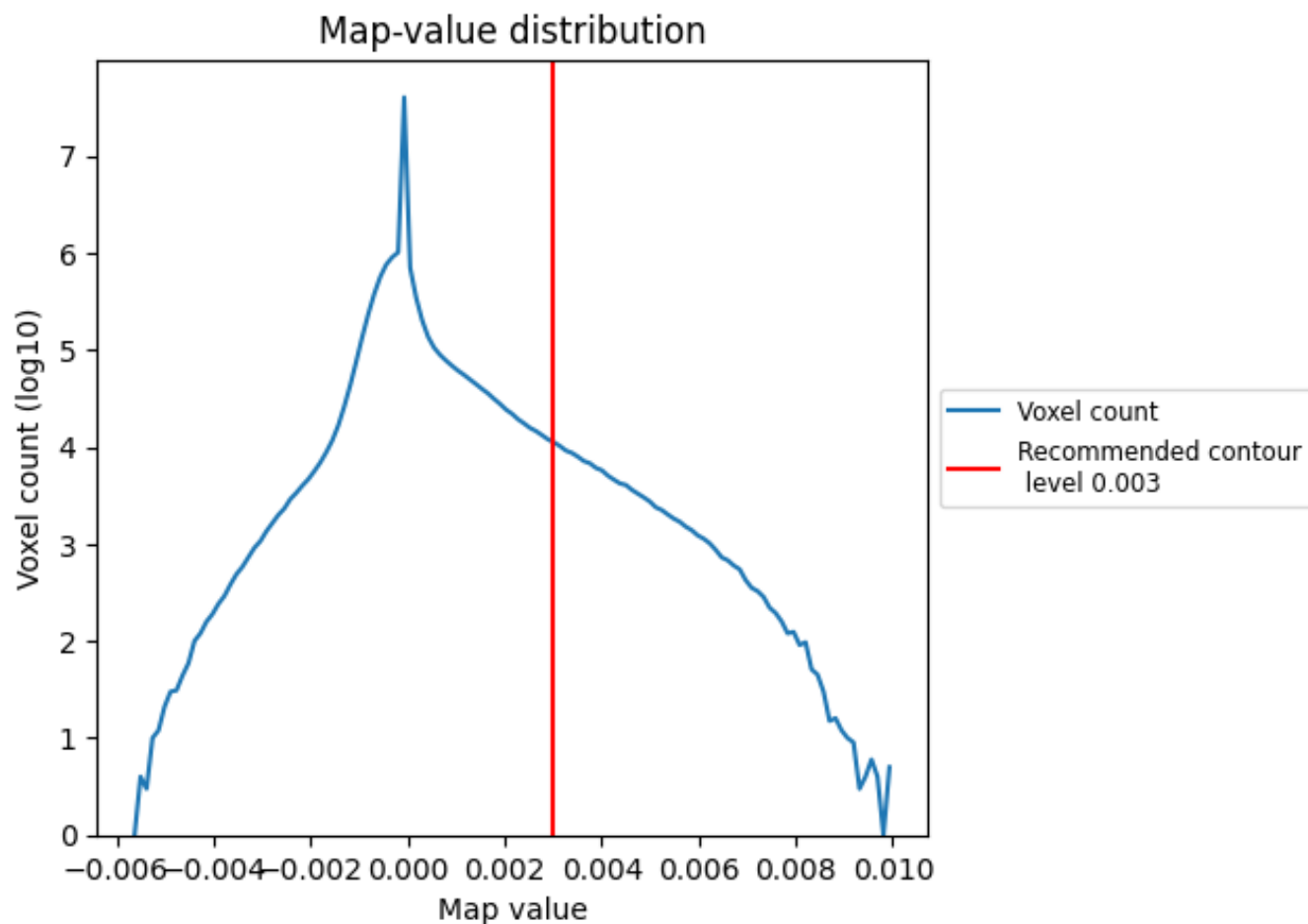
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

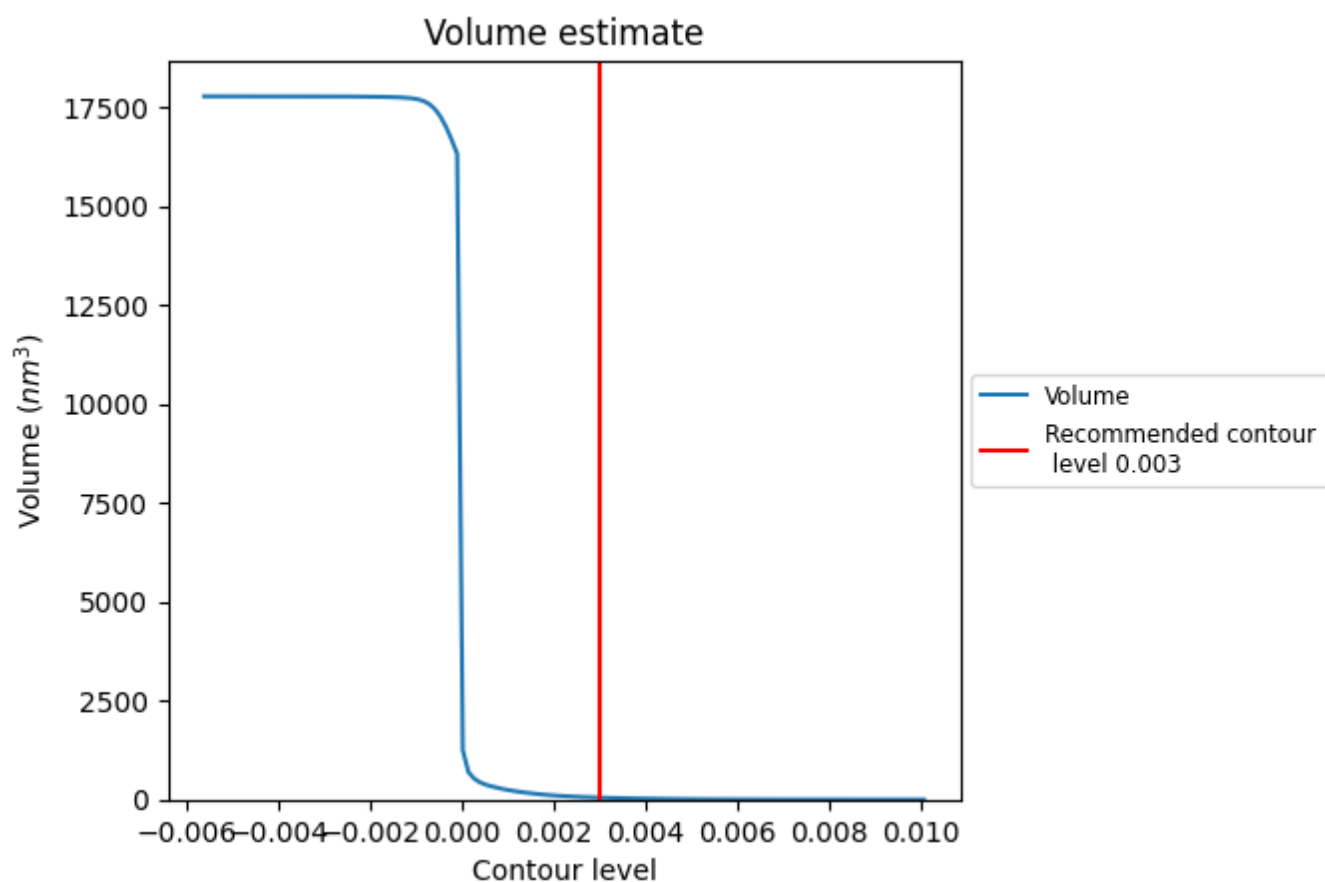
This section contains the results of statistical analysis of the map.

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.

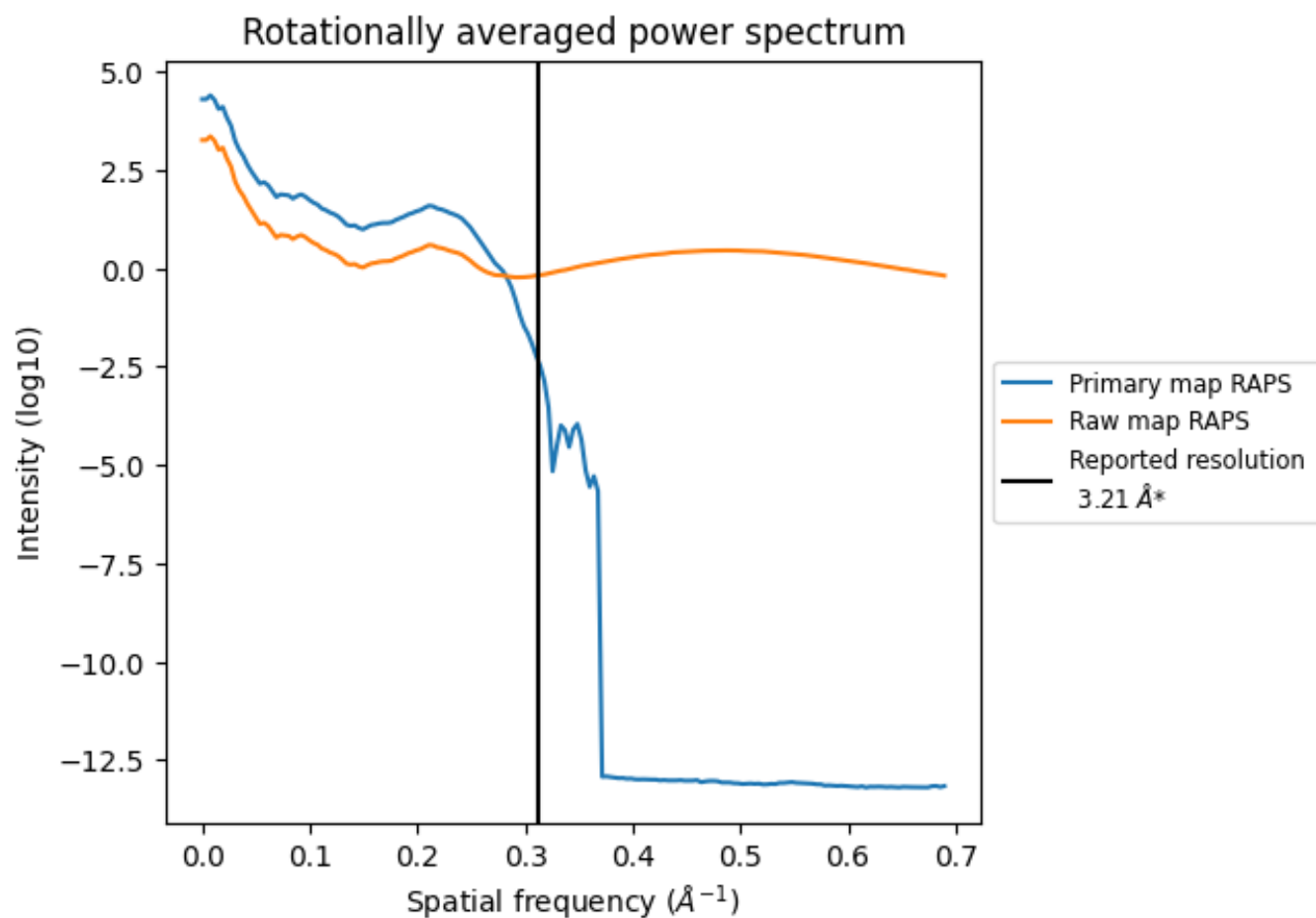
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 44 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 ⓘ

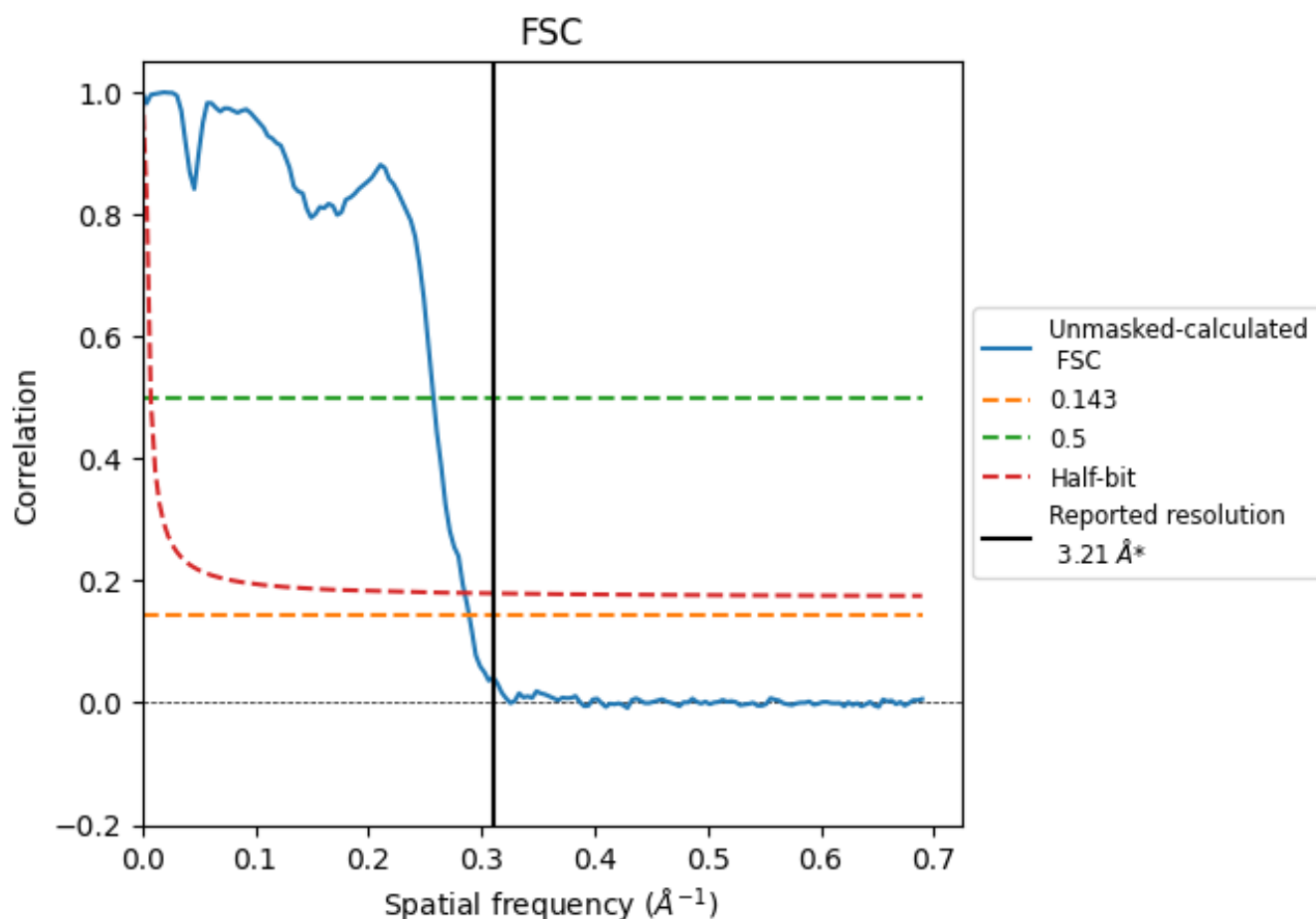


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

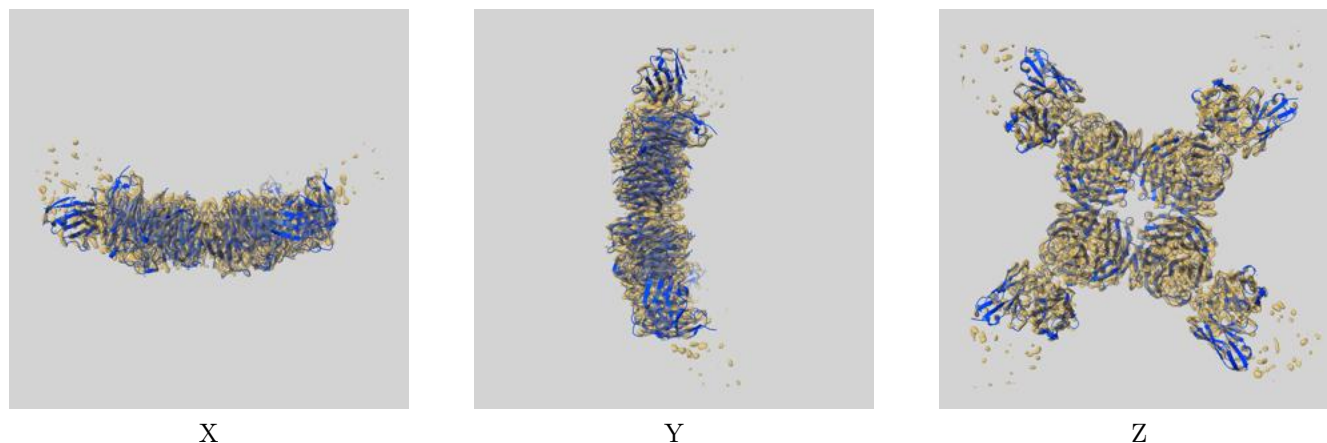
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	3.88	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

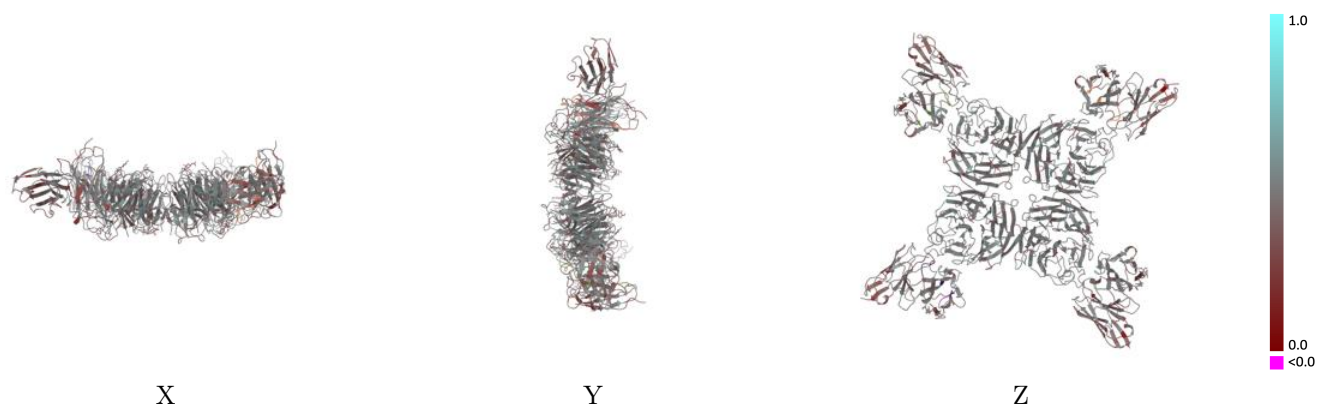
This section contains information regarding the fit between EMDB map EMD-41826 and PDB model 8U1S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



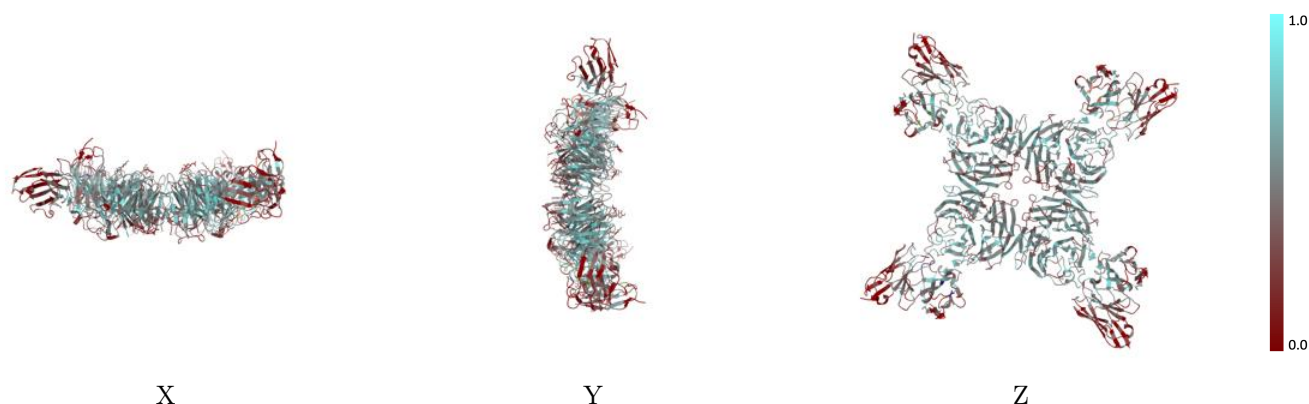
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



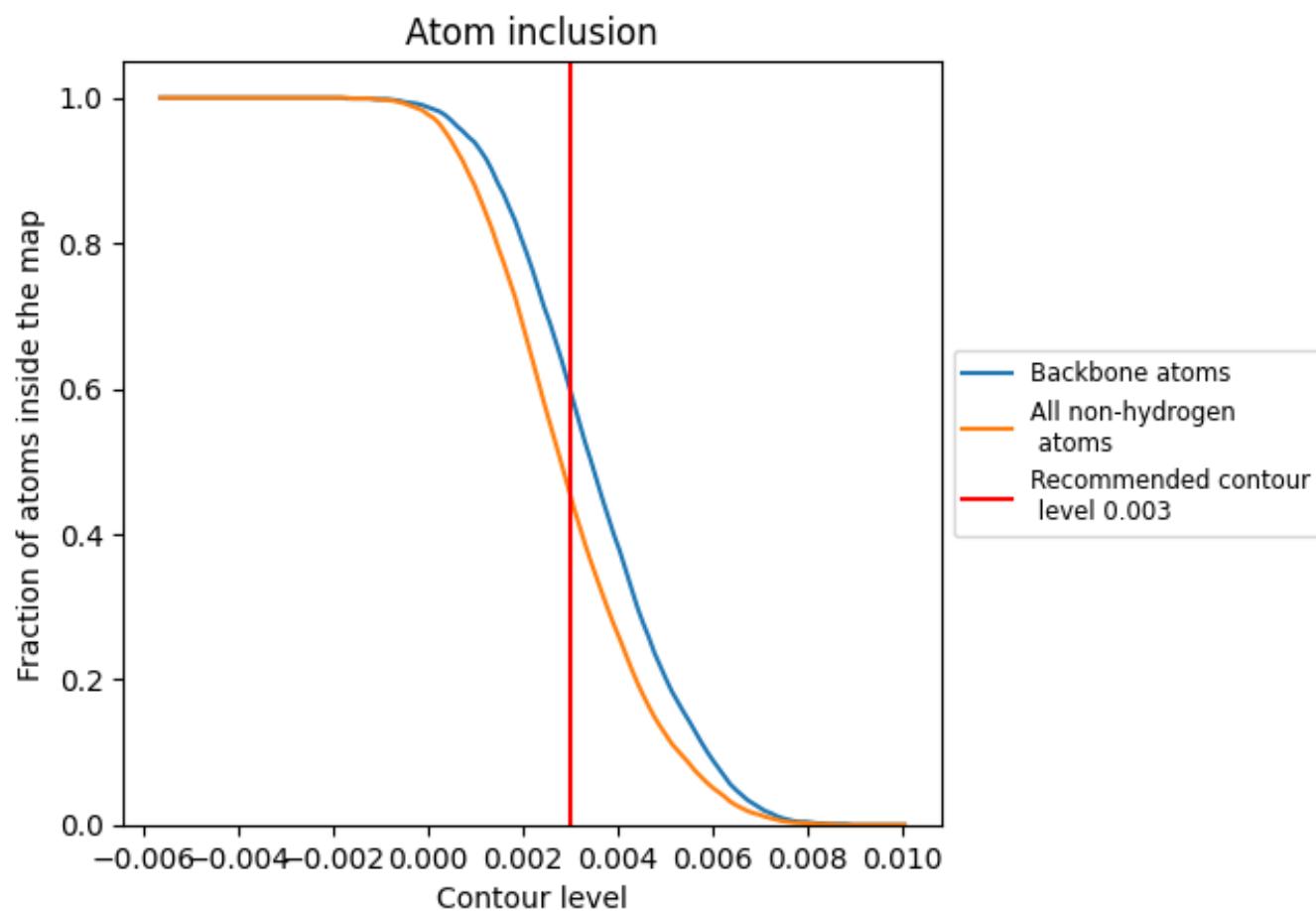
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 46% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4560	0.4400
A	0.5070	0.4580
B	0.5160	0.4570
C	0.5160	0.4560
D	0.5220	0.4570
E	0.4320	0.4210
F	0.3080	0.4010
G	0.4190	0.4220
H	0.4330	0.4280
I	0.3100	0.4090
J	0.4210	0.4270
K	0.3030	0.4010
L	0.3060	0.4010

1.0

0.0

<0.0