



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 02:33 PM EST

PDB ID : 6PSN
EMDB ID : EMD-20459
Title : Anthrax toxin protective antigen channels bound to lethal factor
Authors : Hardenbrook, N.J.; Liu, S.; Zhou, K.; Zhou, Z.H.; Krantz, B.A.
Deposited on : 2019-07-12
Resolution : 4.60 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

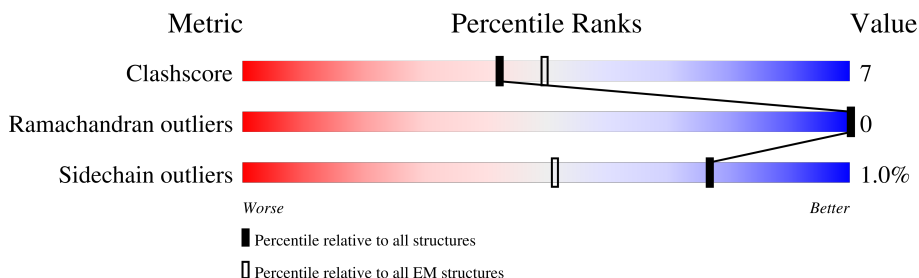
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	568	<div> <div>35%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	B	568	<div> <div>35%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	C	568	<div> <div>35%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	D	568	<div> <div>37%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	E	568	<div> <div>36%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	F	568	<div> <div>36%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	G	568	<div> <div>36%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
2	L	809	<div> <div>8%</div> <div>23%</div> <div>73%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32830 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	B	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	C	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	D	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	E	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	F	562	Total 4431	C 2769	N 765	O 891	S 6	0	0
1	G	562	Total 4431	C 2769	N 765	O 891	S 6	0	0

- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	220	Total 1799	C 1154	N 286	O 356	S 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total 2	Ca 2	0
3	B	2	Total 2	Ca 2	0
3	C	2	Total 2	Ca 2	0
3	D	2	Total 2	Ca 2	0
3	E	2	Total 2	Ca 2	0

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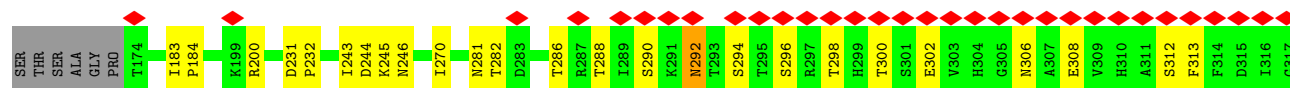
Mol	Chain	Residues	Atoms		AltConf
3	F	2	Total 2	Ca 2	0
3	G	2	Total 2	Ca 2	0

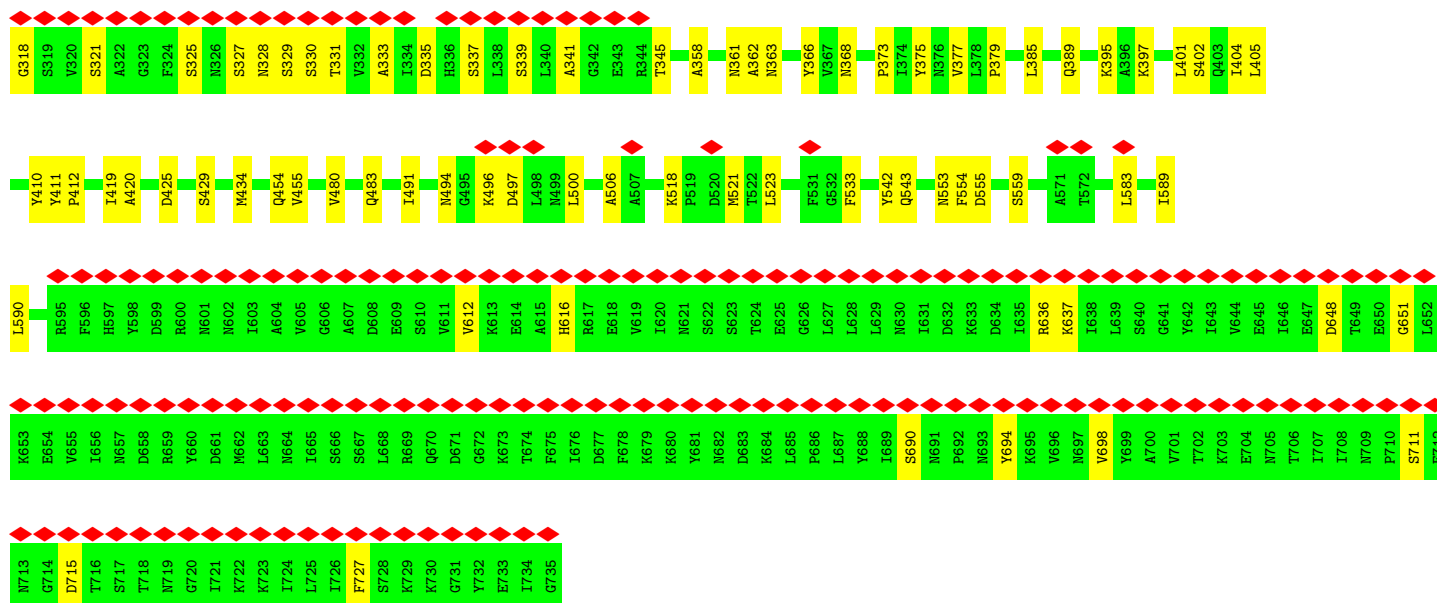
3 Residue-property plots

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.

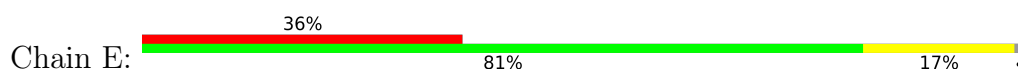
• Molecule 1: Protective antigen



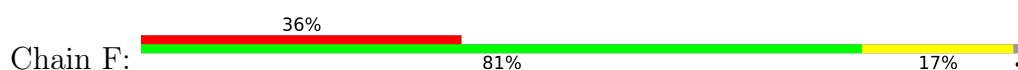


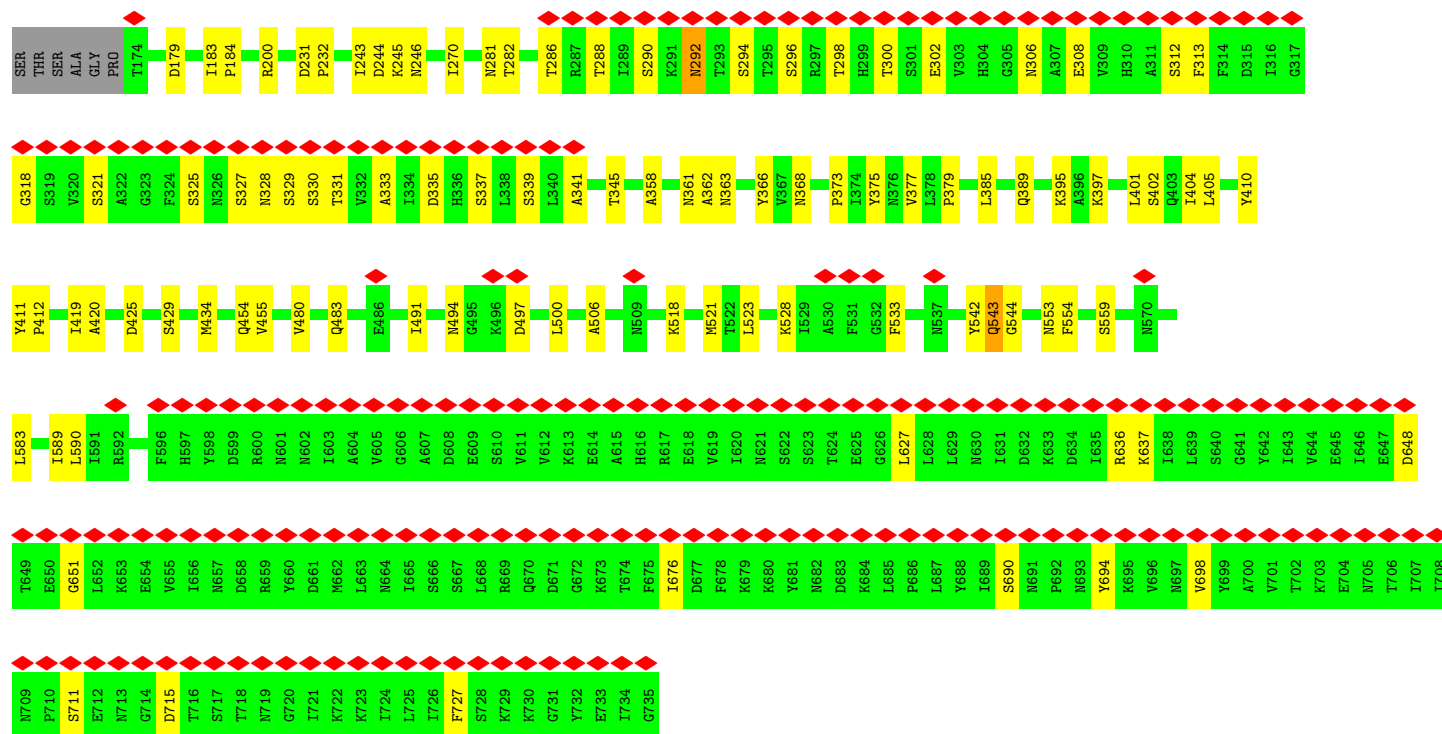


• Molecule 1: Protective antigen

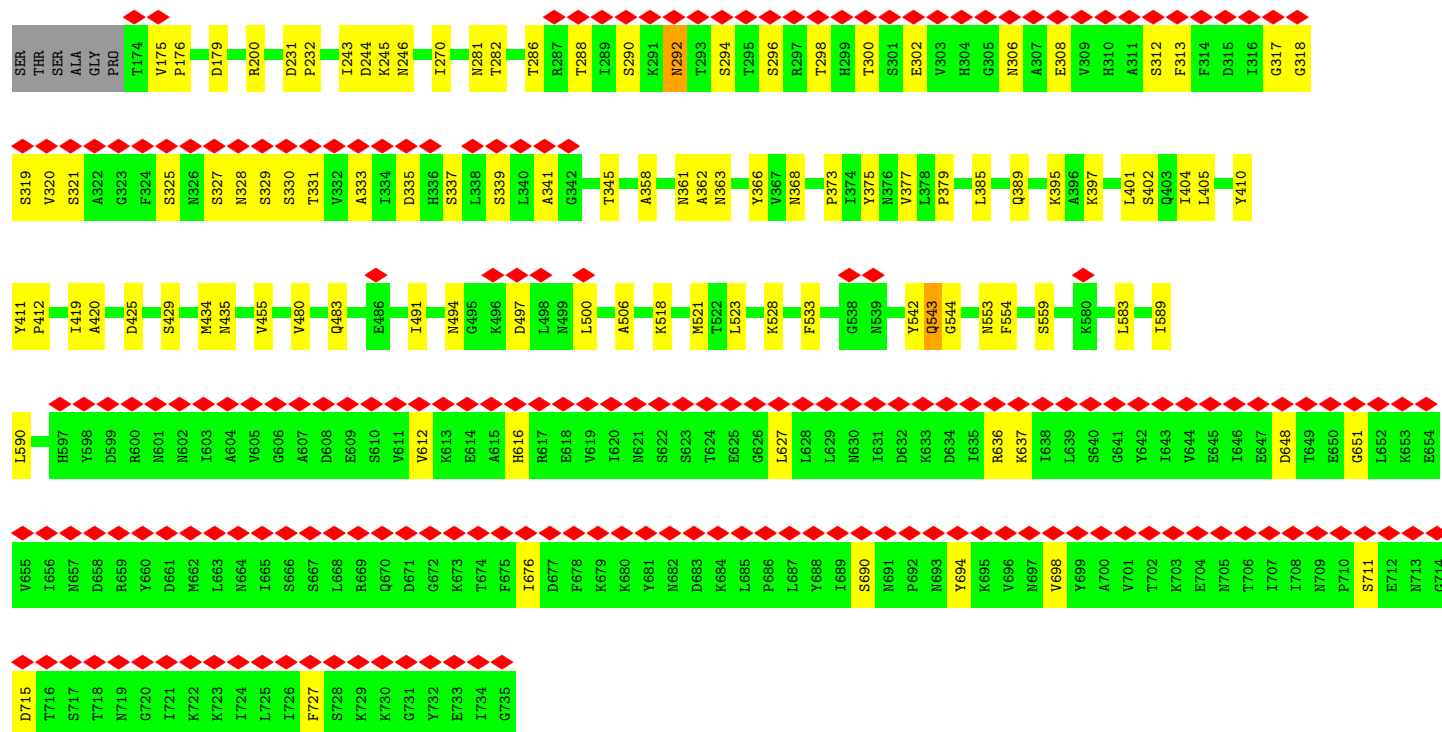
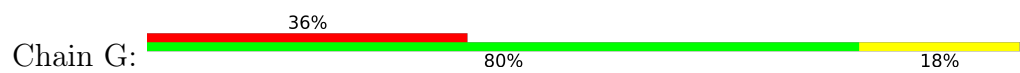


• Molecule 1: Protective antigen





• Molecule 1: Protective antigen



• Molecule 2: Lethal factor



ASN	GLU	ALA	PHE	ALA	GLU	GLY	ASP	LYS	PRO	TYR	GLU	SER	ILE	L114	MET
GLU	ALA	GLY	VAL	GLY	LEU	GLY	LEU	ILE	ALA	LYS	GLU	GLN	ASN	GLY	ASN
PHE	PHE	GLU	GLU	ASP	LYS	ASP	LYS	TYR	ASN	TYR	LEU	GLY	LEU	Y120	LYS
ALA	ARG	LEU	VAL	THR	LYS	THR	VAL	LEU	GLY	LYS	GLY	GLY	GLU	A121	GLY
GLU	GLU	ASN	THR	GLY	ILE	ILE	GLY	GLU	ARG	LYS	LEU	LEU	LEU	E123	ILE
ALA	ASP	ASN	THR	GLN	GLY	GLY	GLY	GLY	ASN	LYS	LEU	LEU	ASP	E124	LYS
PHE	PHE	SER	TYR	TRP	ALA	ARG	ALA	ASP	ASN	ASP	ILE	GLN	GLY	Y125	VAL
ARG	GLY	GLY	VAL	GLN	ILE	ILE	ILE	ASP	ASN	ASP	ILE	GLN	ARG	E126	ILE
LEU	MET	PHE	ASP	LEU	ASN	LEU	GLN	PRO	ASN	GLN	ILE	ILE	MET		SER
HIS	HIS	ILE	GLY	ASN	ASN	LEU	LEU	TYR	ASN	TYR	ASP	ASP	ALA	L129	MET
SER	SER	THR	GLY	ASN	LEU	SER	SER	TYR	ASN	GLY	SER	SER	ALA	Y130	CYS
THR	THR	GLU	GLY	ASN	PRO	THR	ASP	ILE	THR	ILE	SER	ASP	ARG	I131	LYS
ASP	ASP	PHE	ARG	GLN	ASP	ALA	ASP	ILE	ALA	ASN	PHE	GLY	TYR	Q132	THR
HIS	HIS	GLY	PHE	THR	GLY	THR	THR	ASN	THR	GLN	LEU	LEU	LYS	S133	ALA
ALA	ALA	HIS	VAL	ARG	THR	ARG	ARG	GLY	LEU	ARG	SER	TRP	TRP	S134	THR
GLU	GLU	ALA	PHE	ASN	ALA	ALA	ASN	ARG	ALA	ARG	SER	TRP	TRP	E135	ILE
ARG	ARG	VAL	THR	ALA	GLY	GLY	GLY	LEU	GLY	LEU	THR	GLY	GLY	D136	THR
LEU	LEU	ASP	ASP	ALA	TYR	ALA	ASP	GLN	ASP	LEU	THR	GLY	LYS	Y137	LEU
VAL	VAL	ASP	ILE	LEU	LEU	LEU	LEU	ASP	GLY	ILE	GLY	ILE	ILE	E138	GLY
GLN	GLN	VAL	THR	GLY	GLY	GLY	GLY	GLY	VAL	LYS	GLY	GLN	GLY	E139	PRO
LYS	LYS	ALA	LEU	GLY	PRO	GLY	ASP	SER	ASN	GLY	PHE	HIS	TYR	N140	VAL
ASN	ASN	TYR	ASN	LYS	LYS	LYS	THR	THR	LYS	LEU	LEU	TYR	TYR	T141	PHE
ALA	ALA	LEU	ILE	THR	THR	THR	ASP	ASP	ASN	ILE	LYS	GLN	GLN		ILE
PRO	PRO	LEU	ALA	THR	THR	THR	ILE	ASN	ASN	ASP	LEU	TRP	TRP	I151	PRO
LYS	LYS	ASP	GLY	LEU	LEU	LEU	GLN	SER	PRO	SER	GLN	SER	SER	A53	VAL
PHE	PHE	THR	THR	ILE	ILE	ILE	ARG	ASN	ASN	ILE	ASP	SER	SER	Y54	GLY
GLN	GLN	GLN	HIS	PHE	THR	THR	ASN	ILE	ASN	ILE	ASP	LEU	LEU	K55	ALA
PHE	PHE	SER	HIS	ASN	GLY	GLY	ASN	GLY	GLY	ASN	ARG	SER	SER	R157	GLY
ASN	ASN	LEU	ASP	VAL	VAL	VAL	GLY	LEU	ILE	ASP	VAL	GLY	GLY	D158	HIS
GLN	GLN	THR	ILE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ARG	LEU	GLY	I159	GLY
ILE	ILE	ASN	THR	ILE	ILE	ILE	ILE	ILE	ASN	LYS	LYS	ARG	ARG	L160	ASP
LYS	LYS	ASN	TYR	ARG	TYR	ASP	GLY	PHE	GLY	GLY	GLY	GLY	GLY	S161	VAL
PHE	PHE	LYS	GLY	ALA	ALA	VAL	THR	THR	THR	GLN	GLY	GLY	GLY	K162	GLY
ILE	ILE	LYS	VAL	SER	SER	GLN	LYS	LYS	LYS	TYR	GLY	LEU	LEU	I163	GLY
ASN	ASN	ILE	HIS	ASN	ASN	ILE	ASN	ARG	ASN	ARG	LYS	GLY	LEU	N164	MET
SER	SER	ILE	SER	ILE	ILE	ILE	PHE	ASP	PHE	ASP	GLY	LEU	LYS	Q165	HIS
		ASP	LYS	VAL	VAL	VAL	VAL	ILE	THR	ILE	LYS	LEU	LEU	P166	VAL
		ILE	GLY	GLY	GLY	GLY	GLY	GLN	TYR	GLN	GLN	LEU	GLN	Y167	GLU
		PHE	LEU	SER	LEU	LEU	LEU	ASN	SER	ASN	ASN	ASN	ILE	Q168	LYS
		LYS	TYR	ALA	ALA	GLY	ALA	ILE	ILE	ILE	ASN	ARG	PRO		
		GLU	VAL	TYR	VAL	GLY	GLY	SER	SER	ILE	GLY	GLY	GLY	L188	ASN
		GLY	GLU	ILE	ILE	ILE	ILE	TYR	ASN	VAL	VAL	ASP	PRO		
		ASN	SER	SER	SER	LEU	LEU	THR	THR	LEU	LEU	ASP	LYS	L206	ASP
		ASN	ARG	ASN	ASN	ARG	ASN	HIS	MET	HIS	SER	SER	LYS	E207	GLU
		LEU	THR	GLU	GLU	ILE	ILE	GLN	ILE	GLN	GLN	ASP	ASP	A96	ASN
		THR	ILE	TRP	TRP	LYS	VAL	SER	VAL	SER	SER	ASN	ASP	Q208	LYS
		SER	LEU	LEU	LEU	LYS	ALA	ILE	ASP	ILE	PRO	ILE	ILE	M209	ARG
		TYR	LEU	ASN	ASN	LYS	VAL	GLY	ILE	GLY	LEU	ILE	ILE	S98	LYS
		ARG	HIS	GLY	GLY	ASN	VAL	SER	ASN	SER	SER	SER	HIS	S210	ASP
		GLY	ARG	ILE	ILE	ILE	VAL	THR	GLY	THR	GLY	THR	SER	Q214	GLU
		PRO					PRO	LEU	ARG	ARG	LYS	LYS	LEU	D100	GLU
														K101	
														K102	
														K103	
														I107	
														Y108	
														G109	
														K110	
														D111	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63807	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 ($e^-/\text{\AA}^2$)	62.9	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	0.077	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/4508	0.55	0/6116
1	B	0.35	0/4508	0.56	0/6116
1	C	0.35	0/4508	0.55	0/6116
1	D	0.35	0/4508	0.55	0/6116
1	E	0.35	0/4508	0.55	0/6116
1	F	0.35	0/4508	0.55	0/6116
1	G	0.35	0/4508	0.55	0/6116
2	L	0.46	0/1833	0.69	0/2471
All	All	0.35	0/33389	0.56	0/45283

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4372	83	0
1	B	4431	0	4372	85	0
1	C	4431	0	4372	74	0
1	D	4431	0	4372	60	0
1	E	4431	0	4372	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4431	0	4372	62	0
1	G	4431	0	4372	70	0
2	L	1799	0	1778	22	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
All	All	32830	0	32382	466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:PHE:CE1	1:B:542:TYR:HB2	1.94	1.02
1:F:533:PHE:CE1	1:F:542:TYR:HB2	1.96	1.01
1:G:533:PHE:CE1	1:G:542:TYR:HB2	1.96	1.00
1:C:533:PHE:CE1	1:C:542:TYR:HB2	1.96	0.98
1:E:533:PHE:CE1	1:E:542:TYR:HB2	1.97	0.98
1:D:533:PHE:CE1	1:D:542:TYR:HB2	1.98	0.98
1:B:300:THR:HB	1:B:327:SER:HB3	1.49	0.94
1:A:533:PHE:CE1	1:A:542:TYR:HB2	2.04	0.91
1:A:533:PHE:HE1	1:A:542:TYR:CD1	2.02	0.78
1:A:496:LYS:HB2	1:A:542:TYR:OH	1.89	0.73
1:B:242:ARG:HH12	2:L:39:ILE:HG12	1.54	0.73
1:A:209:ASN:HD21	2:L:108:TYR:HA	1.55	0.72
1:B:294:SER:HB2	1:B:333:ALA:HB3	1.73	0.71
1:C:294:SER:HB2	1:C:333:ALA:HB3	1.73	0.70
1:D:533:PHE:HE1	1:D:542:TYR:CD1	2.10	0.70
1:A:294:SER:HB2	1:A:333:ALA:HB3	1.73	0.70
1:F:294:SER:HB2	1:F:333:ALA:HB3	1.73	0.70
1:C:306:ASN:HB3	1:C:321:SER:HB2	1.75	0.69
1:B:306:ASN:HB3	1:B:321:SER:HB2	1.75	0.69
1:B:340:LEU:N	1:C:289:ILE:O	2.23	0.69
1:B:338:LEU:HB2	1:C:291:LYS:HB3	1.72	0.69
1:G:294:SER:HB2	1:G:333:ALA:HB3	1.73	0.69
1:D:294:SER:HB2	1:D:333:ALA:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:SER:HB2	1:E:333:ALA:HB3	1.73	0.69
1:A:306:ASN:HB3	1:A:321:SER:HB2	1.75	0.69
1:D:306:ASN:HB3	1:D:321:SER:HB2	1.75	0.69
1:E:306:ASN:HB3	1:E:321:SER:HB2	1.74	0.68
1:G:306:ASN:HB3	1:G:321:SER:HB2	1.75	0.68
1:F:306:ASN:HB3	1:F:321:SER:HB2	1.74	0.67
1:E:483:GLN:NE2	1:F:244:ASP:OD1	2.28	0.67
1:E:533:PHE:HE1	1:E:542:TYR:CD1	2.13	0.67
1:C:533:PHE:HE1	1:C:542:TYR:CD1	2.12	0.67
1:A:300:THR:HB	1:A:327:SER:HB3	1.76	0.67
1:A:332:VAL:O	1:B:297:ARG:N	2.27	0.67
1:C:300:THR:HB	1:C:327:SER:HB3	1.76	0.67
1:G:533:PHE:HE1	1:G:542:TYR:CD1	2.13	0.66
1:A:303:VAL:O	1:G:325:SER:HA	1.95	0.66
1:F:300:THR:HB	1:F:327:SER:HB3	1.76	0.66
1:E:300:THR:HB	1:E:327:SER:HB3	1.76	0.66
1:D:300:THR:HB	1:D:327:SER:HB3	1.76	0.66
1:G:300:THR:HB	1:G:327:SER:HB3	1.76	0.65
1:F:533:PHE:HE1	1:F:542:TYR:CD1	2.15	0.65
1:A:232:PRO:HD3	1:A:480:VAL:HG11	1.80	0.64
1:B:232:PRO:HD3	1:B:480:VAL:HG11	1.80	0.64
1:G:232:PRO:HD3	1:G:480:VAL:HG11	1.79	0.64
1:C:232:PRO:HD3	1:C:480:VAL:HG11	1.80	0.64
1:E:290:SER:HB2	1:E:337:SER:HB2	1.80	0.64
1:F:290:SER:HB2	1:F:337:SER:HB2	1.80	0.64
1:F:232:PRO:HD3	1:F:480:VAL:HG11	1.79	0.63
1:D:290:SER:HB2	1:D:337:SER:HB2	1.80	0.63
1:A:325:SER:OG	1:B:304:HIS:ND1	2.20	0.63
1:D:302:GLU:HB3	1:D:325:SER:HB2	1.81	0.63
1:E:302:GLU:HB3	1:E:325:SER:HB2	1.81	0.63
1:F:302:GLU:HB3	1:F:325:SER:HB2	1.81	0.63
1:C:290:SER:HB2	1:C:337:SER:HB2	1.80	0.63
1:A:207:ILE:HG23	2:L:108:TYR:HE1	1.63	0.63
1:G:302:GLU:HB3	1:G:325:SER:HB2	1.81	0.63
1:B:288:THR:HB	1:B:339:SER:HB2	1.81	0.63
1:C:288:THR:HB	1:C:339:SER:HB2	1.81	0.63
1:D:232:PRO:HD3	1:D:480:VAL:HG11	1.80	0.63
1:E:288:THR:HB	1:E:339:SER:HB2	1.81	0.63
1:D:288:THR:HB	1:D:339:SER:HB2	1.81	0.63
1:F:288:THR:HB	1:F:339:SER:HB2	1.81	0.63
1:B:483:GLN:NE2	1:C:244:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HB	1:A:339:SER:HB2	1.81	0.62
1:B:290:SER:HB2	1:B:337:SER:HB2	1.80	0.62
1:B:339:SER:HA	1:C:290:SER:HA	1.81	0.62
1:G:290:SER:HB2	1:G:337:SER:HB2	1.80	0.62
1:A:332:VAL:N	1:B:297:ARG:O	2.29	0.62
1:C:483:GLN:NE2	1:D:244:ASP:OD1	2.33	0.62
1:E:232:PRO:HD3	1:E:480:VAL:HG11	1.80	0.62
1:A:272:SER:HB3	1:G:435:ASN:HD22	1.63	0.62
1:C:292:ASN:HD22	1:C:293:THR:N	1.97	0.62
1:G:288:THR:HB	1:G:339:SER:HB2	1.81	0.62
2:L:136:ASP:O	2:L:140:ASN:N	2.31	0.62
1:A:533:PHE:CE1	1:A:542:TYR:CB	2.82	0.62
1:A:302:GLU:HB3	1:A:325:SER:HB2	1.81	0.62
1:A:290:SER:HB2	1:A:337:SER:HB2	1.80	0.62
1:A:324:PHE:O	1:B:305:GLY:N	2.32	0.61
1:B:341:ALA:HA	1:C:288:THR:HA	1.81	0.61
1:B:282:THR:HB	1:B:345:THR:HB	1.83	0.60
1:C:282:THR:HB	1:C:345:THR:HB	1.83	0.60
1:A:282:THR:HB	1:A:345:THR:HB	1.83	0.60
1:A:331:THR:HA	1:B:298:THR:HA	1.83	0.60
1:D:483:GLN:NE2	1:E:244:ASP:OD1	2.33	0.60
1:A:327:SER:HA	1:B:302:GLU:HA	1.82	0.60
1:D:282:THR:HB	1:D:345:THR:HB	1.83	0.60
1:A:483:GLN:NE2	1:B:244:ASP:OD1	2.35	0.60
1:C:533:PHE:CE1	1:C:542:TYR:CB	2.82	0.59
1:E:282:THR:HB	1:E:345:THR:HB	1.83	0.59
1:G:282:THR:HB	1:G:345:THR:HB	1.83	0.59
1:F:282:THR:HB	1:F:345:THR:HB	1.83	0.59
1:B:395:LYS:O	1:B:397:LYS:NZ	2.35	0.59
1:A:325:SER:HA	1:B:304:HIS:HA	1.83	0.58
1:F:483:GLN:NE2	1:G:244:ASP:OD1	2.36	0.58
1:F:425:ASP:HB2	1:F:429:SER:H	1.69	0.58
1:A:425:ASP:HB2	1:A:429:SER:H	1.69	0.58
1:D:425:ASP:HB2	1:D:429:SER:H	1.69	0.58
1:B:425:ASP:HB2	1:B:429:SER:H	1.69	0.58
1:G:292:ASN:HB3	1:G:335:ASP:HB2	1.85	0.58
2:L:93:SER:O	2:L:122:LYS:NZ	2.37	0.58
1:D:292:ASN:HB3	1:D:335:ASP:HB2	1.85	0.58
1:F:395:LYS:O	1:F:397:LYS:NZ	2.35	0.58
1:G:425:ASP:HB2	1:G:429:SER:H	1.69	0.58
2:L:119:VAL:HG23	2:L:131:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:HB3	1:A:335:ASP:HB2	1.85	0.58
1:C:425:ASP:HB2	1:C:429:SER:H	1.69	0.58
1:G:533:PHE:CE1	1:G:542:TYR:CB	2.82	0.58
1:E:395:LYS:O	1:E:397:LYS:NZ	2.35	0.57
1:G:395:LYS:O	1:G:397:LYS:NZ	2.35	0.57
1:E:292:ASN:HB3	1:E:335:ASP:HB2	1.85	0.57
1:E:358:ALA:HB3	1:E:434:MET:HB3	1.86	0.57
1:G:698:VAL:HB	1:G:727:PHE:HB3	1.87	0.57
1:F:698:VAL:HB	1:F:727:PHE:HB3	1.87	0.57
1:D:358:ALA:HB3	1:D:434:MET:HB3	1.86	0.57
1:F:292:ASN:HB3	1:F:335:ASP:HB2	1.85	0.57
1:B:292:ASN:HB3	1:B:335:ASP:HB2	1.85	0.57
1:B:358:ALA:HB3	1:B:434:MET:HB3	1.86	0.57
1:A:698:VAL:HB	1:A:727:PHE:HB3	1.87	0.57
1:E:533:PHE:CE1	1:E:542:TYR:CB	2.82	0.57
1:E:698:VAL:HB	1:E:727:PHE:HB3	1.87	0.57
1:A:358:ALA:HB3	1:A:434:MET:HB3	1.86	0.57
1:A:395:LYS:O	1:A:397:LYS:NZ	2.35	0.57
1:F:358:ALA:HB3	1:F:434:MET:HB3	1.86	0.57
1:C:292:ASN:HB3	1:C:335:ASP:HB2	1.85	0.57
1:B:533:PHE:HE1	1:B:542:TYR:CD1	2.23	0.57
1:B:298:THR:HB	1:B:329:SER:HB2	1.86	0.56
1:E:298:THR:HB	1:E:329:SER:HB2	1.86	0.56
1:E:425:ASP:HB2	1:E:429:SER:H	1.69	0.56
1:B:698:VAL:HB	1:B:727:PHE:HB3	1.87	0.56
1:C:358:ALA:HB3	1:C:434:MET:HB3	1.86	0.56
1:F:298:THR:HB	1:F:329:SER:HB2	1.86	0.56
1:A:298:THR:HB	1:A:329:SER:HB2	1.86	0.56
1:D:395:LYS:O	1:D:397:LYS:NZ	2.35	0.56
1:D:698:VAL:HB	1:D:727:PHE:HB3	1.87	0.56
1:A:310:HIS:HA	1:G:318:GLY:O	2.06	0.56
1:C:298:THR:HB	1:C:329:SER:HB2	1.86	0.56
1:C:698:VAL:HB	1:C:727:PHE:HB3	1.87	0.56
1:D:298:THR:HB	1:D:329:SER:HB2	1.86	0.56
1:G:298:THR:HB	1:G:329:SER:HB2	1.86	0.56
1:B:342:GLY:O	1:C:287:ARG:N	2.29	0.55
1:G:358:ALA:HB3	1:G:434:MET:HB3	1.86	0.55
1:D:533:PHE:CE1	1:D:542:TYR:CB	2.82	0.55
1:F:368:ASN:HB2	1:F:405:LEU:HG	1.89	0.55
2:L:55:LYS:HB3	2:L:133:SER:HB2	1.88	0.55
1:G:368:ASN:HB2	1:G:405:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ASN:HB2	1:E:405:LEU:HG	1.89	0.55
1:D:368:ASN:HB2	1:D:405:LEU:HG	1.89	0.55
1:A:368:ASN:HB2	1:A:405:LEU:HG	1.89	0.55
1:A:197:LYS:HD2	2:L:235:LEU:HG	1.89	0.54
1:C:368:ASN:HB2	1:C:405:LEU:HG	1.89	0.54
1:B:368:ASN:HB2	1:B:405:LEU:HG	1.89	0.54
1:B:533:PHE:CE1	1:B:542:TYR:CB	2.82	0.54
1:F:497:ASP:O	1:F:637:LYS:NZ	2.41	0.54
1:C:395:LYS:O	1:C:397:LYS:NZ	2.35	0.54
1:D:497:ASP:O	1:D:637:LYS:NZ	2.41	0.54
2:L:246:LYS:HG3	2:L:250:GLN:HE21	1.72	0.54
1:D:553:ASN:HB2	1:D:590:LEU:HB3	1.90	0.54
1:A:309:VAL:O	1:G:319:SER:HA	2.08	0.53
1:B:553:ASN:HB2	1:B:590:LEU:HB3	1.90	0.53
1:C:553:ASN:HB2	1:C:590:LEU:HB3	1.90	0.53
1:G:553:ASN:HB2	1:G:590:LEU:HB3	1.90	0.53
1:D:533:PHE:HE1	1:D:542:TYR:HD1	1.55	0.53
1:E:553:ASN:HB2	1:E:590:LEU:HB3	1.90	0.53
1:A:553:ASN:HB2	1:A:590:LEU:HB3	1.90	0.53
1:F:553:ASN:HB2	1:F:590:LEU:HB3	1.90	0.53
1:G:533:PHE:HE1	1:G:542:TYR:HD1	1.55	0.53
1:F:491:ILE:HG12	1:F:589:ILE:HB	1.91	0.53
1:C:497:ASP:O	1:C:637:LYS:NZ	2.41	0.53
1:B:497:ASP:O	1:B:637:LYS:NZ	2.41	0.53
1:F:286:THR:HB	1:F:341:ALA:HB3	1.91	0.53
1:G:286:THR:HB	1:G:341:ALA:HB3	1.91	0.53
1:A:497:ASP:O	1:A:637:LYS:NZ	2.41	0.53
1:E:491:ILE:HG12	1:E:589:ILE:HB	1.91	0.52
1:G:497:ASP:O	1:G:637:LYS:NZ	2.41	0.52
1:C:286:THR:HB	1:C:341:ALA:HB3	1.91	0.52
1:C:292:ASN:HD22	1:C:293:THR:H	1.58	0.52
1:E:497:ASP:O	1:E:637:LYS:NZ	2.41	0.52
1:B:286:THR:HB	1:B:341:ALA:HB3	1.91	0.52
1:A:286:THR:HB	1:A:341:ALA:HB3	1.91	0.52
1:E:286:THR:HB	1:E:341:ALA:HB3	1.91	0.52
1:A:533:PHE:CE1	1:A:542:TYR:CD1	2.91	0.52
2:L:156:SER:HB2	2:L:214:GLN:HB2	1.92	0.52
1:A:178:ARG:NE	2:L:42:HIS:HB3	2.25	0.52
1:B:336:HIS:O	1:C:292:ASN:ND2	2.42	0.52
1:F:533:PHE:CE1	1:F:542:TYR:CB	2.82	0.52
2:L:85:ASP:OD1	2:L:133:SER:OG	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:HB	1:D:341:ALA:HB3	1.91	0.52
1:G:491:ILE:HG12	1:G:589:ILE:HB	1.91	0.52
1:E:533:PHE:HE1	1:E:542:TYR:HD1	1.55	0.51
2:L:102:LYS:HG2	2:L:114:LEU:HD23	1.92	0.51
2:L:31:THR:O	2:L:35:HIS:ND1	2.41	0.51
1:B:491:ILE:HG12	1:B:589:ILE:HB	1.91	0.51
1:D:491:ILE:HG12	1:D:589:ILE:HB	1.91	0.51
1:A:333:ALA:HA	1:B:296:SER:HA	1.93	0.51
1:C:491:ILE:HG12	1:C:589:ILE:HB	1.91	0.51
1:A:491:ILE:HG12	1:A:589:ILE:HB	1.91	0.50
1:B:197:LYS:NZ	2:L:135:GLU:OE1	2.43	0.50
1:A:246:ASN:HB2	1:A:373:PRO:HG3	1.93	0.50
1:C:711:SER:HB2	1:C:715:ASP:HB2	1.94	0.50
1:E:711:SER:HB2	1:E:715:ASP:HB2	1.93	0.50
1:G:246:ASN:HB2	1:G:373:PRO:HG3	1.93	0.50
1:C:302:GLU:HG2	1:C:325:SER:HB2	1.94	0.50
1:D:711:SER:HB2	1:D:715:ASP:HB2	1.94	0.50
1:F:711:SER:HB2	1:F:715:ASP:HB2	1.93	0.50
1:A:307:ALA:O	1:G:321:SER:HA	2.12	0.50
1:E:494:ASN:HB3	1:E:500:LEU:HD23	1.93	0.50
1:C:533:PHE:HE1	1:C:542:TYR:HD1	1.55	0.50
1:B:246:ASN:HB2	1:B:373:PRO:HG3	1.93	0.50
1:D:494:ASN:HB3	1:D:500:LEU:HD23	1.93	0.50
1:F:246:ASN:HB2	1:F:373:PRO:HG3	1.92	0.50
1:A:270:ILE:HB	1:A:361:ASN:HB3	1.94	0.49
1:D:300:THR:O	1:D:327:SER:N	2.45	0.49
1:E:243:ILE:O	1:E:245:LYS:NZ	2.43	0.49
1:F:494:ASN:HB3	1:F:500:LEU:HD23	1.93	0.49
1:A:311:ALA:O	1:G:317:GLY:HA2	2.12	0.49
1:B:483:GLN:HE22	1:C:244:ASP:HA	1.77	0.49
1:B:711:SER:HB2	1:B:715:ASP:HB2	1.94	0.49
1:B:270:ILE:HB	1:B:361:ASN:HB3	1.94	0.49
1:B:494:ASN:HB3	1:B:500:LEU:HD23	1.93	0.49
1:D:243:ILE:O	1:D:245:LYS:NZ	2.42	0.49
1:D:270:ILE:HB	1:D:361:ASN:HB3	1.94	0.49
1:D:496:LYS:HB2	1:D:542:TYR:OH	2.12	0.49
1:A:300:THR:O	1:A:327:SER:N	2.45	0.49
1:B:302:GLU:HB3	1:B:325:SER:HB2	1.94	0.49
1:C:270:ILE:HB	1:C:361:ASN:HB3	1.94	0.49
1:C:494:ASN:HB3	1:C:500:LEU:HD23	1.93	0.49
1:E:246:ASN:HB2	1:E:373:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:ASN:HB3	1:G:500:LEU:HD23	1.93	0.49
1:A:494:ASN:HB3	1:A:500:LEU:HD23	1.93	0.49
1:C:246:ASN:HB2	1:C:373:PRO:HG3	1.92	0.49
1:C:300:THR:O	1:C:327:SER:N	2.45	0.49
1:D:246:ASN:HB2	1:D:373:PRO:HG3	1.93	0.49
1:E:270:ILE:HB	1:E:361:ASN:HB3	1.94	0.49
1:G:711:SER:HB2	1:G:715:ASP:HB2	1.94	0.49
1:G:300:THR:O	1:G:327:SER:N	2.45	0.49
1:G:523:LEU:HA	1:G:583:LEU:HD11	1.94	0.49
1:A:296:SER:O	1:A:330:SER:HA	2.13	0.49
1:G:270:ILE:HB	1:G:361:ASN:HB3	1.94	0.49
1:A:711:SER:HB2	1:A:715:ASP:HB2	1.94	0.49
1:B:296:SER:O	1:B:330:SER:HA	2.13	0.49
1:F:300:THR:O	1:F:327:SER:N	2.45	0.49
1:A:523:LEU:HA	1:A:583:LEU:HD11	1.94	0.49
1:C:296:SER:O	1:C:330:SER:HA	2.13	0.49
1:F:523:LEU:HA	1:F:583:LEU:HD11	1.94	0.49
1:G:296:SER:O	1:G:330:SER:HA	2.13	0.49
1:A:243:ILE:O	1:A:245:LYS:NZ	2.42	0.48
1:B:533:PHE:HE1	1:B:542:TYR:HB2	1.70	0.48
1:F:243:ILE:O	1:F:245:LYS:NZ	2.43	0.48
1:F:533:PHE:HE1	1:F:542:TYR:HD1	1.58	0.48
1:C:523:LEU:HA	1:C:583:LEU:HD11	1.94	0.48
1:F:377:VAL:HB	1:F:402:SER:HB3	1.94	0.48
1:B:377:VAL:HB	1:B:402:SER:HB3	1.94	0.48
1:E:300:THR:O	1:E:327:SER:N	2.45	0.48
1:E:377:VAL:HB	1:E:402:SER:HB3	1.94	0.48
1:F:270:ILE:HB	1:F:361:ASN:HB3	1.94	0.48
1:A:377:VAL:HB	1:A:402:SER:HB3	1.94	0.48
1:D:377:VAL:HB	1:D:402:SER:HB3	1.94	0.48
1:D:523:LEU:HA	1:D:583:LEU:HD11	1.94	0.48
1:E:296:SER:O	1:E:330:SER:HA	2.13	0.48
1:A:454:GLN:NE2	1:B:401:LEU:O	2.47	0.48
1:B:336:HIS:HB2	1:C:293:THR:HG22	1.96	0.48
1:E:454:GLN:NE2	1:F:401:LEU:O	2.47	0.48
1:A:210:ILE:HD11	2:L:188:LEU:HB2	1.96	0.48
1:C:243:ILE:O	1:C:245:LYS:NZ	2.43	0.48
1:D:296:SER:O	1:D:330:SER:HA	2.13	0.48
1:B:523:LEU:HA	1:B:583:LEU:HD11	1.94	0.47
1:E:523:LEU:HA	1:E:583:LEU:HD11	1.94	0.47
1:C:377:VAL:HB	1:C:402:SER:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:SER:O	1:F:330:SER:HA	2.13	0.47
1:D:296:SER:HB2	1:D:331:THR:HB	1.96	0.47
1:E:296:SER:HB2	1:E:331:THR:HB	1.96	0.47
1:G:377:VAL:HB	1:G:402:SER:HB3	1.94	0.47
1:C:296:SER:HB2	1:C:331:THR:HB	1.96	0.47
1:F:296:SER:HB2	1:F:331:THR:HB	1.96	0.47
1:B:483:GLN:HE22	1:C:245:LYS:H	1.62	0.47
1:B:648:ASP:HB3	1:B:651:GLY:H	1.80	0.47
1:E:648:ASP:HB3	1:E:651:GLY:H	1.80	0.47
1:A:648:ASP:HB3	1:A:651:GLY:H	1.80	0.47
1:C:648:ASP:HB3	1:C:651:GLY:H	1.80	0.47
1:G:425:ASP:OD2	1:G:429:SER:OG	2.28	0.46
1:G:648:ASP:HB3	1:G:651:GLY:H	1.80	0.46
1:B:296:SER:HB2	1:B:331:THR:HB	1.96	0.46
1:D:648:ASP:HB3	1:D:651:GLY:H	1.80	0.46
1:G:243:ILE:O	1:G:245:LYS:NZ	2.43	0.46
1:G:296:SER:HB2	1:G:331:THR:HB	1.96	0.46
1:A:296:SER:HB2	1:A:331:THR:HB	1.96	0.46
1:A:506:ALA:HB1	1:A:518:LYS:HZ2	1.81	0.46
1:B:412:PRO:HD3	1:B:419:ILE:HG23	1.98	0.46
1:G:375:TYR:HE1	1:G:404:ILE:HG23	1.81	0.46
1:A:375:TYR:HE1	1:A:404:ILE:HG23	1.81	0.46
1:B:375:TYR:HE1	1:B:404:ILE:HG23	1.81	0.46
1:C:375:TYR:HE1	1:C:404:ILE:HG23	1.81	0.46
1:C:412:PRO:HD3	1:C:419:ILE:HG23	1.98	0.46
1:D:385:LEU:N	1:D:389:GLN:O	2.46	0.46
1:G:506:ALA:HB1	1:G:518:LYS:HZ2	1.81	0.46
1:A:244:ASP:HA	1:G:483:GLN:HE22	1.80	0.46
1:A:479:GLU:HG2	1:B:471:VAL:HG23	1.98	0.46
1:D:375:TYR:HE1	1:D:404:ILE:HG23	1.81	0.46
1:F:648:ASP:HB3	1:F:651:GLY:H	1.80	0.46
1:B:337:SER:HA	1:C:292:ASN:HA	1.98	0.46
1:A:412:PRO:HD3	1:A:419:ILE:HG23	1.98	0.45
1:E:412:PRO:HD3	1:E:419:ILE:HG23	1.98	0.45
1:E:375:TYR:HE1	1:E:404:ILE:HG23	1.81	0.45
1:G:543:GLN:HB3	1:G:544:GLY:H	1.65	0.45
1:A:533:PHE:HE1	1:A:542:TYR:CG	2.33	0.45
1:B:533:PHE:HE1	1:B:542:TYR:HD1	1.63	0.45
2:L:164:ASN:OD1	2:L:165:GLN:N	2.49	0.45
1:B:343:GLU:HA	1:C:285:GLN:O	2.15	0.45
1:F:375:TYR:HE1	1:F:404:ILE:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:PRO:HD3	1:F:419:ILE:HG23	1.98	0.45
1:F:543:GLN:HB3	1:F:544:GLY:H	1.65	0.45
1:B:243:ILE:O	1:B:245:LYS:NZ	2.43	0.45
1:C:506:ALA:HB1	1:C:518:LYS:HZ2	1.82	0.45
1:G:412:PRO:HD3	1:G:419:ILE:HG23	1.98	0.45
1:D:412:PRO:HD3	1:D:419:ILE:HG23	1.98	0.45
1:F:425:ASP:OD2	1:F:429:SER:OG	2.28	0.45
1:F:506:ALA:HB1	1:F:518:LYS:HZ2	1.81	0.45
1:E:366:TYR:HB2	1:E:411:TYR:HB3	1.99	0.44
1:F:183:ILE:HA	1:F:184:PRO:HD3	1.88	0.44
1:E:385:LEU:N	1:E:389:GLN:O	2.46	0.44
1:F:366:TYR:HB2	1:F:411:TYR:HB3	1.99	0.44
1:F:454:GLN:NE2	1:G:401:LEU:O	2.49	0.44
1:B:377:VAL:HG12	1:B:379:PRO:HD3	2.00	0.44
1:D:366:TYR:HB2	1:D:411:TYR:HB3	1.99	0.44
1:F:377:VAL:HG12	1:F:379:PRO:HD3	2.00	0.44
1:E:377:VAL:HG12	1:E:379:PRO:HD3	2.00	0.44
1:C:377:VAL:HG12	1:C:379:PRO:HD3	2.00	0.44
1:D:377:VAL:HG12	1:D:379:PRO:HD3	2.00	0.44
1:A:377:VAL:HG12	1:A:379:PRO:HD3	2.00	0.44
1:E:506:ALA:HB1	1:E:518:LYS:HZ2	1.83	0.44
1:F:554:PHE:HB2	1:F:559:SER:HB2	2.00	0.44
1:B:612:VAL:O	1:B:616:HIS:ND1	2.41	0.44
1:D:612:VAL:O	1:D:616:HIS:ND1	2.41	0.44
1:G:377:VAL:HG12	1:G:379:PRO:HD3	2.00	0.44
1:E:390:THR:HB	1:F:363:ASN:ND2	2.33	0.43
1:B:366:TYR:HB2	1:B:411:TYR:HB3	1.99	0.43
1:C:554:PHE:HB2	1:C:559:SER:HB2	2.00	0.43
1:D:554:PHE:HB2	1:D:559:SER:HB2	2.01	0.43
1:E:425:ASP:OD2	1:E:429:SER:OG	2.28	0.43
1:E:554:PHE:HB2	1:E:559:SER:HB2	2.00	0.43
1:C:366:TYR:HB2	1:C:411:TYR:HB3	1.99	0.43
1:C:454:GLN:NE2	1:D:401:LEU:O	2.51	0.43
1:D:425:ASP:OD2	1:D:429:SER:OG	2.28	0.43
1:B:521:MET:HG3	1:B:583:LEU:HD12	2.01	0.43
1:C:425:ASP:OD2	1:C:429:SER:OG	2.28	0.43
1:E:363:ASN:HA	1:E:419:ILE:O	2.19	0.43
1:G:366:TYR:HB2	1:G:411:TYR:HB3	1.99	0.43
1:A:690:SER:HB3	1:A:694:TYR:HE2	1.84	0.43
1:F:690:SER:HB3	1:F:694:TYR:HE2	1.84	0.43
1:G:554:PHE:HB2	1:G:559:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:HB2	1:A:411:TYR:HB3	1.99	0.43
1:C:521:MET:HG3	1:C:583:LEU:HD12	2.01	0.43
1:G:521:MET:HG3	1:G:583:LEU:HD12	2.01	0.43
2:L:151:ILE:HA	2:L:154:ILE:HD12	2.00	0.43
1:A:612:VAL:O	1:A:616:HIS:ND1	2.41	0.43
1:B:554:PHE:HB2	1:B:559:SER:HB2	2.00	0.43
1:G:363:ASN:HA	1:G:419:ILE:O	2.19	0.43
1:A:244:ASP:OD1	1:G:483:GLN:NE2	2.51	0.43
1:A:521:MET:HG3	1:A:583:LEU:HD12	2.01	0.43
1:D:312:SER:OG	1:D:313:PHE:N	2.52	0.43
1:G:690:SER:HB3	1:G:694:TYR:HE2	1.84	0.43
1:B:298:THR:O	1:B:328:ASN:HA	2.19	0.43
1:C:298:THR:O	1:C:328:ASN:HA	2.19	0.43
1:E:690:SER:HB3	1:E:694:TYR:HE2	1.84	0.43
1:A:312:SER:OG	1:A:313:PHE:N	2.52	0.42
1:A:554:PHE:HB2	1:A:559:SER:HB2	2.00	0.42
1:D:363:ASN:HA	1:D:419:ILE:O	2.19	0.42
1:D:366:TYR:O	1:D:410:TYR:HA	2.19	0.42
1:A:363:ASN:HA	1:A:419:ILE:O	2.19	0.42
1:B:365:ARG:NH2	1:B:416:LEU:O	2.29	0.42
1:B:690:SER:HB3	1:B:694:TYR:HE2	1.84	0.42
1:D:183:ILE:HA	1:D:184:PRO:HD3	1.87	0.42
1:E:298:THR:O	1:E:328:ASN:HA	2.19	0.42
1:E:312:SER:OG	1:E:313:PHE:N	2.52	0.42
1:F:298:THR:O	1:F:328:ASN:HA	2.19	0.42
1:F:385:LEU:N	1:F:389:GLN:O	2.46	0.42
1:G:308:GLU:O	1:G:318:GLY:HA2	2.19	0.42
1:A:231:ASP:OD1	1:A:231:ASP:N	2.53	0.42
1:D:298:THR:O	1:D:328:ASN:HA	2.19	0.42
1:F:366:TYR:O	1:F:410:TYR:HA	2.19	0.42
1:G:405:LEU:HD12	1:G:405:LEU:HA	1.89	0.42
2:L:100:ASP:OD1	2:L:101:LYS:N	2.52	0.42
1:D:690:SER:HB3	1:D:694:TYR:HE2	1.84	0.42
1:G:298:THR:O	1:G:328:ASN:HA	2.19	0.42
1:G:312:SER:OG	1:G:313:PHE:N	2.52	0.42
1:A:298:THR:O	1:A:328:ASN:HA	2.19	0.42
1:B:366:TYR:O	1:B:410:TYR:HA	2.19	0.42
1:C:363:ASN:HA	1:C:419:ILE:O	2.19	0.42
1:C:496:LYS:HB2	1:C:542:TYR:OH	2.19	0.42
1:D:521:MET:HG3	1:D:583:LEU:HD12	2.01	0.42
1:F:308:GLU:O	1:F:318:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:TYR:O	1:G:410:TYR:HA	2.19	0.42
1:A:334:ILE:HG22	1:B:295:THR:OG1	2.19	0.42
1:B:363:ASN:HA	1:B:419:ILE:O	2.19	0.42
1:C:312:SER:OG	1:C:313:PHE:N	2.52	0.42
1:C:366:TYR:O	1:C:410:TYR:HA	2.19	0.42
1:D:308:GLU:O	1:D:318:GLY:HA2	2.19	0.42
1:E:183:ILE:HA	1:E:184:PRO:HD3	1.87	0.42
1:E:366:TYR:O	1:E:410:TYR:HA	2.19	0.42
1:E:379:PRO:HA	1:E:455:VAL:HA	2.02	0.42
1:F:363:ASN:HA	1:F:419:ILE:O	2.19	0.42
1:A:362:ALA:O	1:A:420:ALA:HA	2.20	0.42
1:B:312:SER:OG	1:B:313:PHE:N	2.52	0.42
1:C:308:GLU:O	1:C:318:GLY:HA2	2.20	0.42
1:D:454:GLN:NE2	1:E:401:LEU:O	2.53	0.42
1:D:555:ASP:N	1:D:555:ASP:OD1	2.53	0.42
1:G:612:VAL:O	1:G:616:HIS:ND1	2.41	0.42
1:A:308:GLU:O	1:A:318:GLY:HA2	2.19	0.42
1:B:362:ALA:O	1:B:420:ALA:HA	2.20	0.42
1:E:231:ASP:OD1	1:E:231:ASP:N	2.53	0.42
1:F:521:MET:HG3	1:F:583:LEU:HD12	2.01	0.42
2:L:49:LYS:HB2	2:L:54:VAL:HG23	2.02	0.42
1:A:366:TYR:O	1:A:410:TYR:HA	2.19	0.42
1:B:308:GLU:O	1:B:318:GLY:HA2	2.20	0.42
1:C:231:ASP:OD1	1:C:231:ASP:N	2.53	0.42
1:C:302:GLU:CG	1:C:325:SER:HB2	2.50	0.42
1:D:231:ASP:N	1:D:231:ASP:OD1	2.53	0.42
1:D:379:PRO:HA	1:D:455:VAL:HA	2.02	0.42
1:B:203:LEU:HB3	2:L:44:VAL:HG23	2.02	0.41
1:E:521:MET:HG3	1:E:583:LEU:HD12	2.01	0.41
1:F:379:PRO:HA	1:F:455:VAL:HA	2.02	0.41
1:B:231:ASP:N	1:B:231:ASP:OD1	2.53	0.41
1:C:362:ALA:O	1:C:420:ALA:HA	2.20	0.41
1:C:690:SER:HB3	1:C:694:TYR:HE2	1.84	0.41
1:F:231:ASP:OD1	1:F:231:ASP:N	2.53	0.41
1:G:362:ALA:O	1:G:420:ALA:HA	2.20	0.41
1:G:379:PRO:HA	1:G:455:VAL:HA	2.02	0.41
1:E:496:LYS:HB2	1:E:542:TYR:OH	2.19	0.41
1:F:312:SER:OG	1:F:313:PHE:N	2.52	0.41
1:A:308:GLU:HA	1:G:320:VAL:O	2.20	0.41
1:G:385:LEU:N	1:G:389:GLN:O	2.46	0.41
1:C:379:PRO:HA	1:C:455:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:GLU:O	1:E:318:GLY:HA2	2.19	0.41
1:A:379:PRO:HA	1:A:455:VAL:HA	2.02	0.41
1:C:175:VAL:HA	1:C:176:PRO:HD3	1.95	0.41
1:D:362:ALA:O	1:D:420:ALA:HA	2.20	0.41
1:B:274:ASN:N	1:B:357:THR:O	2.45	0.41
1:B:506:ALA:HB1	1:B:518:LYS:HZ2	1.86	0.41
1:B:222:SER:HB3	1:B:225:LYS:HB2	2.03	0.41
1:D:506:ALA:HB1	1:D:518:LYS:HZ2	1.86	0.41
1:G:528:LYS:HA	1:G:533:PHE:HB2	2.03	0.41
1:B:179:ASP:N	1:B:179:ASP:OD1	2.53	0.41
1:E:362:ALA:O	1:E:420:ALA:HA	2.20	0.41
1:F:179:ASP:N	1:F:179:ASP:OD1	2.53	0.41
1:F:362:ALA:O	1:F:420:ALA:HA	2.20	0.41
1:B:456:TYR:HB2	1:C:403:GLN:HE22	1.85	0.41
1:F:528:LYS:HA	1:F:533:PHE:HB2	2.03	0.41
1:A:179:ASP:OD1	1:A:179:ASP:N	2.53	0.40
1:A:183:ILE:HA	1:A:184:PRO:HD3	1.87	0.40
1:A:528:LYS:HA	1:A:533:PHE:HB2	2.03	0.40
1:C:222:SER:HB3	1:C:225:LYS:HB2	2.03	0.40
1:E:179:ASP:OD1	1:E:179:ASP:N	2.53	0.40
1:G:175:VAL:HA	1:G:176:PRO:HD3	1.95	0.40
1:B:379:PRO:HA	1:B:455:VAL:HA	2.02	0.40
1:C:179:ASP:N	1:C:179:ASP:OD1	2.53	0.40
1:G:627:LEU:HB2	1:G:676:ILE:HB	2.03	0.40
2:L:62:LEU:HD11	2:L:137:TYR:CD1	2.57	0.40
1:B:425:ASP:OD2	1:B:429:SER:OG	2.28	0.40
1:F:627:LEU:HB2	1:F:676:ILE:HB	2.03	0.40
1:G:231:ASP:N	1:G:231:ASP:OD1	2.53	0.40
1:A:222:SER:HB3	1:A:225:LYS:HB2	2.03	0.40
1:B:280:GLN:HB3	1:B:347:ALA:HB3	2.04	0.40
1:C:280:GLN:HB3	1:C:347:ALA:HB3	2.04	0.40
1:E:528:LYS:HA	1:E:533:PHE:HB2	2.03	0.40
1:G:179:ASP:OD1	1:G:179:ASP:N	2.53	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	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	B	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	C	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	D	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	E	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	F	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
1	G	560/568 (99%)	544 (97%)	16 (3%)	0	100	100
2	L	218/809 (27%)	199 (91%)	19 (9%)	0	100	100
All	All	4138/4785 (86%)	4007 (97%)	131 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	494 (99%)	5 (1%)	76	86
1	B	499/505 (99%)	493 (99%)	6 (1%)	71	84
1	C	499/505 (99%)	493 (99%)	6 (1%)	71	84
1	D	499/505 (99%)	494 (99%)	5 (1%)	76	86
1	E	499/505 (99%)	494 (99%)	5 (1%)	76	86
1	F	499/505 (99%)	494 (99%)	5 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	499/505 (99%)	494 (99%)	5 (1%)	76	86
2	L	198/739 (27%)	198 (100%)	0	100	100
All	All	3691/4274 (86%)	3654 (99%)	37 (1%)	77	86

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	281	ASN
1	A	292	ASN
1	A	543	GLN
1	A	636	ARG
1	B	200	ARG
1	B	281	ASN
1	B	292	ASN
1	B	301	SER
1	B	543	GLN
1	B	636	ARG
1	C	200	ARG
1	C	281	ASN
1	C	292	ASN
1	C	302	GLU
1	C	543	GLN
1	C	636	ARG
1	D	200	ARG
1	D	281	ASN
1	D	292	ASN
1	D	543	GLN
1	D	636	ARG
1	E	200	ARG
1	E	281	ASN
1	E	292	ASN
1	E	543	GLN
1	E	636	ARG
1	F	200	ARG
1	F	281	ASN
1	F	292	ASN
1	F	543	GLN
1	F	636	ARG
1	G	200	ARG
1	G	281	ASN

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Mol	Chain	Res	Type
1	G	292	ASN
1	G	543	GLN
1	G	636	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	281	ASN
1	A	292	ASN
1	A	389	GLN
1	A	564	ASN
1	A	584	ASN
1	A	705	ASN
1	B	281	ASN
1	B	292	ASN
1	B	438	GLN
1	B	483	GLN
1	B	564	ASN
1	B	584	ASN
1	B	705	ASN
1	C	281	ASN
1	C	292	ASN
1	C	389	GLN
1	C	564	ASN
1	C	584	ASN
1	C	705	ASN
1	D	281	ASN
1	D	292	ASN
1	D	389	GLN
1	D	564	ASN
1	D	584	ASN
1	D	705	ASN
1	E	281	ASN
1	E	292	ASN
1	E	389	GLN
1	E	564	ASN
1	E	584	ASN
1	E	705	ASN
1	F	281	ASN
1	F	292	ASN
1	F	389	GLN

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Mol	Chain	Res	Type
1	F	564	ASN
1	F	584	ASN
1	F	705	ASN
1	G	281	ASN
1	G	292	ASN
1	G	389	GLN
1	G	483	GLN
1	G	564	ASN
1	G	584	ASN
1	G	705	ASN
2	L	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

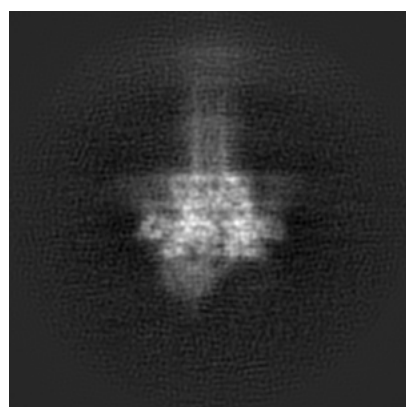
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20459. These allow visual inspection of the internal detail of the map and identification of artifacts.

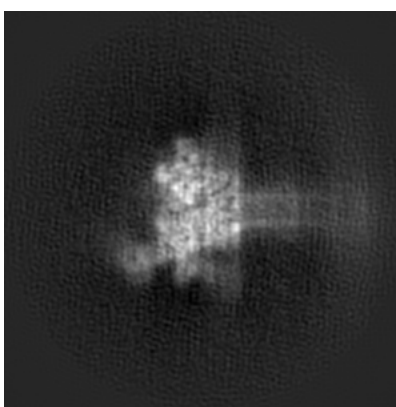
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

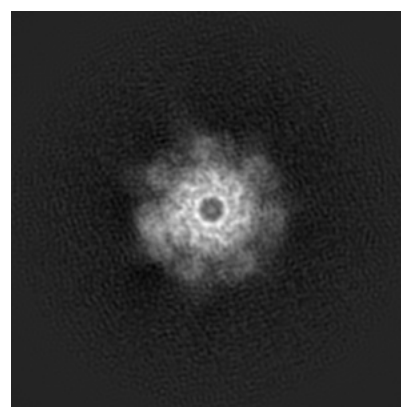
6.1.1 Primary map



X



Y

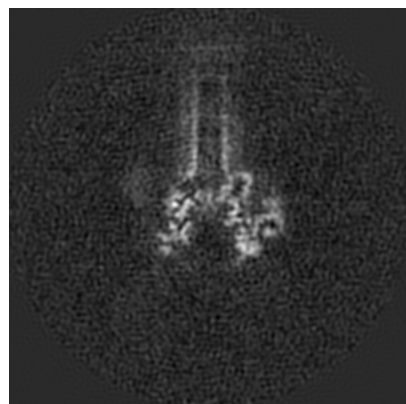


Z

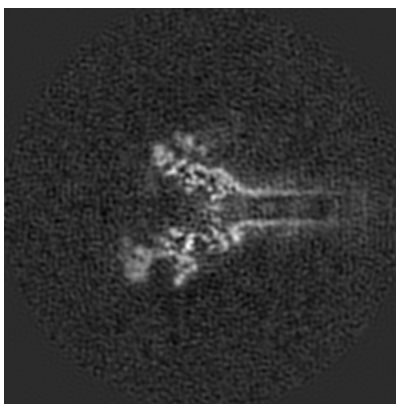
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

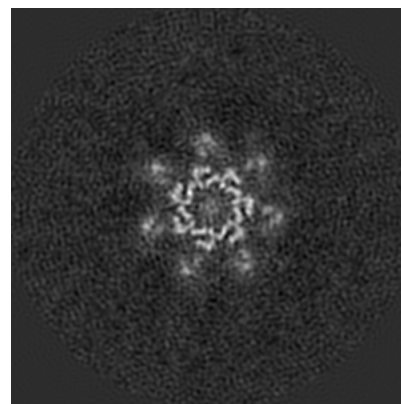
6.2.1 Primary map



X Index: 160



Y Index: 160

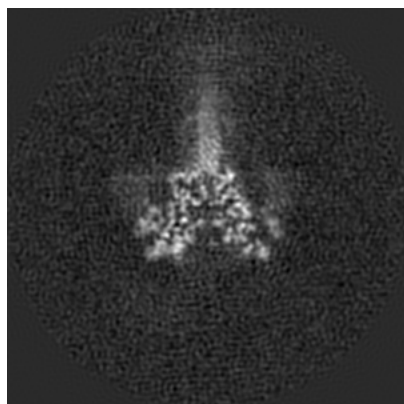


Z Index: 160

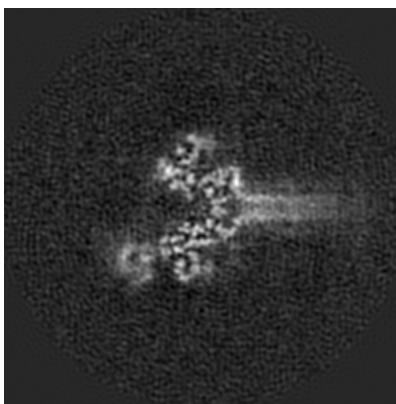
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

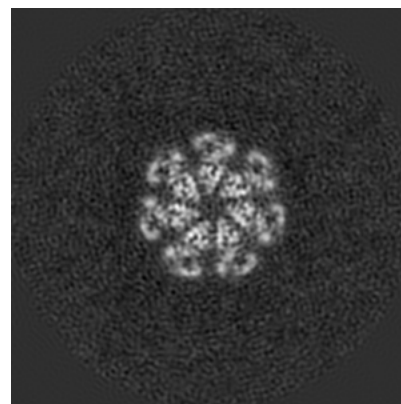
6.3.1 Primary map



X Index: 148



Y Index: 150

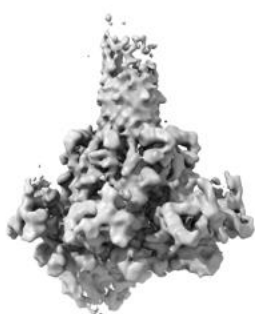


Z Index: 149

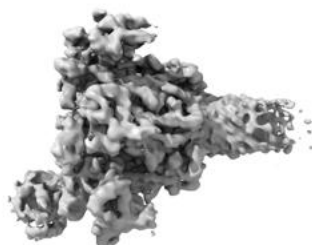
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

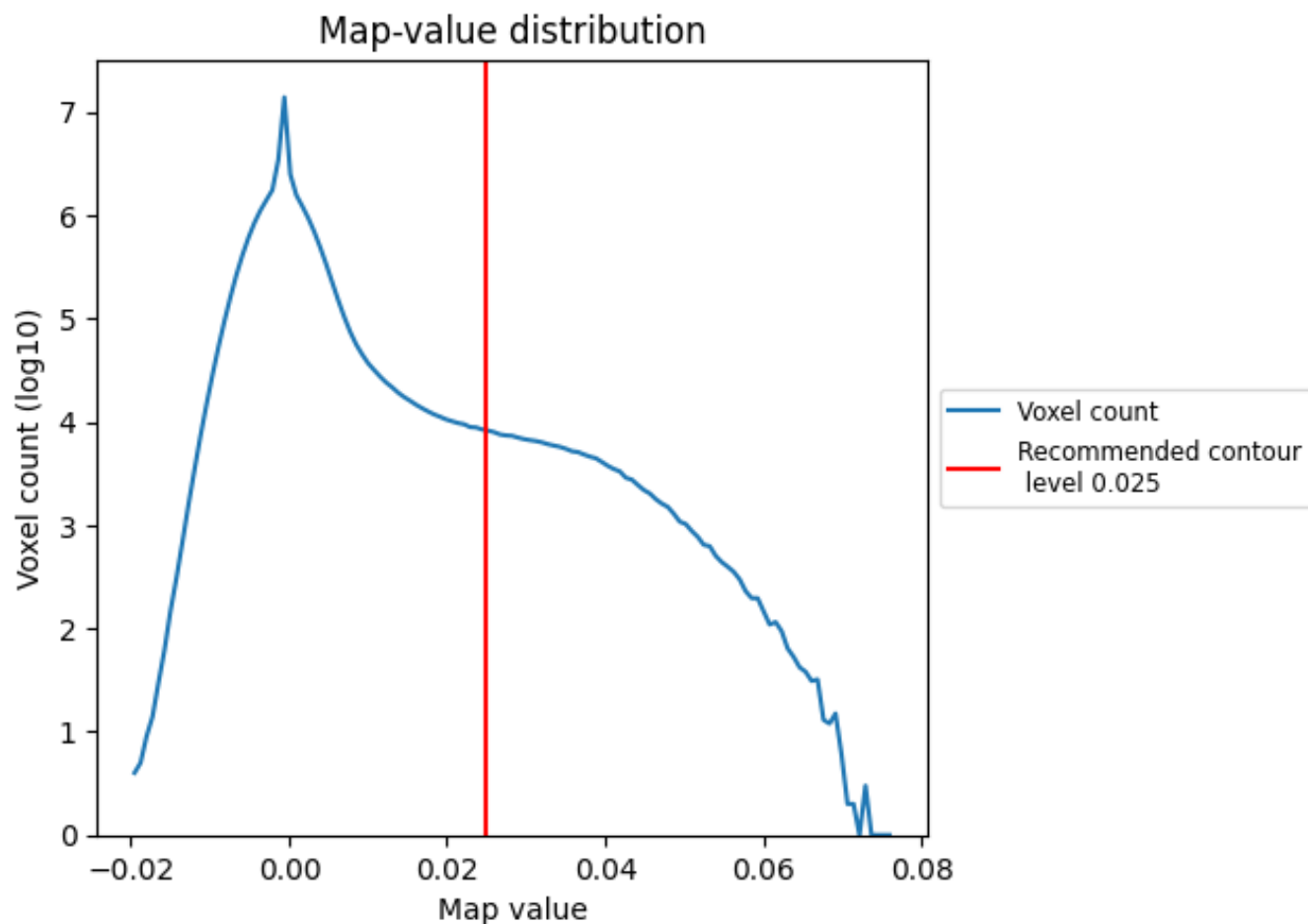
6.5 Mask visualisation

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

7 Map analysis [i](#)

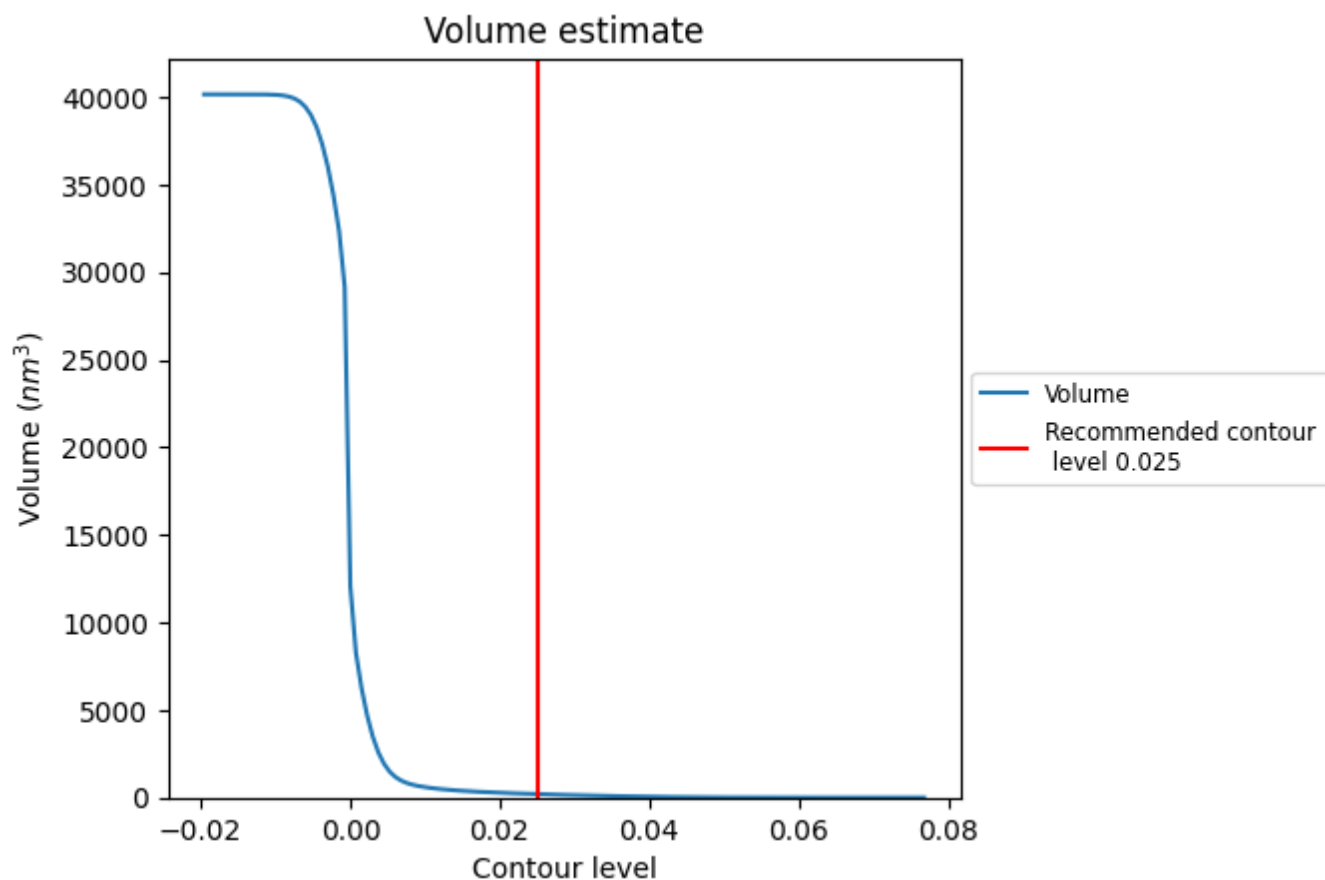
This section contains the results of statistical analysis of the map.

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.

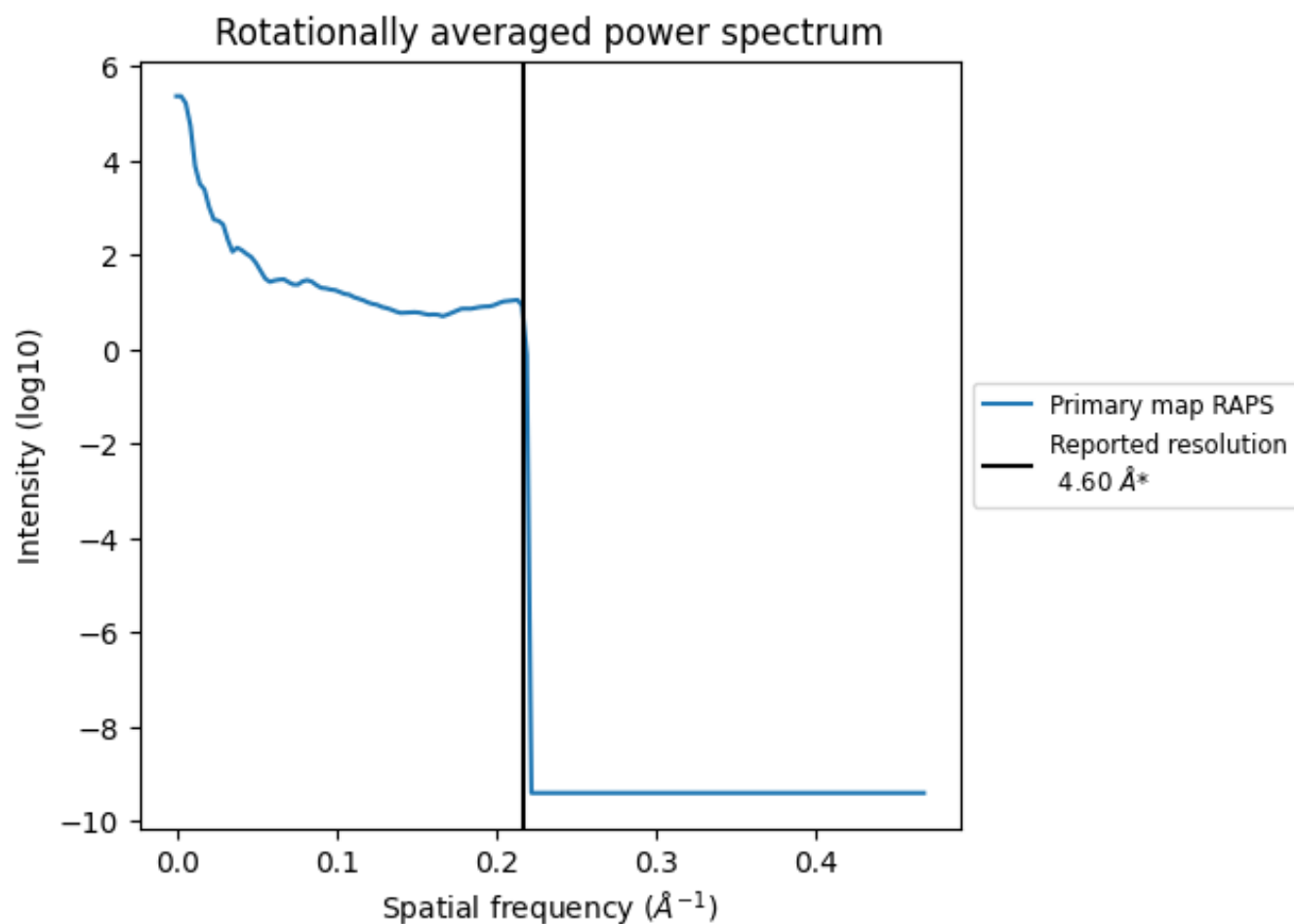
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 0.217 Å⁻¹

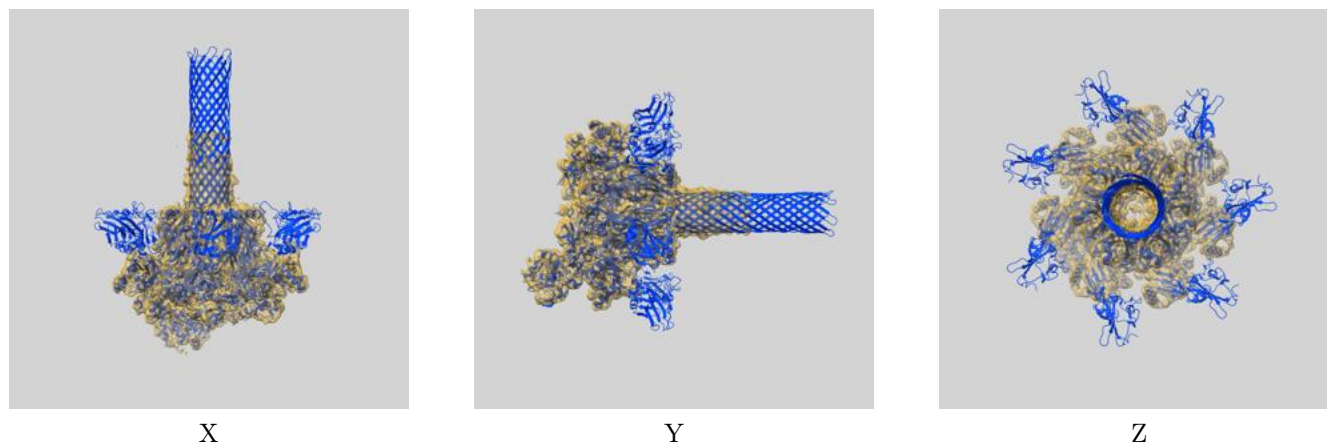
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

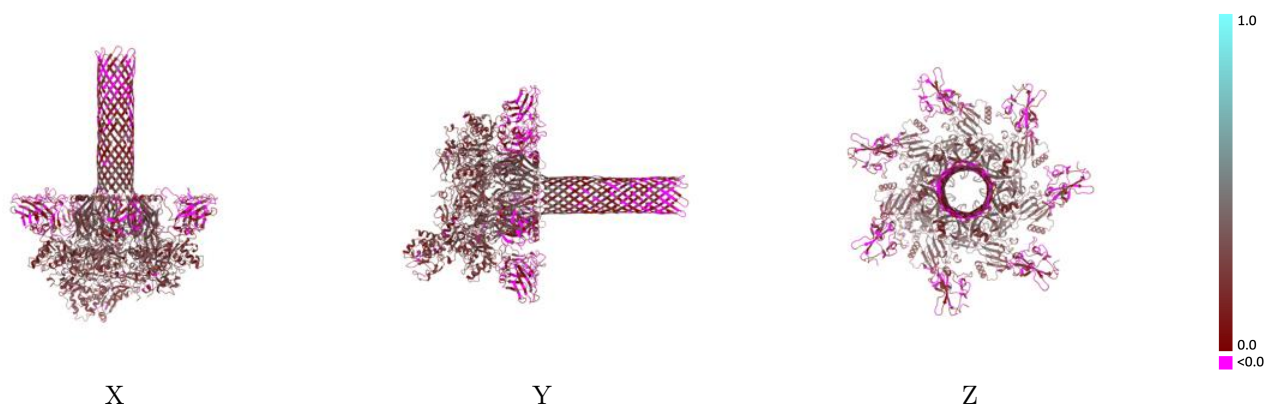
This section contains information regarding the fit between EMDB map EMD-20459 and PDB model 6PSN. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



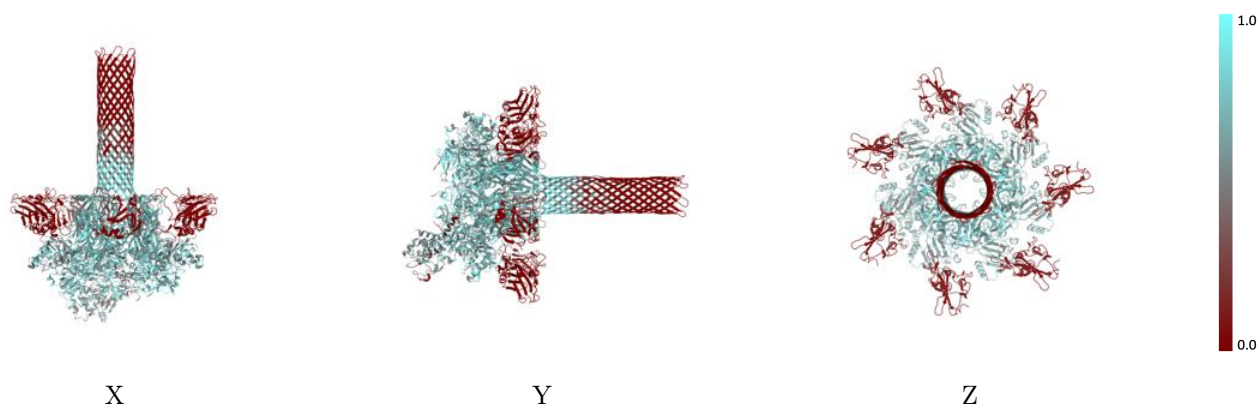
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



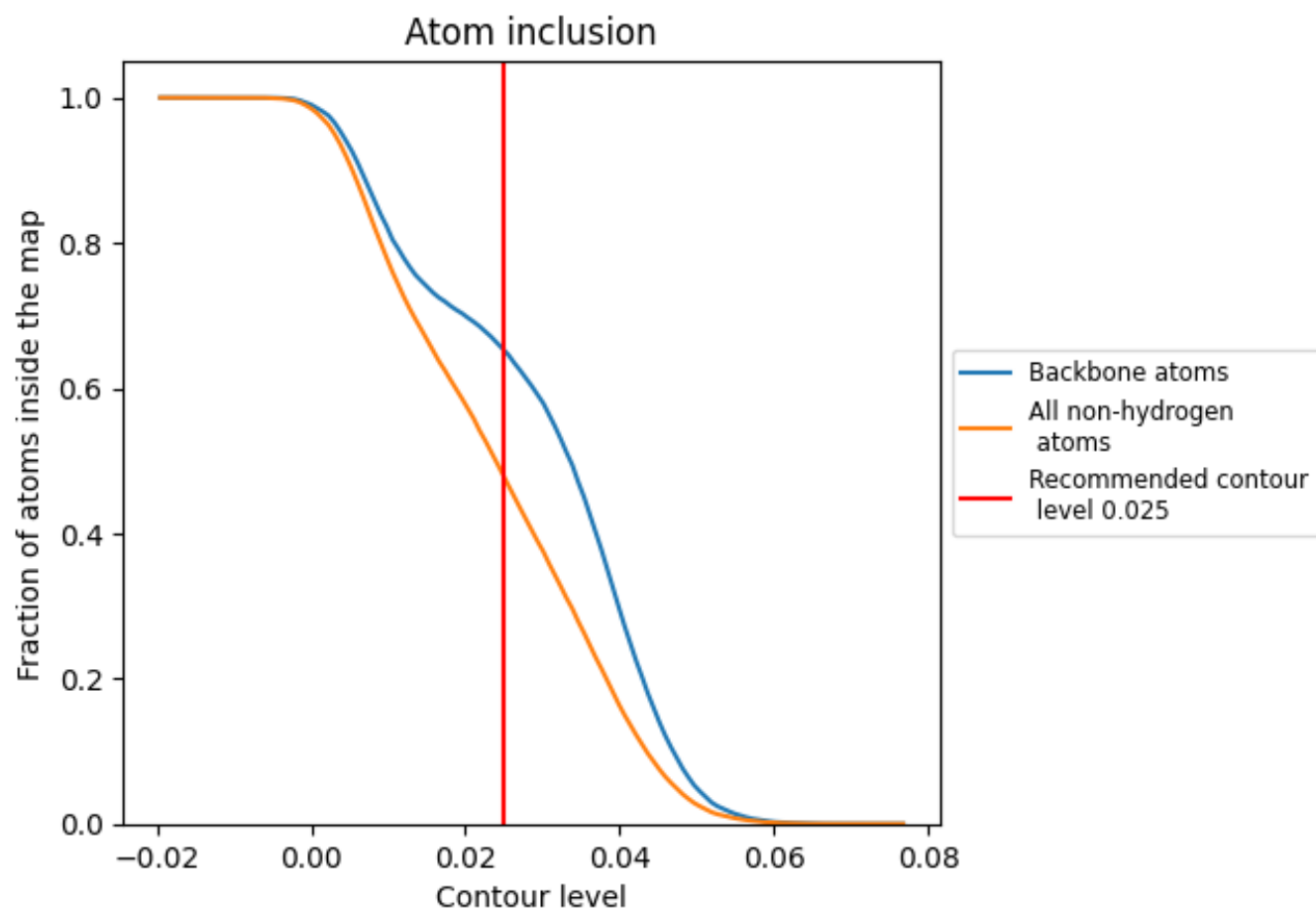
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 48% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4780	<div></div> 0.2010
A	<div></div> 0.4890	<div></div> 0.2100
B	<div></div> 0.4840	<div></div> 0.2100
C	<div></div> 0.4833	<div></div> 0.2020
D	<div></div> 0.4677	<div></div> 0.2020
E	<div></div> 0.4704	<div></div> 0.1970
F	<div></div> 0.4654	<div></div> 0.1990
G	<div></div> 0.4766	<div></div> 0.2000
L	<div></div> 0.5020	<div></div> 0.1770

