



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 6OGD / pdb_00006ogd
EMDB ID : EMD-20053
Title : Cryo-EM structure of YenTcA in its prepore state
Authors : Piper, S.J.; Brillault, L.; Box, J.K.; Landsberg, M.J.
Deposited on : 2019-04-02
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

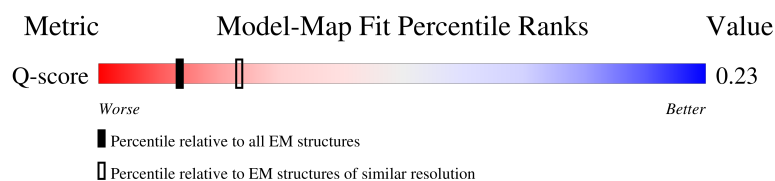
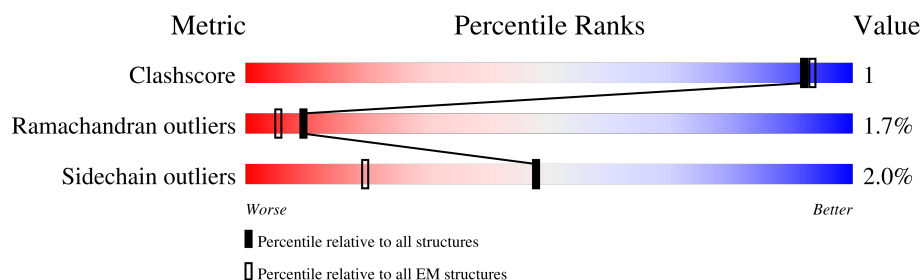
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	1164	
1	D	1164	
1	G	1164	
1	J	1164	

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Mol	Chain	Length	Quality of chain
1	M	1164	
2	B	1364	
2	E	1364	
2	H	1364	
2	K	1364	
2	N	1364	
3	C	633	
3	F	633	
3	I	633	
3	L	633	
3	O	633	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 94125 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 Toxin subunit YenA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			5910	3766	983	1145	16		
1	D	748	Total	C	N	O	S	0	0
			5910	3766	983	1145	16		
1	G	748	Total	C	N	O	S	0	0
			5910	3766	983	1145	16		
1	J	748	Total	C	N	O	S	0	0
			5910	3766	983	1145	16		
1	M	748	Total	C	N	O	S	0	0
			5910	3766	983	1145	16		

- Molecule 2 is a protein called Toxin subunit YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1078	Total	C	N	O	S	0	0
			8742	5535	1489	1688	30		
2	E	1078	Total	C	N	O	S	0	0
			8742	5535	1489	1688	30		
2	H	1078	Total	C	N	O	S	0	0
			8742	5535	1489	1688	30		
2	K	1078	Total	C	N	O	S	0	0
			8742	5535	1489	1688	30		
2	N	1078	Total	C	N	O	S	0	0
			8742	5535	1489	1688	30		

- Molecule 3 is a protein called Chitinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	538	Total	C	N	O	S	0	0
			4173	2641	697	818	17		
3	F	538	Total	C	N	O	S	0	0
			4173	2641	697	818	17		
3	I	538	Total	C	N	O	S	0	0
			4173	2641	697	818	17		

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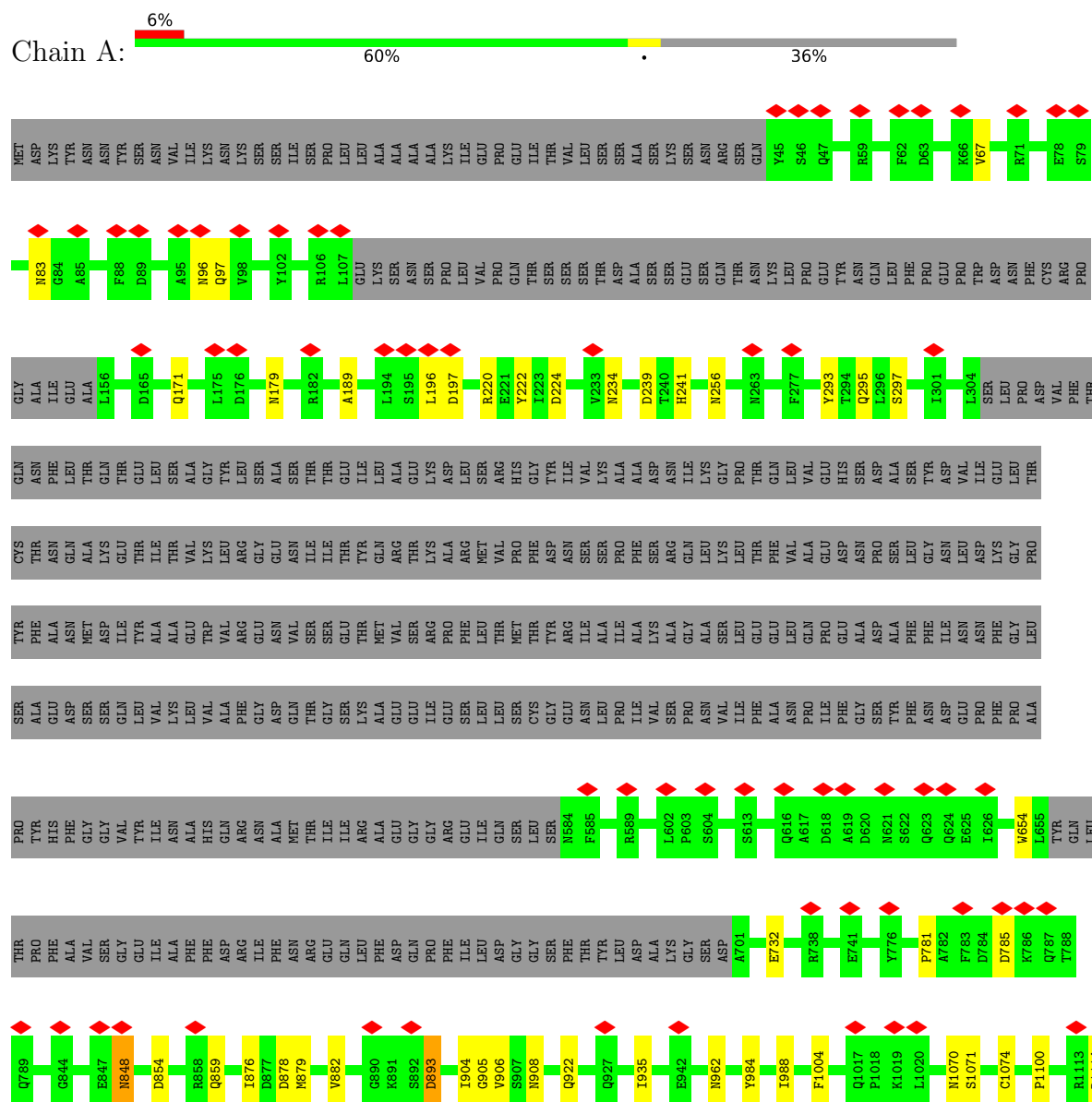
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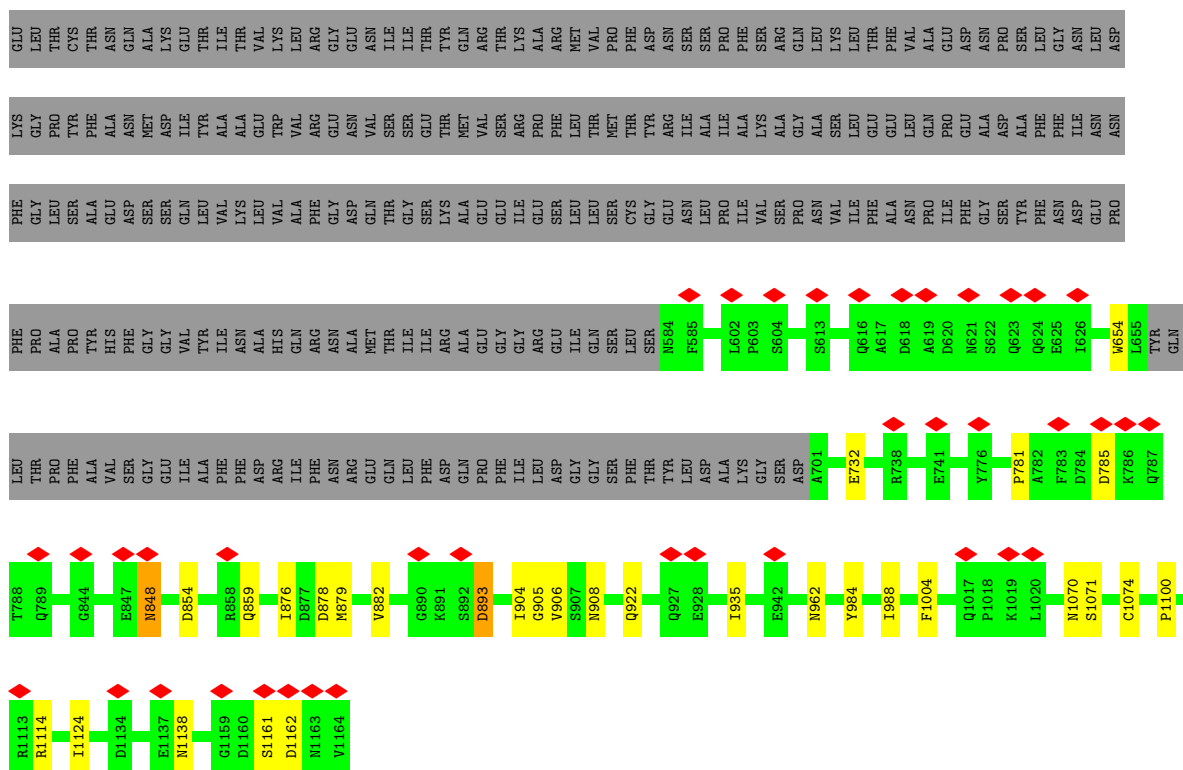
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	538	Total	C	N	O	S	0	0
			4173	2641	697	818	17		
3	O	538	Total	C	N	O	S	0	0
			4173	2641	697	818	17		

3 Residue-property plots

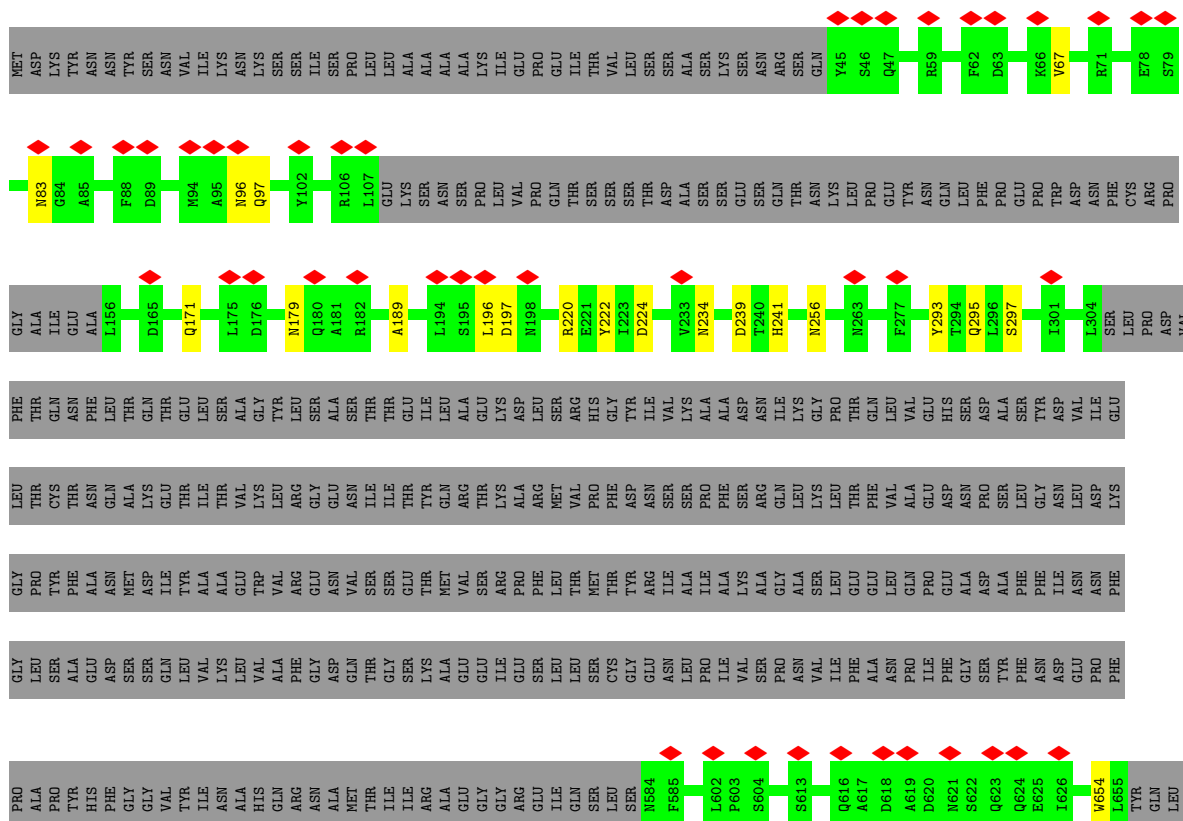
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

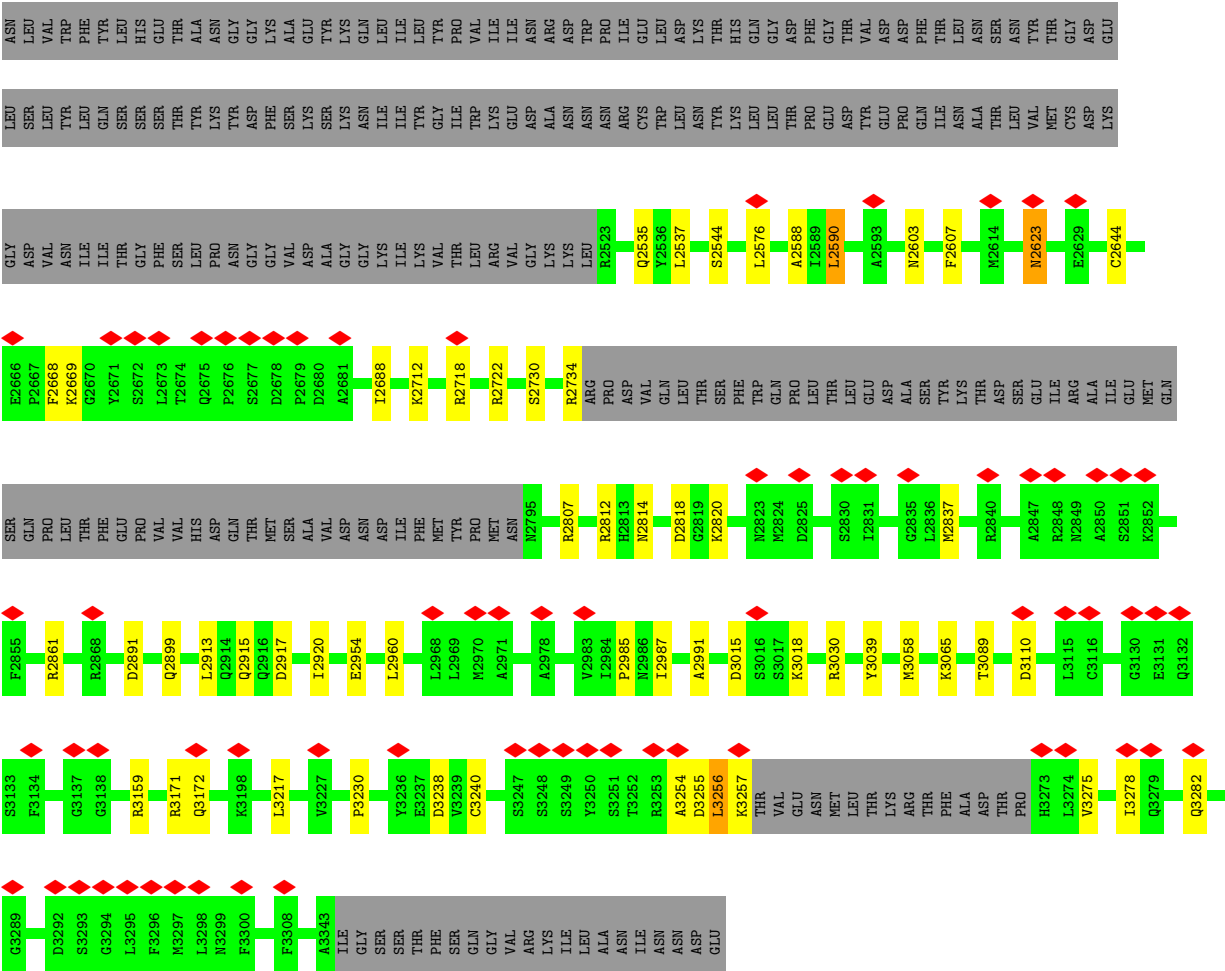
• Molecule 1: Toxin subunit YenA1



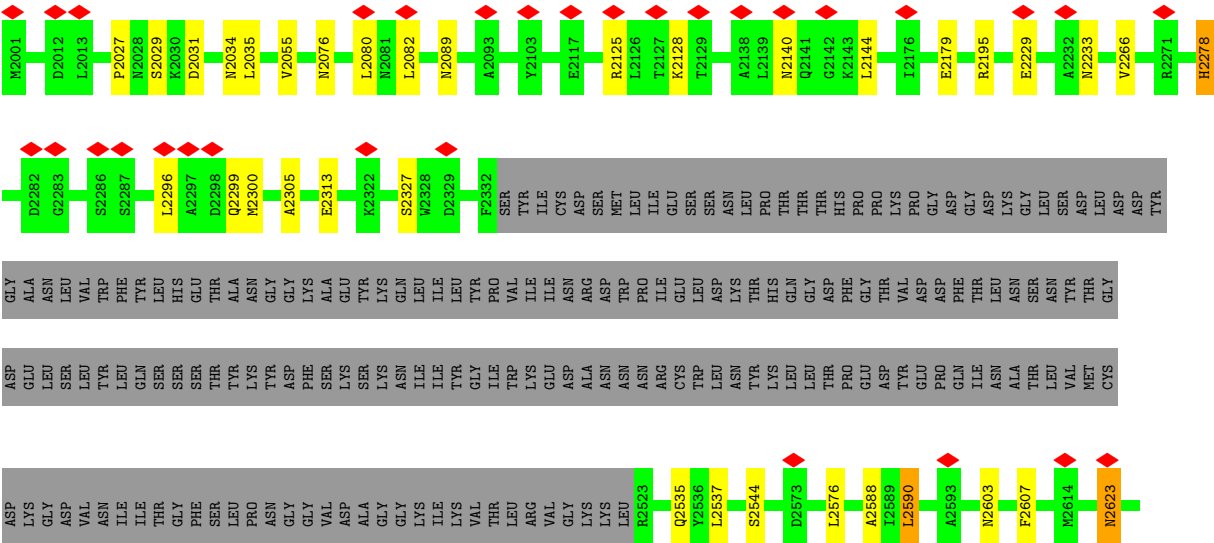


- Molecule 1: Toxin subunit YenA1

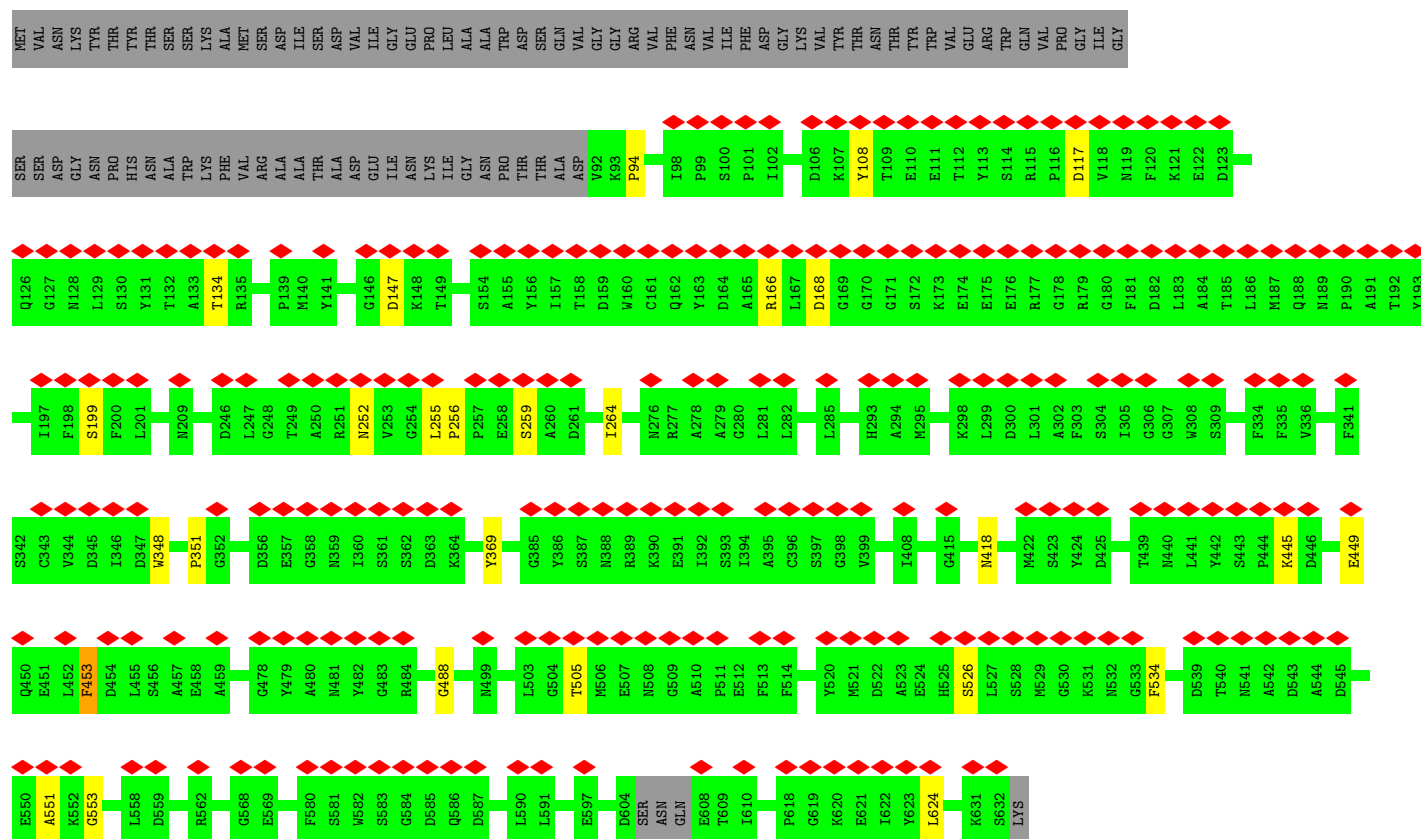
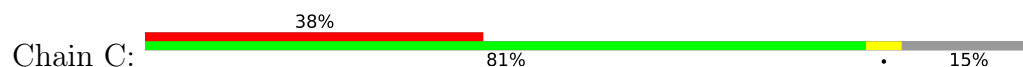




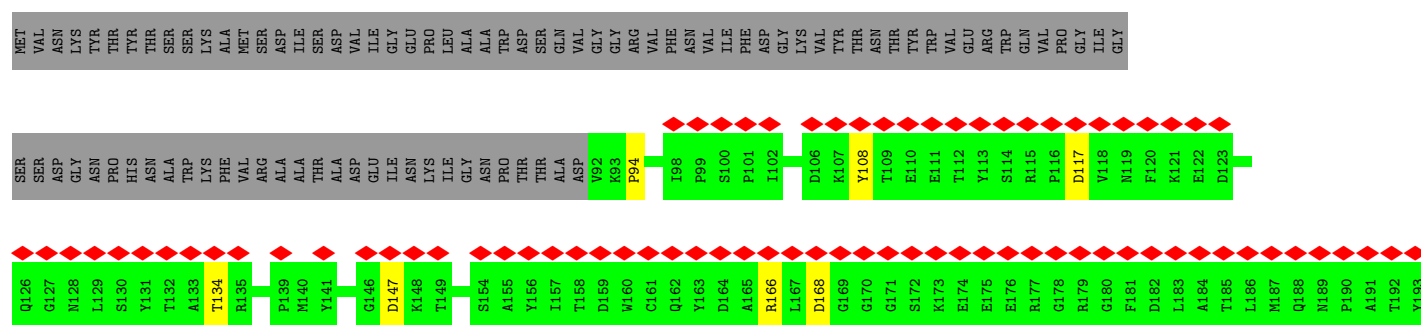
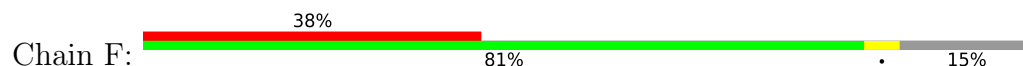
● Molecule 2: Toxin subunit YenA2

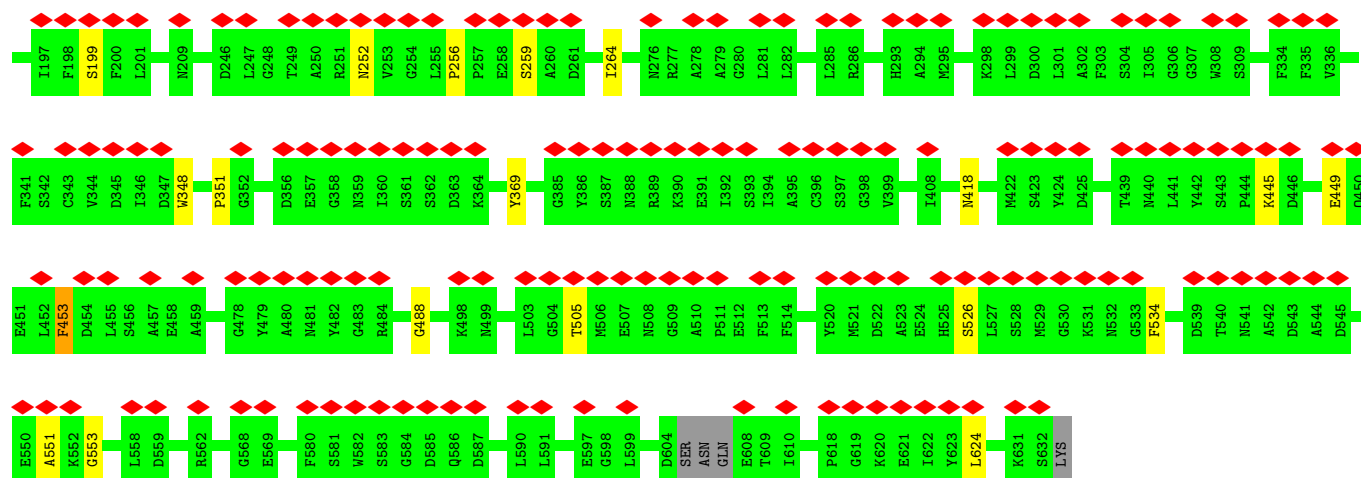


- Molecule 3: Chitinase 2

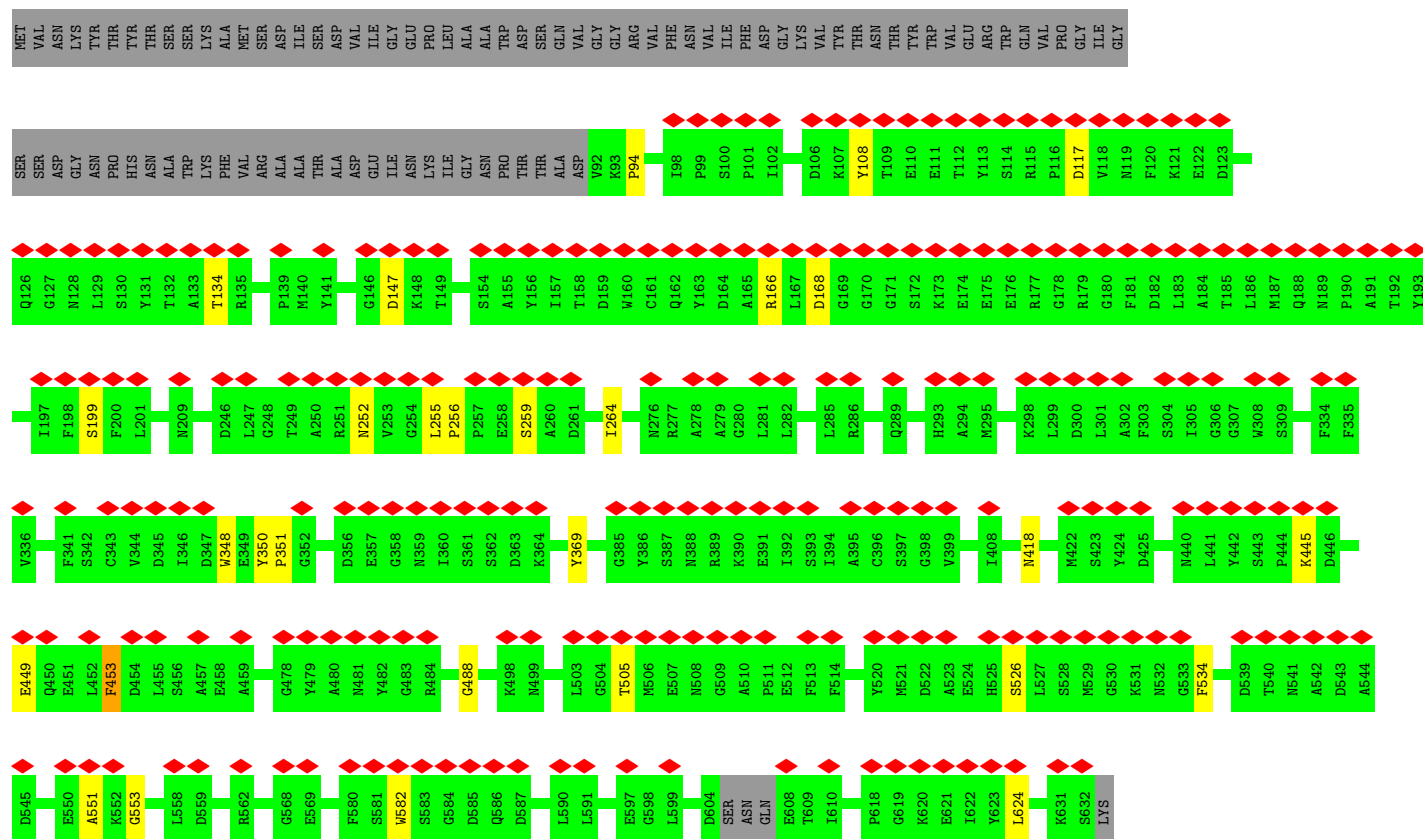
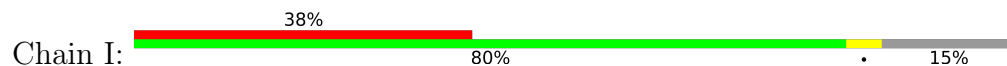


- Molecule 3: Chitinase 2

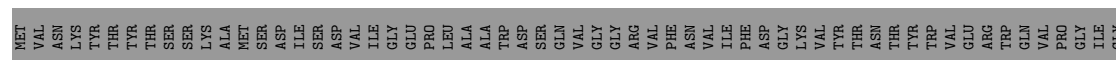
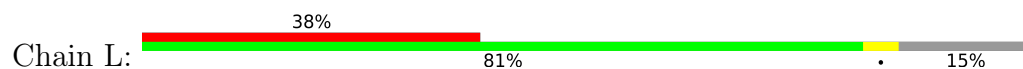


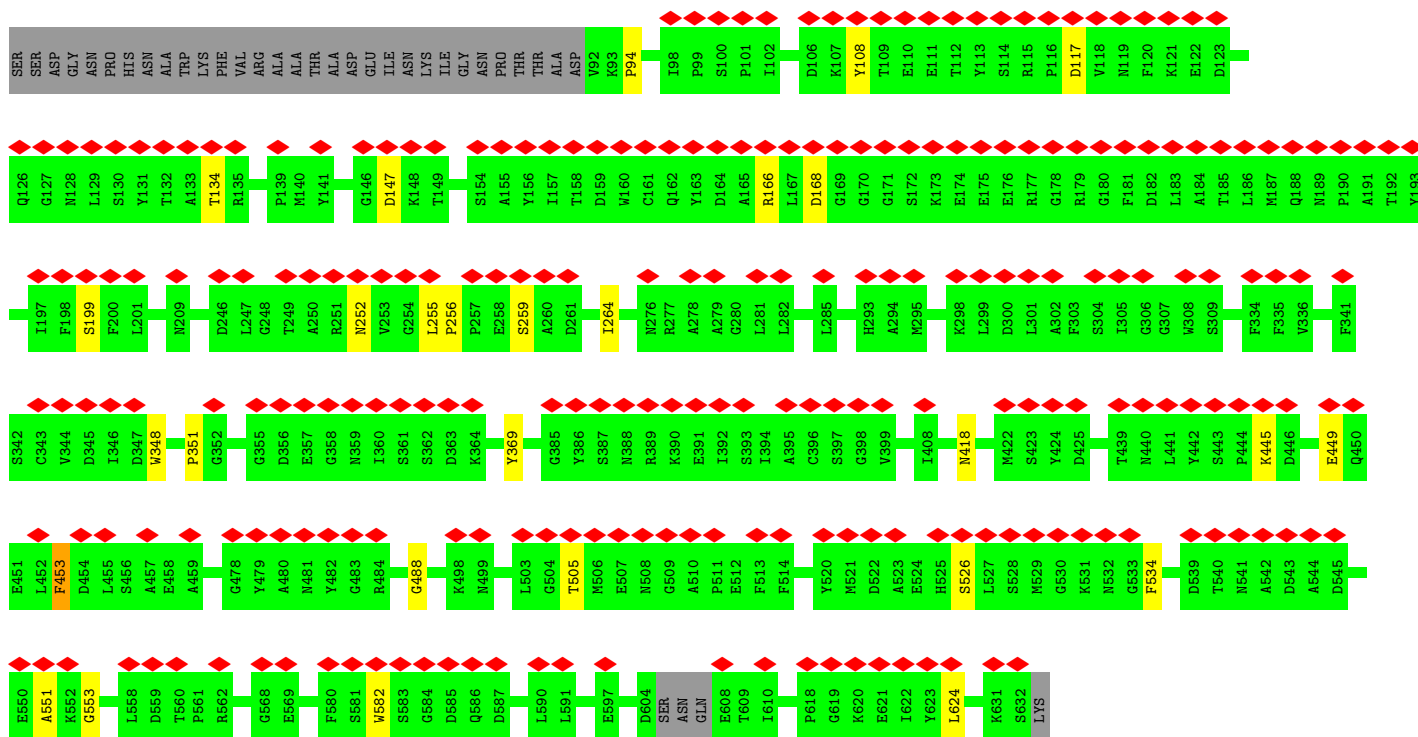


• Molecule 3: Chitinase 2

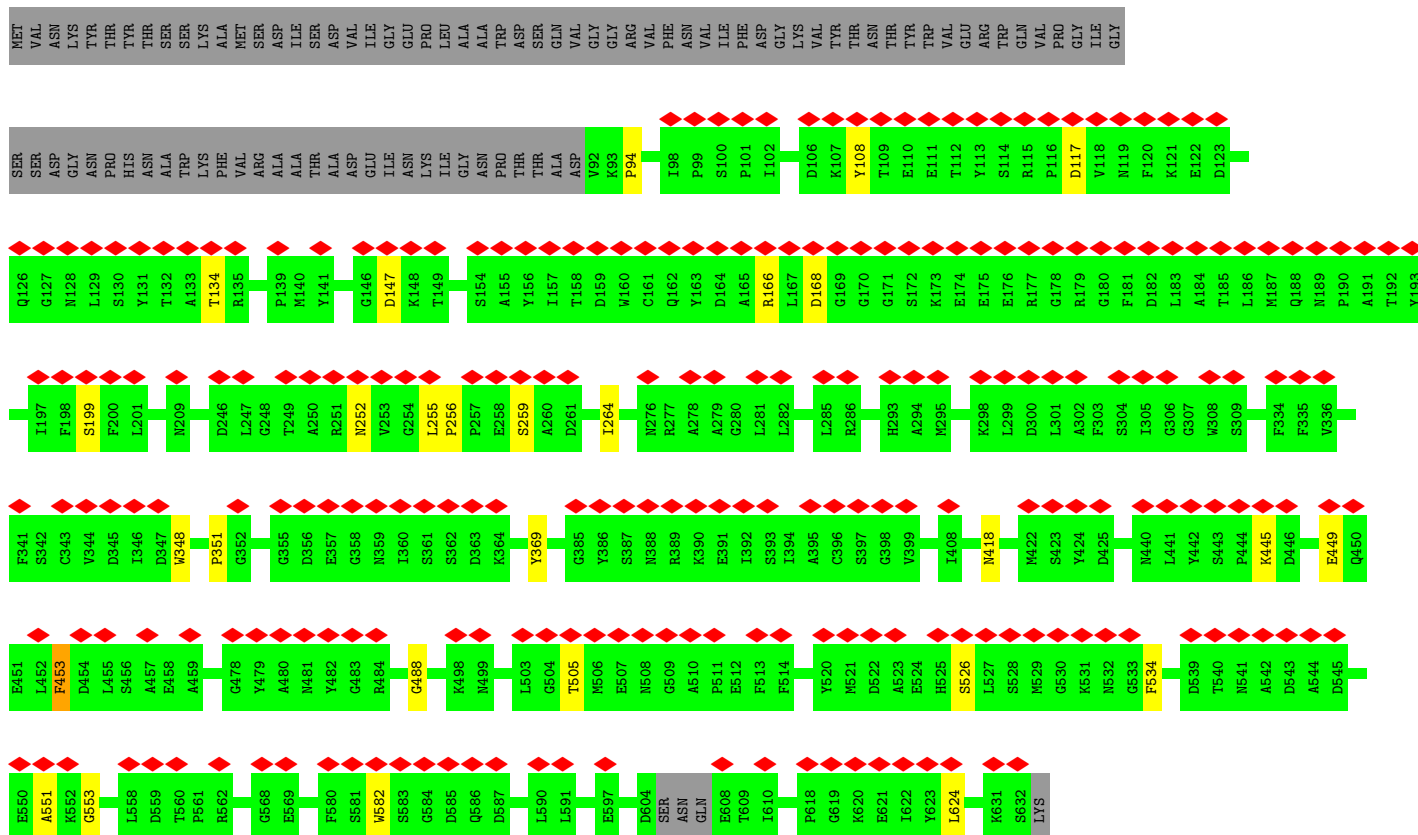
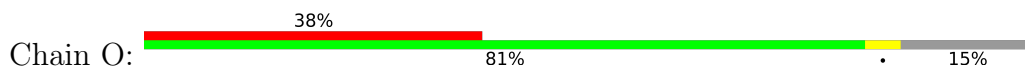


• Molecule 3: Chitinase 2





- Molecule 3: Chitinase 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	9856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	58.496	Depositor
Minimum map value	-45.992	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.654	Depositor
Recommended contour level	7.5	Depositor
Map size (Å)	557.44, 557.44, 557.44	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	0/6007	1.42	14/8156 (0.2%)
1	D	0.84	0/6007	1.42	14/8156 (0.2%)
1	G	0.84	0/6007	1.42	14/8156 (0.2%)
1	J	0.84	0/6007	1.42	15/8156 (0.2%)
1	M	0.84	0/6007	1.42	14/8156 (0.2%)
2	B	0.86	1/8915 (0.0%)	1.42	20/12066 (0.2%)
2	E	0.86	1/8915 (0.0%)	1.42	24/12066 (0.2%)
2	H	0.86	1/8915 (0.0%)	1.42	20/12066 (0.2%)
2	K	0.86	1/8915 (0.0%)	1.42	24/12066 (0.2%)
2	N	0.86	1/8915 (0.0%)	1.42	18/12066 (0.1%)
3	C	0.90	1/4271 (0.0%)	1.46	16/5778 (0.3%)
3	F	0.90	1/4271 (0.0%)	1.46	14/5778 (0.2%)
3	I	0.90	1/4271 (0.0%)	1.46	20/5778 (0.3%)
3	L	0.90	1/4271 (0.0%)	1.46	18/5778 (0.3%)
3	O	0.90	1/4271 (0.0%)	1.46	18/5778 (0.3%)
All	All	0.86	10/95965 (0.0%)	1.43	263/130000 (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
1	A	0	3
1	D	0	3
1	G	0	3
1	J	0	3
1	M	0	3
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
2	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
3	I	0	1
3	L	0	1
3	O	0	1
All	All	0	30

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	256	PRO	CA-C	5.29	1.54	1.51
2	N	2820	LYS	CA-CB	5.25	1.57	1.53
2	K	2820	LYS	CA-CB	5.22	1.57	1.53
2	E	2820	LYS	CA-CB	5.21	1.57	1.53
3	O	256	PRO	CA-C	5.21	1.54	1.51
2	B	2820	LYS	CA-CB	5.21	1.57	1.53
2	H	2820	LYS	CA-CB	5.19	1.57	1.53
3	C	256	PRO	CA-C	5.17	1.54	1.51
3	F	256	PRO	CA-C	5.13	1.54	1.51
3	I	256	PRO	CA-C	5.13	1.54	1.51

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2029	SER	N-CA-C	7.43	120.12	110.53
2	K	2029	SER	N-CA-C	7.42	120.11	110.53
2	E	2029	SER	N-CA-C	7.40	120.07	110.53
2	B	2029	SER	N-CA-C	7.39	120.06	110.53
2	N	2029	SER	N-CA-C	7.39	120.06	110.53
3	L	117	ASP	CA-CB-CG	6.96	119.56	112.60
3	C	117	ASP	CA-CB-CG	6.94	119.54	112.60
3	O	117	ASP	CA-CB-CG	6.92	119.52	112.60
3	F	117	ASP	CA-CB-CG	6.91	119.51	112.60
3	I	117	ASP	CA-CB-CG	6.89	119.49	112.60
2	B	2985	PRO	CA-C-N	6.61	130.36	120.31
2	B	2985	PRO	C-N-CA	6.61	130.36	120.31
2	N	2985	PRO	CA-C-N	6.60	130.35	120.31
2	N	2985	PRO	C-N-CA	6.60	130.35	120.31
2	K	2985	PRO	CA-C-N	6.60	130.34	120.31
2	K	2985	PRO	C-N-CA	6.60	130.34	120.31
2	E	2985	PRO	CA-C-N	6.60	130.34	120.31
2	E	2985	PRO	C-N-CA	6.60	130.34	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2985	PRO	CA-C-N	6.59	130.32	120.31
2	H	2985	PRO	C-N-CA	6.59	130.32	120.31
2	K	2891	ASP	CA-CB-CG	6.23	118.83	112.60
2	N	2891	ASP	CA-CB-CG	6.23	118.83	112.60
2	B	2891	ASP	CA-CB-CG	6.22	118.82	112.60
2	H	2891	ASP	CA-CB-CG	6.22	118.82	112.60
2	E	2891	ASP	CA-CB-CG	6.21	118.81	112.60
3	I	453	PHE	CA-CB-CG	6.10	119.90	113.80
3	L	453	PHE	CA-CB-CG	6.08	119.88	113.80
3	C	453	PHE	CA-CB-CG	6.07	119.87	113.80
3	F	453	PHE	CA-CB-CG	6.05	119.85	113.80
3	O	453	PHE	CA-CB-CG	6.04	119.83	113.80
3	I	168	ASP	CA-CB-CG	5.95	118.55	112.60
3	F	168	ASP	CA-CB-CG	5.93	118.53	112.60
3	C	168	ASP	CA-CB-CG	5.93	118.53	112.60
3	O	168	ASP	CA-CB-CG	5.92	118.52	112.60
3	L	168	ASP	CA-CB-CG	5.91	118.51	112.60
2	E	2917	ASP	CA-CB-CG	5.88	118.48	112.60
2	K	2917	ASP	CA-CB-CG	5.87	118.47	112.60
2	B	2917	ASP	CA-CB-CG	5.86	118.46	112.60
2	H	2917	ASP	CA-CB-CG	5.85	118.45	112.60
2	N	2917	ASP	CA-CB-CG	5.83	118.43	112.60
1	M	239	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	239	ASP	CA-CB-CG	5.70	118.30	112.60
1	G	239	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	239	ASP	CA-CB-CG	5.68	118.28	112.60
1	J	239	ASP	CA-CB-CG	5.67	118.27	112.60
3	I	418	ASN	CA-CB-CG	5.59	118.19	112.60
3	C	418	ASN	CA-CB-CG	5.55	118.15	112.60
1	M	1004	PHE	CA-CB-CG	5.55	119.35	113.80
3	O	418	ASN	CA-CB-CG	5.54	118.14	112.60
3	F	418	ASN	CA-CB-CG	5.53	118.13	112.60
3	L	418	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	1004	PHE	CA-CB-CG	5.51	119.31	113.80
1	G	1004	PHE	CA-CB-CG	5.51	119.31	113.80
1	D	1004	PHE	CA-CB-CG	5.50	119.30	113.80
1	G	1100	PRO	N-CA-C	5.49	117.40	110.70
1	J	1004	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	1100	PRO	N-CA-C	5.48	117.39	110.70
1	D	1100	PRO	N-CA-C	5.48	117.38	110.70
1	M	1100	PRO	N-CA-C	5.46	117.37	110.70
1	J	1100	PRO	N-CA-C	5.45	117.35	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2623	ASN	CA-CB-CG	5.44	118.04	112.60
2	B	2623	ASN	CA-CB-CG	5.40	118.00	112.60
1	M	893	ASP	CA-CB-CG	5.40	118.00	112.60
2	N	2623	ASN	CA-CB-CG	5.39	117.99	112.60
2	K	2623	ASN	CA-CB-CG	5.39	117.99	112.60
2	K	2588	ALA	N-CA-C	5.38	118.63	111.75
2	E	2623	ASN	CA-CB-CG	5.38	117.97	112.60
1	G	893	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	893	ASP	CA-CB-CG	5.36	117.96	112.60
1	J	893	ASP	CA-CB-CG	5.36	117.96	112.60
2	E	2576	LEU	CB-CA-C	5.36	117.86	111.22
3	I	526	SER	N-CA-C	5.36	119.39	112.86
2	E	2588	ALA	N-CA-C	5.35	118.59	111.75
2	N	2576	LEU	CB-CA-C	5.34	117.85	111.22
2	B	2588	ALA	N-CA-C	5.34	118.59	111.75
1	D	893	ASP	CA-CB-CG	5.34	117.94	112.60
2	K	2668	PHE	CA-C-N	5.34	131.74	121.54
2	K	2668	PHE	C-N-CA	5.34	131.74	121.54
2	H	2668	PHE	CA-C-N	5.34	131.74	121.54
2	H	2668	PHE	C-N-CA	5.34	131.74	121.54
2	N	2668	PHE	CA-C-N	5.33	131.73	121.54
2	N	2668	PHE	C-N-CA	5.33	131.73	121.54
3	O	526	SER	N-CA-C	5.33	119.37	112.86
2	E	2668	PHE	CA-C-N	5.33	131.72	121.54
2	E	2668	PHE	C-N-CA	5.33	131.72	121.54
1	G	1070	ASN	CA-CB-CG	5.33	117.93	112.60
2	B	2576	LEU	CB-CA-C	5.33	117.83	111.22
1	J	1070	ASN	CA-CB-CG	5.33	117.93	112.60
2	B	2668	PHE	CA-C-N	5.33	131.72	121.54
2	B	2668	PHE	C-N-CA	5.33	131.72	121.54
2	H	2588	ALA	N-CA-C	5.32	118.56	111.75
2	N	2588	ALA	N-CA-C	5.32	118.56	111.75
3	L	526	SER	N-CA-C	5.32	119.35	112.86
3	C	526	SER	N-CA-C	5.32	119.34	112.86
2	H	2576	LEU	CB-CA-C	5.31	117.81	111.22
1	D	1070	ASN	CA-CB-CG	5.31	117.91	112.60
3	F	526	SER	N-CA-C	5.31	119.33	112.86
2	K	2576	LEU	CB-CA-C	5.31	117.80	111.22
1	M	1070	ASN	CA-CB-CG	5.30	117.91	112.60
1	A	1070	ASN	CA-CB-CG	5.30	117.90	112.60
3	F	259	SER	CA-C-N	5.29	128.85	121.02
3	F	259	SER	C-N-CA	5.29	128.85	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	259	SER	CA-C-N	5.28	128.84	121.02
3	O	259	SER	C-N-CA	5.28	128.84	121.02
3	I	259	SER	CA-C-N	5.26	128.81	121.02
3	I	259	SER	C-N-CA	5.26	128.81	121.02
3	C	259	SER	CA-C-N	5.26	128.80	121.02
3	C	259	SER	C-N-CA	5.26	128.80	121.02
3	L	259	SER	CA-C-N	5.25	128.80	121.02
3	L	259	SER	C-N-CA	5.25	128.80	121.02
2	N	2278	HIS	CB-CG-CD2	-5.22	124.41	131.20
2	H	2278	HIS	CB-CG-CD2	-5.20	124.43	131.20
3	O	624	LEU	CA-C-N	5.20	128.23	120.90
3	O	624	LEU	C-N-CA	5.20	128.23	120.90
1	J	171	GLN	OE1-CD-NE2	-5.19	117.41	122.60
3	L	624	LEU	CA-C-N	5.19	128.22	120.90
3	L	624	LEU	C-N-CA	5.19	128.22	120.90
2	B	2278	HIS	CB-CG-CD2	-5.19	124.46	131.20
2	K	2278	HIS	CB-CG-CD2	-5.19	124.46	131.20
3	I	624	LEU	CA-C-N	5.18	128.21	120.90
3	I	624	LEU	C-N-CA	5.18	128.21	120.90
2	K	2035	LEU	CA-C-N	5.18	127.48	120.38
2	K	2035	LEU	C-N-CA	5.18	127.48	120.38
3	L	488	GLY	CA-C-N	5.18	124.89	119.92
3	L	488	GLY	C-N-CA	5.18	124.89	119.92
2	E	2278	HIS	CB-CG-CD2	-5.18	124.47	131.20
2	K	2089	ASN	CA-CB-CG	5.18	117.78	112.60
3	L	147	ASP	CA-CB-CG	5.18	117.78	112.60
3	C	624	LEU	CA-C-N	5.17	128.19	120.90
3	C	624	LEU	C-N-CA	5.17	128.19	120.90
1	D	67	VAL	N-CA-C	5.17	115.69	110.05
3	F	488	GLY	CA-C-N	5.17	124.89	119.92
3	F	488	GLY	C-N-CA	5.17	124.89	119.92
1	M	67	VAL	N-CA-C	5.17	115.69	110.05
3	C	488	GLY	CA-C-N	5.17	124.88	119.92
3	C	488	GLY	C-N-CA	5.17	124.88	119.92
1	J	67	VAL	N-CA-C	5.17	115.68	110.05
2	E	2089	ASN	CA-CB-CG	5.17	117.77	112.60
3	F	147	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	67	VAL	N-CA-C	5.16	115.68	110.05
1	D	171	GLN	OE1-CD-NE2	-5.16	117.44	122.60
3	F	624	LEU	CA-C-N	5.16	128.18	120.90
3	F	624	LEU	C-N-CA	5.16	128.18	120.90
1	G	171	GLN	OE1-CD-NE2	-5.16	117.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ASP	CA-CB-CG	5.16	117.76	112.60
2	N	2089	ASN	CA-CB-CG	5.16	117.75	112.60
1	A	171	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	D	189	ALA	CA-C-N	5.15	130.61	121.80
1	D	189	ALA	C-N-CA	5.15	130.61	121.80
3	I	488	GLY	CA-C-N	5.15	124.86	119.92
3	I	488	GLY	C-N-CA	5.15	124.86	119.92
2	B	2089	ASN	CA-CB-CG	5.15	117.75	112.60
2	H	2861	ARG	N-CA-C	5.14	117.17	110.43
3	I	147	ASP	CA-CB-CG	5.14	117.75	112.60
3	O	147	ASP	CA-CB-CG	5.14	117.75	112.60
1	G	67	VAL	N-CA-C	5.14	115.66	110.05
1	G	785	ASP	CA-C-N	5.14	127.68	120.28
1	G	785	ASP	C-N-CA	5.14	127.68	120.28
2	E	2035	LEU	CA-C-N	5.14	127.42	120.38
2	E	2035	LEU	C-N-CA	5.14	127.42	120.38
1	M	785	ASP	CA-C-N	5.14	127.68	120.28
1	M	785	ASP	C-N-CA	5.14	127.68	120.28
2	N	2861	ARG	N-CA-C	5.14	117.16	110.43
1	M	171	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	E	2861	ARG	N-CA-C	5.13	117.15	110.43
2	H	2089	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	2861	ARG	N-CA-C	5.13	117.15	110.43
3	O	488	GLY	CA-C-N	5.12	124.84	119.92
3	O	488	GLY	C-N-CA	5.12	124.84	119.92
1	A	785	ASP	CA-C-N	5.12	127.65	120.28
1	A	785	ASP	C-N-CA	5.12	127.65	120.28
1	J	189	ALA	CA-C-N	5.12	130.55	121.80
1	J	189	ALA	C-N-CA	5.12	130.55	121.80
1	A	189	ALA	CA-C-N	5.12	130.55	121.80
1	A	189	ALA	C-N-CA	5.12	130.55	121.80
1	M	189	ALA	CA-C-N	5.11	130.54	121.80
1	M	189	ALA	C-N-CA	5.11	130.54	121.80
1	D	785	ASP	CA-C-N	5.11	127.64	120.28
1	D	785	ASP	C-N-CA	5.11	127.64	120.28
1	G	189	ALA	CA-C-N	5.11	130.54	121.80
1	G	189	ALA	C-N-CA	5.11	130.54	121.80
1	J	785	ASP	CA-C-N	5.11	127.64	120.28
1	J	785	ASP	C-N-CA	5.11	127.64	120.28
1	D	224	ASP	CA-C-N	5.10	127.07	120.44
1	D	224	ASP	C-N-CA	5.10	127.07	120.44
1	J	224	ASP	CA-C-N	5.09	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	224	ASP	C-N-CA	5.09	127.06	120.44
1	A	224	ASP	CA-C-N	5.09	127.06	120.44
1	A	224	ASP	C-N-CA	5.09	127.06	120.44
2	K	2861	ARG	N-CA-C	5.09	117.10	110.43
1	M	224	ASP	CA-C-N	5.08	127.04	120.44
1	M	224	ASP	C-N-CA	5.08	127.04	120.44
3	L	255	LEU	CA-C-N	5.07	123.36	119.66
3	L	255	LEU	C-N-CA	5.07	123.36	119.66
1	G	224	ASP	CA-C-N	5.07	127.03	120.44
1	G	224	ASP	C-N-CA	5.07	127.03	120.44
3	I	255	LEU	CA-C-N	5.07	123.36	119.66
3	I	255	LEU	C-N-CA	5.07	123.36	119.66
2	B	3238	ASP	CA-CB-CG	5.07	117.67	112.60
2	K	3238	ASP	CA-CB-CG	5.07	117.67	112.60
3	C	255	LEU	CA-C-N	5.06	123.36	119.66
3	C	255	LEU	C-N-CA	5.06	123.36	119.66
2	E	3238	ASP	CA-CB-CG	5.06	117.66	112.60
2	N	3238	ASP	CA-CB-CG	5.06	117.66	112.60
3	O	255	LEU	CA-C-N	5.05	123.35	119.66
3	O	255	LEU	C-N-CA	5.05	123.35	119.66
2	E	2677	SER	CA-C-N	5.05	129.38	122.06
2	E	2677	SER	C-N-CA	5.05	129.38	122.06
1	G	882	VAL	N-CA-C	5.05	115.91	110.21
1	M	882	VAL	N-CA-C	5.04	115.91	110.21
1	A	882	VAL	N-CA-C	5.04	115.90	110.21
1	J	882	VAL	N-CA-C	5.04	115.90	110.21
3	O	199	SER	CA-C-N	5.04	130.76	121.70
3	O	199	SER	C-N-CA	5.04	130.76	121.70
2	B	2031	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	882	VAL	N-CA-C	5.03	115.89	110.21
2	E	2031	ASP	CA-CB-CG	5.03	117.63	112.60
2	H	3238	ASP	CA-CB-CG	5.03	117.63	112.60
2	K	2031	ASP	CA-CB-CG	5.03	117.63	112.60
2	N	2677	SER	CA-C-N	5.03	129.35	122.06
2	N	2677	SER	C-N-CA	5.03	129.35	122.06
2	N	2031	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	2535	GLN	OE1-CD-NE2	-5.03	117.57	122.60
2	H	2607	PHE	CA-C-N	5.02	127.01	120.28
2	H	2607	PHE	C-N-CA	5.02	127.01	120.28
3	O	582	TRP	CA-C-N	5.02	130.74	121.70
3	O	582	TRP	C-N-CA	5.02	130.74	121.70
2	K	2076	ASN	CA-C-N	5.02	127.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2076	ASN	C-N-CA	5.02	127.01	120.28
2	B	2677	SER	CA-C-N	5.02	129.34	122.06
2	B	2677	SER	C-N-CA	5.02	129.34	122.06
1	J	1162	ASP	CA-CB-CG	5.02	117.62	112.60
2	H	2535	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	K	2535	GLN	OE1-CD-NE2	-5.02	117.58	122.60
2	E	2076	ASN	CA-C-N	5.01	127.00	120.28
2	E	2076	ASN	C-N-CA	5.01	127.00	120.28
3	F	199	SER	CA-C-N	5.01	130.73	121.70
3	F	199	SER	C-N-CA	5.01	130.73	121.70
2	H	2076	ASN	CA-C-N	5.01	127.00	120.28
2	H	2076	ASN	C-N-CA	5.01	127.00	120.28
3	C	199	SER	CA-C-N	5.01	130.72	121.70
3	C	199	SER	C-N-CA	5.01	130.72	121.70
3	I	582	TRP	CA-C-N	5.01	130.72	121.70
3	I	582	TRP	C-N-CA	5.01	130.72	121.70
3	L	582	TRP	CA-C-N	5.01	130.72	121.70
3	L	582	TRP	C-N-CA	5.01	130.72	121.70
2	B	2607	PHE	CA-C-N	5.01	126.99	120.28
2	B	2607	PHE	C-N-CA	5.01	126.99	120.28
3	I	199	SER	CA-C-N	5.01	130.72	121.70
3	I	199	SER	C-N-CA	5.01	130.72	121.70
2	K	2677	SER	CA-C-N	5.01	129.32	122.06
2	K	2677	SER	C-N-CA	5.01	129.32	122.06
2	E	2535	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	E	2607	PHE	CA-C-N	5.01	126.99	120.28
2	E	2607	PHE	C-N-CA	5.01	126.99	120.28
2	H	2031	ASP	CA-CB-CG	5.01	117.61	112.60
2	N	2535	GLN	OE1-CD-NE2	-5.01	117.59	122.60
3	I	350	TYR	CA-C-N	5.00	124.78	119.28
3	I	350	TYR	C-N-CA	5.00	124.78	119.28
2	K	2607	PHE	CA-C-N	5.00	126.98	120.28
2	K	2607	PHE	C-N-CA	5.00	126.98	120.28
3	L	199	SER	CA-C-N	5.00	130.71	121.70
3	L	199	SER	C-N-CA	5.00	130.71	121.70

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1114	ARG	Sidechain
1	A	241	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	984	TYR	Sidechain
2	B	2718	ARG	Sidechain
2	B	2807	ARG	Sidechain
3	C	369	TYR	Sidechain
1	D	1114	ARG	Sidechain
1	D	241	HIS	Peptide
1	D	984	TYR	Sidechain
2	E	2718	ARG	Sidechain
2	E	2807	ARG	Sidechain
3	F	369	TYR	Sidechain
1	G	1114	ARG	Sidechain
1	G	241	HIS	Peptide
1	G	984	TYR	Sidechain
2	H	2718	ARG	Sidechain
2	H	2807	ARG	Sidechain
3	I	369	TYR	Sidechain
1	J	1114	ARG	Sidechain
1	J	241	HIS	Peptide
1	J	984	TYR	Sidechain
2	K	2718	ARG	Sidechain
2	K	2807	ARG	Sidechain
3	L	369	TYR	Sidechain
1	M	1114	ARG	Sidechain
1	M	241	HIS	Peptide
1	M	984	TYR	Sidechain
2	N	2718	ARG	Sidechain
2	N	2807	ARG	Sidechain
3	O	369	TYR	Sidechain

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	5910	0	5971	11	0
1	D	5910	0	5971	12	0
1	G	5910	0	5971	12	0
1	J	5910	0	5971	10	0
1	M	5910	0	5971	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8742	0	8563	94	0
2	E	8742	0	8563	97	0
2	H	8742	0	8563	88	0
2	K	8742	0	8563	92	0
2	N	8742	0	8563	94	0
3	C	4173	0	4010	1	0
3	F	4173	0	4010	1	0
3	I	4173	0	4010	1	0
3	L	4173	0	4010	1	0
3	O	4173	0	4010	1	0
All	All	94125	0	92720	273	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 1.

All (273) 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:B:2812:ARG:HD2	2:E:2055:VAL:CB	1.62	1.28
2:K:2812:ARG:HD2	2:N:2055:VAL:CB	1.66	1.25
2:B:2812:ARG:HD2	2:E:2055:VAL:CG1	1.67	1.23
2:E:2812:ARG:HD2	2:H:2055:VAL:CB	1.67	1.22
2:K:2812:ARG:HD2	2:N:2055:VAL:CG1	1.69	1.21
2:E:3255:ASP:N	1:G:908:ASN:OD1	1.73	1.20
2:H:2812:ARG:HD2	2:K:2055:VAL:CG1	1.70	1.20
2:E:2812:ARG:HD2	2:H:2055:VAL:CG1	1.72	1.20
2:H:2812:ARG:HD2	2:K:2055:VAL:CB	1.70	1.20
2:B:2055:VAL:CB	2:N:2812:ARG:HD2	1.72	1.19
2:B:2055:VAL:CG1	2:N:2812:ARG:HD2	1.72	1.17
2:B:3255:ASP:N	1:D:908:ASN:OD1	1.75	1.17
2:K:3255:ASP:N	1:M:908:ASN:OD1	1.77	1.15
1:A:908:ASN:OD1	2:N:3255:ASP:N	1.76	1.14
2:H:3255:ASP:N	1:J:908:ASN:OD1	1.80	1.14
2:B:2812:ARG:HD2	2:E:2055:VAL:HB	1.32	1.09
2:E:3172:GLN:HG3	2:H:3278:ILE:CG1	1.82	1.09
2:B:3278:ILE:CG1	2:N:3172:GLN:HG3	1.81	1.09
2:K:2812:ARG:HD2	2:N:2055:VAL:HB	1.36	1.07
2:K:3172:GLN:HG3	2:N:3278:ILE:CG1	1.85	1.07
2:B:3172:GLN:HG3	2:E:3278:ILE:CG1	1.85	1.06
2:H:3172:GLN:HG3	2:K:3278:ILE:CG1	1.85	1.05
2:E:2812:ARG:HD2	2:H:2055:VAL:HB	1.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3172:GLN:HG3	2:N:3278:ILE:HG12	1.40	1.03
2:H:2812:ARG:HD2	2:K:2055:VAL:HB	1.39	1.03
2:B:3278:ILE:CD1	2:N:3172:GLN:HG3	1.89	1.02
2:B:2055:VAL:HB	2:N:2812:ARG:HD2	1.40	1.02
2:E:3172:GLN:HG3	2:H:3278:ILE:HG12	1.36	1.02
2:H:2812:ARG:HD2	2:K:2055:VAL:HG11	1.42	1.01
2:H:3172:GLN:HG3	2:K:3278:ILE:HG12	1.42	1.00
2:B:2812:ARG:CD	2:E:2055:VAL:HB	1.91	1.00
2:B:3172:GLN:HG3	2:E:3278:ILE:HG12	1.40	1.00
2:K:2812:ARG:HD2	2:N:2055:VAL:HG11	1.43	1.00
2:B:3278:ILE:HG12	2:N:3172:GLN:HG3	1.39	0.99
2:H:3172:GLN:HG3	2:K:3278:ILE:CD1	1.92	0.99
2:K:3172:GLN:HG3	2:N:3278:ILE:CD1	1.93	0.99
2:B:2812:ARG:HD2	2:E:2055:VAL:HG11	1.42	0.99
2:B:2055:VAL:HG11	2:N:2812:ARG:HD2	1.43	0.98
2:E:2812:ARG:HD2	2:H:2055:VAL:HG11	1.46	0.98
2:E:3172:GLN:HG3	2:H:3278:ILE:CD1	1.93	0.98
2:E:3172:GLN:CG	2:H:3278:ILE:HG12	1.95	0.96
2:E:2812:ARG:CD	2:H:2055:VAL:HB	1.95	0.96
2:B:3172:GLN:HG3	2:E:3278:ILE:CD1	1.95	0.96
2:K:2812:ARG:CD	2:N:2055:VAL:HB	1.95	0.95
2:B:3278:ILE:HG12	2:N:3172:GLN:CG	1.95	0.95
2:K:3172:GLN:CG	2:N:3278:ILE:HG12	1.97	0.94
2:E:3110:ASP:OD1	1:G:922:GLN:NE2	2.02	0.92
2:B:3110:ASP:OD1	1:D:922:GLN:NE2	2.01	0.92
2:H:3172:GLN:CG	2:K:3278:ILE:HG12	1.99	0.92
1:A:922:GLN:NE2	2:N:3110:ASP:OD1	2.00	0.92
2:B:3172:GLN:CG	2:E:3278:ILE:HG12	1.99	0.91
2:K:3110:ASP:OD1	1:M:922:GLN:NE2	2.04	0.90
2:H:2812:ARG:CD	2:K:2055:VAL:HB	1.99	0.90
2:B:2055:VAL:HB	2:N:2812:ARG:CD	2.01	0.90
2:H:3110:ASP:OD1	1:J:922:GLN:NE2	2.04	0.90
2:B:2812:ARG:CD	2:E:2055:VAL:CG1	2.49	0.90
2:B:3278:ILE:HD11	2:N:3172:GLN:HG3	1.56	0.87
2:E:2812:ARG:CD	2:H:2055:VAL:CG1	2.55	0.84
2:K:2812:ARG:CD	2:N:2055:VAL:CG1	2.52	0.84
2:H:3172:GLN:HG3	2:K:3278:ILE:HD11	1.57	0.83
2:B:2812:ARG:CG	2:E:2055:VAL:HB	2.08	0.83
2:E:3172:GLN:H	2:H:3278:ILE:HD11	1.44	0.83
2:K:3172:GLN:HG3	2:N:3278:ILE:HD11	1.59	0.83
2:H:2812:ARG:CD	2:K:2055:VAL:CG1	2.54	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3172:GLN:HG3	2:E:3278:ILE:HD11	1.62	0.81
2:B:3278:ILE:HD11	2:N:3172:GLN:H	1.45	0.81
2:B:2812:ARG:CD	2:E:2055:VAL:HG11	2.10	0.81
2:B:3172:GLN:H	2:E:3278:ILE:HD11	1.46	0.81
2:B:2055:VAL:CG1	2:N:2812:ARG:CD	2.56	0.81
2:E:3172:GLN:HG3	2:H:3278:ILE:HD11	1.62	0.80
2:E:2730:SER:OG	2:H:2080:LEU:HD11	1.82	0.79
2:K:2812:ARG:CD	2:N:2055:VAL:HG11	2.13	0.79
2:E:3257:LYS:HB2	1:G:905:GLY:HA3	1.65	0.79
2:K:2812:ARG:CG	2:N:2055:VAL:HB	2.12	0.79
2:K:3172:GLN:H	2:N:3278:ILE:HD11	1.47	0.79
2:H:2812:ARG:CD	2:K:2055:VAL:HG11	2.14	0.78
2:B:2080:LEU:HD11	2:N:2730:SER:OG	1.84	0.77
2:E:2812:ARG:CD	2:H:2055:VAL:HG11	2.15	0.77
2:H:3172:GLN:H	2:K:3278:ILE:HD11	1.48	0.77
2:B:3278:ILE:CG1	2:N:3172:GLN:CG	2.59	0.76
2:B:2730:SER:OG	2:E:2080:LEU:HD11	1.84	0.76
2:E:2812:ARG:CG	2:H:2055:VAL:HB	2.14	0.76
2:H:2812:ARG:CG	2:K:2055:VAL:HB	2.15	0.76
2:K:3257:LYS:HB2	1:M:905:GLY:HA3	1.68	0.76
2:B:2055:VAL:HG11	2:N:2812:ARG:CD	2.15	0.76
2:K:2730:SER:OG	2:N:2080:LEU:HD11	1.84	0.76
2:H:3172:GLN:CG	2:K:3278:ILE:CG1	2.63	0.74
2:B:2055:VAL:HB	2:N:2812:ARG:CG	2.17	0.74
2:H:2730:SER:OG	2:K:2080:LEU:HD11	1.88	0.74
2:B:3058:MET:HB3	2:N:2920:ILE:HD11	1.69	0.73
2:B:3257:LYS:HB2	1:D:905:GLY:HA3	1.69	0.73
1:A:905:GLY:HA3	2:N:3257:LYS:HB2	1.68	0.73
2:K:3172:GLN:CG	2:N:3278:ILE:CG1	2.62	0.73
2:K:2920:ILE:HD11	2:N:3058:MET:HB3	1.71	0.72
2:B:2920:ILE:HD11	2:E:3058:MET:HB3	1.70	0.72
2:H:3257:LYS:HB2	1:J:905:GLY:HA3	1.71	0.72
2:H:2920:ILE:HD11	2:K:3058:MET:HB3	1.72	0.72
2:E:2920:ILE:HD11	2:H:3058:MET:HB3	1.72	0.71
2:E:3172:GLN:CG	2:H:3278:ILE:CG1	2.61	0.70
2:E:2812:ARG:CD	2:H:2055:VAL:CB	2.55	0.69
2:B:3278:ILE:HD11	2:N:3172:GLN:N	2.07	0.69
2:E:3172:GLN:N	2:H:3278:ILE:HD11	2.07	0.69
2:B:3172:GLN:N	2:E:3278:ILE:HD11	2.08	0.68
2:B:2913:LEU:HD13	2:E:3065:LYS:HB2	1.77	0.67
2:K:3172:GLN:N	2:N:3278:ILE:HD11	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3172:GLN:N	2:K:3278:ILE:HD11	2.09	0.66
2:B:3065:LYS:HB2	2:N:2913:LEU:HD13	1.76	0.65
2:B:3172:GLN:CG	2:E:3278:ILE:CG1	2.64	0.65
2:K:2913:LEU:HD13	2:N:3065:LYS:HB2	1.79	0.64
2:H:2913:LEU:HD13	2:K:3065:LYS:HB2	1.79	0.64
2:K:2812:ARG:CD	2:N:2055:VAL:CB	2.54	0.64
2:E:2913:LEU:HD13	2:H:3065:LYS:HB2	1.80	0.62
2:B:2913:LEU:HD13	2:E:3065:LYS:CB	2.31	0.60
2:B:3065:LYS:CB	2:N:2913:LEU:HD13	2.32	0.60
1:A:908:ASN:HB2	2:N:3254:ALA:HB1	1.84	0.59
2:E:3255:ASP:CB	1:G:908:ASN:OD1	2.50	0.59
2:B:2991:ALA:HB1	2:N:2987:ILE:HD11	1.83	0.59
2:K:3255:ASP:CB	1:M:908:ASN:OD1	2.51	0.59
2:E:3254:ALA:HB1	1:G:908:ASN:HB2	1.85	0.59
2:B:2644:CYS:HB3	2:E:2082:LEU:HD11	1.84	0.58
2:B:2954:GLU:OE2	2:E:3030:ARG:NH2	2.32	0.58
2:K:2913:LEU:HD13	2:N:3065:LYS:CB	2.34	0.58
2:B:2812:ARG:HD2	2:E:2055:VAL:CG2	2.34	0.58
2:B:3254:ALA:HB1	1:D:908:ASN:HB2	1.87	0.57
2:H:2913:LEU:HD13	2:K:3065:LYS:CB	2.34	0.57
2:E:3254:ALA:HB1	1:G:908:ASN:CB	2.35	0.57
2:E:2987:ILE:HD11	2:H:2991:ALA:HB1	1.86	0.57
2:K:2987:ILE:HD11	2:N:2991:ALA:HB1	1.86	0.57
2:B:3030:ARG:NH2	2:N:2954:GLU:OE2	2.34	0.57
2:E:2913:LEU:HD13	2:H:3065:LYS:CB	2.35	0.57
1:A:848:ASN:CG	2:K:3159:ARG:HH11	2.13	0.56
2:H:2987:ILE:HD11	2:K:2991:ALA:HB1	1.86	0.56
2:B:3255:ASP:CB	1:D:908:ASN:OD1	2.53	0.56
2:E:2954:GLU:OE2	2:H:3030:ARG:NH2	2.34	0.56
1:D:848:ASN:CG	2:N:3159:ARG:HH11	2.14	0.56
2:K:2644:CYS:HB3	2:N:2082:LEU:HD11	1.87	0.56
2:B:3254:ALA:HB1	1:D:908:ASN:CB	2.36	0.55
2:E:3159:ARG:HH11	1:J:848:ASN:CG	2.14	0.55
1:A:908:ASN:OD1	2:N:3255:ASP:CB	2.55	0.55
2:H:3255:ASP:CB	1:J:908:ASN:OD1	2.54	0.55
2:K:2954:GLU:OE2	2:N:3030:ARG:NH2	2.36	0.55
1:A:908:ASN:CB	2:N:3254:ALA:HB1	2.36	0.55
2:E:3256:LEU:HG	1:G:906:VAL:HB	1.87	0.54
2:K:3254:ALA:HB1	1:M:908:ASN:HB2	1.89	0.54
2:B:3159:ARG:HH11	1:G:848:ASN:CG	2.15	0.54
2:E:2644:CYS:HB3	2:H:2082:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3254:ALA:HB1	1:J:908:ASN:HB2	1.90	0.53
2:B:2987:ILE:HD11	2:E:2991:ALA:HB1	1.89	0.53
2:B:3256:LEU:HG	1:D:906:VAL:HB	1.91	0.53
1:A:906:VAL:HB	2:N:3256:LEU:HG	1.89	0.52
2:E:2812:ARG:HD2	2:H:2055:VAL:CG2	2.38	0.52
2:H:2644:CYS:HB3	2:K:2082:LEU:HD11	1.89	0.52
2:K:3256:LEU:HG	1:M:906:VAL:HB	1.91	0.52
2:H:2954:GLU:OE2	2:K:3030:ARG:NH2	2.34	0.52
2:B:3278:ILE:CG1	2:N:3172:GLN:NE2	2.74	0.51
2:E:3172:GLN:N	2:H:3278:ILE:CD1	2.73	0.51
2:K:2960:LEU:HD22	2:N:3015:ASP:CG	2.35	0.51
2:B:2644:CYS:CB	2:E:2082:LEU:HD11	2.41	0.51
2:B:2082:LEU:HD11	2:N:2644:CYS:HB3	1.93	0.51
2:B:3278:ILE:CD1	2:N:3172:GLN:N	2.73	0.51
2:K:3254:ALA:HB1	1:M:908:ASN:CB	2.40	0.51
2:B:2960:LEU:HD22	2:E:3015:ASP:CG	2.37	0.50
2:H:3159:ARG:HH11	1:M:848:ASN:CG	2.19	0.50
2:E:3018:LYS:HG3	2:N:2140:ASN:OD1	2.12	0.50
2:H:2140:ASN:OD1	2:N:3018:LYS:HG3	2.12	0.50
2:H:3254:ALA:HB1	1:J:908:ASN:CB	2.42	0.50
2:K:2644:CYS:CB	2:N:2082:LEU:HD11	2.42	0.50
2:H:2644:CYS:CB	2:K:2082:LEU:HD11	2.42	0.49
2:E:2960:LEU:HD22	2:H:3015:ASP:CG	2.37	0.49
2:K:3172:GLN:NE2	2:N:3278:ILE:CG1	2.75	0.49
2:B:3172:GLN:N	2:E:3278:ILE:CD1	2.75	0.49
2:H:3256:LEU:HG	1:J:906:VAL:HB	1.94	0.49
2:E:2644:CYS:CB	2:H:2082:LEU:HD11	2.44	0.48
2:E:3172:GLN:NE2	2:H:3278:ILE:CG1	2.76	0.48
2:H:3172:GLN:N	2:K:3278:ILE:CD1	2.77	0.48
2:B:3015:ASP:CG	2:N:2960:LEU:HD22	2.37	0.48
2:H:3172:GLN:NE2	2:K:3278:ILE:CG1	2.76	0.48
2:H:2960:LEU:HD22	2:K:3015:ASP:CG	2.39	0.48
2:B:3278:ILE:HG13	2:N:3172:GLN:NE2	2.29	0.48
2:K:2960:LEU:HD22	2:N:3015:ASP:HB3	1.96	0.48
2:K:2812:ARG:HD2	2:N:2055:VAL:CG2	2.38	0.47
3:I:348:TRP:CH2	3:I:351:PRO:HA	2.50	0.47
3:L:348:TRP:CH2	3:L:351:PRO:HA	2.50	0.47
3:O:348:TRP:CH2	3:O:351:PRO:HA	2.50	0.47
3:F:348:TRP:CH2	3:F:351:PRO:HA	2.50	0.47
2:B:2812:ARG:HG2	2:E:2055:VAL:HB	1.93	0.47
2:E:2140:ASN:OD1	2:K:3018:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3171:ARG:HA	2:E:3278:ILE:CD1	2.44	0.46
2:B:3254:ALA:HB1	1:D:908:ASN:CG	2.40	0.46
2:K:2960:LEU:HD22	2:N:3015:ASP:CB	2.46	0.46
2:B:2960:LEU:HD22	2:E:3015:ASP:HB3	1.97	0.46
2:E:3171:ARG:HA	2:H:3278:ILE:CD1	2.45	0.46
3:C:348:TRP:CH2	3:C:351:PRO:HA	2.50	0.46
2:B:3278:ILE:CG1	2:N:3172:GLN:CD	2.89	0.46
2:K:3172:GLN:N	2:N:3278:ILE:CD1	2.76	0.46
2:B:2812:ARG:NE	2:E:2055:VAL:CG1	2.79	0.46
2:B:3171:ARG:HA	2:E:3278:ILE:HD13	1.98	0.46
2:E:3171:ARG:HA	2:H:3278:ILE:HD13	1.98	0.46
2:B:2960:LEU:HD22	2:E:3015:ASP:CB	2.46	0.46
2:B:3172:GLN:NE2	2:E:3278:ILE:CG1	2.80	0.46
2:B:2082:LEU:HD11	2:N:2644:CYS:CB	2.46	0.45
2:K:3172:GLN:NE2	2:N:3278:ILE:HG12	2.32	0.45
2:B:3278:ILE:HG12	2:N:3172:GLN:NE2	2.32	0.45
2:B:2920:ILE:CD1	2:E:3058:MET:HB3	2.43	0.45
2:E:2960:LEU:HD22	2:H:3015:ASP:HB3	1.99	0.45
2:E:3172:GLN:CD	2:H:3278:ILE:CG1	2.90	0.45
2:K:3172:GLN:NE2	2:N:3278:ILE:HG13	2.32	0.45
2:H:3172:GLN:NE2	2:K:3278:ILE:HG13	2.32	0.45
2:E:3172:GLN:NE2	2:H:3278:ILE:HG12	2.33	0.44
2:K:3171:ARG:HA	2:N:3278:ILE:CD1	2.48	0.44
2:H:2960:LEU:HD22	2:K:3015:ASP:HB3	2.00	0.44
2:B:3278:ILE:HG12	2:N:3172:GLN:CD	2.43	0.44
2:E:3254:ALA:HB1	1:G:908:ASN:CG	2.42	0.44
2:B:3018:LYS:HG3	2:K:2140:ASN:OD1	2.18	0.44
2:E:3172:GLN:CD	2:H:3278:ILE:HG12	2.42	0.44
2:H:2837:MET:SD	2:K:3078:MET:HG3	2.57	0.44
1:A:908:ASN:CG	2:N:3254:ALA:HB1	2.43	0.43
2:B:3078:MET:HG3	2:N:2837:MET:SD	2.58	0.43
2:K:3172:GLN:CD	2:N:3278:ILE:CG1	2.91	0.43
2:B:3255:ASP:CA	1:D:908:ASN:OD1	2.63	0.43
2:B:3278:ILE:CD1	2:N:3171:ARG:HA	2.48	0.43
2:E:3172:GLN:NE2	2:H:3278:ILE:HG13	2.33	0.43
1:A:196:LEU:HG	1:A:197:ASP:H	1.84	0.43
2:E:2960:LEU:HD22	2:H:3015:ASP:CB	2.49	0.43
2:H:3171:ARG:HA	2:K:3278:ILE:CD1	2.48	0.43
2:B:2933:GLN:HB2	2:E:3044:TRP:HE1	1.83	0.43
2:B:2998:GLY:H	2:N:2981:LEU:HD21	1.84	0.43
1:D:196:LEU:HG	1:D:197:ASP:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2812:ARG:HG2	2:N:2055:VAL:HB	1.96	0.43
2:B:2055:VAL:CG2	2:N:2812:ARG:HD2	2.42	0.43
2:B:2954:GLU:CD	2:E:3030:ARG:HH21	2.26	0.42
2:H:2920:ILE:CD1	2:K:3058:MET:HB3	2.46	0.42
1:G:196:LEU:HG	1:G:197:ASP:H	1.84	0.42
2:H:3172:GLN:CD	2:K:3278:ILE:CG1	2.92	0.42
1:J:196:LEU:HG	1:J:197:ASP:H	1.84	0.42
2:E:2920:ILE:CD1	2:H:3058:MET:HB3	2.46	0.42
2:E:3255:ASP:CA	1:G:908:ASN:OD1	2.60	0.42
2:H:3172:GLN:NE2	2:K:3278:ILE:HG12	2.34	0.42
2:K:3171:ARG:HA	2:N:3278:ILE:HD13	2.01	0.42
2:K:2920:ILE:CD1	2:N:3058:MET:HB3	2.45	0.42
2:K:2812:ARG:NE	2:N:2055:VAL:CG1	2.83	0.41
2:N:2590:LEU:C	2:N:2590:LEU:HD12	2.45	0.41
1:A:1071:SER:HA	1:A:1074:CYS:SG	2.61	0.41
2:B:3058:MET:HB3	2:N:2920:ILE:CD1	2.44	0.41
2:E:2976:THR:HG23	2:N:2194:TYR:OH	2.20	0.41
2:K:3254:ALA:HB1	1:M:908:ASN:CG	2.46	0.41
1:M:196:LEU:HG	1:M:197:ASP:H	1.84	0.41
2:B:3278:ILE:HD13	2:N:3171:ARG:HA	2.02	0.41
2:B:2590:LEU:C	2:B:2590:LEU:HD12	2.45	0.41
1:J:1071:SER:HA	1:J:1074:CYS:SG	2.61	0.41
2:K:2590:LEU:HD12	2:K:2590:LEU:C	2.45	0.41
2:K:3172:GLN:CD	2:N:3278:ILE:HG12	2.43	0.41
2:B:2837:MET:SD	2:E:3078:MET:HG3	2.61	0.41
2:H:3171:ARG:HA	2:K:3278:ILE:HD13	2.03	0.41
2:B:2140:ASN:OD1	2:H:3018:LYS:HG3	2.20	0.41
2:B:3278:ILE:HG12	2:N:3172:GLN:HE21	1.86	0.41
2:B:3172:GLN:CD	2:E:3278:ILE:CG1	2.94	0.41
1:D:1071:SER:HA	1:D:1074:CYS:SG	2.61	0.41
2:E:2590:LEU:C	2:E:2590:LEU:HD12	2.45	0.41
2:H:2590:LEU:HD12	2:H:2590:LEU:C	2.45	0.41
2:B:3172:GLN:NE2	2:E:3278:ILE:HG13	2.35	0.40
1:G:1071:SER:HA	1:G:1074:CYS:SG	2.61	0.40
2:H:2960:LEU:HD22	2:K:3015:ASP:CB	2.51	0.40
2:K:3172:GLN:HE21	2:N:3278:ILE:HG12	1.86	0.40
1:M:1071:SER:HA	1:M:1074:CYS:SG	2.61	0.40
2:H:2812:ARG:HD2	2:K:2055:VAL:CG2	2.44	0.40
2:B:3172:GLN:NE2	2:E:3278:ILE:HG12	2.36	0.40
2:H:2229:GLU:HG3	2:N:3000:PRO:HG3	2.03	0.40
2:B:2730:SER:CB	2:E:2080:LEU:HD21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3172:GLN:CD	2:E:3278:ILE:HG12	2.47	0.40
2:E:2229:GLU:HG3	2:K:3000:PRO:HG3	2.04	0.40
2:E:2812:ARG:NE	2:H:2055:VAL:CG1	2.84	0.40
2:K:2837:MET:SD	2:N:3078:MET:HG3	2.60	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	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	10	42
1	D	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	10	42
1	G	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	10	42
1	J	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	10	42
1	M	740/1164 (64%)	665 (90%)	66 (9%)	9 (1%)	10	42
2	B	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	6	31
2	E	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	6	31
2	H	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	6	31
2	K	1070/1364 (78%)	934 (87%)	115 (11%)	21 (2%)	6	31
2	N	1070/1364 (78%)	934 (87%)	116 (11%)	20 (2%)	6	32
3	C	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	7	35
3	F	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	7	35
3	I	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	7	35
3	L	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	7	35
3	O	534/633 (84%)	475 (89%)	50 (9%)	9 (2%)	7	35
All	All	11720/15805 (74%)	10370 (88%)	1156 (10%)	194 (2%)	9	35

All (194) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2669	LYS
2	E	2669	LYS
2	H	2669	LYS
2	K	2669	LYS
2	N	2669	LYS
1	A	295	GLN
1	A	297	SER
1	A	1161	SER
2	B	2712	LYS
2	B	3275	VAL
3	C	551	ALA
1	D	295	GLN
1	D	297	SER
1	D	1161	SER
2	E	2712	LYS
2	E	3275	VAL
3	F	551	ALA
1	G	295	GLN
1	G	297	SER
1	G	1161	SER
2	H	2712	LYS
2	H	3275	VAL
3	I	551	ALA
1	J	295	GLN
1	J	297	SER
1	J	1161	SER
2	K	2712	LYS
2	K	3275	VAL
3	L	551	ALA
1	M	295	GLN
1	M	297	SER
1	M	1161	SER
2	N	2712	LYS
2	N	3275	VAL
3	O	551	ALA
2	B	2125	ARG
2	B	2299	GLN
2	B	2537	LEU
3	C	108	TYR
2	E	2125	ARG
2	E	2299	GLN
2	E	2537	LEU

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Mol	Chain	Res	Type
3	F	108	TYR
2	H	2125	ARG
2	H	2299	GLN
2	H	2537	LEU
3	I	108	TYR
2	K	2125	ARG
2	K	2299	GLN
2	K	2537	LEU
3	L	108	TYR
2	N	2125	ARG
2	N	2299	GLN
2	N	2537	LEU
3	O	108	TYR
1	A	234	ASN
2	B	2179	GLU
2	B	2266	VAL
2	B	2296	LEU
2	B	2327	SER
2	B	2818	ASP
2	B	3230	PRO
2	B	3240	CYS
2	B	3282	GLN
3	C	94	PRO
3	C	166	ARG
3	C	252	ASN
3	C	445	LYS
3	C	449	GLU
3	C	553	GLY
1	D	234	ASN
2	E	2179	GLU
2	E	2266	VAL
2	E	2296	LEU
2	E	2327	SER
2	E	2818	ASP
2	E	3230	PRO
2	E	3240	CYS
2	E	3282	GLN
3	F	94	PRO
3	F	166	ARG
3	F	252	ASN
3	F	445	LYS
3	F	449	GLU

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Mol	Chain	Res	Type
3	F	553	GLY
1	G	234	ASN
2	H	2179	GLU
2	H	2266	VAL
2	H	2296	LEU
2	H	2327	SER
2	H	2818	ASP
2	H	3230	PRO
2	H	3240	CYS
2	H	3282	GLN
3	I	94	PRO
3	I	166	ARG
3	I	252	ASN
3	I	445	LYS
3	I	449	GLU
3	I	553	GLY
1	J	234	ASN
2	K	2179	GLU
2	K	2266	VAL
2	K	2296	LEU
2	K	2327	SER
2	K	2818	ASP
2	K	3230	PRO
2	K	3240	CYS
2	K	3282	GLN
3	L	94	PRO
3	L	166	ARG
3	L	252	ASN
3	L	445	LYS
3	L	449	GLU
3	L	553	GLY
1	M	234	ASN
2	N	2179	GLU
2	N	2266	VAL
2	N	2296	LEU
2	N	2327	SER
2	N	2818	ASP
2	N	3230	PRO
2	N	3240	CYS
2	N	3282	GLN
3	O	94	PRO
3	O	166	ARG

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Mol	Chain	Res	Type
3	O	252	ASN
3	O	445	LYS
3	O	449	GLU
3	O	553	GLY
1	A	854	ASP
1	A	879	MET
2	B	2128	LYS
2	B	2305	ALA
2	B	2313	GLU
2	B	2814	ASN
1	D	854	ASP
1	D	879	MET
2	E	2128	LYS
2	E	2305	ALA
2	E	2313	GLU
2	E	2814	ASN
1	G	854	ASP
1	G	879	MET
2	H	2128	LYS
2	H	2305	ALA
2	H	2313	GLU
2	H	2814	ASN
1	J	854	ASP
1	J	879	MET
2	K	2128	LYS
2	K	2305	ALA
2	K	2313	GLU
2	K	2814	ASN
1	M	854	ASP
1	M	879	MET
2	N	2128	LYS
2	N	2305	ALA
2	N	2313	GLU
2	N	2814	ASN
2	B	2027	PRO
2	B	2300	MET
2	B	2544	SER
2	E	2027	PRO
2	E	2300	MET
2	E	2544	SER
2	H	2027	PRO
2	H	2300	MET

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Mol	Chain	Res	Type
2	H	2544	SER
2	K	2027	PRO
2	K	2300	MET
2	K	2544	SER
2	N	2027	PRO
2	N	2544	SER
1	A	781	PRO
1	D	781	PRO
1	G	781	PRO
1	J	781	PRO
1	M	781	PRO
1	A	876	ILE
1	A	904	ILE
3	C	264	ILE
1	D	876	ILE
1	D	904	ILE
3	F	264	ILE
1	G	876	ILE
1	G	904	ILE
3	I	264	ILE
1	J	876	ILE
1	J	904	ILE
3	L	264	ILE
1	M	876	ILE
1	M	904	ILE
3	O	264	ILE

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	664/1022 (65%)	645 (97%)	19 (3%)	37	58
1	D	664/1022 (65%)	645 (97%)	19 (3%)	37	58
1	G	664/1022 (65%)	645 (97%)	19 (3%)	37	58
1	J	664/1022 (65%)	645 (97%)	19 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	664/1022 (65%)	645 (97%)	19 (3%)	37	58
2	B	953/1209 (79%)	935 (98%)	18 (2%)	50	66
2	E	953/1209 (79%)	935 (98%)	18 (2%)	50	66
2	H	953/1209 (79%)	935 (98%)	18 (2%)	50	66
2	K	953/1209 (79%)	935 (98%)	18 (2%)	50	66
2	N	953/1209 (79%)	935 (98%)	18 (2%)	50	66
3	C	441/520 (85%)	437 (99%)	4 (1%)	70	76
3	F	441/520 (85%)	437 (99%)	4 (1%)	70	76
3	I	441/520 (85%)	437 (99%)	4 (1%)	70	76
3	L	441/520 (85%)	437 (99%)	4 (1%)	70	76
3	O	441/520 (85%)	437 (99%)	4 (1%)	70	76
All	All	10290/13755 (75%)	10085 (98%)	205 (2%)	48	66

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	ASN
1	A	97	GLN
1	A	179	ASN
1	A	220	ARG
1	A	222	TYR
1	A	256	ASN
1	A	293	TYR
1	A	654	TRP
1	A	732	GLU
1	A	848	ASN
1	A	859	GLN
1	A	878	ASP
1	A	893	ASP
1	A	935	ILE
1	A	962	ASN
1	A	988	ILE
1	A	1124	ILE
1	A	1138	ASN
2	B	2034	ASN
2	B	2144	LEU
2	B	2195	ARG

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Mol	Chain	Res	Type
2	B	2229	GLU
2	B	2233	ASN
2	B	2278	HIS
2	B	2590	LEU
2	B	2603	ASN
2	B	2623	ASN
2	B	2688	ILE
2	B	2722	ARG
2	B	2734	ARG
2	B	2899	GLN
2	B	2915	GLN
2	B	3039	TYR
2	B	3089	THR
2	B	3217	LEU
2	B	3256	LEU
3	C	134	THR
3	C	453	PHE
3	C	505	THR
3	C	534	PHE
1	D	83	ASN
1	D	96	ASN
1	D	97	GLN
1	D	179	ASN
1	D	220	ARG
1	D	222	TYR
1	D	256	ASN
1	D	293	TYR
1	D	654	TRP
1	D	732	GLU
1	D	848	ASN
1	D	859	GLN
1	D	878	ASP
1	D	893	ASP
1	D	935	ILE
1	D	962	ASN
1	D	988	ILE
1	D	1124	ILE
1	D	1138	ASN
2	E	2034	ASN
2	E	2144	LEU
2	E	2195	ARG
2	E	2229	GLU

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Mol	Chain	Res	Type
2	E	2233	ASN
2	E	2278	HIS
2	E	2590	LEU
2	E	2603	ASN
2	E	2623	ASN
2	E	2688	ILE
2	E	2722	ARG
2	E	2734	ARG
2	E	2899	GLN
2	E	2915	GLN
2	E	3039	TYR
2	E	3089	THR
2	E	3217	LEU
2	E	3256	LEU
3	F	134	THR
3	F	453	PHE
3	F	505	THR
3	F	534	PHE
1	G	83	ASN
1	G	96	ASN
1	G	97	GLN
1	G	179	ASN
1	G	220	ARG
1	G	222	TYR
1	G	256	ASN
1	G	293	TYR
1	G	654	TRP
1	G	732	GLU
1	G	848	ASN
1	G	859	GLN
1	G	878	ASP
1	G	893	ASP
1	G	935	ILE
1	G	962	ASN
1	G	988	ILE
1	G	1124	ILE
1	G	1138	ASN
2	H	2034	ASN
2	H	2144	LEU
2	H	2195	ARG
2	H	2229	GLU
2	H	2233	ASN

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Mol	Chain	Res	Type
2	H	2278	HIS
2	H	2590	LEU
2	H	2603	ASN
2	H	2623	ASN
2	H	2688	ILE
2	H	2722	ARG
2	H	2734	ARG
2	H	2899	GLN
2	H	2915	GLN
2	H	3039	TYR
2	H	3089	THR
2	H	3217	LEU
2	H	3256	LEU
3	I	134	THR
3	I	453	PHE
3	I	505	THR
3	I	534	PHE
1	J	83	ASN
1	J	96	ASN
1	J	97	GLN
1	J	179	ASN
1	J	220	ARG
1	J	222	TYR
1	J	256	ASN
1	J	293	TYR
1	J	654	TRP
1	J	732	GLU
1	J	848	ASN
1	J	859	GLN
1	J	878	ASP
1	J	893	ASP
1	J	935	ILE
1	J	962	ASN
1	J	988	ILE
1	J	1124	ILE
1	J	1138	ASN
2	K	2034	ASN
2	K	2144	LEU
2	K	2195	ARG
2	K	2229	GLU
2	K	2233	ASN
2	K	2278	HIS

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Mol	Chain	Res	Type
2	K	2590	LEU
2	K	2603	ASN
2	K	2623	ASN
2	K	2688	ILE
2	K	2722	ARG
2	K	2734	ARG
2	K	2899	GLN
2	K	2915	GLN
2	K	3039	TYR
2	K	3089	THR
2	K	3217	LEU
2	K	3256	LEU
3	L	134	THR
3	L	453	PHE
3	L	505	THR
3	L	534	PHE
1	M	83	ASN
1	M	96	ASN
1	M	97	GLN
1	M	179	ASN
1	M	220	ARG
1	M	222	TYR
1	M	256	ASN
1	M	293	TYR
1	M	654	TRP
1	M	732	GLU
1	M	848	ASN
1	M	859	GLN
1	M	878	ASP
1	M	893	ASP
1	M	935	ILE
1	M	962	ASN
1	M	988	ILE
1	M	1124	ILE
1	M	1138	ASN
2	N	2034	ASN
2	N	2144	LEU
2	N	2195	ARG
2	N	2229	GLU
2	N	2233	ASN
2	N	2278	HIS
2	N	2590	LEU

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Mol	Chain	Res	Type
2	N	2603	ASN
2	N	2623	ASN
2	N	2688	ILE
2	N	2722	ARG
2	N	2734	ARG
2	N	2899	GLN
2	N	2915	GLN
2	N	3039	TYR
2	N	3089	THR
2	N	3217	LEU
2	N	3256	LEU
3	O	134	THR
3	O	453	PHE
3	O	505	THR
3	O	534	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (239) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	225	GLN
1	A	234	ASN
1	A	241	HIS
1	A	300	GLN
1	A	754	GLN
1	A	843	ASN
1	A	859	GLN
1	A	873	ASN
1	A	933	GLN
1	A	963	GLN
1	A	966	ASN
1	A	1011	ASN
1	A	1043	ASN
1	A	1070	ASN
1	A	1099	ASN
2	B	2024	GLN
2	B	2028	ASN
2	B	2072	GLN
2	B	2076	ASN
2	B	2089	ASN
2	B	2109	ASN
2	B	2134	GLN

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Mol	Chain	Res	Type
2	B	2180	ASN
2	B	2192	GLN
2	B	2205	GLN
2	B	2582	ASN
2	B	2696	ASN
2	B	2714	GLN
2	B	2916	GLN
2	B	2966	ASN
2	B	2986	ASN
2	B	2996	HIS
2	B	3013	GLN
2	B	3033	GLN
2	B	3051	GLN
2	B	3059	GLN
2	B	3090	ASN
2	B	3172	GLN
2	B	3283	GLN
2	B	3327	ASN
2	B	3337	HIS
3	C	97	ASN
3	C	119	ASN
3	C	143	HIS
3	C	407	ASN
3	C	410	GLN
3	C	495	GLN
1	D	47	GLN
1	D	225	GLN
1	D	241	HIS
1	D	300	GLN
1	D	754	GLN
1	D	843	ASN
1	D	859	GLN
1	D	873	ASN
1	D	933	GLN
1	D	963	GLN
1	D	966	ASN
1	D	1011	ASN
1	D	1043	ASN
1	D	1070	ASN
1	D	1099	ASN
2	E	2024	GLN
2	E	2028	ASN

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Mol	Chain	Res	Type
2	E	2076	ASN
2	E	2089	ASN
2	E	2090	GLN
2	E	2109	ASN
2	E	2134	GLN
2	E	2192	GLN
2	E	2205	GLN
2	E	2696	ASN
2	E	2714	GLN
2	E	2916	GLN
2	E	2933	GLN
2	E	2966	ASN
2	E	2986	ASN
2	E	2996	HIS
2	E	3013	GLN
2	E	3033	GLN
2	E	3051	GLN
2	E	3059	GLN
2	E	3090	ASN
2	E	3172	GLN
2	E	3273	HIS
2	E	3279	GLN
2	E	3283	GLN
2	E	3327	ASN
2	E	3337	HIS
3	F	97	ASN
3	F	119	ASN
3	F	143	HIS
3	F	209	ASN
3	F	407	ASN
3	F	410	GLN
3	F	495	GLN
1	G	47	GLN
1	G	225	GLN
1	G	241	HIS
1	G	300	GLN
1	G	754	GLN
1	G	843	ASN
1	G	859	GLN
1	G	873	ASN
1	G	933	GLN
1	G	963	GLN

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Mol	Chain	Res	Type
1	G	966	ASN
1	G	1011	ASN
1	G	1043	ASN
1	G	1070	ASN
1	G	1099	ASN
2	H	2024	GLN
2	H	2028	ASN
2	H	2072	GLN
2	H	2076	ASN
2	H	2089	ASN
2	H	2109	ASN
2	H	2111	GLN
2	H	2134	GLN
2	H	2180	ASN
2	H	2192	GLN
2	H	2205	GLN
2	H	2582	ASN
2	H	2696	ASN
2	H	2714	GLN
2	H	2933	GLN
2	H	2961	GLN
2	H	2966	ASN
2	H	2986	ASN
2	H	2996	HIS
2	H	3013	GLN
2	H	3051	GLN
2	H	3059	GLN
2	H	3090	ASN
2	H	3172	GLN
2	H	3204	ASN
2	H	3283	GLN
2	H	3327	ASN
2	H	3337	HIS
3	I	97	ASN
3	I	119	ASN
3	I	143	HIS
3	I	209	ASN
3	I	407	ASN
3	I	410	GLN
3	I	495	GLN
1	J	47	GLN
1	J	225	GLN

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Continued from previous page...

Mol	Chain	Res	Type
1	J	234	ASN
1	J	241	HIS
1	J	300	GLN
1	J	754	GLN
1	J	811	ASN
1	J	843	ASN
1	J	859	GLN
1	J	873	ASN
1	J	933	GLN
1	J	1011	ASN
1	J	1043	ASN
1	J	1070	ASN
1	J	1099	ASN
2	K	2024	GLN
2	K	2028	ASN
2	K	2072	GLN
2	K	2076	ASN
2	K	2089	ASN
2	K	2109	ASN
2	K	2134	GLN
2	K	2180	ASN
2	K	2192	GLN
2	K	2205	GLN
2	K	2696	ASN
2	K	2714	GLN
2	K	2961	GLN
2	K	2966	ASN
2	K	2986	ASN
2	K	2996	HIS
2	K	3013	GLN
2	K	3051	GLN
2	K	3059	GLN
2	K	3090	ASN
2	K	3172	GLN
2	K	3273	HIS
2	K	3279	GLN
2	K	3283	GLN
2	K	3327	ASN
2	K	3337	HIS
3	L	97	ASN
3	L	119	ASN
3	L	143	HIS

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Mol	Chain	Res	Type
3	L	407	ASN
3	L	410	GLN
3	L	495	GLN
1	M	47	GLN
1	M	225	GLN
1	M	241	HIS
1	M	300	GLN
1	M	754	GLN
1	M	843	ASN
1	M	859	GLN
1	M	873	ASN
1	M	963	GLN
1	M	966	ASN
1	M	1011	ASN
1	M	1043	ASN
1	M	1070	ASN
1	M	1099	ASN
2	N	2024	GLN
2	N	2028	ASN
2	N	2076	ASN
2	N	2089	ASN
2	N	2090	GLN
2	N	2109	ASN
2	N	2134	GLN
2	N	2173	GLN
2	N	2180	ASN
2	N	2192	GLN
2	N	2205	GLN
2	N	2582	ASN
2	N	2696	ASN
2	N	2714	GLN
2	N	2961	GLN
2	N	2966	ASN
2	N	2986	ASN
2	N	2996	HIS
2	N	3051	GLN
2	N	3059	GLN
2	N	3090	ASN
2	N	3172	GLN
2	N	3204	ASN
2	N	3283	GLN
2	N	3327	ASN

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Mol	Chain	Res	Type
2	N	3337	HIS
3	O	97	ASN
3	O	119	ASN
3	O	407	ASN
3	O	410	GLN
3	O	495	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

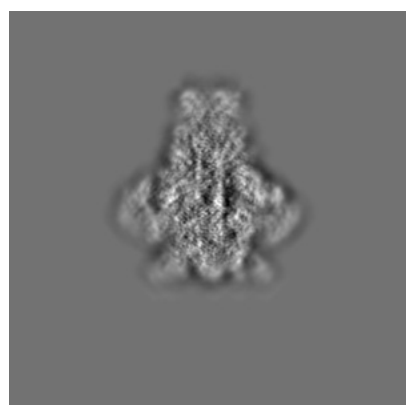
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20053. These allow visual inspection of the internal detail of the map and identification of artifacts.

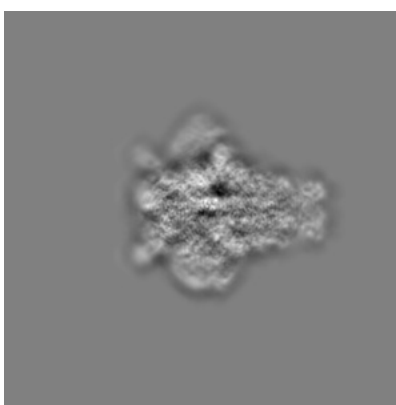
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

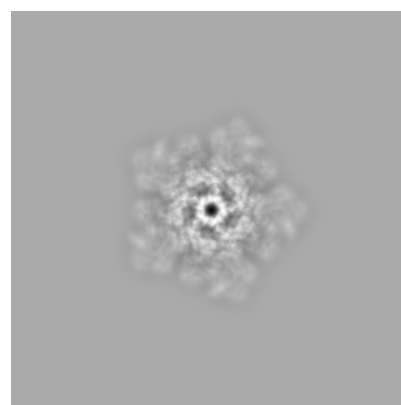
6.1.1 Primary map



X



Y

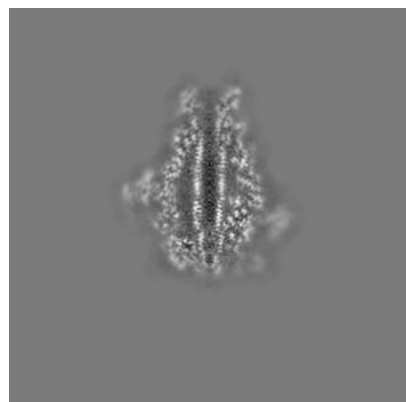


Z

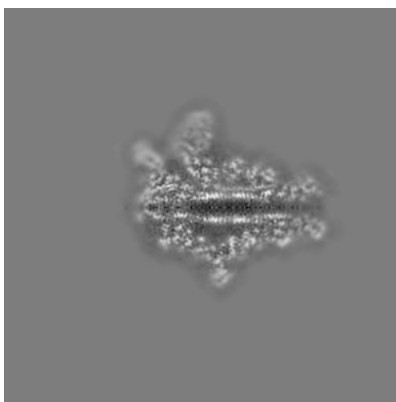
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

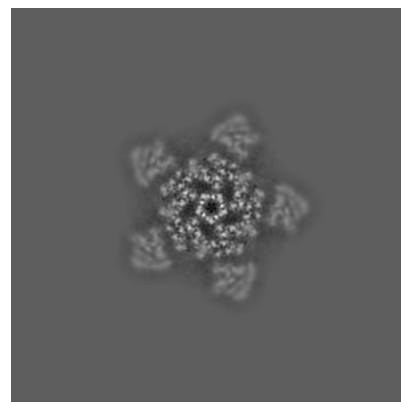
6.2.1 Primary map



X Index: 208



Y Index: 208

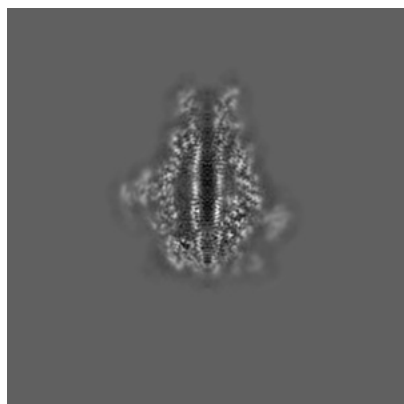


Z Index: 208

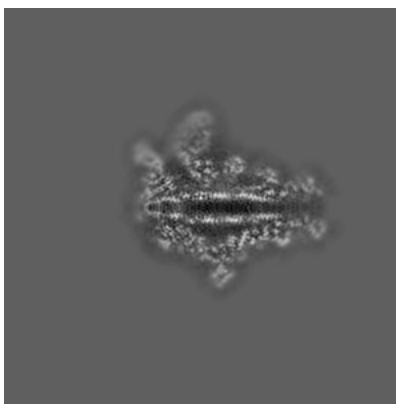
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

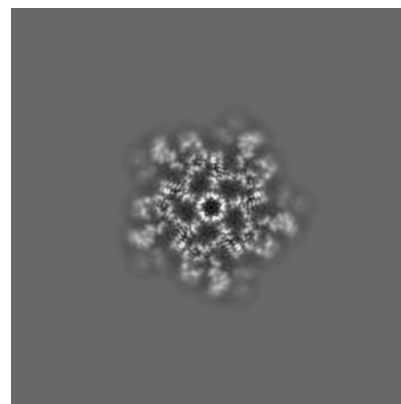
6.3.1 Primary map



X Index: 209



Y Index: 206

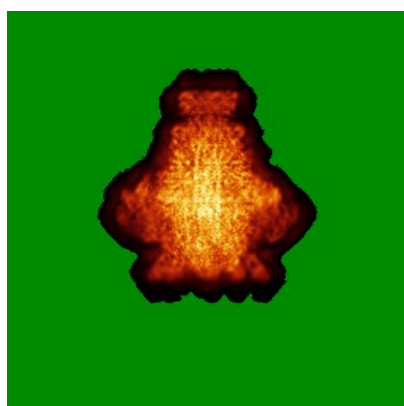


Z Index: 218

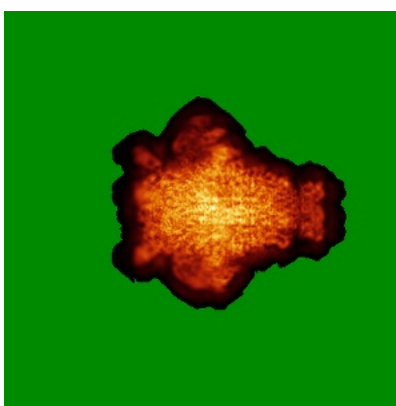
The images above show the largest variance slices of the map in three orthogonal directions.

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

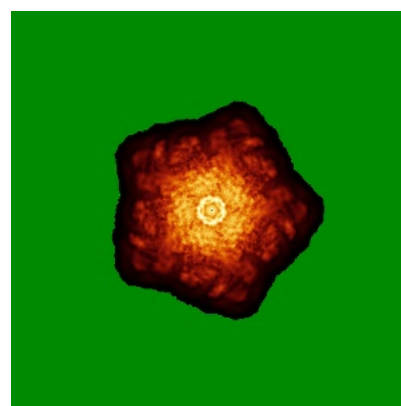
6.4.1 Primary map



X



Y

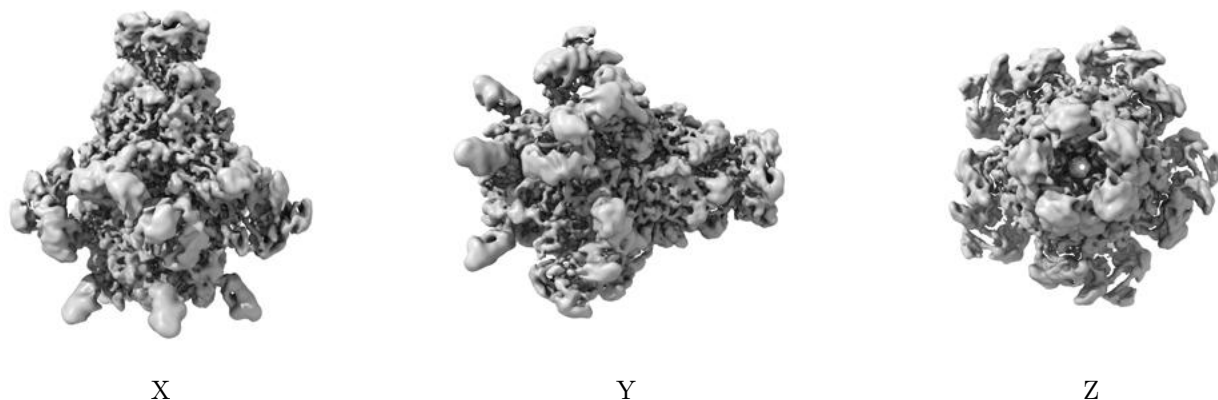


Z

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 7.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

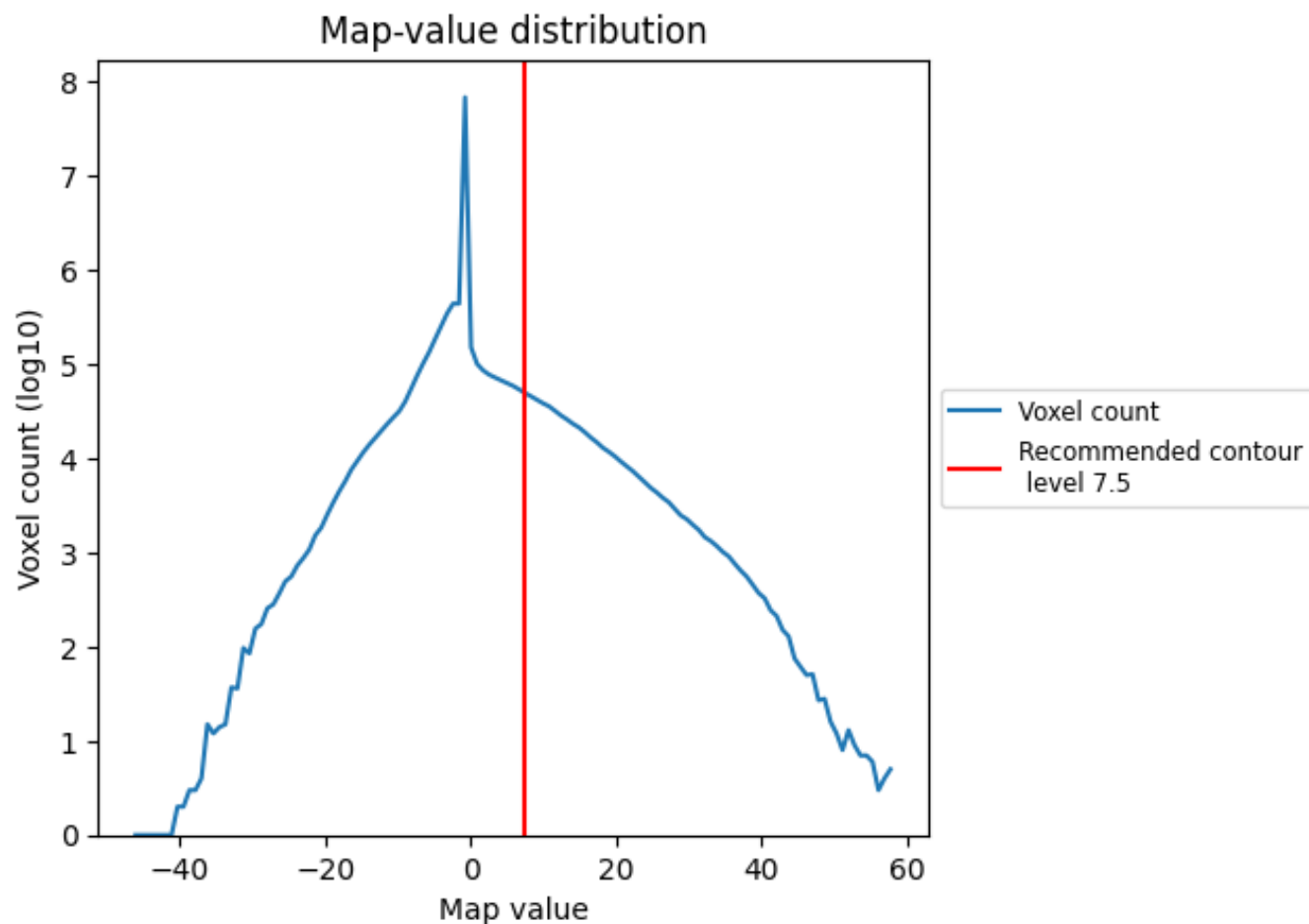
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

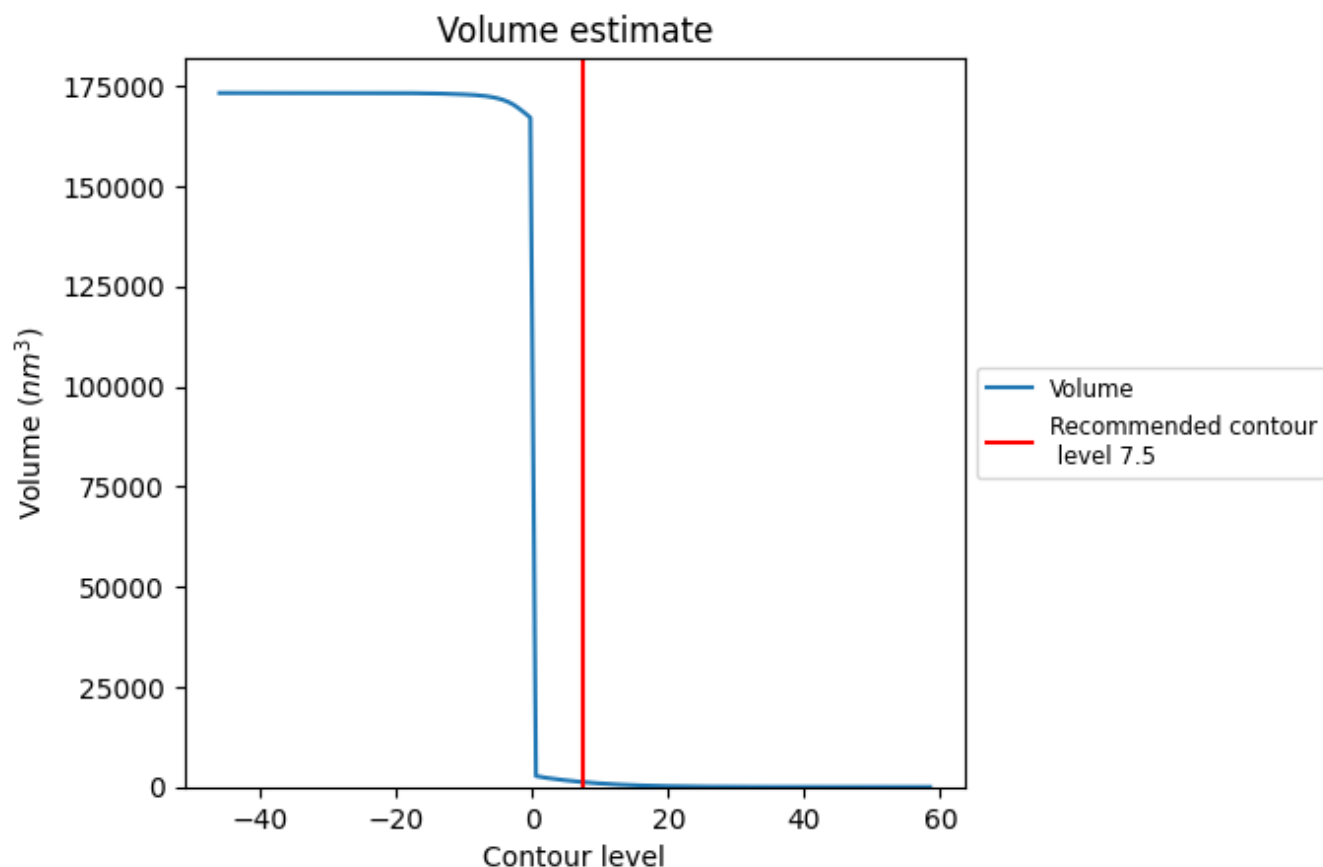
This section contains the results of statistical analysis of the map.

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.

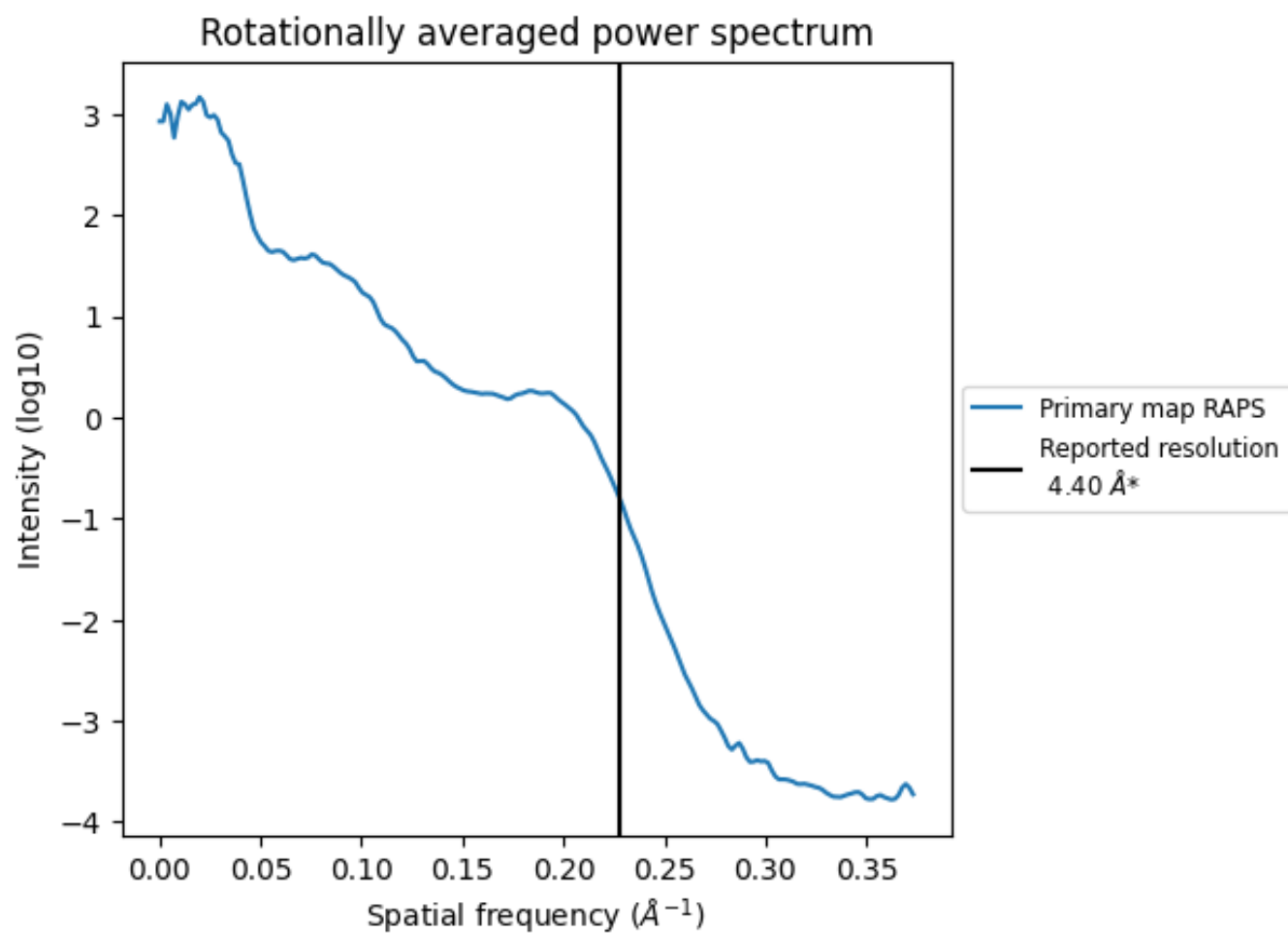
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1210 nm³; this corresponds to an approximate mass of 1093 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 ⓘ

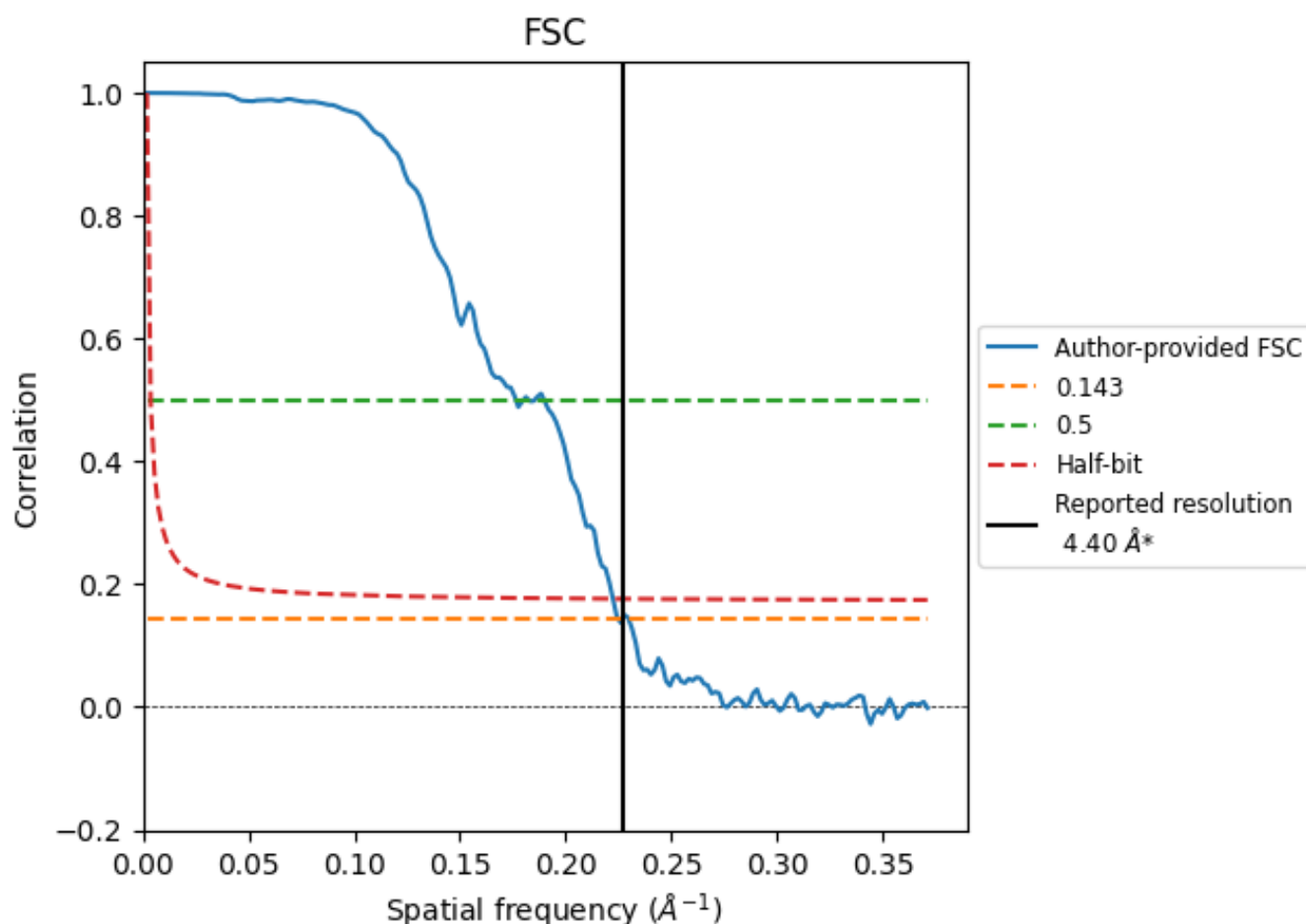


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

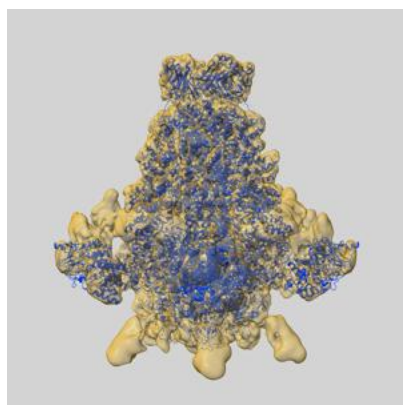
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.44	5.67	4.49
Unmasked-calculated*	-	-	-

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

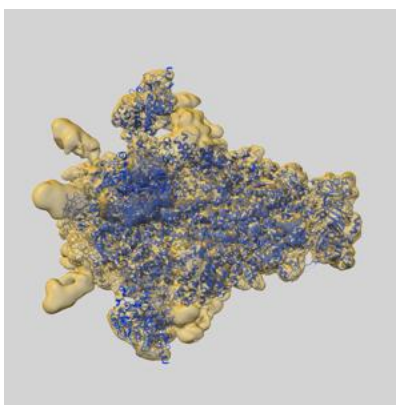
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20053 and PDB model 6OGD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

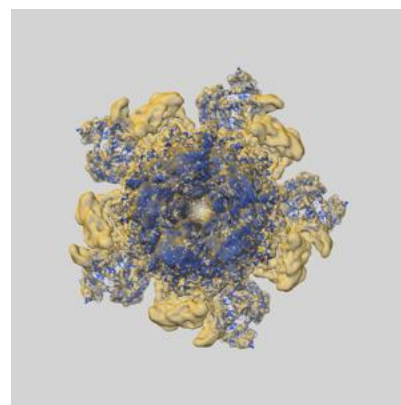
9.1 Map-model overlay [i](#)



X



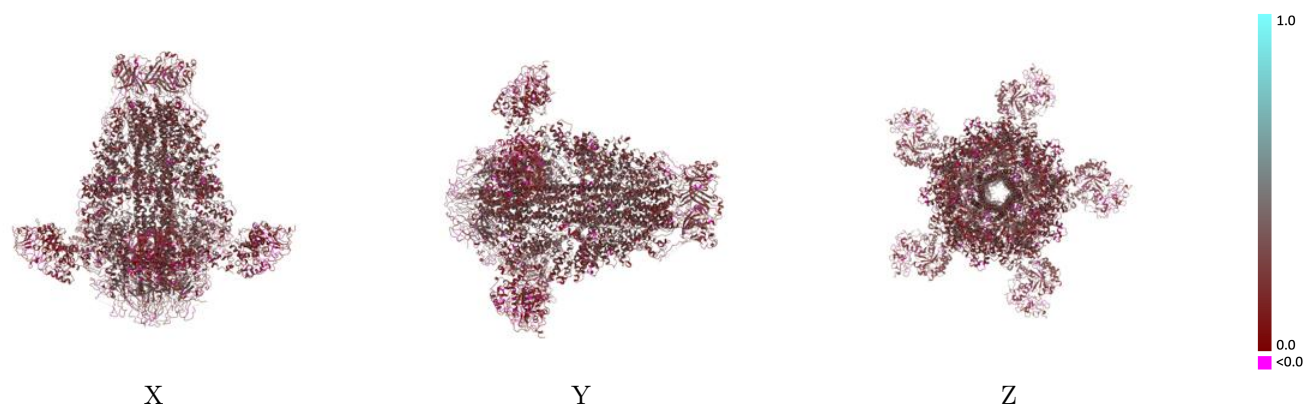
Y



Z

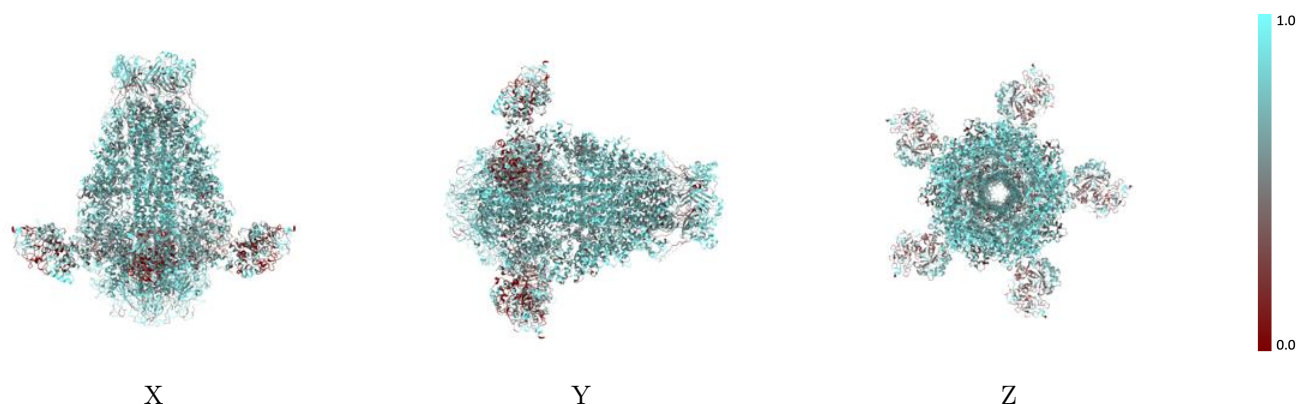
The images above show the 3D surface view of the map at the recommended contour level 7.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



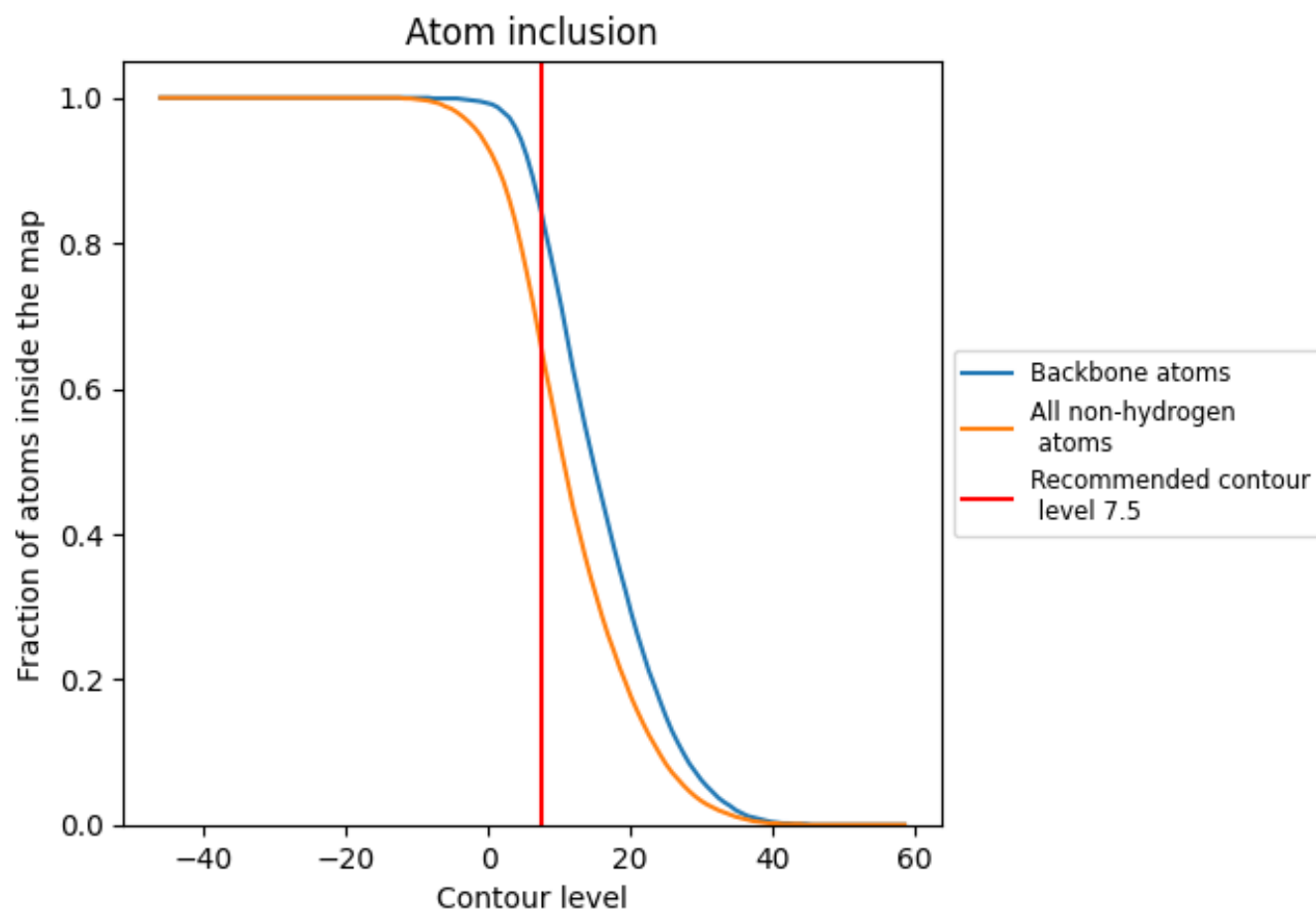
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (7.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.2300
A	0.7130	0.2370
B	0.7110	0.2640
C	0.4590	0.1490
D	0.7130	0.2380
E	0.7120	0.2630
F	0.4580	0.1470
G	0.7130	0.2390
H	0.7130	0.2630
I	0.4550	0.1480
J	0.7120	0.2380
K	0.7110	0.2640
L	0.4580	0.1480
M	0.7120	0.2380
N	0.7120	0.2640
O	0.4590	0.1490

1.0

0.0

<0.0