



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:46 PM UTC

PDB ID : 9LC0 / pdb_00009lc0
EMDB ID : EMD-62961
Title : tail complex of mature phage N4
Authors : Liu, H.; Chen, W.
Deposited on : 2025-01-03
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

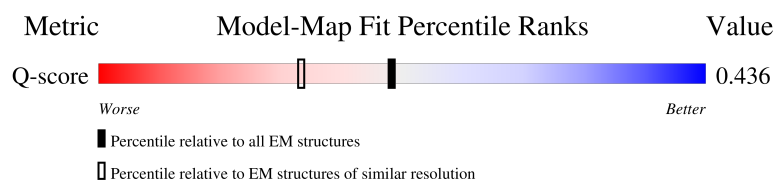
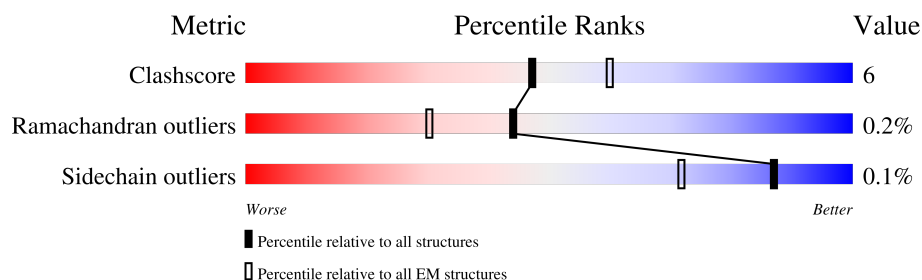
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	556	5% 10% . 87%
1	B	556	5% 13% . 84%
1	C	556	5% 11% 5% 84%
1	D	556	5% 9% . 88%

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Mol	Chain	Length	Quality of chain
1	E	556	
1	F	556	
1	G	556	
1	L	556	
1	Q	556	
1	V	556	
1	a	556	
1	f	556	
2	M	417	
2	R	417	
3	I	1382	
3	N	1382	
4	H	236	
4	J	236	
4	O	236	
4	S	236	
5	K	299	
5	P	299	
5	T	299	
5	U	299	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 51753 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 60 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	73	Total	C	N	O	S	0	0
			589	379	96	110	4		
1	B	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	C	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	D	69	Total	C	N	O	S	0	0
			559	361	92	103	3		
1	E	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	F	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	G	73	Total	C	N	O	S	0	0
			589	379	96	110	4		
1	L	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	Q	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	V	69	Total	C	N	O	S	0	0
			559	361	92	103	3		
1	a	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	f	88	Total	C	N	O	S	0	0
			703	450	115	133	5		

- Molecule 2 is a protein called Gp64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	415	Total	C	N	O	S	0	0
			3384	2213	537	616	18		
2	R	415	Total	C	N	O	S	0	0
			3384	2213	537	616	18		

- Molecule 3 is a protein called Non-contractile tail sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1381	Total	C	N	O	S	0	0
			10866	6904	1831	2082	49		
3	N	1190	Total	C	N	O	S	0	0
			9403	5989	1583	1789	42		

- Molecule 4 is a protein called 30 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	236	Total	C	N	O	S	0	0
			1911	1201	327	374	9		
4	O	236	Total	C	N	O	S	0	0
			1911	1201	327	374	9		
4	S	236	Total	C	N	O	S	0	0
			1911	1201	327	374	9		
4	H	236	Total	C	N	O	S	0	0
			1911	1201	327	374	9		

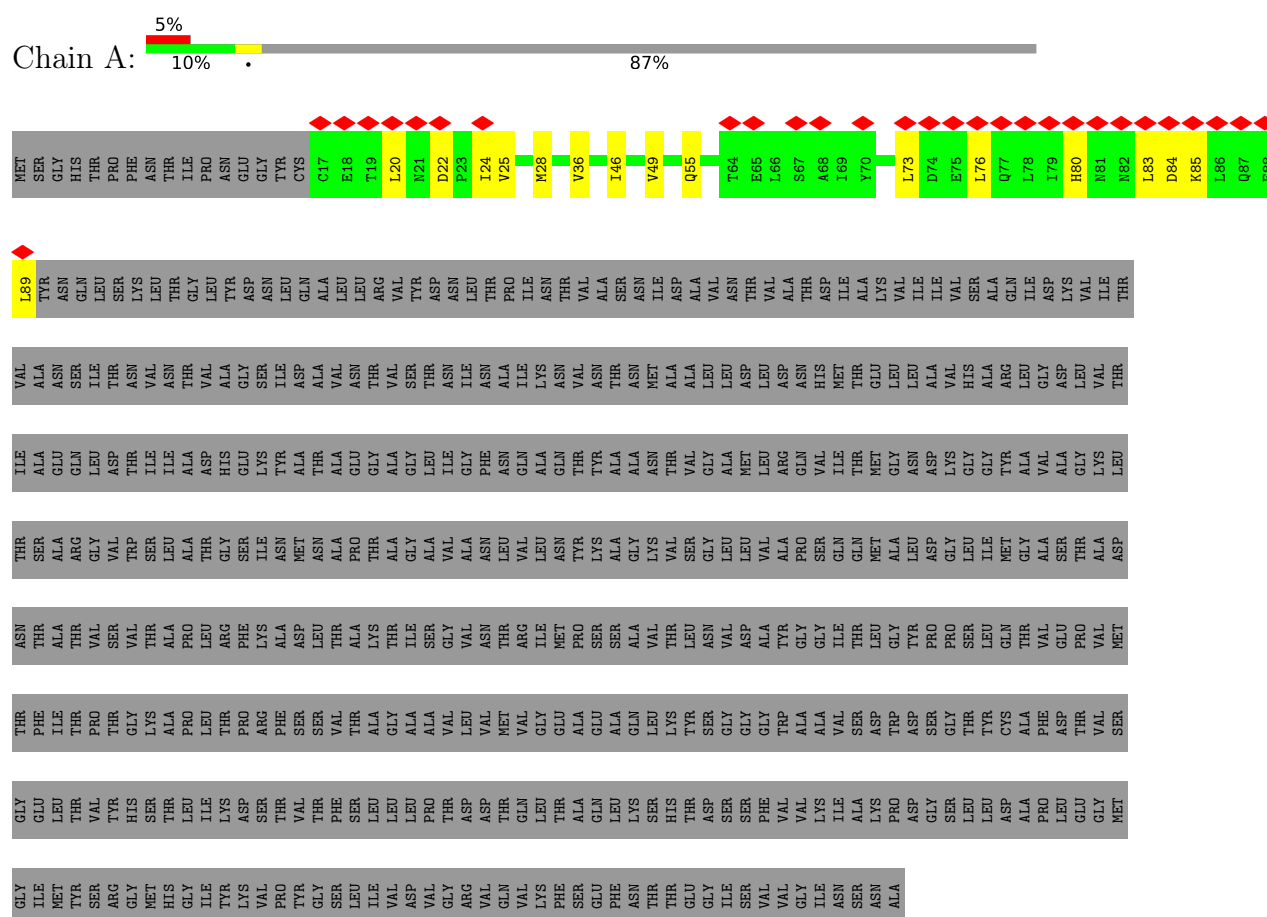
- Molecule 5 is a protein called Gp54.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	298	Total	C	N	O	S	0	0
			2262	1408	381	463	10		
5	P	298	Total	C	N	O	S	0	0
			2262	1408	381	463	10		
5	T	298	Total	C	N	O	S	0	0
			2262	1408	381	463	10		
5	U	298	Total	C	N	O	S	0	0
			2262	1408	381	463	10		

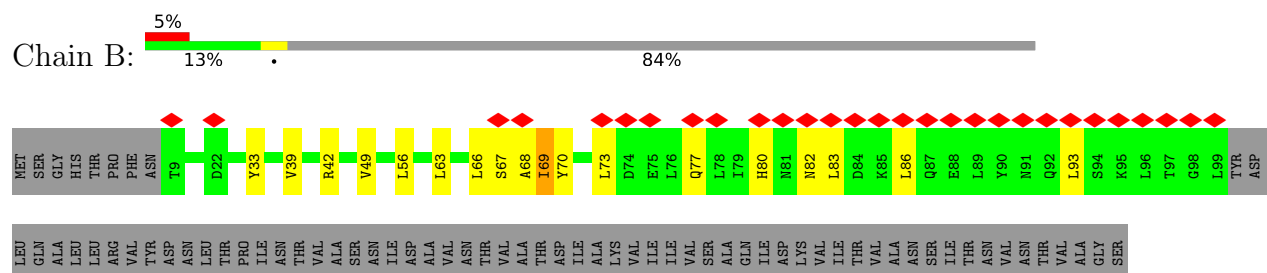
3 Residue-property plots

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: 60 kDa protein

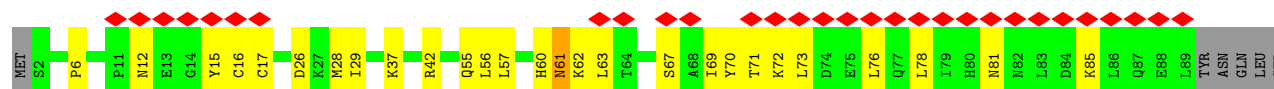


• Molecule 1: 60 kDa protein



PRO	THR	PHE	ALA	ASN	TYR	ILE
THR	THR	PHE	THR	ASP	ASP	ASP
VAL	VAL	VAL	THR	ASP	ALA	VAL
LEU	LEU	THR	ALA	PRO	GLU	THR
ILE	LEU	ALA	LYS	THR	GLY	VAL
VAL	LEU	GLY	ILE	ALA	ALA	VAL
VAL	PRO	ALA	SER	ALA	LEU	VAL
GLY	THR	VAL	GLY	VAL	ILE	ASN
ARG	ASP	LEU	VAL	ALA	GLY	ILE
VAL	ASP	VAL	ASN	ASN	PHE	ASN
GLN	THR	MET	THR	LEU	ASN	ALA
VAL	GLN	VAL	ARG	VAL	ILE	LYS
LYS	LEU	GLY	ILE	LEU	GLN	ALA
PHE	THR	GLU	MET	ASN	GLN	VAL
SER	ALA	ALA	PRO	TYR	THR	VAL
GLU	GLN	GLU	SER	LYS	TYR	ASN
PHE	LEU	ALA	SER	ALA	ALA	THR
ASN	LYS	GLN	ALA	GLY	ALA	ASN
THR	SER	LEU	VAL	LYS	VAL	MET
THR	HIS	THR	THR	VAL	THR	ALA
GLU	THR	TYR	LEU	SER	VAL	ALA
GLY	ASP	SER	ASN	GLY	GLY	LEU
ILE	SER	GLY	VAL	LEU	ALA	LEU
VAL	SER	GLY	ASP	LEU	MET	ASP
VAL	PHE	GLY	THR	VAL	ARG	ASN
GLY	VAL	ALA	TYR	ALA	GLN	ASN
ILE	LYS	ALA	GLY	SER	VAL	HIS
ASN	ILE	VAL	ILE	GLN	ILE	MET
SER	ALA	SER	THR	GLN	THR	THR
ASN	LYS	ASP	LEU	MET	MET	GLU
ALA	PRO	ASP	TYR	LEU	ASN	LEU
	GLY	SER	PRO	ASP	ALA	VAL
	SER	GLY	PRO	GLY	LYS	VAL
	LEU	THR	SER	THR	VAL	ASP
	LEU	THR	LEU	SER	THR	ILE
	ASP	PHE	THR	GLY	THR	ALA
	PRO	LEU	VAL	ALA	VAL	GLU
	LEU	ASP	GLU	SER	ALA	GLN
	GLU	THR	THR	THR	ARG	LEU
	GLY	VAL	VAL	VAL	VAL	THR
	GLY	GLY	THR	THR	TRP	THR
	ILE	GLU	PHE	THR	SER	ILE
	MET	LEU	ILE	ALA	ALA	ILE
	TYR	THR	THR	THR	ARG	GLN
	SER	VAL	PRO	VAL	GLY	LEU
	ARG	TYR	THR	SER	VAL	ASP
	GLY	HIS	GLY	VAL	THR	THR
	MET	SER	LYS	THR	SER	ILE
	HIS	THR	ALA	ALA	ALA	ILE
	GLY	LEU	PRO	PRO	ALA	ALA
	ILE	ILE	LEU	LEU	THR	THR
	TYR	LYS	THR	ARG	GLY	ASP
	LYS	ASP	PRO	PHE	SER	GLU
	VAL	SER	ARG	LYS	THR	LYS

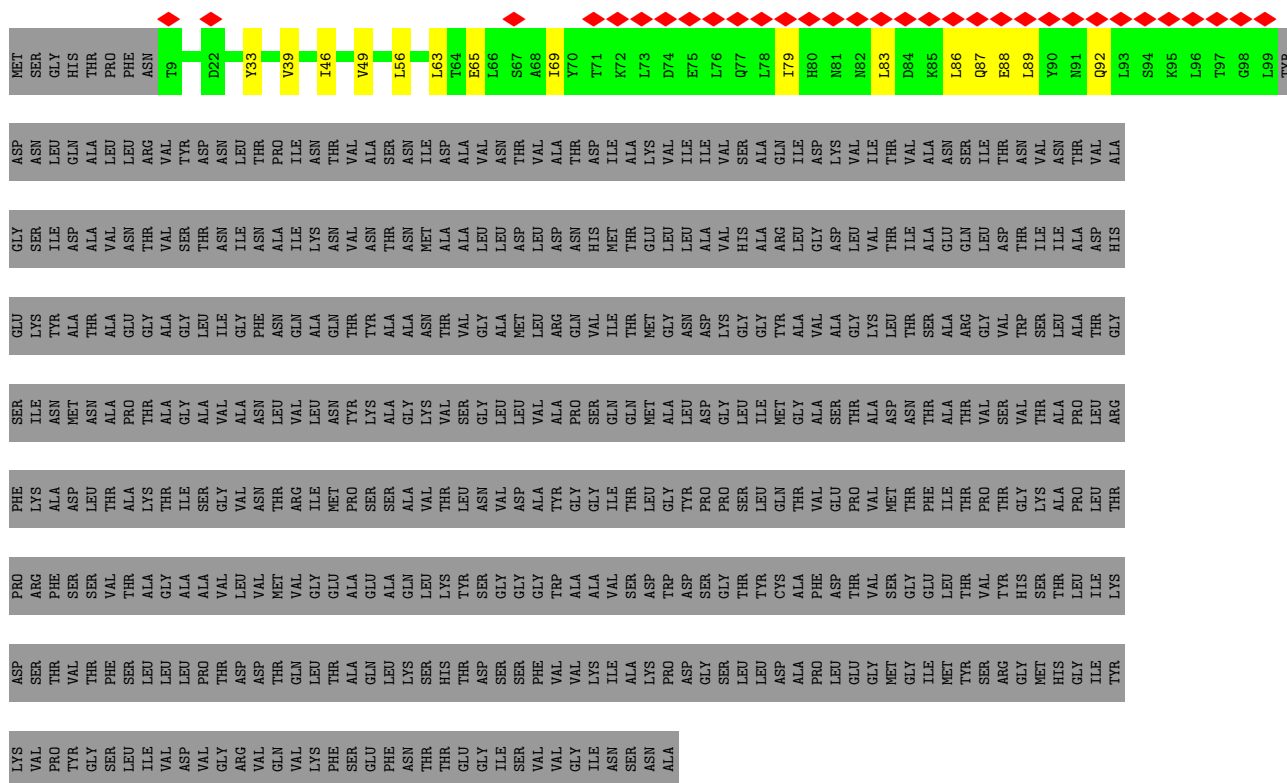
- Molecule 1: 60 kDa protein



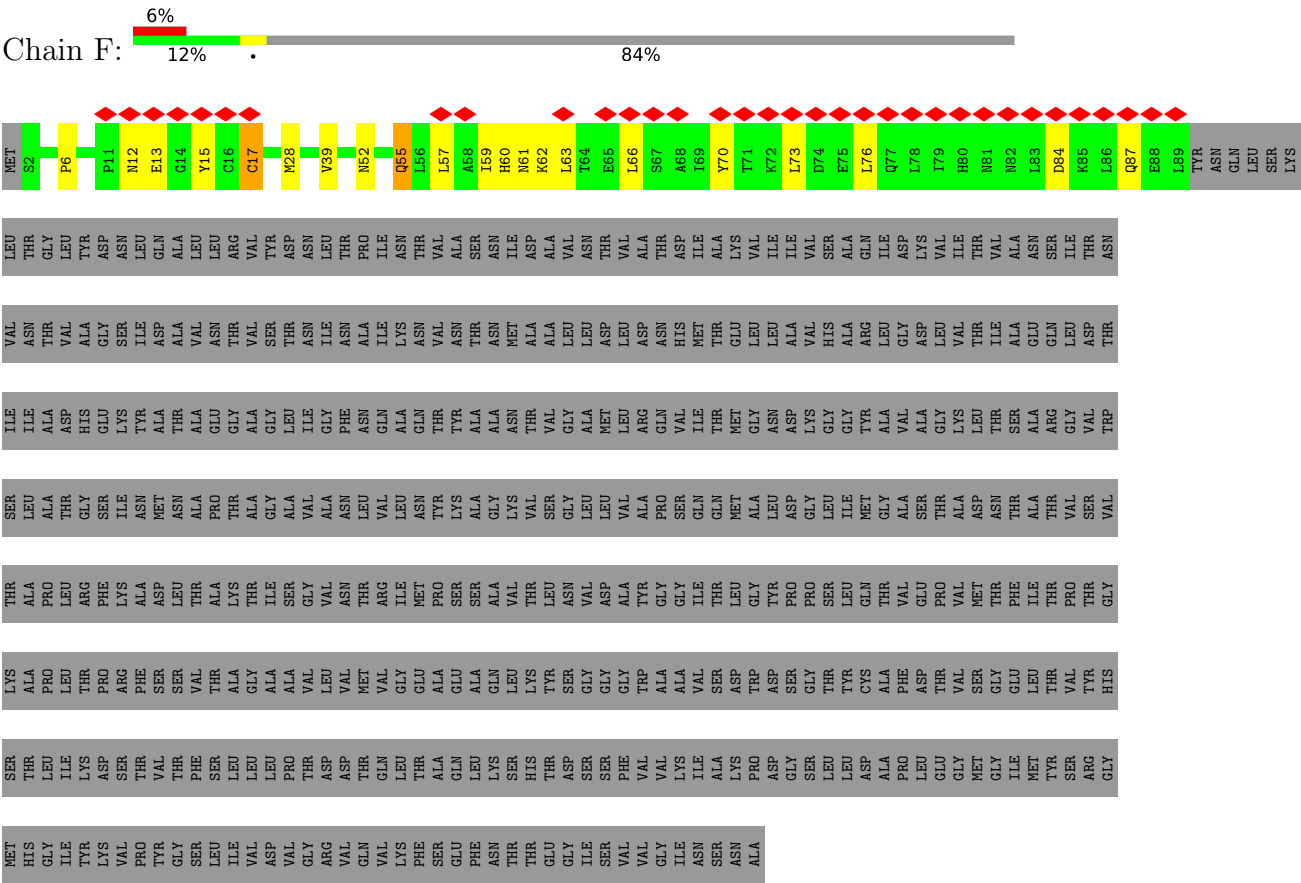
GLY	GLY	HIS	GLY	VAL	TRP	THR	ASN	LYS
MET	LYS	SER	THR	THR	LEU	LEU	ILE	LEU
HIS	ALA	THR	ALA	ALA	LEU	ILE	ASN	THR
ILE	PRO	LEU	PRO	PRO	ALA	ASP	THR	GLY
ILE	LEU	ILE	LEU	LEU	THR	HIS	ALA	TYR
TYR	THR	LYS	ARG	ARG	GLY	ASP	ALA	ASP
LYS	PRO	ASP	PHE	PHE	SER	GLU	LYS	ASN
VAL	ARG	SER	ARG	ILE	ILE	THR	THR	GLN
PRO	PHE	THR	ALA	ALA	ASN	TYR	ILE	LEU
TYR	SER	VAL	SER	ASP	MET	ASP	ASP	GLN
GLY	THR	THR	SER	LEU	ASN	THR	ALA	ALA
SER	PHE	THR	VAL	THR	ASN	ALA	VAL	LEU
LEU	THR	SER	THR	ALA	PRO	GLU	ASN	LEU
ILE	ALA	LEU	LYS	LYS	THR	GLY	THR	ARG
VAL	GLY	LEU	THR	ILE	GLY	ALA	VAL	VAL
ASP	ALA	LEU	ILE	ILE	GLY	GLY	SER	TYR
VAL	VAL	PRO	VAL	GLY	ALA	LEU	THR	ASP
VAL	THR	THR	THR	GLY	VAL	ILE	ASN	ASN
GLY	VAL	THR	VAL	GLY	VAL	THR	ILE	ASN
ARG	LEU	ASP	VAL	VAL	VAL	GLY	GLY	LEU
VAL	VAL	ASP	VAL	ASN	ASN	PHE	ILE	THR
GLN	THR	THR	MET	ARG	LEU	THR	ASN	PRO
VAL	VAL	GLN	THR	THR	VAL	GLN	ILE	ILE
VAL	VAL	GLN	VAL	ILE	LEU	ALA	LYS	ASN
PHE	GLU	THR	GLY	MET	ASN	GLN	ASN	THR
THR	THR	THR	LEU	THR	VAL	THR	THR	VAL
THR	THR	HIS	LYS	THR	VAL	THR	THR	VAL
GLY	GLY	THR	THR	LEU	GLY	VAL	VAL	ALA
GLU	GLU	ASP	SER	ASN	GLY	THR	LEU	ASN
ILE	ILE	SER	GLY	VAL	LEU	ALA	ASP	THR
VAL	ASN	ILE	ILE	ILE	GLN	ILE	MET	ILE
SER	SER	ALA	SER	THR	GLN	THR	THR	LYS
ASN	ASN	LYS	ASP	GLN	MET	MET	GLU	ALA
ALA	ALA	PRO	TRP	GLY	ALA	GLY	LEU	VAL
		ASP	ASP	TYR	LEU	ASN	LEU	ILE
		GLY	SER	PRO	GLY	VAL	ALA	THR
		LEU	GLY	PRO	GLY	LYS	VAL	VAL
		LEU	THR	SER	LEU	GLY	HIS	SER
		ASP	CYS	GLN	ILE	GLY	ALA	GLN
		ALA	ALA	THR	MET	TYR	ARG	ILE
		PRO	PHE	VAL	SER	VAL	GLY	ASN
		LEU	ASP	GLU	SER	ALA	ASP	LYS
		GLY	THR	PRO	THR	GLY	LEU	THR
		VAL	VAL	VAL	ALA	LYS	VAL	ILE
		SER	SER	MET	ASP	LEU	THR	THR
		GLY	GLY	THR	ASN	THR	ILE	VAL
		ILE	ILE	PHE	THR	SER	ALA	THR
		MET	LEU	ILE	THR	ALA	GLU	ASN
		TYR	THR	THR	THR	ARG	GLN	SER
		SER	VAL	PRO	SER	GLY	LEU	THR

- Molecule 1: 60 kDa protein

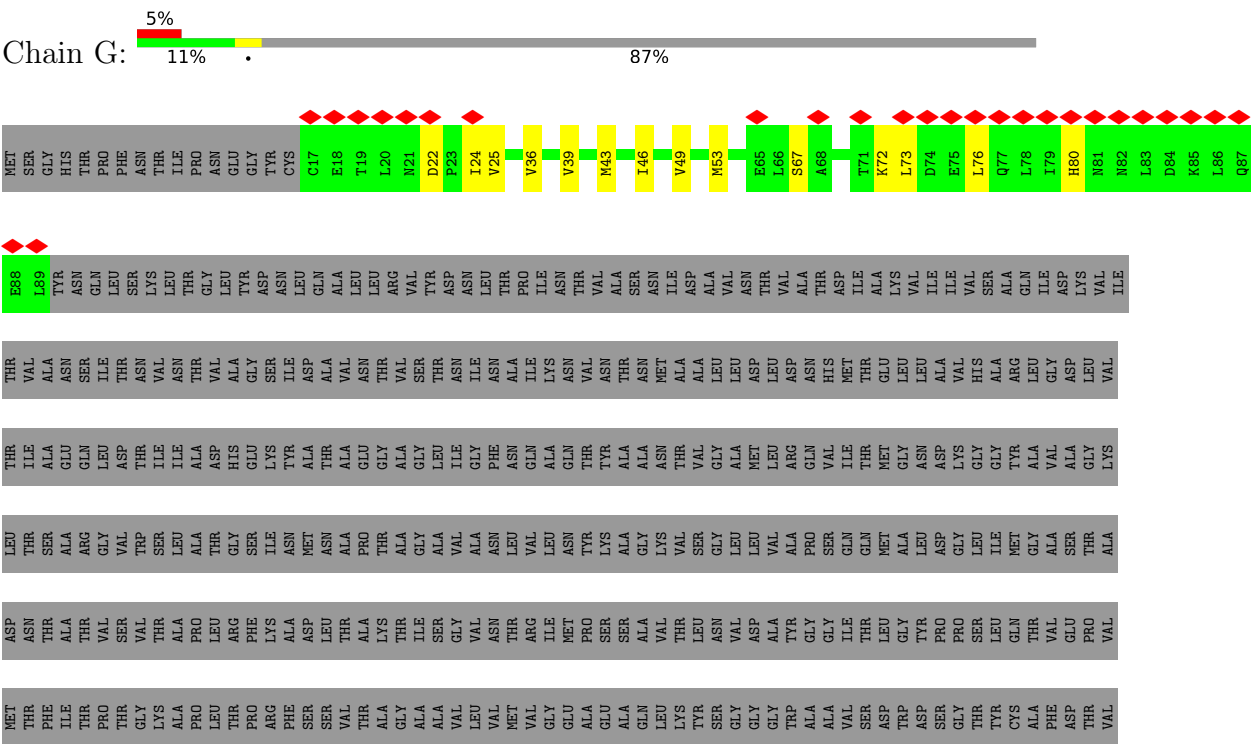


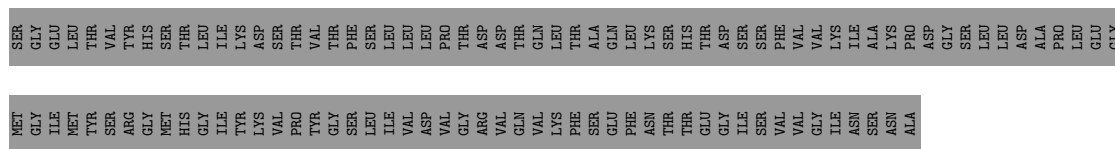


● Molecule 1: 60 kDa protein

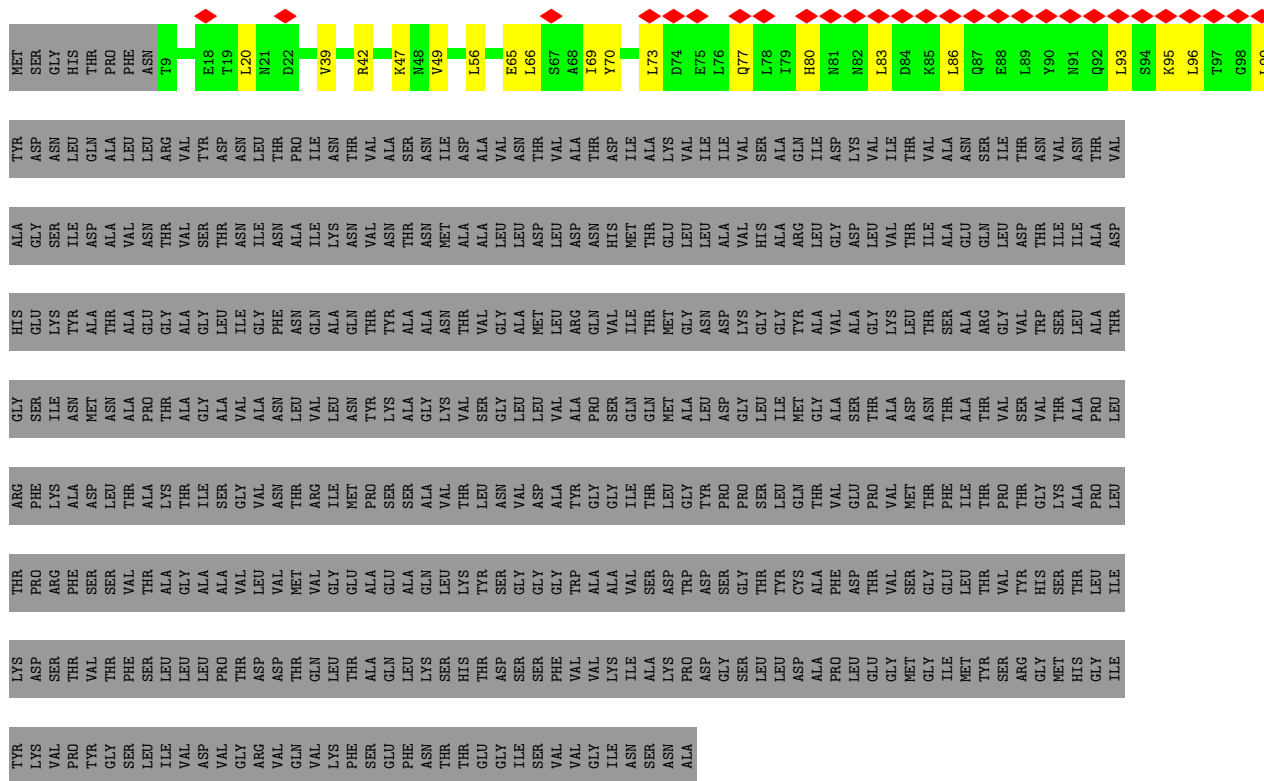


● Molecule 1: 60 kDa protein

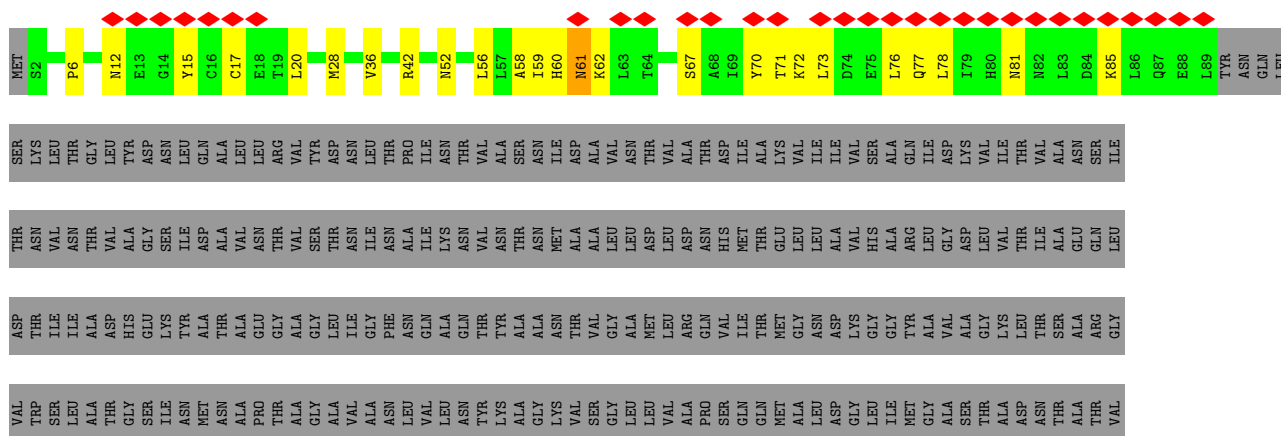




- Molecule 1: 60 kDa protein

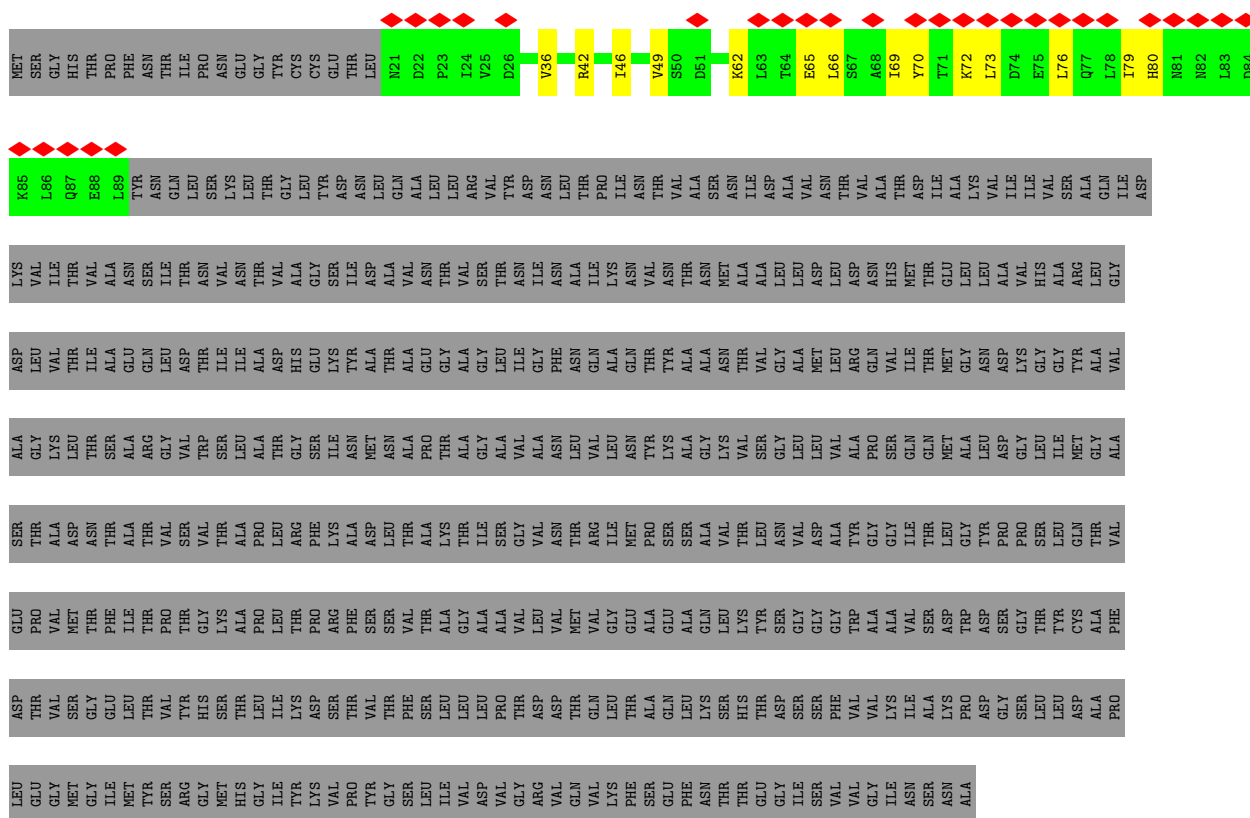


- Molecule 1: 60 kDa protein

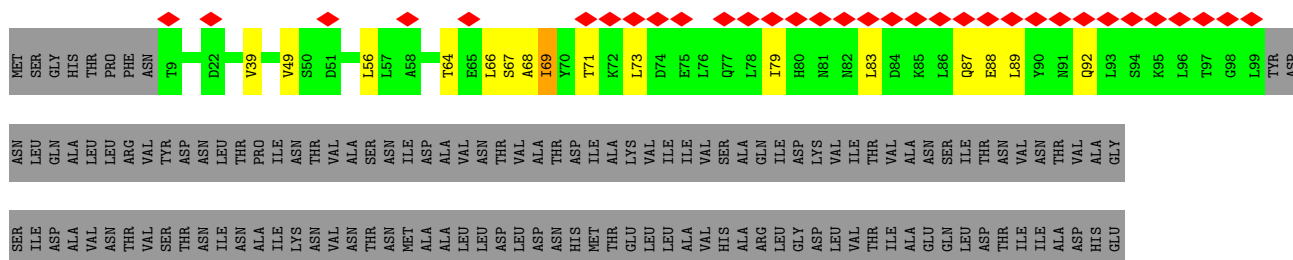


[illegible]

- Molecule 1: 60 kDa protein



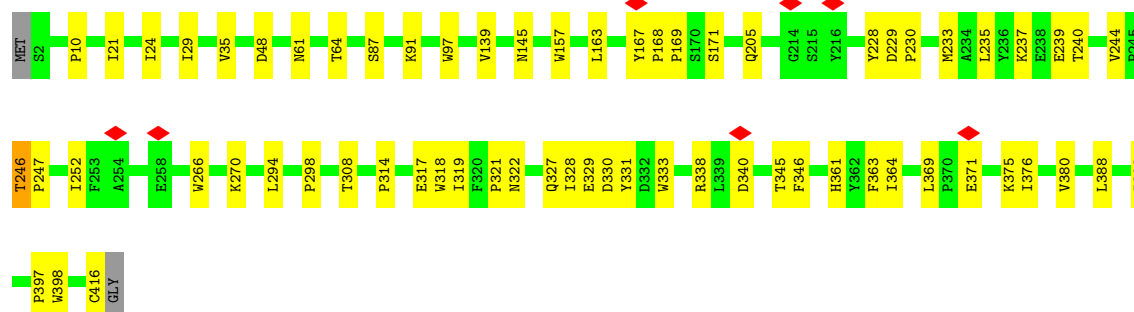
- Molecule 1: 60 kDa protein





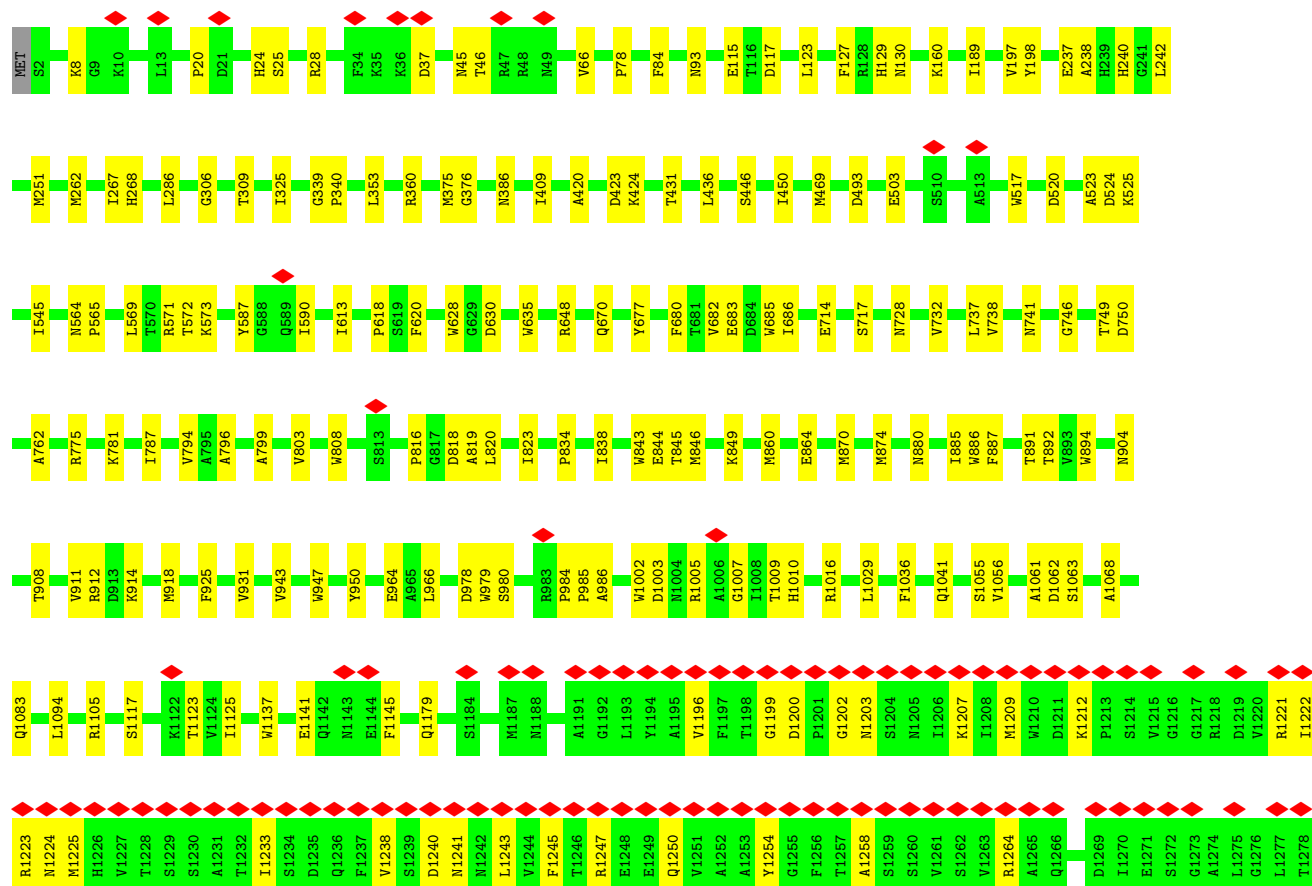
• Molecule 2: Gp64

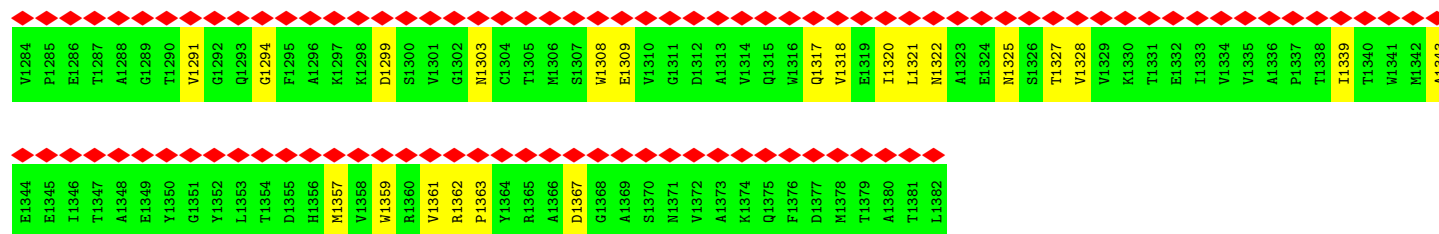
Chain R: 84% 16%



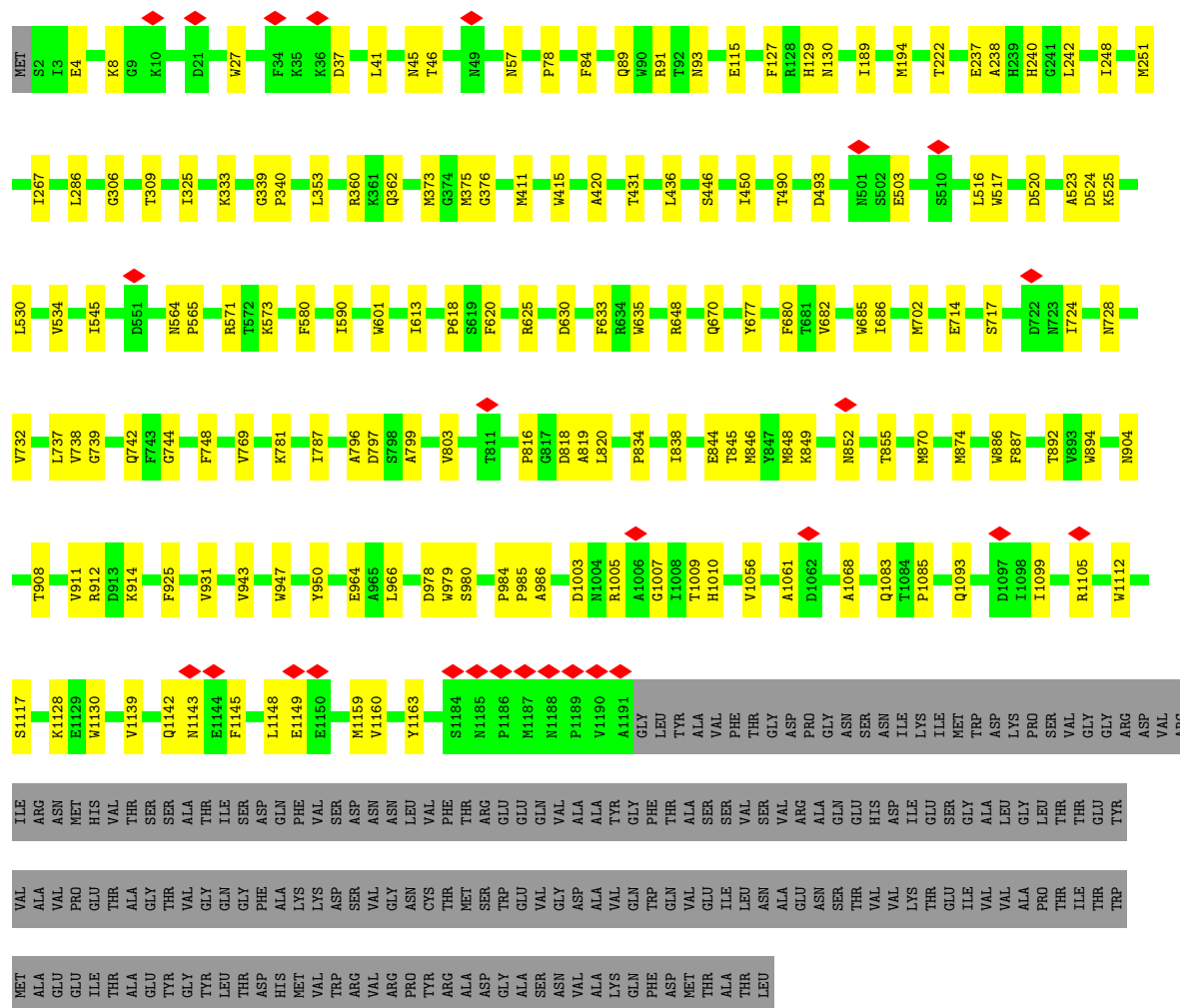
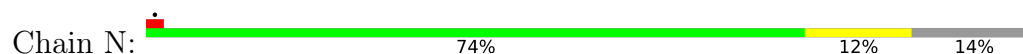
• Molecule 3: Non-contractile tail sheath

Chain I: 15% 85% 15%

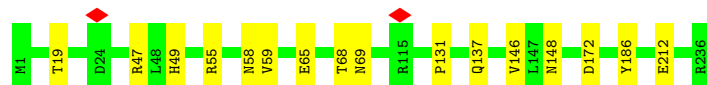




• Molecule 3: Non-contractile tail sheath

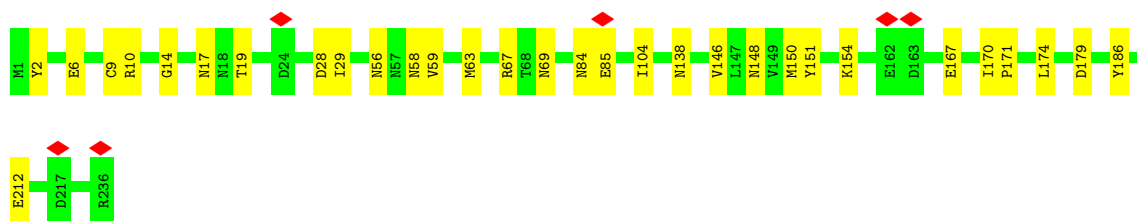


• Molecule 4: 30 kDa protein



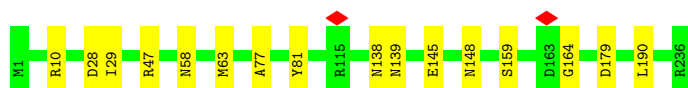
• Molecule 4: 30 kDa protein

Chain O:  87% 13%



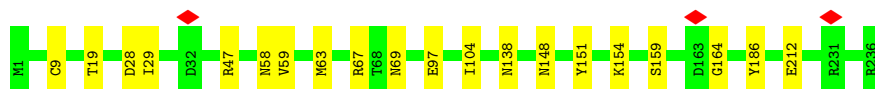
- Molecule 4: 30 kDa protein

Chain S:  93% 7%



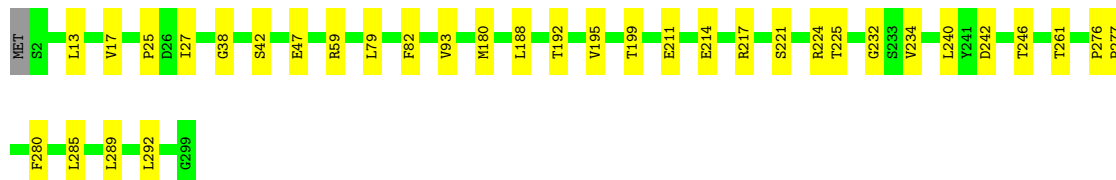
- Molecule 4: 30 kDa protein

Chain H:  92% 8%



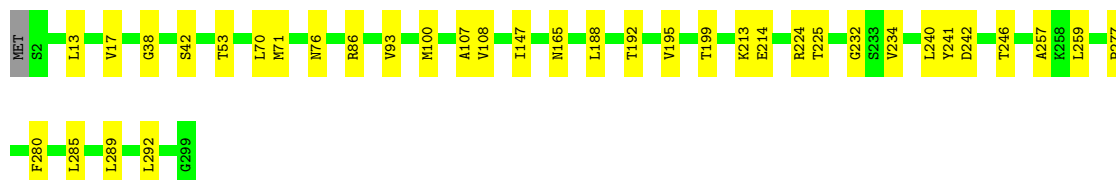
- Molecule 5: Gp54

Chain K:  88% 11%



- Molecule 5: Gp54

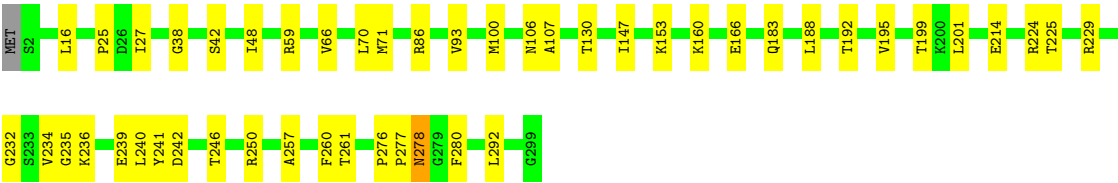
Chain P:  88% 12%



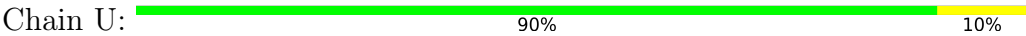
- Molecule 5: Gp54

Chain T:  84% 16%





• Molecule 5: Gp54



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.334	Depositor
Minimum map value	-45.213	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.815	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/597	0.37	0/808
1	B	0.16	0/740	0.33	0/1003
1	C	0.27	0/716	0.48	0/972
1	D	0.12	0/567	0.34	0/767
1	E	0.18	0/740	0.33	0/1003
1	F	0.23	0/716	0.54	1/972 (0.1%)
1	G	0.13	0/597	0.34	0/808
1	L	0.21	0/740	0.38	0/1003
1	Q	0.25	0/716	0.49	0/972
1	V	0.13	0/567	0.32	0/767
1	a	0.17	0/740	0.34	0/1003
1	f	0.22	0/716	0.45	0/972
2	M	0.18	0/3499	0.40	1/4784 (0.0%)
2	R	0.17	0/3499	0.39	1/4784 (0.0%)
3	I	0.17	0/11163	0.38	0/15218
3	N	0.17	0/9670	0.38	0/13182
4	H	0.19	0/1952	0.37	0/2654
4	J	0.19	0/1952	0.35	0/2654
4	O	0.19	0/1952	0.38	0/2654
4	S	0.19	0/1952	0.36	0/2654
5	K	0.22	0/2289	0.39	0/3103
5	P	0.24	0/2289	0.41	0/3103
5	T	0.23	0/2289	0.39	0/3103
5	U	0.23	0/2289	0.40	0/3103
All	All	0.19	0/52947	0.39	3/72046 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	R	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	GLU	N-CA-C	-7.87	102.69	111.82
2	R	246	THR	C-N-CD	-5.53	102.33	125.00
2	M	246	THR	C-N-CD	-5.04	104.35	125.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	246	THR	Peptide
2	R	246	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	589	0	609	12	0
1	B	729	0	747	23	0
1	C	703	0	707	27	0
1	D	559	0	580	12	0
1	E	729	0	747	14	0
1	F	703	0	707	19	0
1	G	589	0	609	13	0
1	L	729	0	747	21	0
1	Q	703	0	707	22	0
1	V	559	0	580	12	0
1	a	729	0	747	13	0
1	f	703	0	707	17	0
2	M	3384	0	3272	48	0
2	R	3384	0	3272	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	10866	0	10396	138	0
3	N	9403	0	8990	110	0
4	H	1911	0	1844	18	0
4	J	1911	0	1844	15	0
4	O	1911	0	1844	29	0
4	S	1911	0	1844	11	0
5	K	2262	0	2260	24	0
5	P	2262	0	2260	27	0
5	T	2262	0	2260	40	0
5	U	2262	0	2260	25	0
All	All	51753	0	50540	611	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 6.

All (611) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1139:VAL:HG22	3:N:1142:GLN:HE22	1.43	0.83
1:B:67:SER:HA	1:C:55:GLN:HE22	1.42	0.83
3:I:1224:ASN:HB3	3:I:1233:ILE:HD12	1.61	0.83
2:R:416:CYS:HB3	4:H:9:CYS:HB3	1.65	0.79
3:I:816:PRO:HB3	3:I:820:LEU:HD23	1.68	0.76
3:I:894:TRP:HB2	3:I:947:TRP:HB2	1.69	0.75
1:L:66:LEU:HD13	1:Q:56:LEU:HD21	1.70	0.74
1:f:11:PRO:HG3	1:f:20:LEU:HD12	1.70	0.74
2:R:24:ILE:HD11	3:I:573:LYS:HB2	1.68	0.74
2:M:24:ILE:HD11	3:N:573:LYS:HB2	1.69	0.73
3:I:1196:VAL:HG21	3:I:1209:MET:HE3	1.68	0.73
3:N:493:ASP:OD2	3:N:571:ARG:NH1	2.23	0.72
5:T:183:GLN:HG3	5:U:188:LEU:HD22	1.72	0.71
3:N:852:ASN:ND2	3:N:855:THR:OG1	2.23	0.70
3:N:240:HIS:HD2	3:N:333:LYS:HG2	1.56	0.69
3:N:870:MET:HG2	3:N:874:MET:HE2	1.75	0.69
3:I:1221:ARG:HD3	3:I:1223:ARG:HH21	1.55	0.69
3:I:864:GLU:HG3	3:I:918:MET:HE3	1.75	0.69
2:R:416:CYS:CB	4:H:9:CYS:HB3	2.23	0.68
2:M:317:GLU:O	2:M:322:ASN:ND2	2.22	0.68
2:M:331:TYR:HH	2:M:398:TRP:CD1	2.11	0.68
4:J:212:GLU:OE2	4:H:47:ARG:NH1	2.27	0.68
2:R:319:ILE:HG22	2:R:321:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1238:VAL:HB	3:I:1243:LEU:HD22	1.75	0.67
4:S:10:ARG:NH1	4:S:179:ASP:OD2	2.27	0.67
1:G:73:LEU:HD11	1:L:69:ILE:HG12	1.75	0.67
3:N:89:GLN:HE21	3:N:91:ARG:HH21	1.42	0.67
5:P:165:ASN:ND2	5:T:166:GLU:OE2	2.28	0.67
2:M:319:ILE:HG22	2:M:321:PRO:HD2	1.77	0.67
2:M:330:ASP:HB2	2:M:333:TRP:HD1	1.61	0.66
1:f:53:MET:O	1:f:57:LEU:HG	1.96	0.66
1:A:24:ILE:HG13	1:A:25:VAL:HG23	1.78	0.65
1:G:24:ILE:HG13	1:G:25:VAL:HG23	1.79	0.65
3:N:852:ASN:ND2	3:N:855:THR:HG1	1.95	0.65
5:T:277:PRO:HD2	5:T:280:PHE:HD2	1.62	0.65
1:B:63:LEU:HD21	1:C:56:LEU:HD11	1.79	0.64
3:N:803:VAL:HG21	3:N:844:GLU:HA	1.79	0.64
4:O:10:ARG:NH1	4:O:179:ASP:OD2	2.30	0.64
3:N:545:ILE:HG13	3:N:590:ILE:HG21	1.79	0.64
2:M:381:ASP:OD1	3:N:41:LEU:HB2	1.98	0.64
3:N:648:ARG:NH2	3:N:714:GLU:OE1	2.31	0.64
2:R:317:GLU:O	2:R:322:ASN:ND2	2.23	0.63
2:M:63:GLU:HG3	2:M:67:LYS:HE3	1.79	0.63
3:I:286:LEU:HG	3:I:325:ILE:HD11	1.80	0.63
3:I:870:MET:HG2	3:I:874:MET:HE2	1.80	0.63
3:I:648:ARG:NH2	3:I:714:GLU:OE2	2.31	0.63
3:I:1212:LYS:HE3	3:I:1241:ASN:HB3	1.78	0.63
5:K:214:GLU:OE1	5:K:224:ARG:NH1	2.31	0.63
3:N:286:LEU:HG	3:N:325:ILE:HD11	1.79	0.63
3:N:816:PRO:HB3	3:N:820:LEU:HD23	1.80	0.63
3:I:838:ILE:HD13	3:I:886:TRP:HB2	1.79	0.63
3:I:738:VAL:HA	3:I:838:ILE:HB	1.81	0.62
3:I:493:ASP:OD2	3:I:571:ARG:NH1	2.32	0.62
3:N:490:THR:HG22	3:N:516:LEU:HB3	1.80	0.62
3:I:818:ASP:OD1	3:I:819:ALA:N	2.33	0.62
4:J:58:ASN:OD1	4:J:59:VAL:N	2.32	0.62
4:H:58:ASN:HD21	4:H:148:ASN:HD21	1.45	0.62
2:R:331:TYR:OH	2:R:398:TRP:NE1	2.33	0.62
3:I:545:ILE:HG13	3:I:590:ILE:HG21	1.81	0.62
1:Q:70:TYR:HA	1:Q:73:LEU:HG	1.81	0.61
3:I:587:TYR:HB2	3:I:590:ILE:HD11	1.81	0.61
3:I:1317:GLN:HB3	3:I:1362:ARG:HB3	1.80	0.61
3:N:739:GLY:HA3	3:N:744:GLY:HA3	1.82	0.61
2:R:331:TYR:HH	2:R:398:TRP:CD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:845:THR:HG22	3:N:911:VAL:HG21	1.82	0.61
1:E:33:TYR:HE1	1:F:28:MET:HE2	1.66	0.61
1:E:63:LEU:HD22	1:F:52:ASN:HD22	1.66	0.61
1:Q:12:ASN:HB2	1:Q:15:TYR:O	2.00	0.61
3:I:1320:ILE:HD11	3:I:1339:ILE:HD13	1.83	0.61
1:A:76:LEU:HD21	1:C:76:LEU:HD13	1.82	0.60
5:T:261:THR:HG21	5:U:259:LEU:HD21	1.82	0.60
1:V:66:LEU:HD13	1:a:66:LEU:HD21	1.83	0.60
4:H:104:ILE:HD11	4:H:154:LYS:HB3	1.83	0.60
2:R:330:ASP:HB2	2:R:333:TRP:HD1	1.65	0.60
1:A:73:LEU:HD11	1:B:69:ILE:HG12	1.82	0.60
2:M:9:MET:HE3	3:N:601:TRP:HE1	1.67	0.60
5:K:277:PRO:HD2	5:K:280:PHE:HD2	1.67	0.60
1:F:6:PRO:HD2	4:J:58:ASN:ND2	2.16	0.60
3:I:115:GLU:OE1	3:I:360:ARG:NH2	2.35	0.60
3:I:1199:GLY:HA2	3:I:1362:ARG:HD3	1.84	0.60
1:A:84:ASP:OD1	1:A:85:LYS:N	2.34	0.60
3:N:564:ASN:HB3	3:N:565:PRO:HD3	1.84	0.60
1:D:50:SER:HA	1:D:53:MET:HE3	1.84	0.59
3:N:986:ALA:HB3	3:N:1003:ASP:HB2	1.83	0.59
1:a:73:LEU:HD21	1:f:62:LYS:HG3	1.85	0.59
3:I:564:ASN:HB3	3:I:565:PRO:HD3	1.84	0.59
3:I:803:VAL:HG21	3:I:844:GLU:HA	1.83	0.59
1:a:68:ALA:O	1:a:71:THR:N	2.35	0.59
3:N:894:TRP:HB2	3:N:947:TRP:HB2	1.85	0.59
3:N:848:MET:HA	3:N:852:ASN:HB2	1.84	0.59
3:I:849:LYS:HG2	3:I:904:ASN:HD22	1.68	0.59
1:C:70:TYR:HA	1:C:73:LEU:HG	1.84	0.58
1:B:83:LEU:HD13	1:C:72:LYS:HD2	1.84	0.58
2:R:329:GLU:HG2	2:R:363:PHE:HB2	1.86	0.58
5:T:100:MET:HE1	5:U:99:THR:HG21	1.84	0.58
3:I:741:ASN:HD21	3:I:843:TRP:HE3	1.50	0.58
5:P:13:LEU:HD12	5:U:160:LYS:HE3	1.84	0.58
2:R:48:ASP:HB3	2:R:64:THR:HG21	1.84	0.58
1:B:67:SER:HA	1:C:55:GLN:NE2	2.18	0.58
3:I:986:ALA:HB3	3:I:1003:ASP:HB2	1.86	0.58
2:R:237:LYS:HE3	2:R:244:VAL:HG23	1.86	0.57
3:N:115:GLU:OE1	3:N:360:ARG:NH2	2.37	0.57
2:R:327:GLN:HB3	2:R:363:PHE:HE1	1.68	0.57
3:N:738:VAL:HA	3:N:838:ILE:HB	1.86	0.57
2:M:48:ASP:HB3	2:M:64:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:838:ILE:HD11	3:I:966:LEU:HD11	1.85	0.57
5:U:214:GLU:OE1	5:U:224:ARG:NH1	2.37	0.57
4:O:104:ILE:HD11	4:O:154:LYS:HB3	1.86	0.57
1:C:12:ASN:HB2	1:C:15:TYR:O	2.05	0.57
1:G:80:HIS:CE1	1:L:86:LEU:HD11	2.40	0.57
3:N:1083:GLN:HB2	3:N:1105:ARG:HD2	1.86	0.57
5:K:93:VAL:HG21	5:P:86:ARG:HB3	1.87	0.57
1:L:93:LEU:HD13	1:Q:78:LEU:HD12	1.86	0.57
2:M:237:LYS:HE3	2:M:244:VAL:HG13	1.85	0.57
2:M:347:ASP:OD1	2:M:351:ASN:ND2	2.37	0.57
4:O:28:ASP:OD1	4:O:29:ILE:N	2.38	0.57
4:H:59:VAL:HG23	4:H:151:TYR:HE1	1.68	0.57
5:P:232:GLY:O	5:P:234:VAL:N	2.38	0.56
5:P:292:LEU:HD11	5:T:257:ALA:HB1	1.87	0.56
1:D:84:ASP:HB3	1:E:86:LEU:HD11	1.87	0.56
4:S:58:ASN:HD21	4:S:148:ASN:HD21	1.54	0.56
3:I:912:ARG:HH11	3:I:980:SER:HB2	1.70	0.56
4:S:63:MET:HE1	4:S:138:ASN:HB3	1.86	0.56
5:P:285:LEU:O	5:P:289:LEU:HG	2.05	0.56
4:O:67:ARG:NH1	4:O:69:ASN:O	2.39	0.56
5:K:232:GLY:O	5:K:234:VAL:N	2.37	0.56
4:H:19:THR:HG21	4:H:186:TYR:HE2	1.71	0.56
5:T:240:LEU:HD11	5:U:241:TYR:CD1	2.40	0.56
1:Q:60:HIS:O	1:Q:61:ASN:HB2	2.06	0.56
2:R:48:ASP:O	2:R:61:ASN:HB2	2.06	0.56
3:N:912:ARG:HH11	3:N:980:SER:HB2	1.70	0.56
5:T:278:ASN:O	5:T:278:ASN:ND2	2.37	0.56
3:I:127:PHE:HB3	3:I:353:LEU:HD23	1.88	0.55
3:N:737:LEU:HD11	3:N:834:PRO:HB3	1.87	0.55
2:M:208:GLU:HG2	2:M:210:TRP:CH2	2.41	0.55
3:I:1083:GLN:HB2	3:I:1105:ARG:HD2	1.88	0.55
5:T:232:GLY:O	5:T:234:VAL:N	2.38	0.55
5:U:232:GLY:O	5:U:234:VAL:N	2.39	0.55
3:N:237:GLU:HG2	3:N:238:ALA:H	1.71	0.55
1:C:60:HIS:HA	1:C:63:LEU:HG	1.88	0.55
3:N:985:PRO:HG2	3:N:1056:VAL:HG13	1.88	0.55
1:F:60:HIS:O	1:F:62:LYS:N	2.40	0.55
2:M:21:ILE:HA	2:M:24:ILE:HG22	1.88	0.55
3:I:503:GLU:HG2	3:I:517:TRP:HZ2	1.71	0.55
3:N:222:THR:OG1	5:K:47:GLU:OE1	2.24	0.55
1:B:68:ALA:O	1:B:69:ILE:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:242:LEU:HD22	3:N:267:ILE:HD13	1.89	0.54
1:E:89:LEU:O	1:E:92:GLN:N	2.41	0.54
5:P:93:VAL:HG21	5:T:86:ARG:HB3	1.89	0.54
2:M:48:ASP:O	2:M:61:ASN:HB2	2.06	0.54
3:I:242:LEU:HD22	3:I:267:ILE:HD13	1.88	0.54
3:N:849:LYS:HG2	3:N:904:ASN:HD22	1.72	0.54
1:L:83:LEU:HA	1:L:86:LEU:HD12	1.88	0.54
1:a:89:LEU:O	1:a:92:GLN:N	2.40	0.54
3:N:838:ILE:HD11	3:N:966:LEU:HD11	1.89	0.54
3:I:237:GLU:HG2	3:I:238:ALA:H	1.71	0.54
3:I:1137:TRP:CH2	3:I:1141:GLU:HB3	2.43	0.54
3:N:1128:LYS:HE3	3:N:1130:TRP:HE1	1.73	0.54
2:R:331:TYR:HH	2:R:398:TRP:NE1	2.06	0.54
3:I:1123:THR:HG22	3:I:1125:ILE:HG23	1.90	0.54
2:M:327:GLN:HB3	2:M:363:PHE:HE1	1.71	0.54
4:O:58:ASN:HD21	4:O:148:ASN:HD21	1.54	0.54
4:S:47:ARG:NH1	4:H:212:GLU:OE2	2.41	0.54
5:K:13:LEU:HD12	5:T:160:LYS:HE3	1.89	0.54
5:K:261:THR:HG21	5:P:259:LEU:HD21	1.89	0.53
5:K:292:LEU:HD11	5:P:257:ALA:HB1	1.90	0.53
1:F:12:ASN:HB3	1:F:15:TYR:HA	1.90	0.53
5:K:240:LEU:HD11	5:P:241:TYR:CD1	2.43	0.53
5:P:240:LEU:HD11	5:T:241:TYR:CD1	2.42	0.53
5:T:214:GLU:OE1	5:T:224:ARG:NH1	2.41	0.53
3:I:746:GLY:HA2	3:I:749:THR:HG22	1.89	0.53
3:I:845:THR:HG22	3:I:911:VAL:HG21	1.91	0.53
1:D:70:TYR:HA	1:D:73:LEU:HG	1.90	0.53
1:A:55:GLN:OE1	1:C:57:LEU:HD13	2.08	0.53
3:N:93:ASN:O	3:N:240:HIS:ND1	2.42	0.53
4:H:67:ARG:NH1	4:H:69:ASN:O	2.42	0.53
5:P:277:PRO:HD2	5:P:280:PHE:HD2	1.74	0.53
5:T:292:LEU:HD11	5:U:257:ALA:HB1	1.91	0.53
1:F:84:ASP:HA	1:F:87:GLN:HE21	1.74	0.52
2:R:21:ILE:HA	2:R:24:ILE:HG22	1.91	0.52
3:I:66:VAL:O	3:I:386:ASN:ND2	2.41	0.52
3:I:620:PHE:O	3:I:635:TRP:HA	2.10	0.52
3:N:78:PRO:HA	3:N:84:PHE:HA	1.90	0.52
3:N:503:GLU:HG2	3:N:517:TRP:HZ2	1.74	0.52
2:R:397:PRO:HD2	3:I:376:GLY:O	2.10	0.52
3:I:737:LEU:HD13	3:I:834:PRO:HB3	1.90	0.52
1:a:68:ALA:O	1:a:69:ILE:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1202:GLY:HA2	3:I:1258:ALA:HB3	1.91	0.52
2:R:327:GLN:HG2	2:R:361:HIS:HB2	1.91	0.52
3:N:127:PHE:HB3	3:N:353:LEU:HD23	1.90	0.52
4:S:63:MET:HG3	4:S:145:GLU:HG2	1.92	0.52
3:N:129:HIS:CG	3:N:130:ASN:H	2.28	0.52
2:R:163:LEU:HD22	2:R:169:PRO:HB2	1.92	0.52
2:R:233:MET:O	2:R:237:LYS:HG2	2.09	0.52
2:R:397:PRO:HD3	3:I:375:MET:HE2	1.91	0.52
2:M:19:GLU:O	2:M:23:GLU:HG2	2.10	0.52
3:I:979:TRP:CD1	3:I:979:TRP:H	2.28	0.52
3:N:838:ILE:HD13	3:N:886:TRP:HB2	1.91	0.52
1:Q:77:GLN:C	1:Q:78:LEU:HD23	2.35	0.51
1:G:67:SER:HA	1:L:65:GLU:OE1	2.11	0.51
3:I:682:VAL:O	3:I:686:ILE:HG12	2.11	0.51
2:M:10:PRO:HG3	3:N:613:ILE:HD13	1.93	0.51
5:P:13:LEU:HD11	5:U:160:LYS:HG2	1.92	0.51
2:R:10:PRO:HG3	3:I:613:ILE:HD13	1.93	0.51
3:I:781:LYS:NZ	3:I:964:GLU:OE2	2.44	0.51
3:I:892:THR:HG22	3:I:908:THR:HG21	1.93	0.51
1:L:65:GLU:O	1:L:69:ILE:HG13	2.11	0.51
3:N:37:ASP:N	3:N:37:ASP:OD1	2.44	0.51
3:N:57:ASN:OD1	3:N:362:GLN:NE2	2.44	0.51
1:V:65:GLU:O	1:V:69:ILE:HD12	2.09	0.51
3:N:248:ILE:HG21	3:N:251:MET:HE2	1.91	0.51
2:M:416:CYS:HG	4:O:9:CYS:HB3	1.76	0.50
3:N:620:PHE:O	3:N:635:TRP:HA	2.11	0.50
3:N:846:MET:O	3:N:849:LYS:HG3	2.11	0.50
3:N:1139:VAL:HG22	3:N:1142:GLN:NE2	2.21	0.50
1:G:43:MET:HE2	1:L:42:ARG:HB2	1.92	0.50
3:I:1359:TRP:HD1	3:I:1361:VAL:HG13	1.76	0.50
3:I:1222:ILE:HD11	3:I:1243:LEU:HD21	1.92	0.50
3:N:796:ALA:HB3	3:N:799:ALA:HB2	1.94	0.50
3:N:818:ASP:OD1	3:N:819:ALA:N	2.44	0.50
1:A:80:HIS:HD1	1:A:83:LEU:HD12	1.77	0.50
3:N:1112:TRP:HB2	3:N:1163:TYR:HB2	1.94	0.50
1:B:33:TYR:HE1	1:C:28:MET:HE2	1.77	0.50
2:M:329:GLU:HG2	2:M:363:PHE:HB2	1.93	0.50
2:M:342:VAL:O	2:M:345:THR:HG22	2.11	0.50
3:I:117:ASP:OD2	3:I:360:ARG:NH1	2.44	0.50
1:L:83:LEU:HD13	1:Q:72:LYS:HD2	1.92	0.50
2:M:167:TYR:HB3	2:M:168:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:157:TRP:HA	2:R:228:TYR:HD2	1.77	0.50
3:I:808:TRP:HB3	3:I:870:MET:HE1	1.94	0.50
3:I:1117:SER:HB2	3:I:1145:PHE:HZ	1.77	0.50
3:N:1142:GLN:HB2	3:N:1148:LEU:O	2.12	0.50
3:I:251:MET:HG2	3:I:262:MET:HG3	1.92	0.50
3:I:846:MET:O	3:I:849:LYS:HG3	2.11	0.50
3:I:1179:GLN:O	3:I:1179:GLN:HG2	2.12	0.50
3:I:1303:ASN:OD1	3:I:1343:ALA:N	2.45	0.50
2:M:327:GLN:HG2	2:M:361:HIS:HB2	1.92	0.50
1:V:72:LYS:HB3	1:V:76:LEU:HD13	1.93	0.49
3:I:45:ASN:O	3:I:46:THR:OG1	2.24	0.49
3:I:749:THR:OG1	3:I:750:ASP:N	2.38	0.49
3:N:781:LYS:NZ	3:N:964:GLU:OE1	2.45	0.49
1:F:6:PRO:HD2	4:J:58:ASN:HD22	1.77	0.49
2:M:170:SER:OG	3:N:411:MET:SD	2.65	0.49
1:f:70:TYR:HA	1:f:73:LEU:HG	1.95	0.49
4:O:84:ASN:OD1	4:O:85:GLU:N	2.45	0.49
5:K:211:GLU:HG3	5:P:213:LYS:HG2	1.94	0.49
1:D:66:LEU:HD21	1:F:66:LEU:HD13	1.94	0.49
1:V:70:TYR:HA	1:V:73:LEU:HG	1.94	0.49
3:N:633:PHE:CE1	3:N:702:MET:HE1	2.47	0.49
2:M:233:MET:O	2:M:237:LYS:HG2	2.13	0.49
5:T:235:GLY:O	5:T:239:GLU:HG3	2.13	0.49
1:V:69:ILE:HD11	1:f:70:TYR:HB2	1.94	0.49
3:N:682:VAL:O	3:N:686:ILE:HG12	2.12	0.49
1:B:33:TYR:CE1	1:C:28:MET:HE2	2.46	0.49
1:A:36:VAL:HG13	1:B:39:VAL:HG21	1.94	0.49
1:D:72:LYS:HB3	1:D:76:LEU:HD13	1.94	0.49
4:H:59:VAL:HG23	4:H:151:TYR:CE1	2.46	0.49
5:P:214:GLU:OE1	5:P:224:ARG:NH1	2.46	0.49
1:C:29:ILE:HG22	1:C:29:ILE:O	2.12	0.48
2:R:205:GLN:HE21	2:R:294:LEU:HB2	1.77	0.48
2:R:252:ILE:HD11	2:R:308:THR:OG1	2.13	0.48
3:I:25:SER:OG	4:H:97:GLU:OE2	2.28	0.48
3:I:683:GLU:OE2	3:I:775:ARG:NH1	2.46	0.48
3:N:373:MET:HG2	3:N:375:MET:H	1.77	0.48
1:C:42:ARG:HG3	1:C:42:ARG:HH11	1.78	0.48
1:E:83:LEU:HD21	1:F:76:LEU:HD21	1.96	0.48
2:M:331:TYR:OH	2:M:398:TRP:NE1	2.46	0.48
3:N:1142:GLN:HG2	3:N:1143:ASN:OD1	2.12	0.48
4:J:47:ARG:NH1	4:O:212:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:LEU:O	1:F:60:HIS:HB3	2.13	0.48
1:B:33:TYR:CE2	4:O:146:VAL:HG21	2.48	0.48
2:R:167:TYR:HB3	2:R:168:PRO:HD3	1.94	0.48
3:I:796:ALA:HB3	3:I:799:ALA:HB2	1.93	0.48
3:I:1318:VAL:HG22	3:I:1361:VAL:HG12	1.94	0.48
1:B:68:ALA:O	1:B:70:TYR:N	2.47	0.48
1:V:46:ILE:HG23	1:a:49:VAL:HG21	1.94	0.48
2:R:346:PHE:HE1	2:R:392:ILE:HG13	1.79	0.48
4:O:63:MET:HE1	4:O:138:ASN:HB3	1.96	0.48
1:L:93:LEU:HD23	1:L:96:LEU:HD12	1.96	0.48
1:V:49:VAL:HG11	1:a:56:LEU:HD21	1.95	0.48
2:M:252:ILE:HD11	2:M:308:THR:OG1	2.13	0.48
1:A:22:ASP:OD1	1:A:22:ASP:N	2.47	0.48
1:G:36:VAL:HG13	1:L:39:VAL:HG21	1.96	0.48
3:N:1010:HIS:CD2	3:N:1061:ALA:HB2	2.48	0.48
1:f:63:LEU:O	1:f:64:THR:C	2.57	0.48
4:O:19:THR:HG21	4:O:186:TYR:HE2	1.77	0.48
3:I:37:ASP:N	3:I:37:ASP:OD1	2.44	0.47
3:I:237:GLU:HG2	3:I:238:ALA:N	2.29	0.47
4:O:59:VAL:HG23	4:O:151:TYR:CE1	2.49	0.47
4:S:28:ASP:OD1	4:S:29:ILE:N	2.47	0.47
3:N:89:GLN:NE2	3:N:91:ARG:HH21	2.11	0.47
1:C:15:TYR:CE2	1:C:17:CYS:HB2	2.49	0.47
1:G:22:ASP:N	1:G:22:ASP:OD1	2.48	0.47
3:I:1016:ARG:HH22	3:I:1055:SER:HG	1.61	0.47
4:J:58:ASN:HD21	4:J:148:ASN:ND2	2.12	0.47
3:I:8:LYS:HD2	3:I:8:LYS:O	2.14	0.47
3:N:45:ASN:O	3:N:46:THR:OG1	2.24	0.47
4:H:63:MET:CE	4:H:138:ASN:HD22	2.27	0.47
3:I:1245:PHE:HE2	3:I:1250:GLN:HB3	1.78	0.47
4:H:159:SER:HB3	4:H:164:GLY:HA3	1.96	0.47
1:D:80:HIS:HB2	1:E:79:ILE:HG12	1.95	0.47
1:Q:58:ALA:O	1:Q:61:ASN:HB3	2.15	0.47
3:I:1094:LEU:H	3:I:1094:LEU:HD12	1.80	0.47
4:O:170:ILE:HG13	4:O:171:PRO:HD2	1.97	0.47
5:T:48:ILE:HG13	5:U:125:GLN:HE21	1.79	0.47
1:F:84:ASP:HA	1:F:87:GLN:NE2	2.30	0.47
3:N:630:ASP:OD2	3:N:787:ILE:HG13	2.15	0.47
1:C:26:ASP:OD2	4:J:68:THR:OG1	2.30	0.47
1:F:60:HIS:C	1:F:62:LYS:H	2.23	0.47
1:G:46:ILE:HG23	1:L:49:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:237:GLU:HG2	3:N:238:ALA:N	2.30	0.47
3:N:618:PRO:HG2	3:N:717:SER:HB3	1.96	0.47
1:V:42:ARG:HB2	1:f:43:MET:HE2	1.97	0.47
2:R:87:SER:HB3	3:I:436:LEU:HD11	1.97	0.47
3:I:446:SER:O	3:I:450:ILE:HG12	2.15	0.47
3:I:523:ALA:O	3:I:525:LYS:HG2	2.14	0.47
5:P:195:VAL:O	5:P:199:THR:HG23	2.15	0.47
5:T:195:VAL:O	5:T:199:THR:HG23	2.15	0.47
3:I:78:PRO:HA	3:I:84:PHE:HA	1.97	0.46
3:I:808:TRP:HB3	3:I:870:MET:CE	2.45	0.46
1:D:46:ILE:HG23	1:E:49:VAL:HG21	1.97	0.46
3:I:1203:ASN:HA	3:I:1247:ARG:HE	1.79	0.46
3:N:530:LEU:O	3:N:534:VAL:HG23	2.15	0.46
3:N:931:VAL:HG21	3:N:950:TYR:HE2	1.79	0.46
3:N:420:ALA:HB2	3:N:431:THR:HG22	1.97	0.46
3:N:523:ALA:O	3:N:525:LYS:HG2	2.15	0.46
5:T:93:VAL:HG21	5:U:86:ARG:HB3	1.97	0.46
1:C:67:SER:O	1:C:71:THR:HG23	2.16	0.46
2:M:145:ASN:OD1	2:M:171:SER:OG	2.33	0.46
3:I:978:ASP:OD2	3:I:1063:SER:OG	2.27	0.46
3:N:4:GLU:O	3:N:8:LYS:HG2	2.16	0.46
5:P:147:ILE:HD13	5:T:153:LYS:HB2	1.98	0.46
5:U:38:GLY:HA3	5:U:42:SER:HB3	1.98	0.46
1:B:93:LEU:HD13	1:C:78:LEU:HD13	1.96	0.46
2:M:318:TRP:O	2:M:319:ILE:HD13	2.15	0.46
2:M:331:TYR:HH	2:M:398:TRP:NE1	2.13	0.46
1:A:85:LYS:O	1:A:89:LEU:N	2.41	0.46
1:Q:81:ASN:HB3	1:Q:85:LYS:NZ	2.30	0.46
3:I:24:HIS:HB3	3:I:28:ARG:HE	1.81	0.46
3:N:625:ARG:NH1	3:N:724:ILE:O	2.48	0.46
1:G:76:LEU:HD21	1:Q:76:LEU:HD13	1.98	0.46
2:R:318:TRP:O	2:R:319:ILE:HD13	2.15	0.46
4:O:58:ASN:OD1	4:O:59:VAL:N	2.48	0.46
2:M:87:SER:HB3	3:N:436:LEU:HD11	1.99	0.46
2:M:21:ILE:O	2:M:24:ILE:HG22	2.16	0.45
3:N:728:ASN:O	3:N:732:VAL:HG22	2.15	0.45
3:N:306:GLY:O	3:N:309:THR:HG22	2.16	0.45
3:N:978:ASP:OD1	3:N:979:TRP:N	2.49	0.45
3:N:1142:GLN:HG3	3:N:1149:GLU:O	2.16	0.45
1:E:46:ILE:HG23	1:F:39:VAL:HG21	1.98	0.45
1:Q:73:LEU:HD23	1:Q:76:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:340:ASP:OD1	2:R:340:ASP:N	2.46	0.45
1:D:49:VAL:HG11	1:E:56:LEU:HD21	1.98	0.45
1:L:73:LEU:HD12	1:Q:62:LYS:HG3	1.99	0.45
3:I:129:HIS:CG	3:I:130:ASN:H	2.34	0.45
3:N:979:TRP:CD1	3:N:979:TRP:H	2.33	0.45
3:N:1139:VAL:CG2	3:N:1142:GLN:HE22	2.22	0.45
1:a:64:THR:HA	1:a:67:SER:OG	2.17	0.45
3:I:93:ASN:O	3:I:240:HIS:ND1	2.49	0.45
3:I:1299:ASP:OD1	3:I:1303:ASN:N	2.50	0.45
1:Q:28:MET:HE2	1:Q:28:MET:HA	1.97	0.45
2:R:145:ASN:OD1	2:R:171:SER:OG	2.34	0.45
5:T:229:ARG:HH11	5:T:229:ARG:HG3	1.82	0.45
3:N:670:GLN:HB3	3:N:677:TYR:CZ	2.52	0.45
5:K:59:ARG:O	5:P:76:ASN:ND2	2.45	0.45
3:I:1294:GLY:HA2	3:I:1308:TRP:HB3	1.99	0.45
1:B:83:LEU:HD23	1:B:86:LEU:HD12	1.98	0.45
1:V:36:VAL:HG13	1:a:39:VAL:HG21	1.98	0.45
4:S:159:SER:HB3	4:S:164:GLY:HA3	1.98	0.45
3:I:1010:HIS:CD2	3:I:1061:ALA:HB2	2.52	0.44
3:N:682:VAL:HA	3:N:685:TRP:CD1	2.52	0.44
5:K:13:LEU:O	5:K:17:VAL:HG22	2.16	0.44
5:T:59:ARG:O	5:U:76:ASN:ND2	2.46	0.44
1:B:66:LEU:O	1:C:55:GLN:NE2	2.50	0.44
1:C:61:ASN:O	1:C:62:LYS:HD3	2.17	0.44
3:I:420:ALA:HB2	3:I:431:THR:HG22	1.99	0.44
3:I:618:PRO:HG2	3:I:717:SER:HB3	1.99	0.44
1:Q:67:SER:O	1:Q:71:THR:HG23	2.16	0.44
1:L:47:LYS:HE3	3:I:20:PRO:HD3	2.00	0.44
1:a:66:LEU:O	1:f:59:ILE:HD11	2.17	0.44
2:R:376:ILE:O	2:R:380:VAL:HG23	2.17	0.44
4:O:167:GLU:CD	4:O:167:GLU:H	2.25	0.44
1:f:63:LEU:O	1:f:66:LEU:N	2.51	0.44
5:T:38:GLY:HA3	5:T:42:SER:HB3	1.99	0.44
1:E:33:TYR:CE1	1:F:28:MET:HE2	2.49	0.44
1:G:49:VAL:HG11	1:L:56:LEU:HD21	1.98	0.44
1:V:62:LYS:HD2	1:f:63:LEU:HD22	1.99	0.44
3:I:339:GLY:HA2	3:I:340:PRO:HD3	1.86	0.44
5:U:203:THR:HA	5:U:206:ILE:HD12	2.00	0.44
1:L:20:LEU:HA	1:L:42:ARG:NH1	2.33	0.44
2:M:32:MET:HE1	3:N:580:PHE:HD2	1.83	0.44
2:M:397:PRO:HD3	3:N:375:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:197:VAL:HG22	3:I:198:TYR:CD2	2.52	0.44
3:N:524:ASP:O	3:N:525:LYS:HD2	2.17	0.44
5:P:188:LEU:O	5:P:192:THR:HG23	2.18	0.44
5:U:195:VAL:O	5:U:199:THR:HG23	2.18	0.44
1:B:73:LEU:O	1:B:77:GLN:HG3	2.17	0.44
2:R:369:LEU:O	2:R:371:GLU:N	2.51	0.44
3:I:630:ASP:OD2	3:I:787:ILE:HG13	2.18	0.44
3:I:834:PRO:O	3:I:880:ASN:ND2	2.51	0.44
3:N:129:HIS:CG	3:N:130:ASN:N	2.86	0.44
3:N:1009:THR:HG23	3:N:1010:HIS:CD2	2.53	0.44
2:M:416:CYS:SG	4:O:9:CYS:HB3	2.58	0.44
2:R:416:CYS:SG	4:H:9:CYS:HB3	2.58	0.44
3:I:1291:VAL:HG11	3:I:1361:VAL:HG21	2.00	0.44
3:N:339:GLY:HA2	3:N:340:PRO:HD3	1.85	0.44
3:N:446:SER:O	3:N:450:ILE:HG12	2.18	0.44
5:K:188:LEU:O	5:K:192:THR:HG23	2.18	0.44
5:U:188:LEU:O	5:U:192:THR:HG23	2.18	0.44
1:B:70:TYR:HA	1:B:73:LEU:HD23	1.99	0.43
2:M:397:PRO:HD2	3:N:376:GLY:O	2.17	0.43
2:R:229:ASP:OD1	2:R:230:PRO:HD2	2.18	0.43
3:I:1225:MET:HE3	3:I:1264:ARG:HB3	2.00	0.43
4:J:49:HIS:CE1	4:J:55:ARG:HD2	2.53	0.43
3:I:469:MET:HE2	3:I:469:MET:HB3	1.93	0.43
4:J:58:ASN:HD21	4:J:148:ASN:HD21	1.66	0.43
4:S:190:LEU:HD23	4:S:190:LEU:HA	1.87	0.43
1:D:86:LEU:HB3	1:F:87:GLN:NE2	2.32	0.43
2:M:181:LEU:HD22	2:M:278:ILE:HD11	2.00	0.43
2:M:410:TYR:CE1	3:N:41:LEU:HG	2.53	0.43
3:I:931:VAL:HG21	3:I:950:TYR:CE2	2.53	0.43
3:N:887:PHE:CE2	3:N:925:PHE:HB3	2.54	0.43
3:N:1117:SER:HB2	3:N:1145:PHE:CZ	2.53	0.43
5:K:217:ARG:NE	5:K:221:SER:OG	2.40	0.43
1:A:49:VAL:HG11	1:B:56:LEU:HD21	2.00	0.43
1:Q:58:ALA:O	1:Q:59:ILE:C	2.61	0.43
3:I:569:LEU:O	3:I:572:THR:OG1	2.35	0.43
1:E:65:GLU:O	1:E:69:ILE:HG13	2.19	0.43
1:a:87:GLN:HG2	1:a:88:GLU:N	2.34	0.43
2:M:366:PHE:HE1	2:M:398:TRP:CZ3	2.35	0.43
3:I:887:PHE:CE2	3:I:925:PHE:HB3	2.53	0.43
5:K:13:LEU:CD1	5:T:160:LYS:HE3	2.48	0.43
1:F:60:HIS:C	1:F:62:LYS:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:LEU:O	1:L:77:GLN:HG3	2.18	0.43
2:M:369:LEU:O	2:M:371:GLU:N	2.51	0.43
1:D:36:VAL:HG13	1:E:39:VAL:HG21	1.99	0.43
1:a:83:LEU:HD21	1:f:76:LEU:HD21	2.01	0.43
3:I:306:GLY:O	3:I:309:THR:HG22	2.18	0.43
3:I:860:MET:N	3:I:860:MET:HE2	2.34	0.43
3:I:1207:LYS:HA	3:I:1243:LEU:O	2.19	0.43
3:I:1209:MET:HE1	3:I:1367:ASP:HB2	2.01	0.43
3:N:892:THR:HG22	3:N:908:THR:HG21	2.01	0.43
5:K:285:LEU:O	5:K:289:LEU:HG	2.19	0.43
1:L:80:HIS:HA	1:L:83:LEU:HG	2.00	0.43
1:V:80:HIS:HB2	1:a:79:ILE:HG12	2.01	0.43
3:I:985:PRO:HG2	3:I:1056:VAL:HG13	2.01	0.43
3:N:520:ASP:OD1	3:N:520:ASP:N	2.50	0.43
3:N:931:VAL:HG21	3:N:950:TYR:CE2	2.53	0.43
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.83	0.43
1:C:6:PRO:HD2	4:O:58:ASN:ND2	2.34	0.43
1:C:37:LYS:NZ	4:J:65:GLU:OE1	2.44	0.43
2:M:416:CYS:HG	4:O:9:CYS:CB	2.31	0.43
2:R:139:VAL:HG22	3:I:409:ILE:HG21	2.01	0.43
3:I:1200:ASP:HB2	3:I:1203:ASN:HB2	2.00	0.43
5:P:108:VAL:HG21	5:T:106:ASN:HB3	2.00	0.43
1:C:60:HIS:C	1:C:62:LYS:H	2.26	0.43
1:G:39:VAL:HG21	1:Q:36:VAL:HG13	2.01	0.43
1:Q:52:ASN:O	1:Q:56:LEU:HB2	2.18	0.43
2:M:157:TRP:HA	2:M:228:TYR:HD2	1.84	0.43
2:R:328:ILE:HG21	2:R:345:THR:HG23	2.00	0.43
3:I:670:GLN:HB3	3:I:677:TYR:CZ	2.54	0.43
3:I:682:VAL:HA	3:I:685:TRP:CD1	2.54	0.43
5:P:71:MET:HE1	5:P:100:MET:HG3	2.01	0.43
1:A:46:ILE:HG23	1:B:49:VAL:HG21	2.01	0.42
1:B:80:HIS:HB2	1:C:69:ILE:HD11	2.00	0.42
1:C:72:LYS:O	1:C:76:LEU:HG	2.19	0.42
1:F:70:TYR:HA	1:F:73:LEU:HG	2.01	0.42
1:f:83:LEU:HA	1:f:86:LEU:HD12	2.00	0.42
2:R:29:ILE:HG12	2:R:35:VAL:HG12	2.01	0.42
3:I:524:ASP:O	3:I:525:LYS:HD2	2.19	0.42
5:P:70:LEU:HD12	5:P:107:ALA:HB2	2.01	0.42
5:T:48:ILE:HG13	5:U:125:GLN:NE2	2.34	0.42
3:N:130:ASN:OD1	3:N:189:ILE:HG21	2.20	0.42
1:A:20:LEU:HD22	1:A:28:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:333:TRP:HZ3	2:R:338:ARG:HH11	1.65	0.42
3:I:750:ASP:N	3:I:762:ALA:O	2.53	0.42
3:I:1002:TRP:HH2	3:I:1029:LEU:HD21	1.83	0.42
3:N:943:VAL:O	3:N:943:VAL:HG12	2.19	0.42
3:I:860:MET:HB3	3:I:914:LYS:NZ	2.35	0.42
3:I:1322:ASN:HA	3:I:1357:MET:HG3	2.01	0.42
1:L:42:ARG:HH11	1:L:42:ARG:HG2	1.83	0.42
4:O:59:VAL:HG23	4:O:151:TYR:HE1	1.84	0.42
5:P:242:ASP:O	5:P:246:THR:HG23	2.19	0.42
5:U:242:ASP:O	5:U:246:THR:HG23	2.19	0.42
1:E:87:GLN:HG2	1:E:88:GLU:N	2.34	0.42
2:R:21:ILE:O	2:R:24:ILE:HG22	2.18	0.42
2:R:91:LYS:NZ	3:I:423:ASP:OD2	2.41	0.42
2:R:364:ILE:HG22	2:R:380:VAL:HG13	2.01	0.42
3:I:160:LYS:HD3	3:I:160:LYS:HA	1.87	0.42
3:I:1309:GLU:CD	3:I:1309:GLU:H	2.28	0.42
4:O:56:ASN:HB3	4:O:150:MET:HE3	2.02	0.42
5:P:38:GLY:HA3	5:P:42:SER:HB3	2.02	0.42
5:T:147:ILE:HD13	5:U:153:LYS:HB2	2.02	0.42
5:U:84:ASN:O	5:U:86:ARG:N	2.51	0.42
1:C:81:ASN:HB3	1:C:85:LYS:NZ	2.35	0.42
1:G:72:LYS:HB3	1:G:76:LEU:HD13	2.02	0.42
2:R:375:LYS:HB3	2:R:375:LYS:HE3	1.76	0.42
3:I:1009:THR:HG23	3:I:1010:HIS:CD2	2.55	0.42
5:K:195:VAL:O	5:K:199:THR:HG23	2.19	0.42
3:N:748:PHE:HA	3:N:769:VAL:HG21	2.02	0.42
5:U:276:PRO:HA	5:U:277:PRO:HD3	1.91	0.42
3:I:943:VAL:HG12	3:I:943:VAL:O	2.19	0.42
3:I:1233:ILE:HD13	3:I:1250:GLN:HA	2.01	0.42
5:K:79:LEU:HA	5:K:82:PHE:HB3	2.01	0.42
3:I:1117:SER:HB2	3:I:1145:PHE:CZ	2.54	0.42
3:I:1291:VAL:HG22	3:I:1363:PRO:HB3	2.02	0.42
3:N:1005:ARG:HG3	3:N:1007:GLY:H	1.85	0.42
5:T:16:LEU:O	5:U:160:LYS:NZ	2.48	0.42
5:T:70:LEU:HD12	5:T:107:ALA:HB2	2.02	0.42
1:G:49:VAL:HG12	1:G:53:MET:HE1	2.02	0.41
3:I:520:ASP:OD1	3:I:520:ASP:N	2.52	0.41
3:I:794:VAL:HG12	3:I:823:ILE:HD12	2.01	0.41
3:I:891:THR:HG22	3:I:950:TYR:OH	2.20	0.41
5:U:100:MET:HE2	5:U:100:MET:HB3	1.99	0.41
1:B:83:LEU:HA	1:B:86:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:LEU:HD23	1:F:63:LEU:HA	1.90	0.41
5:K:180:MET:HE2	5:K:180:MET:HB2	1.87	0.41
5:P:277:PRO:HD2	5:P:280:PHE:CD2	2.52	0.41
5:T:276:PRO:HA	5:T:277:PRO:HD3	1.91	0.41
1:B:33:TYR:HE2	4:O:146:VAL:HG21	1.85	0.41
1:D:60:HIS:HA	1:D:63:LEU:HG	2.02	0.41
1:Q:6:PRO:HD2	4:H:58:ASN:ND2	2.35	0.41
1:Q:72:LYS:O	1:Q:76:LEU:HG	2.20	0.41
1:f:84:ASP:O	1:f:87:GLN:NE2	2.53	0.41
2:M:416:CYS:SG	4:O:9:CYS:SG	3.18	0.41
4:O:2:TYR:HD2	4:O:6:GLU:HB2	1.84	0.41
5:K:242:ASP:O	5:K:246:THR:HG23	2.20	0.41
5:P:53:THR:HG21	5:T:66:VAL:HG22	2.02	0.41
5:T:100:MET:O	5:T:100:MET:HG2	2.21	0.41
2:M:229:ASP:OD1	2:M:230:PRO:HD2	2.20	0.41
3:I:267:ILE:HG22	3:I:268:HIS:O	2.20	0.41
3:N:27:TRP:HZ3	4:J:131:PRO:HB2	1.86	0.41
3:N:130:ASN:OD1	3:N:189:ILE:HD13	2.19	0.41
3:N:194:MET:HE3	3:N:194:MET:HB3	1.77	0.41
4:O:174:LEU:HD23	4:O:174:LEU:HA	1.87	0.41
5:T:236:LYS:HD3	5:T:236:LYS:HA	1.92	0.41
1:L:70:TYR:HA	1:L:73:LEU:HD23	2.00	0.41
5:K:38:GLY:HA3	5:K:42:SER:HB3	2.02	0.41
1:C:12:ASN:ND2	1:C:16:CYS:O	2.53	0.41
1:Q:15:TYR:CE2	1:Q:17:CYS:HB2	2.56	0.41
3:N:530:LEU:HD23	3:N:530:LEU:HA	1.88	0.41
4:J:19:THR:HG21	4:J:186:TYR:HE2	1.84	0.41
1:D:80:HIS:CD2	1:D:83:LEU:HD12	2.56	0.41
1:E:33:TYR:CE2	4:J:146:VAL:HG21	2.56	0.41
1:Q:20:LEU:HD22	4:S:139:ASN:HB2	2.02	0.41
2:M:415:VAL:O	2:M:416:CYS:SG	2.79	0.41
4:O:14:GLY:O	4:O:17:ASN:ND2	2.54	0.41
4:O:58:ASN:HD21	4:O:148:ASN:ND2	2.18	0.41
1:f:63:LEU:HD23	1:f:63:LEU:HA	1.90	0.41
2:R:298:PRO:HG3	2:R:333:TRP:NE1	2.35	0.41
1:C:73:LEU:HD23	1:C:76:LEU:HD12	2.03	0.41
1:Q:42:ARG:HG3	1:Q:42:ARG:HH11	1.86	0.41
2:M:298:PRO:HG3	2:M:333:TRP:NE1	2.36	0.41
2:R:314:PRO:HD2	2:R:318:TRP:CH2	2.56	0.41
3:I:1036:PHE:CE2	3:I:1041:GLN:HG2	2.56	0.41
3:I:1062:ASP:OD1	3:I:1063:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1203:ASN:HA	3:I:1247:ARG:NE	2.36	0.41
3:I:1321:LEU:HB3	3:I:1328:VAL:HG22	2.02	0.41
3:N:411:MET:O	3:N:415:TRP:NE1	2.46	0.41
3:N:680:PHE:CE2	3:N:685:TRP:HB3	2.55	0.41
3:N:984:PRO:HD3	3:N:1068:ALA:HB3	2.01	0.41
3:N:1093:GLN:HE21	3:N:1099:ILE:HG13	1.85	0.41
4:O:63:MET:HE3	4:O:63:MET:HB3	1.77	0.41
4:H:28:ASP:OD1	4:H:29:ILE:N	2.54	0.41
5:K:289:LEU:HD22	5:T:260:PHE:CE1	2.56	0.41
1:B:82:ASN:O	1:B:86:LEU:HG	2.21	0.41
2:M:370:PRO:HB3	2:M:405:ARG:HH11	1.85	0.41
2:R:97:TRP:CE3	3:I:424:LYS:HE2	2.56	0.41
3:I:728:ASN:O	3:I:732:VAL:HG22	2.21	0.41
3:I:984:PRO:HD3	3:I:1068:ALA:HB3	2.03	0.41
3:I:1233:ILE:HD11	3:I:1254:TYR:CE1	2.56	0.41
3:N:1159:MET:HE3	3:N:1159:MET:HB2	1.96	0.41
4:J:69:ASN:OD1	4:J:137:GLN:HG2	2.21	0.41
4:O:63:MET:HE2	4:O:138:ASN:HD22	1.86	0.41
5:T:71:MET:HB3	5:T:71:MET:HE3	1.70	0.41
5:T:188:LEU:O	5:T:192:THR:HG23	2.21	0.41
5:T:242:ASP:O	5:T:246:THR:HG23	2.20	0.41
1:F:55:GLN:O	1:F:59:ILE:HG13	2.21	0.40
1:L:95:LYS:O	1:L:99:LEU:HG	2.20	0.40
2:M:410:TYR:HE1	3:N:41:LEU:HG	1.86	0.40
2:R:266:TRP:O	2:R:270:LYS:HG2	2.20	0.40
2:R:388:LEU:HD23	2:R:388:LEU:HA	1.87	0.40
3:I:680:PHE:CE2	3:I:685:TRP:HB3	2.56	0.40
3:I:885:ILE:O	3:I:925:PHE:HA	2.21	0.40
3:N:914:LYS:HD2	3:N:914:LYS:HA	1.97	0.40
4:J:172:ASP:OD2	4:H:154:LYS:HD3	2.22	0.40
4:S:77:ALA:O	4:S:81:TYR:HB3	2.21	0.40
5:K:25:PRO:HB2	5:K:27:ILE:HD12	2.03	0.40
5:P:13:LEU:O	5:P:17:VAL:HG22	2.20	0.40
5:T:25:PRO:HB2	5:T:27:ILE:HD12	2.02	0.40
1:V:49:VAL:HG21	1:f:46:ILE:HG23	2.03	0.40
2:R:235:LEU:HD23	2:R:235:LEU:HA	1.94	0.40
5:T:130:THR:HG22	5:U:135:LEU:HD12	2.02	0.40
2:R:239:GLU:O	2:R:240:THR:OG1	2.33	0.40
3:I:628:TRP:HE1	3:I:682:VAL:HG11	1.85	0.40
3:N:1085:PRO:HG2	3:N:1160:VAL:HG12	2.03	0.40
4:H:58:ASN:HD21	4:H:148:ASN:ND2	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:6:PRO:HD2	4:S:58:ASN:ND2	2.36	0.40
1:f:42:ARG:HB3	1:f:45:PHE:HD2	1.86	0.40
2:M:272:GLY:HA3	2:M:317:GLU:HG3	2.04	0.40
3:I:123:LEU:HD23	3:I:123:LEU:HA	1.94	0.40
3:I:130:ASN:OD1	3:I:189:ILE:HG21	2.21	0.40
3:I:1005:ARG:HG3	3:I:1007:GLY:H	1.86	0.40
3:I:1238:VAL:HG12	3:I:1240:ASP:H	1.86	0.40
3:I:1325:ASN:ND2	3:I:1327:THR:OG1	2.53	0.40
5:T:201:LEU:HD23	5:U:206:ILE:HG13	2.03	0.40
3:N:742:GLN:HE21	3:N:797:ASP:HA	1.86	0.40
3:N:1117:SER:HB2	3:N:1145:PHE:HZ	1.86	0.40
4:O:84:ASN:OD1	4:O:85:GLU:HG3	2.21	0.40
5:K:276:PRO:HA	5:K:277:PRO:HD3	1.91	0.40
5:T:246:THR:O	5:T:250:ARG:HG2	2.22	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	71/556 (13%)	67 (94%)	4 (6%)	0	100	100
1	B	89/556 (16%)	83 (93%)	5 (6%)	1 (1%)	11	43
1	C	86/556 (16%)	74 (86%)	11 (13%)	1 (1%)	10	42
1	D	67/556 (12%)	63 (94%)	3 (4%)	1 (2%)	8	37
1	E	89/556 (16%)	85 (96%)	4 (4%)	0	100	100
1	F	86/556 (16%)	76 (88%)	8 (9%)	2 (2%)	5	29
1	G	71/556 (13%)	65 (92%)	6 (8%)	0	100	100
1	L	89/556 (16%)	86 (97%)	3 (3%)	0	100	100
1	Q	86/556 (16%)	74 (86%)	11 (13%)	1 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	67/556 (12%)	62 (92%)	4 (6%)	1 (2%)	8	37
1	a	89/556 (16%)	83 (93%)	5 (6%)	1 (1%)	11	43
1	f	86/556 (16%)	77 (90%)	9 (10%)	0	100	100
2	M	413/417 (99%)	385 (93%)	27 (6%)	1 (0%)	43	73
2	R	413/417 (99%)	391 (95%)	21 (5%)	1 (0%)	43	73
3	I	1379/1382 (100%)	1314 (95%)	65 (5%)	0	100	100
3	N	1188/1382 (86%)	1122 (94%)	66 (6%)	0	100	100
4	H	234/236 (99%)	228 (97%)	6 (3%)	0	100	100
4	J	234/236 (99%)	224 (96%)	10 (4%)	0	100	100
4	O	234/236 (99%)	227 (97%)	7 (3%)	0	100	100
4	S	234/236 (99%)	227 (97%)	7 (3%)	0	100	100
5	K	296/299 (99%)	284 (96%)	11 (4%)	1 (0%)	36	68
5	P	296/299 (99%)	288 (97%)	7 (2%)	1 (0%)	36	68
5	T	296/299 (99%)	287 (97%)	8 (3%)	1 (0%)	36	68
5	U	296/299 (99%)	287 (97%)	8 (3%)	1 (0%)	36	68
All	All	6489/12410 (52%)	6159 (95%)	316 (5%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	61	ASN
2	M	247	PRO
2	R	247	PRO
1	C	61	ASN
1	F	17	CYS
1	F	61	ASN
1	B	69	ILE
5	P	225	THR
5	K	225	THR
5	T	225	THR
5	U	225	THR
1	D	79	ILE
1	V	79	ILE
1	a	69	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	68/455 (15%)	68 (100%)	0	100	100
1	B	84/455 (18%)	84 (100%)	0	100	100
1	C	81/455 (18%)	81 (100%)	0	100	100
1	D	64/455 (14%)	64 (100%)	0	100	100
1	E	84/455 (18%)	84 (100%)	0	100	100
1	F	81/455 (18%)	79 (98%)	2 (2%)	42	69
1	G	68/455 (15%)	68 (100%)	0	100	100
1	L	84/455 (18%)	84 (100%)	0	100	100
1	Q	81/455 (18%)	81 (100%)	0	100	100
1	V	64/455 (14%)	64 (100%)	0	100	100
1	a	84/455 (18%)	84 (100%)	0	100	100
1	f	81/455 (18%)	80 (99%)	1 (1%)	63	79
2	M	370/371 (100%)	370 (100%)	0	100	100
2	R	370/371 (100%)	370 (100%)	0	100	100
3	I	1154/1155 (100%)	1154 (100%)	0	100	100
3	N	997/1155 (86%)	997 (100%)	0	100	100
4	H	209/209 (100%)	209 (100%)	0	100	100
4	J	209/209 (100%)	209 (100%)	0	100	100
4	O	209/209 (100%)	209 (100%)	0	100	100
4	S	209/209 (100%)	209 (100%)	0	100	100
5	K	243/244 (100%)	243 (100%)	0	100	100
5	P	243/244 (100%)	243 (100%)	0	100	100
5	T	243/244 (100%)	242 (100%)	1 (0%)	84	86
5	U	243/244 (100%)	243 (100%)	0	100	100
All	All	5623/10324 (54%)	5619 (100%)	4 (0%)	87	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	17	CYS
1	F	55	GLN
1	f	55	GLN
5	T	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	60	HIS
1	C	55	GLN
1	D	80	HIS
1	E	21	ASN
1	E	82	ASN
1	F	52	ASN
1	F	61	ASN
1	F	87	GLN
1	G	52	ASN
1	Q	4	HIS
1	Q	80	HIS
1	Q	81	ASN
1	V	52	ASN
1	a	52	ASN
1	f	87	GLN
2	M	36	HIS
2	M	273	GLN
2	M	394	HIS
2	R	36	HIS
3	I	33	GLN
3	I	110	HIS
3	I	239	HIS
3	I	370	GLN
3	I	742	GLN
3	I	852	ASN
3	I	877	ASN
3	I	880	ASN
3	I	901	ASN
3	I	904	ASN
3	I	1142	GLN
3	N	89	GLN
3	N	110	HIS
3	N	119	ASN
3	N	261	GLN

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Mol	Chain	Res	Type
3	N	343	GLN
3	N	370	GLN
3	N	536	GLN
3	N	711	GLN
3	N	841	ASN
3	N	901	ASN
3	N	1010	HIS
3	N	1043	ASN
3	N	1155	HIS
4	J	49	HIS
4	J	148	ASN
4	O	13	ASN
4	O	123	ASN
4	O	148	ASN
4	O	227	ASN
4	S	120	ASN
4	S	123	ASN
4	S	148	ASN
4	H	138	ASN
4	H	139	ASN
4	H	148	ASN
4	H	227	ASN
5	U	77	HIS

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.

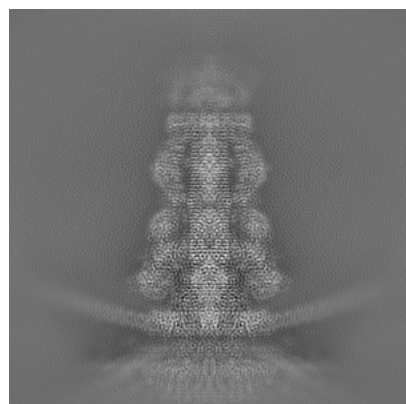
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62961. These allow visual inspection of the internal detail of the map and identification of artifacts.

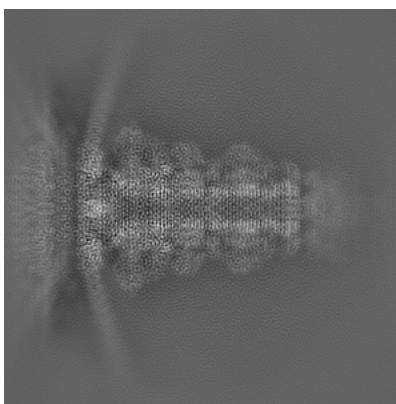
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

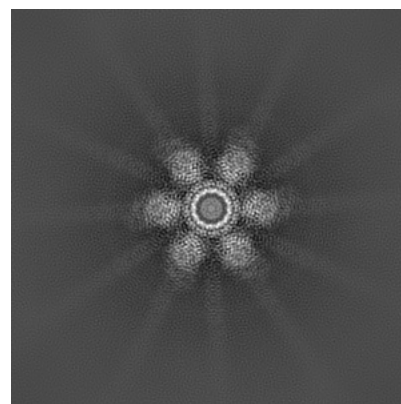
6.1.1 Primary map



X

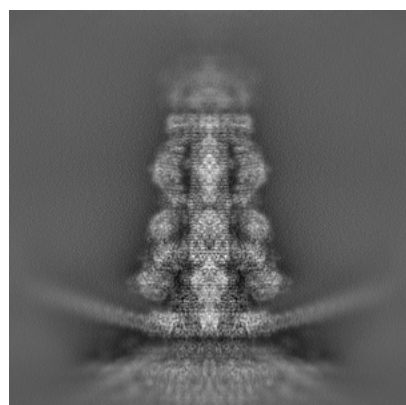


Y

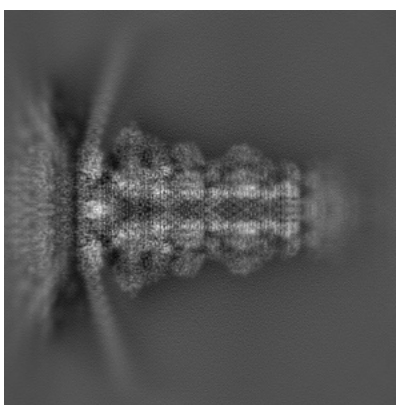


Z

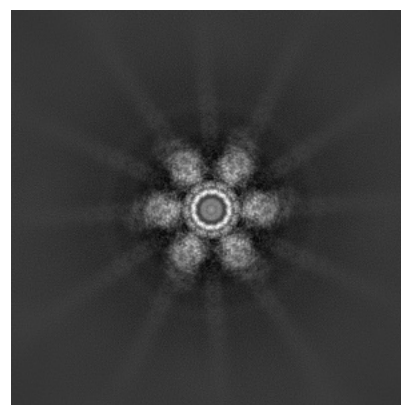
6.1.2 Raw map



X



Y



Z

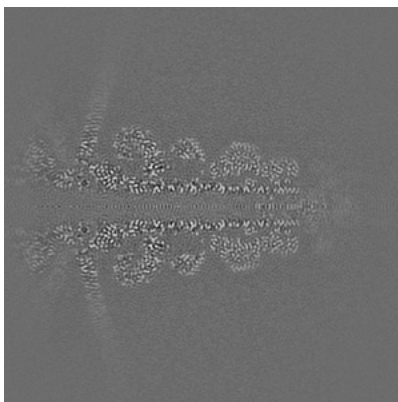
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

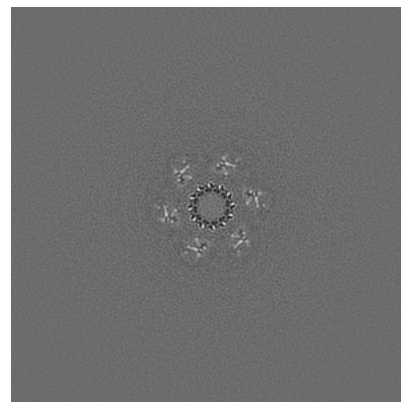
6.2.1 Primary map



X Index: 240

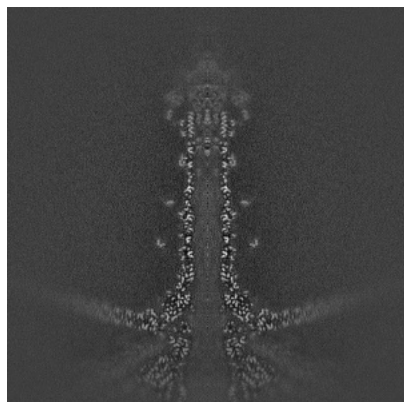


Y Index: 240

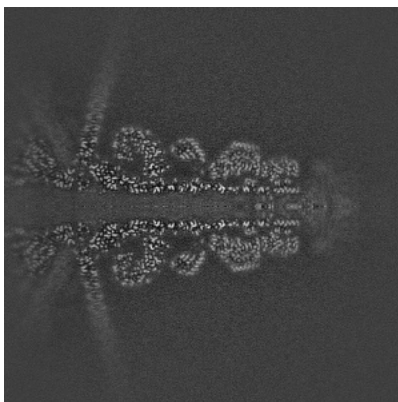


Z Index: 240

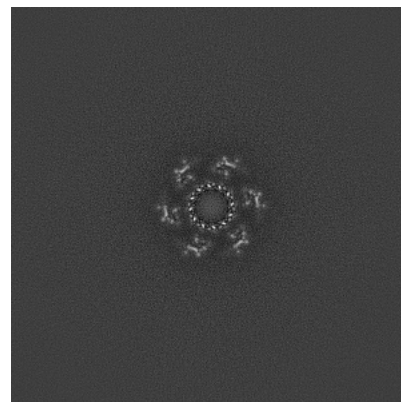
6.2.2 Raw map



X Index: 240



Y Index: 240

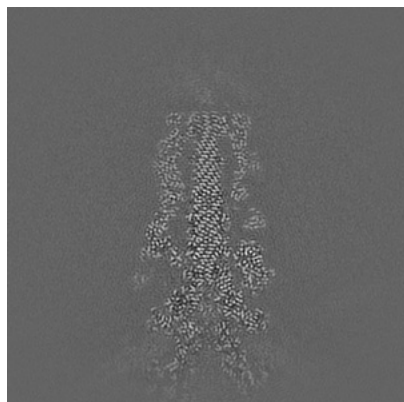


Z Index: 240

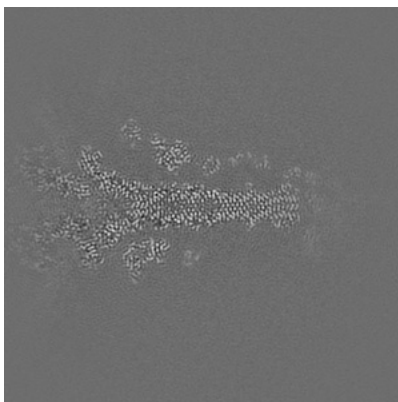
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

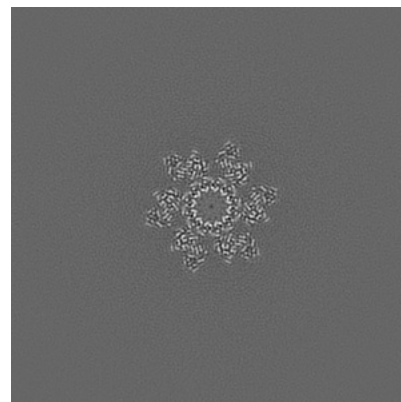
6.3.1 Primary map



X Index: 220

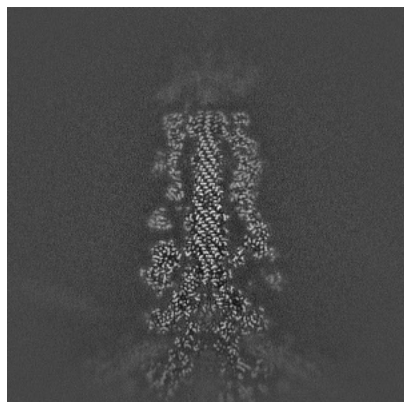


Y Index: 258

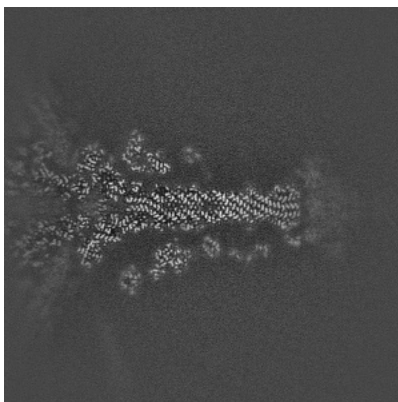


Z Index: 189

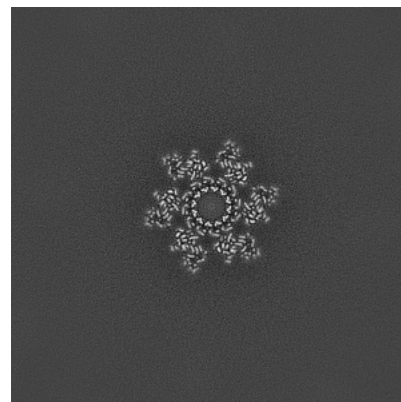
6.3.2 Raw map



X Index: 260



Y Index: 221

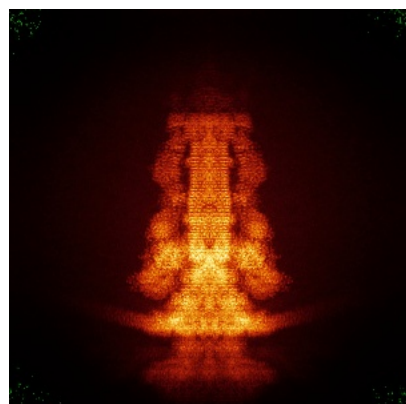


Z Index: 189

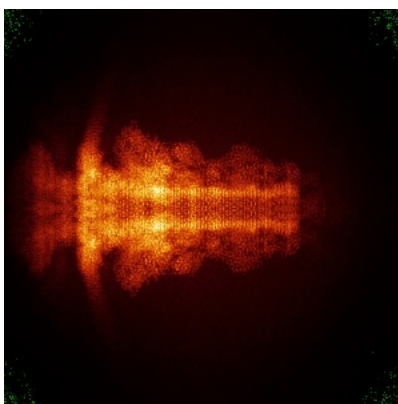
The images above show the largest variance slices of the map in three orthogonal directions.

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

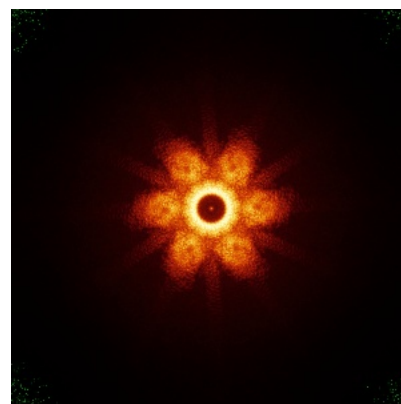
6.4.1 Primary map



X

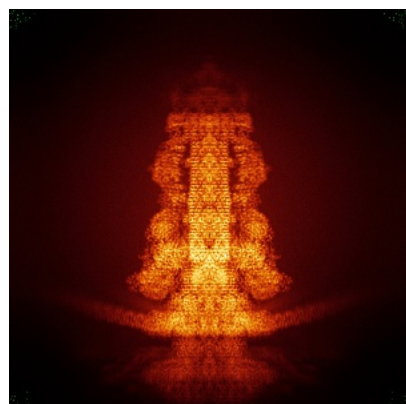


Y

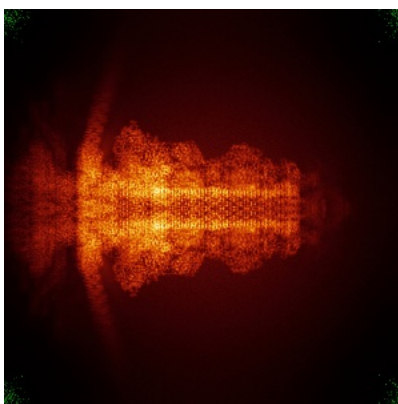


Z

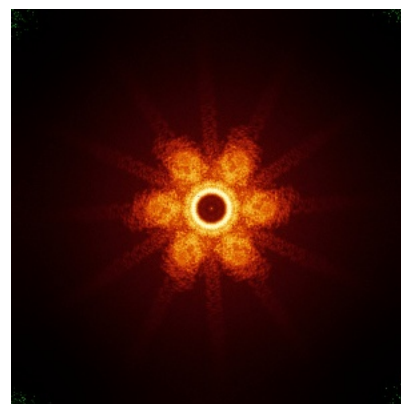
6.4.2 Raw map



X



Y

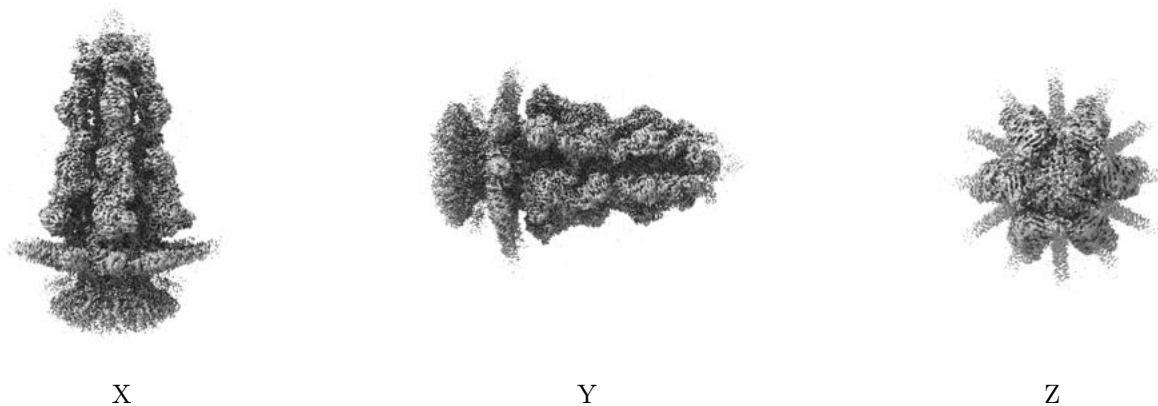


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

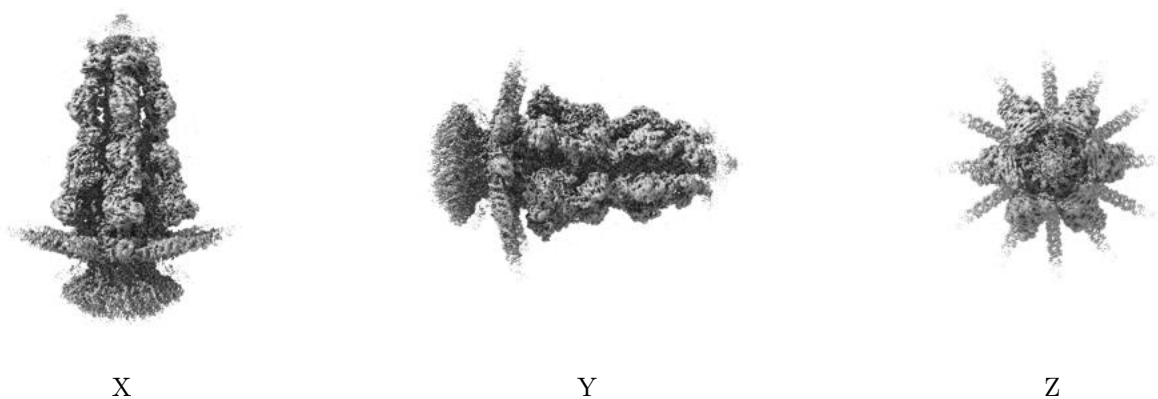
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

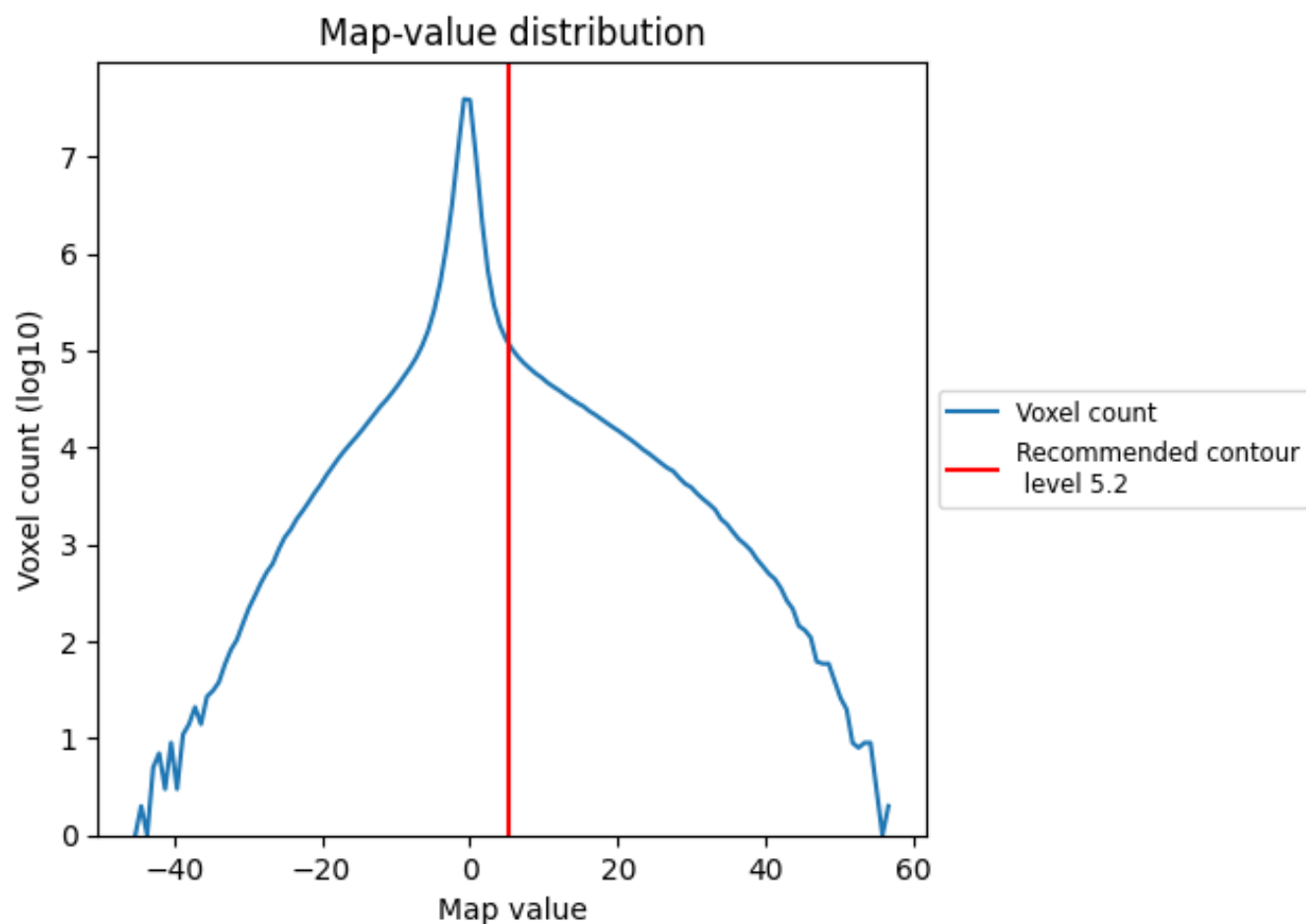
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

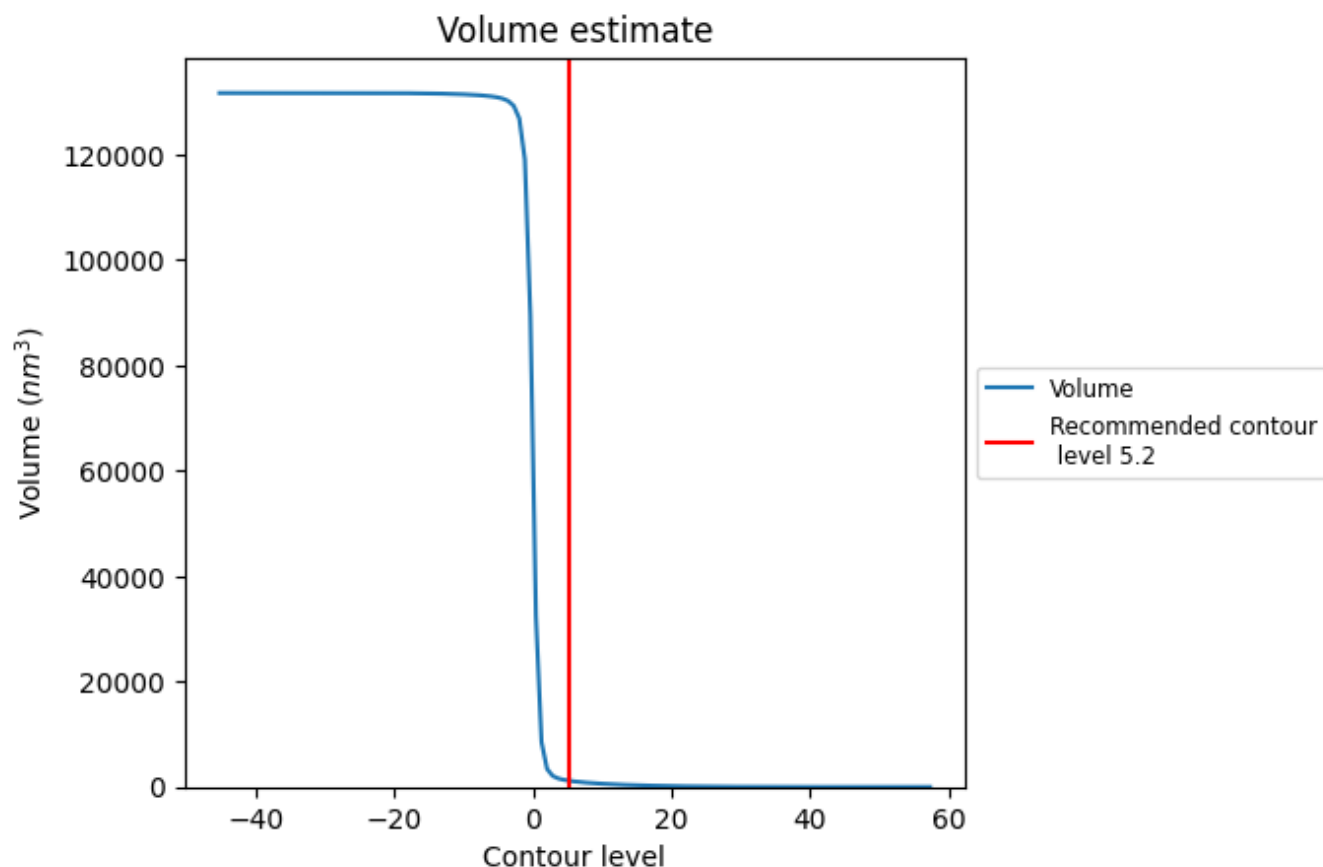
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

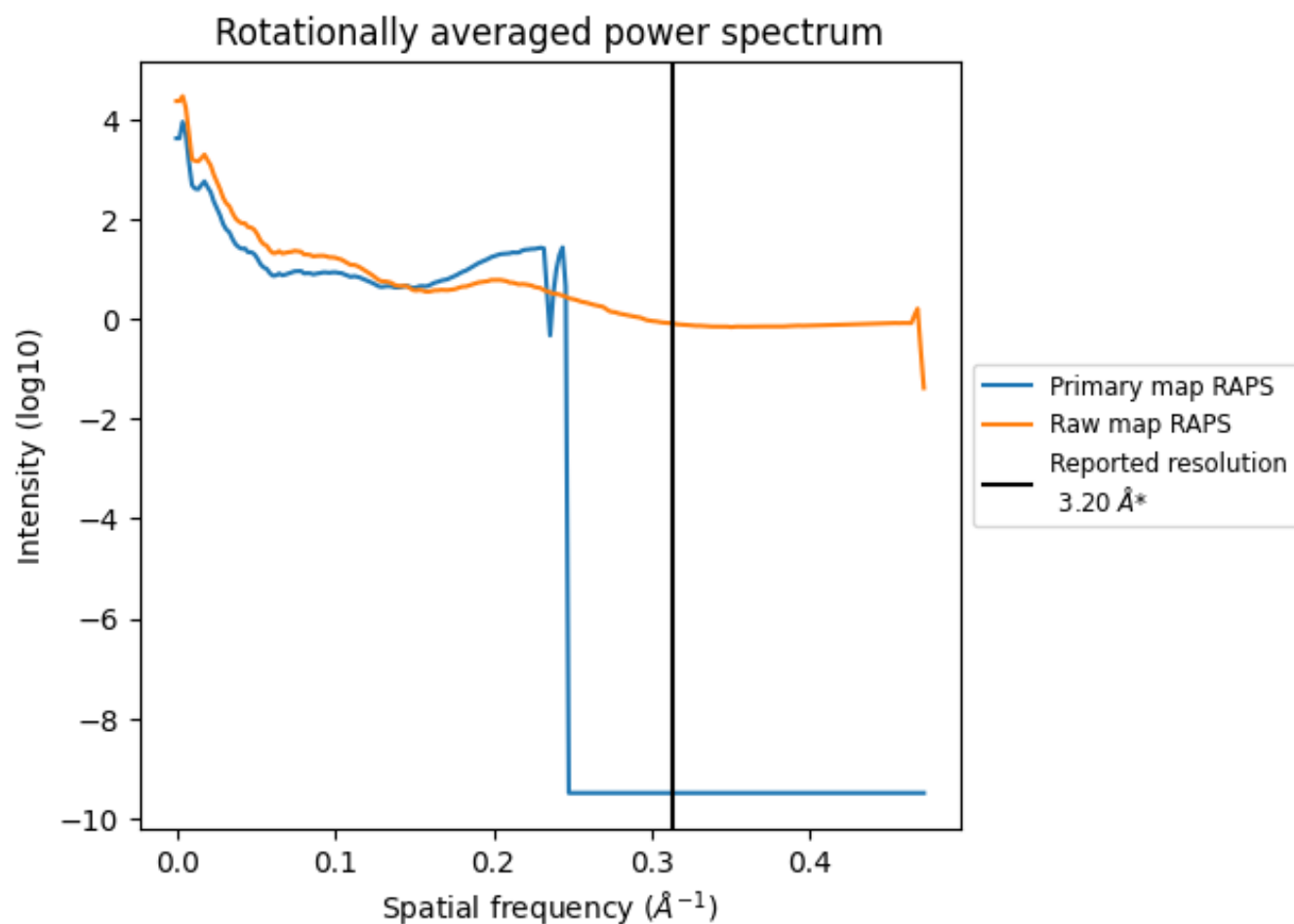
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1187 nm^3 ; this corresponds to an approximate mass of 1072 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

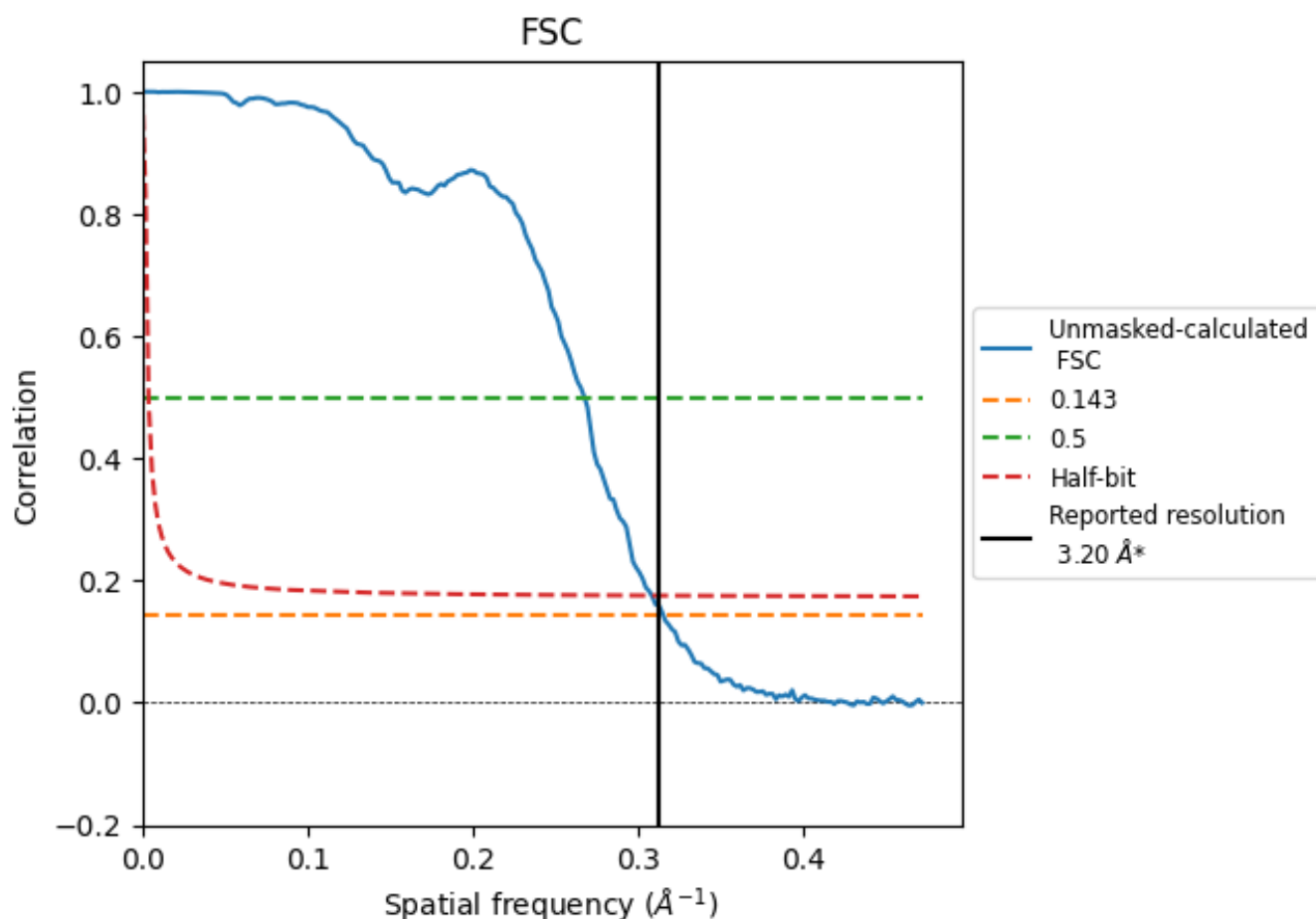


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.74	3.25

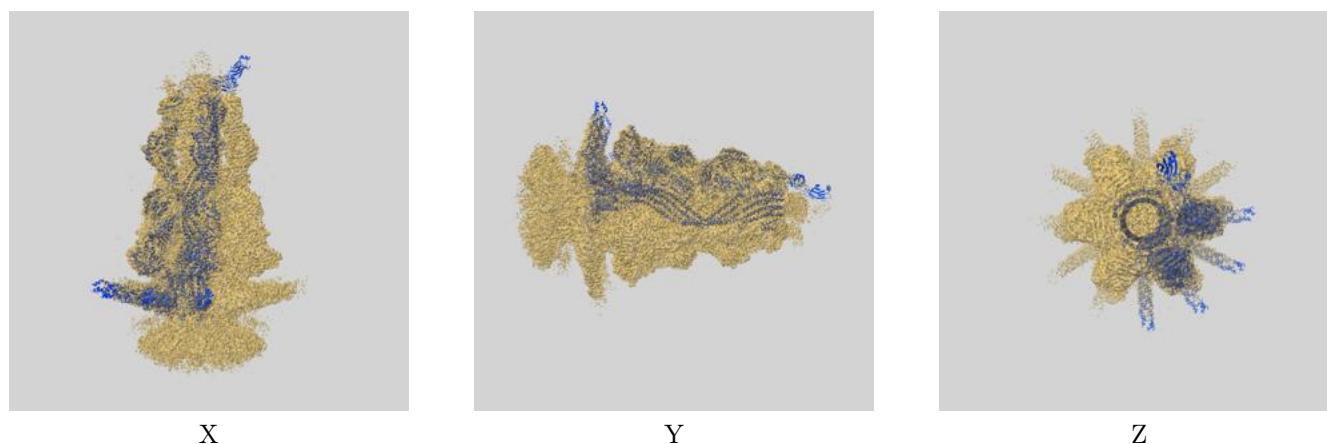
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

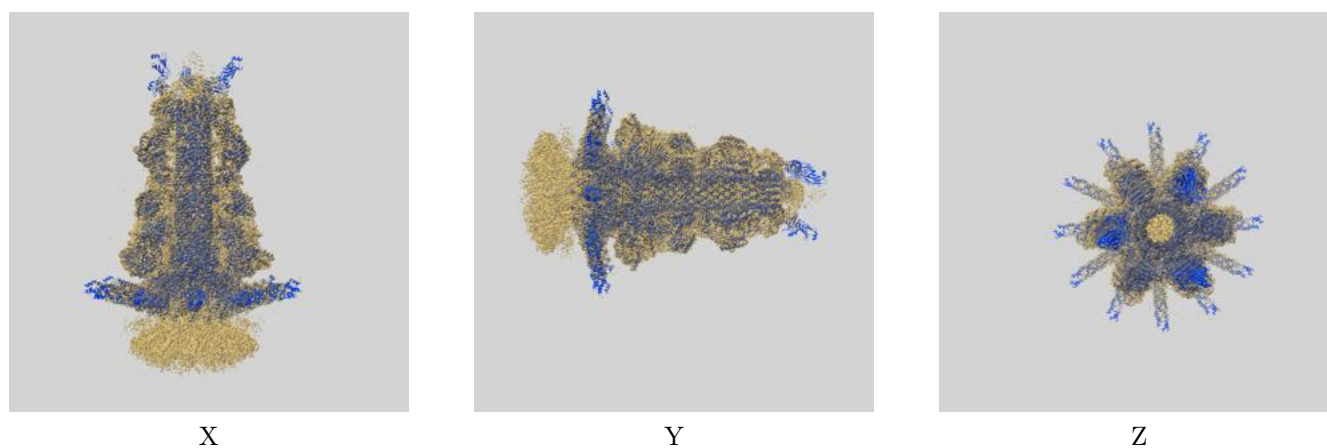
This section contains information regarding the fit between EMDB map EMD-62961 and PDB model 9LC0. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

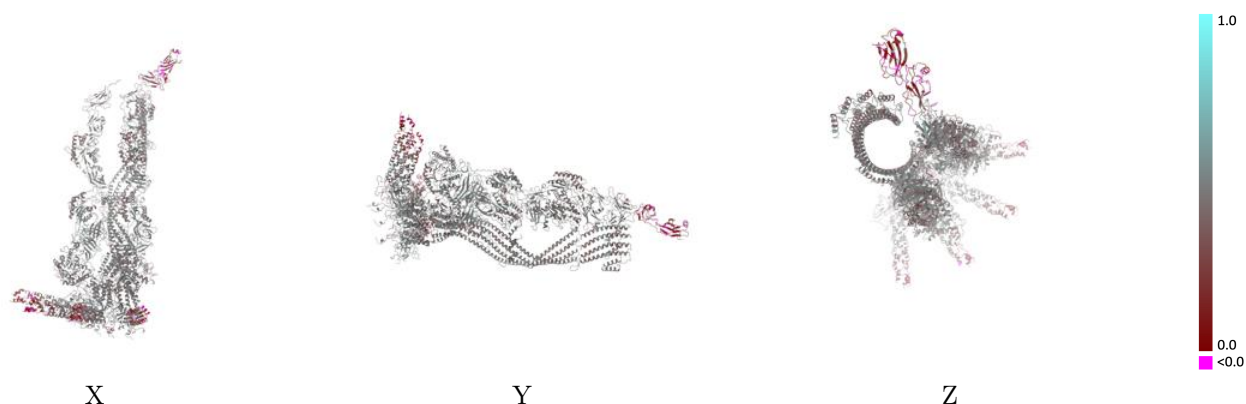


9.1.2 Map-model assembly overlay [i](#)



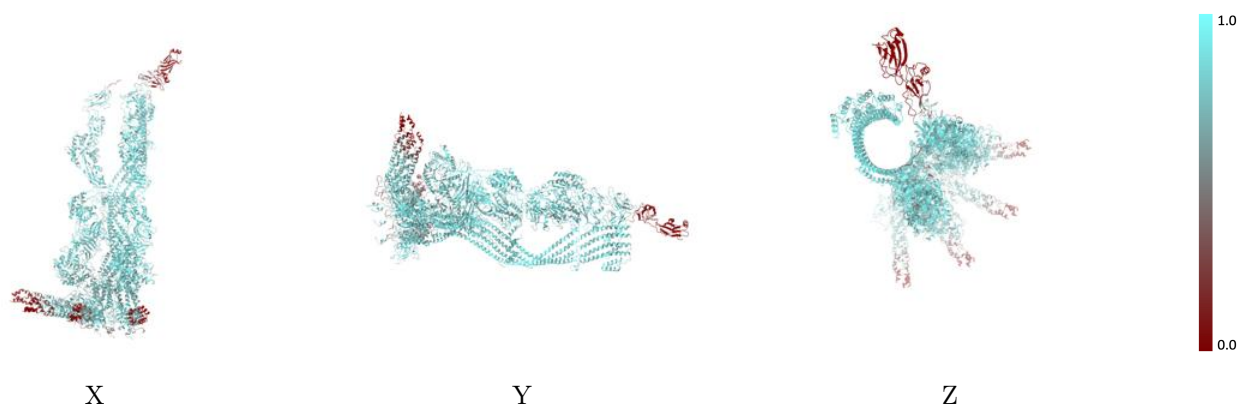
The images above show the 3D surface view of the map at the recommended contour level 5.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



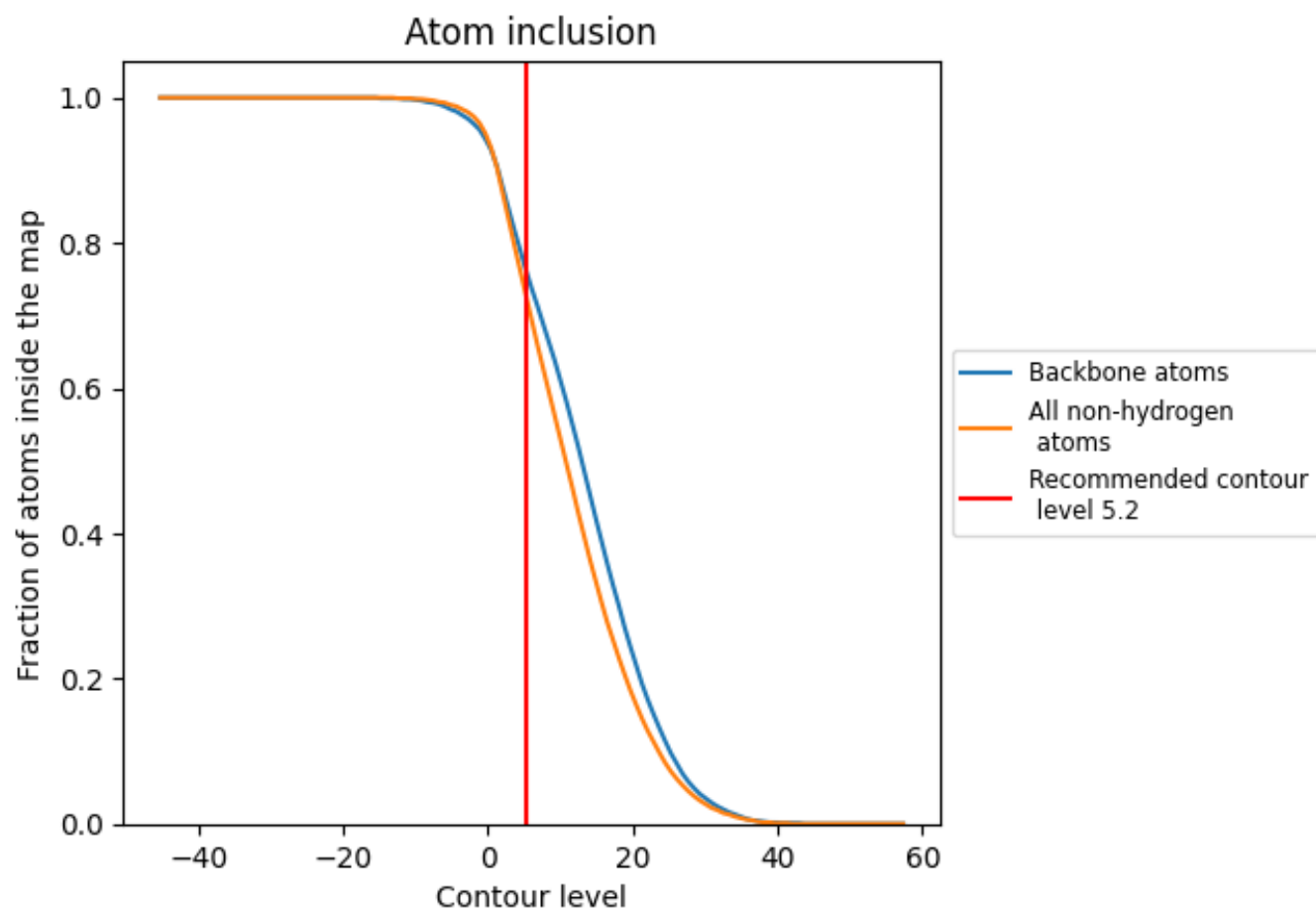
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.4360
A	 0.4710	 0.3390
B	 0.5290	 0.3640
C	 0.5310	 0.3630
D	 0.4640	 0.3270
E	 0.5170	 0.3690
F	 0.5010	 0.3600
G	 0.4950	 0.3350
H	 0.7820	 0.4650
I	 0.6980	 0.4230
J	 0.7900	 0.4690
K	 0.8190	 0.4550
L	 0.5320	 0.3680
M	 0.7940	 0.4570
N	 0.7920	 0.4610
O	 0.7730	 0.4650
P	 0.8090	 0.4540
Q	 0.5340	 0.3580
R	 0.7880	 0.4590
S	 0.7890	 0.4720
T	 0.8170	 0.4540
U	 0.8180	 0.4550
V	 0.4480	 0.3340
a	 0.5120	 0.3590
f	 0.4920	 0.3610

