



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:49 AM UTC

PDB ID : 9EFK / pdb_00009efk
EMDB ID : EMD-47975
Title : Cryo-EM structure of the portal-tail complex of LME-1 phage
Authors : Deme, J.C.; Lea, S.M.
Deposited on : 2024-11-20
Resolution : 1.90 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:

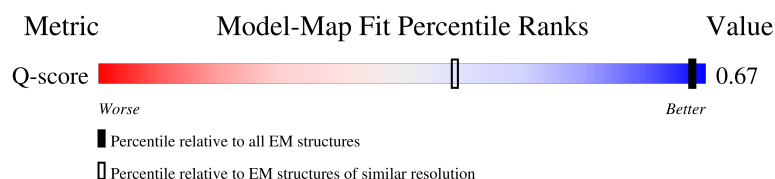
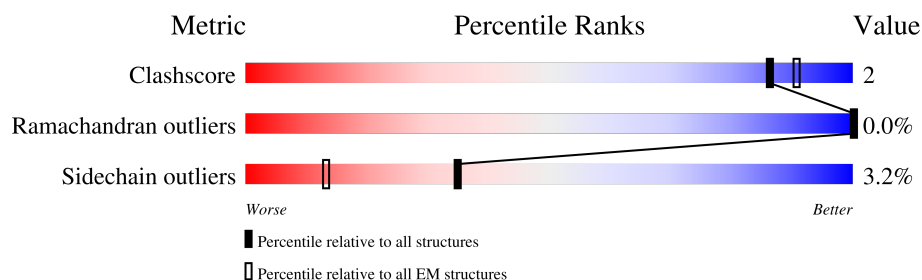
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 1.90 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	1185 (1.40 - 2.40)

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	554	7% 83% 10% • 6%
1	B	554	9% 84% 9% • 6%
1	C	554	8% 81% 11% • 6%
1	D	554	10% 84% 8% • 6%

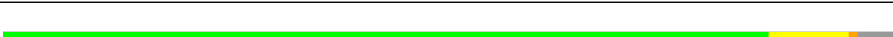
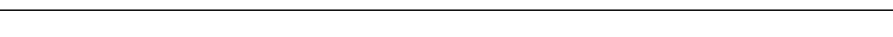
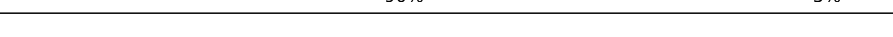
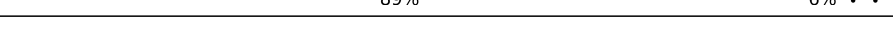
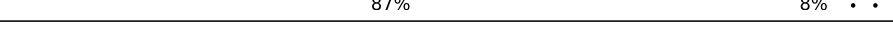
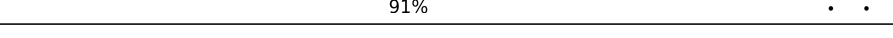
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Mol	Chain	Length	Quality of chain
1	E	554	
1	F	554	
1	G	554	
1	H	554	
1	I	554	
1	J	554	
1	K	554	
1	L	554	
2	M	818	
2	N	818	
2	O	818	
2	P	818	
2	Q	818	
2	R	818	
3	AE	658	
3	AF	658	
3	AG	658	
3	AN	658	
3	AO	658	
3	AP	658	
3	AW	658	
3	AX	658	
3	AY	658	
3	BF	658	
3	BG	658	

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Mol	Chain	Length	Quality of chain
3	BH	658	
3	BO	658	
3	BP	658	
3	BQ	658	
3	BX	658	
3	BY	658	
3	BZ	658	
4	AA	201	
4	AB	201	
4	AC	201	
4	AD	201	
4	S	201	
4	T	201	
4	U	201	
4	V	201	
4	W	201	
4	X	201	
4	Y	201	
4	Z	201	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 129576 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 orf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	B	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	C	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	D	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	E	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	F	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	G	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	H	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	I	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	J	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	K	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	L	519	Total 4128	C 2626	N 705	O 778	S 19	0	0

- Molecule 2 is a protein called orf18.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0
2	N	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0
2	O	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		
2	Q	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		
2	R	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		

- Molecule 3 is a protein called orf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AE	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AF	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AG	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AN	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AO	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AP	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AW	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AX	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AY	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BF	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BG	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BH	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BO	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BP	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BQ	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BX	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BY	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BZ	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		

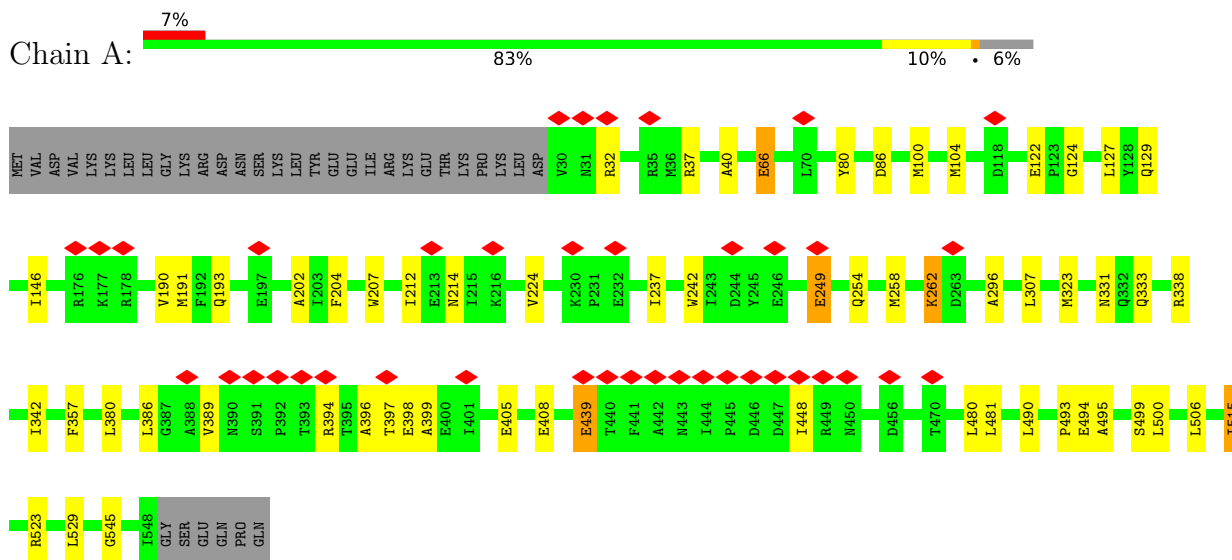
- Molecule 4 is a protein called orf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AC	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AD	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	S	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	X	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	U	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	V	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	W	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	Y	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	Z	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AA	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AB	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		

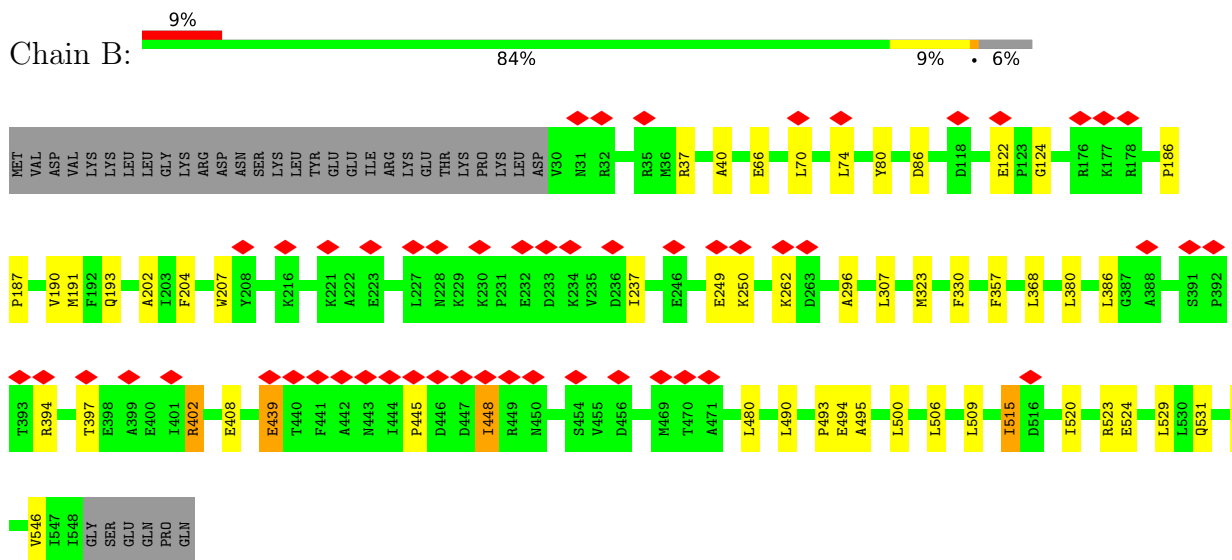
3 Residue-property plots

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.

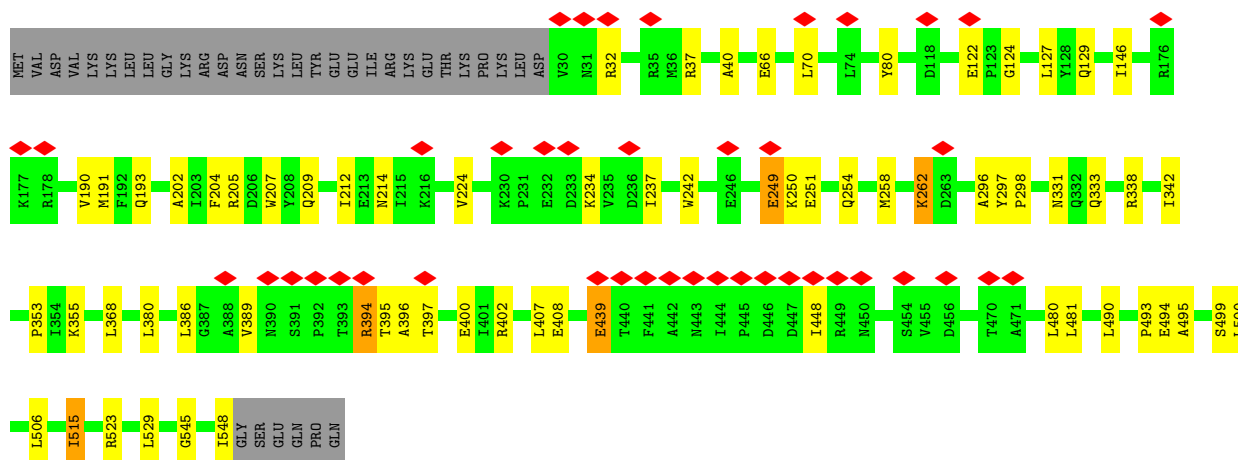
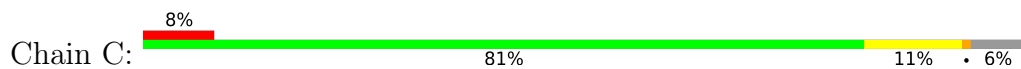
- Molecule 1: orf12



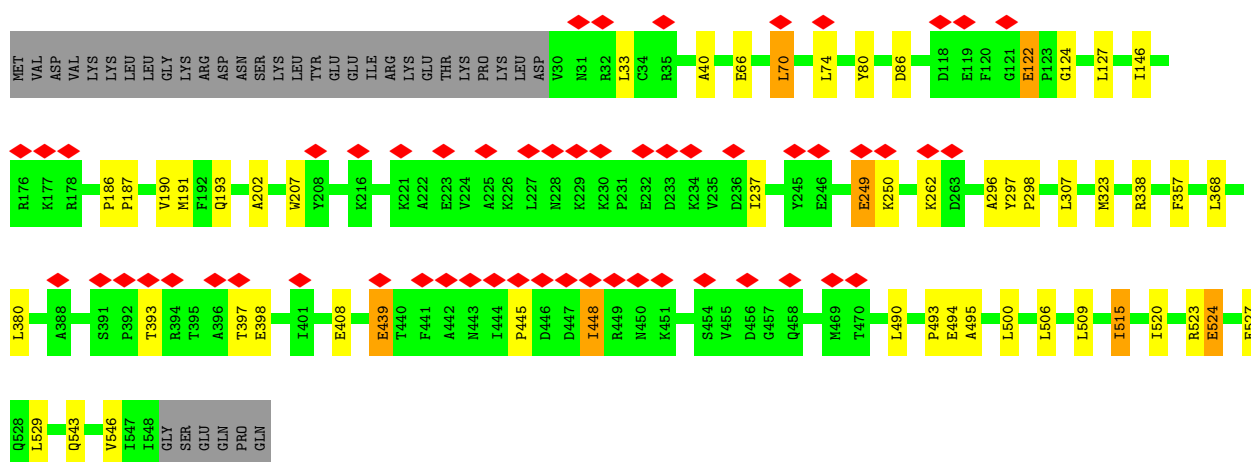
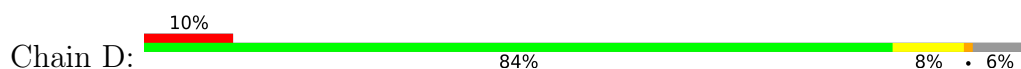
- Molecule 1: orf12



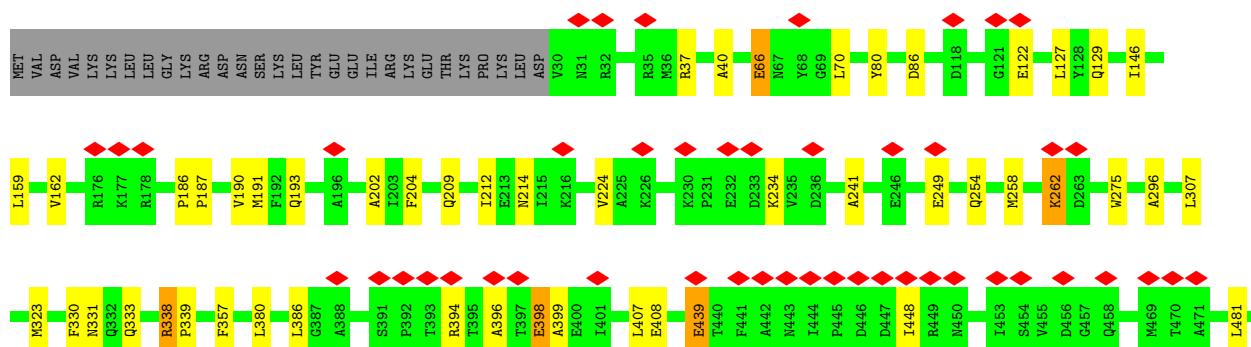
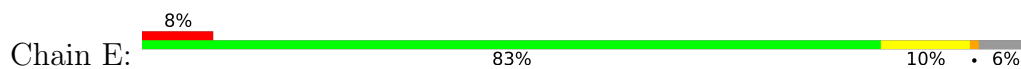
- Molecule 1: orf12



• Molecule 1: orf12

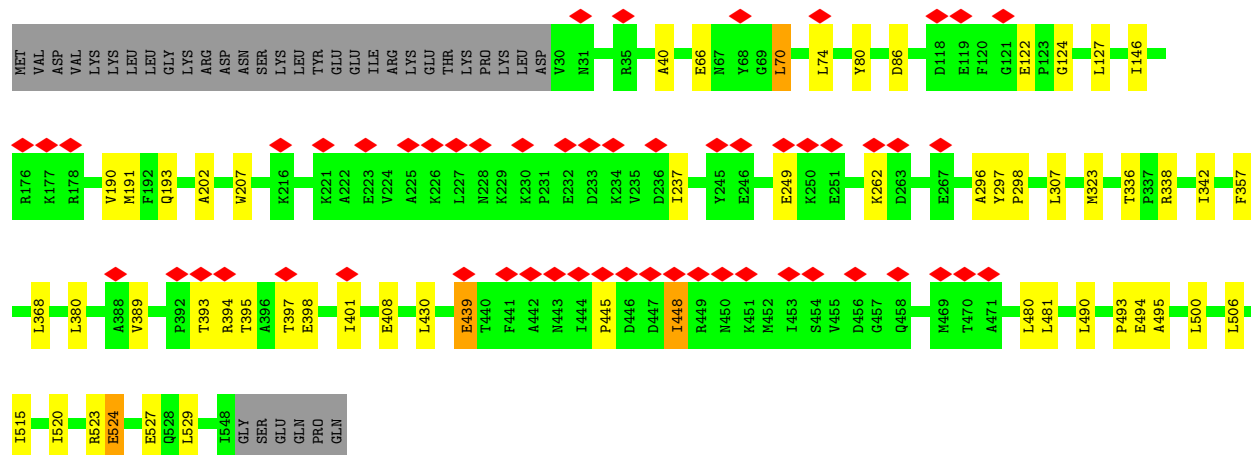
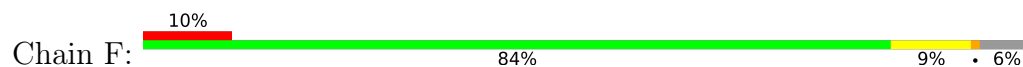


• Molecule 1: orf12

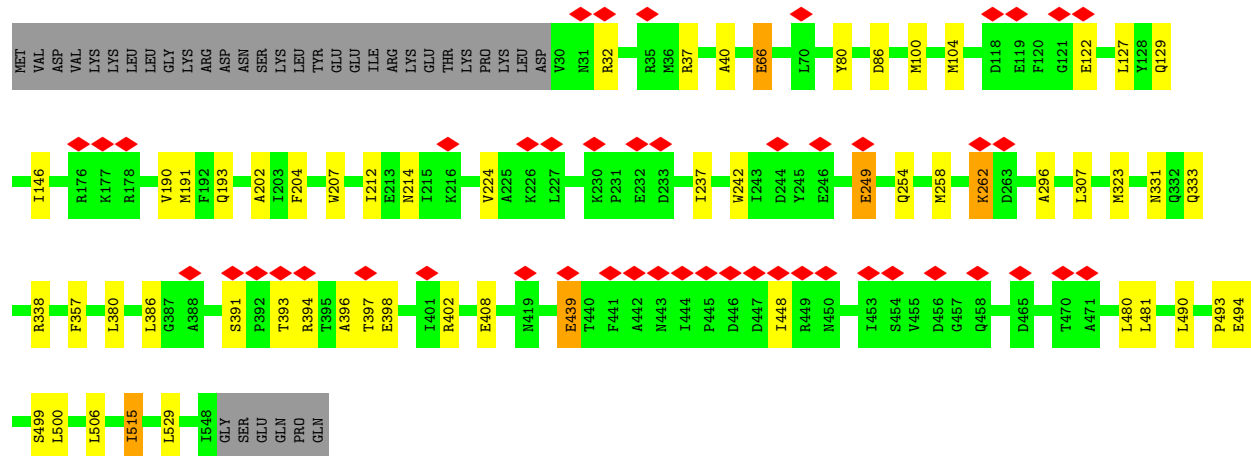
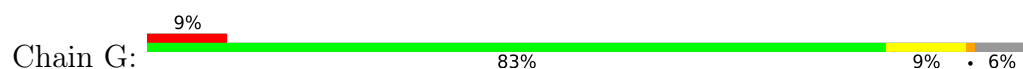




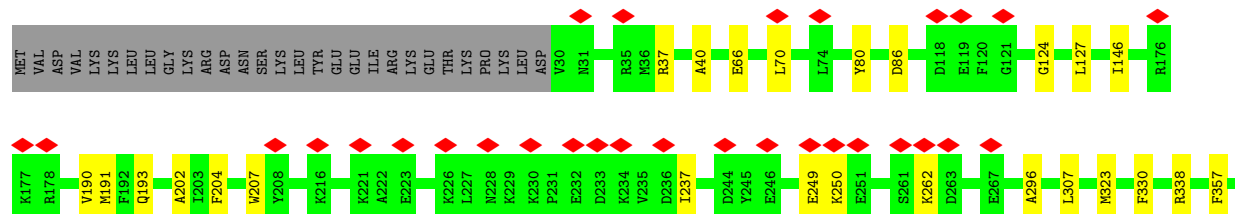
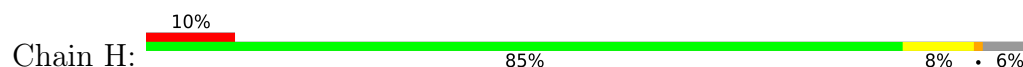
- Molecule 1: orf12

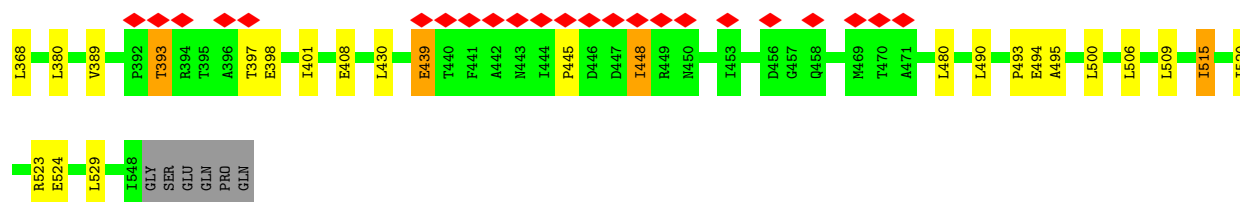


- Molecule 1: orf12

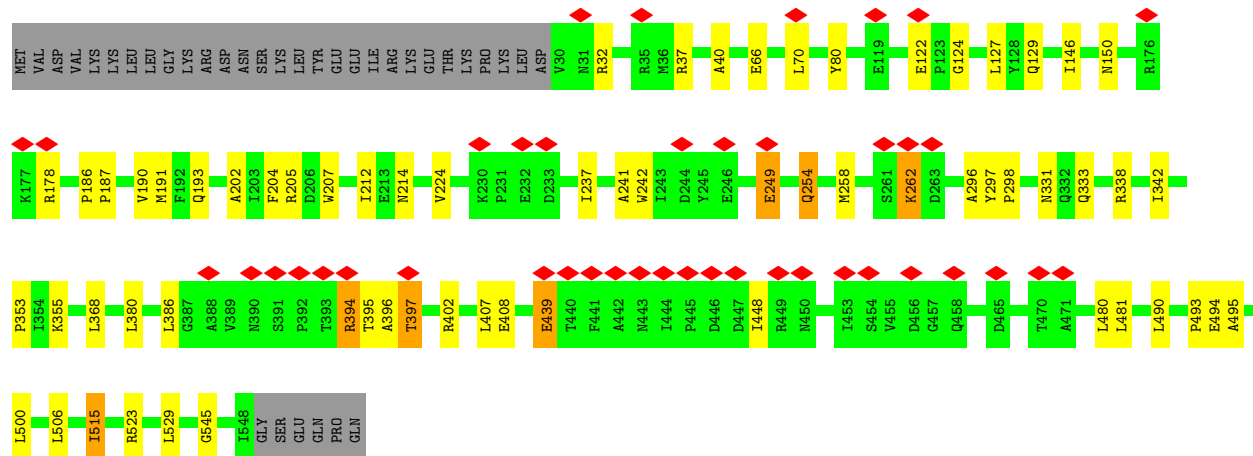
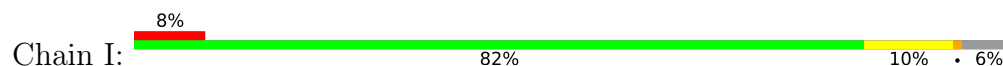


- Molecule 1: orf12

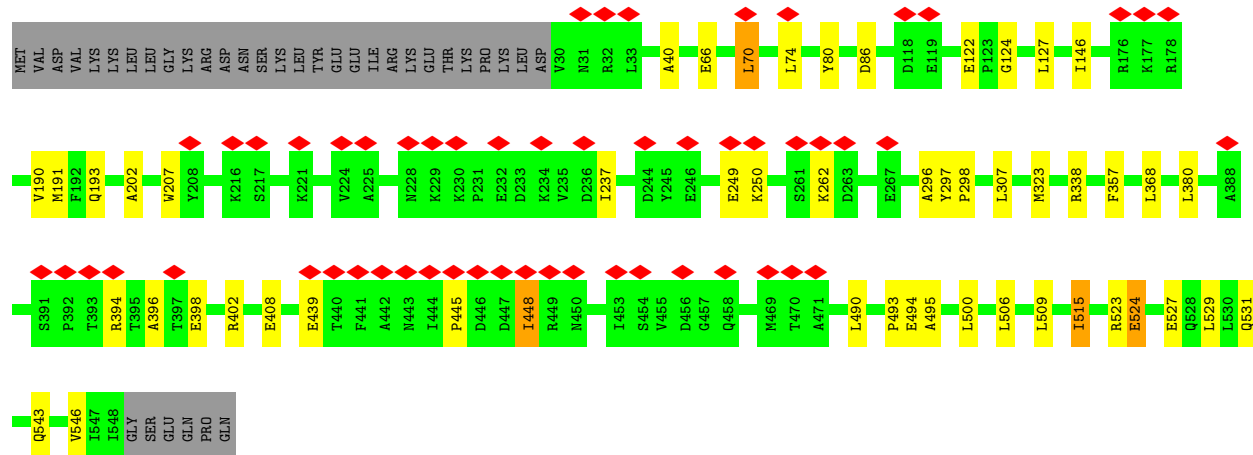
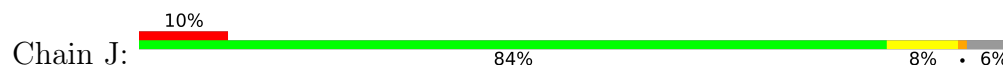




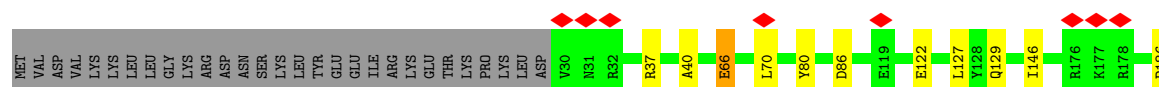
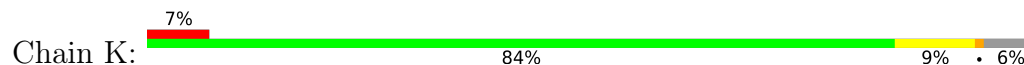
• Molecule 1: orf12

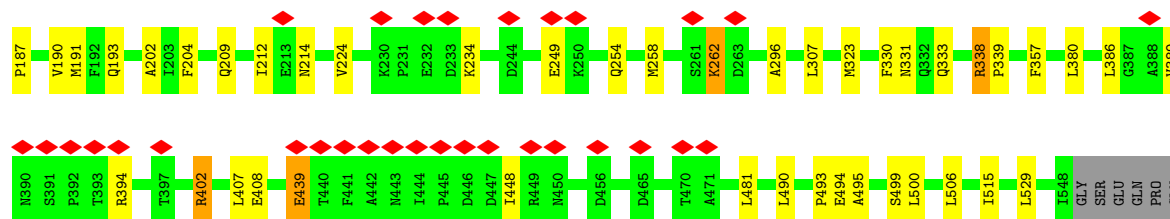


• Molecule 1: orf12

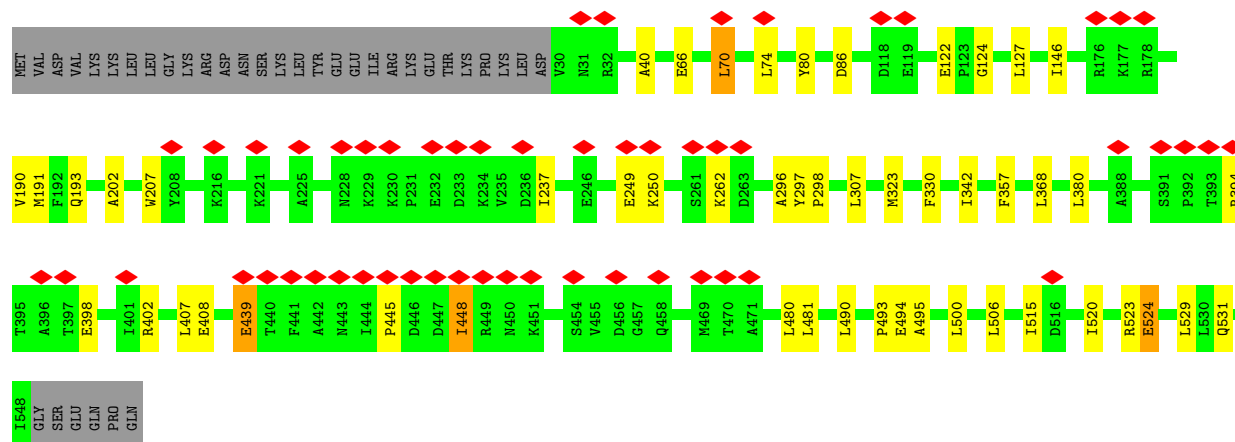
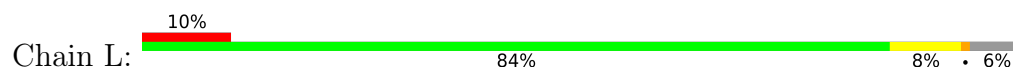


• Molecule 1: orf12

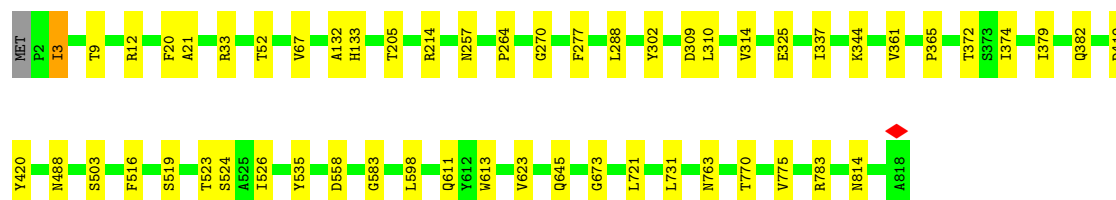




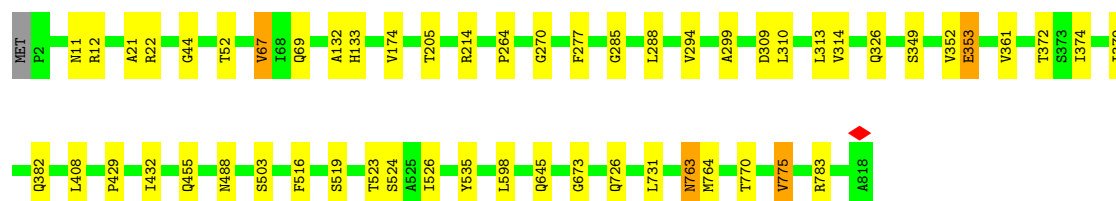
- Molecule 1: orf12



- Molecule 2: orf18



- Molecule 2: orf18



- Molecule 2: orf18



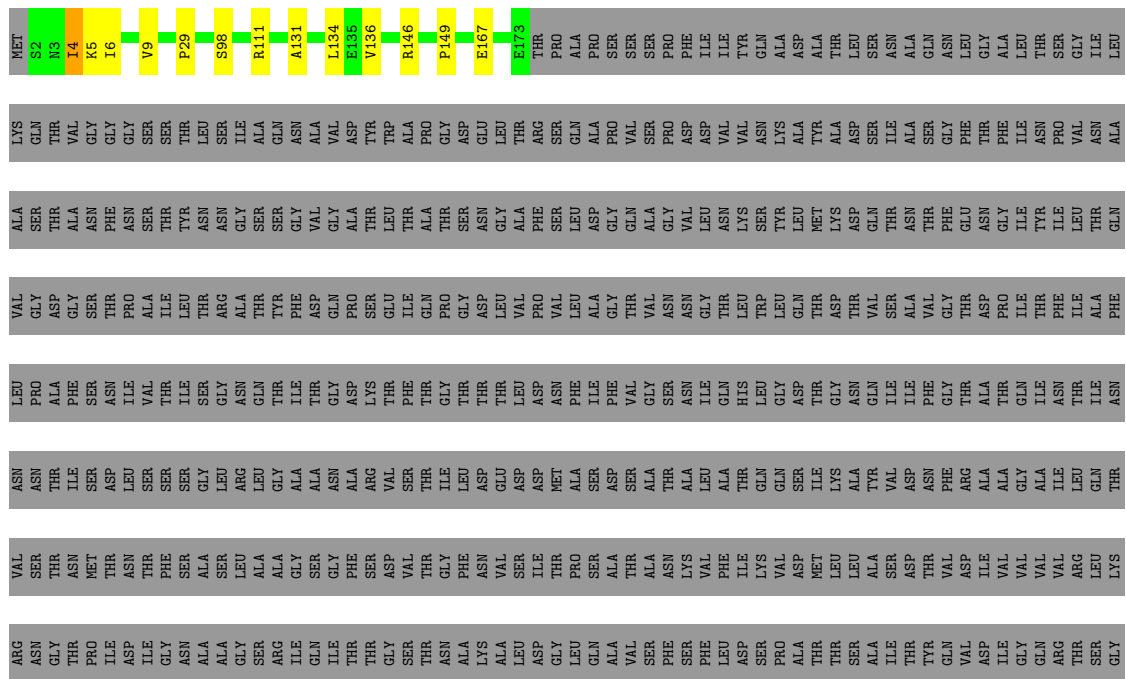


[illegible]

Chain AX: 24% 1% 74%

[illegible]

Chain AY: 25% . 74%



SER	ALA	VAL	GLY	ILE	VAL	VAL	ASN	ARG	SER	GLY	ALA	ASP	VAL	ASP	SER	SER	SER	TYR	THR	ARG	GLY	ALA	ALA	SER	THR	ILE	THR	THR	GLY
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• Molecule 3: orf22



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• Molecule 3: orf22



MET	S2	I6	E34	T90	L100	G107	R111	M116	A131	L134	I171	D172	E173	THR	PRO	ALA	PRO	SER	SER	SER	PRO	PHE	ILE	ILE	ILE	GLN	ALA	ASP	THR	LEU	SER	ASN	ILE	ASN	GLN	GLY	ALA	LEU	THR	SER	PRO	GLY	THR	VAL		
GLY	GLY	GLY	SER	THR	ALA	ASN	VAL	ASP	PRO	GLY	GLU	LEU	THR	ARG	SER	GLN	ALA	VAL	GLN	LEU	GLY	ASP	VAL	VAL	VAL	ASN	GLY	ASP	THR	LEU	GLY	THR	ASN	GLN	SER	GLY	ALA	THR	THR	THR	THR	THR	THR	THR	THR	
ASN	PHE	ASN	SER	ASN	SER	GLY	GLY	ALA	THR	THR	ASN	GLY	ALA	PHE	LEU	ASP	GLY	GLN	LEU	ALA	PHE	LEU	GLY	ASN	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	THR	PRO	ALA	ARG	THR	PHE	GLN	PRO	THR	PRO	ASP	VAL	VAL	VAL	ALA	THR	GLY	VAL	GLN	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	ASN	ILE	VAL	GLY	GLN	ILE	THR	LYS	PHE	GLY	THR	LEU	ASP	ASN	PHE	ILE	PHE	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	ASP	LEU	SER	LEU	LEU	ALA	ASN	ARG	VAL	ILE	GLU	ASP	ASP	MET	ALA	ASP	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
MET	THR	ASN	THR	SER	ALA	SER	GLY	SER	THR	PHE	ASN	VAL	ILE	THR	PRO	SER	ALA	ALA	ASN	LYS	VAL	PHE	THR	ILE	ILE	LYS	VAL	VAL	MET	LEU	LYS	ALA	TYR	ASP	ASN	PHE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	

- Molecule 3: orf22

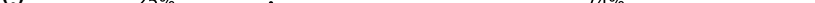
[illegible]

- Molecule 3: orf22

[illegible]

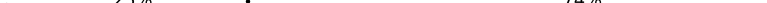
[illegible]

- Molecule 3: orf22

Chain BQ:  25% 74%

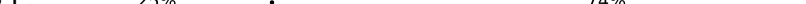
[illegible]

- Molecule 3: orf22

Chain BX:  25% . 74%

[illegible]

- Molecule 3: orf22

Chain BY:  25% 74%

[illegible]

- Molecule 3: orf22

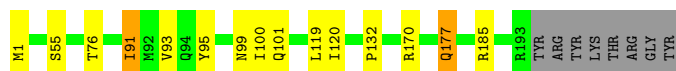
Chain BZ: 25% 74%

[illegible]



- Molecule 4: orf17

Chain V: 89% 6% . .



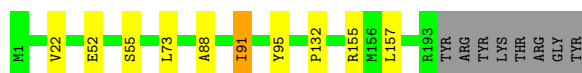
- Molecule 4: orf17

Chain W: 89% 6% .



- Molecule 4: orf17

Chain Y: 91% . .



- Molecule 4: orf17

Chain Z: 87% 7% . .



- Molecule 4: orf17

Chain AA: 91% . . .



- Molecule 4: orf17

Chain AB: 89% 6% . .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88530	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 ($e^-/\text{\AA}^2$)	52.9	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.337	Depositor
Minimum map value	-0.451	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	702.4, 702.4, 702.4	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.878, 0.878, 0.878	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/4223	0.29	0/5744
1	B	0.18	0/4223	0.28	0/5744
1	C	0.19	0/4223	0.31	1/5744 (0.0%)
1	D	0.19	0/4223	0.29	0/5744
1	E	0.19	0/4223	0.30	0/5744
1	F	0.19	0/4223	0.29	0/5744
1	G	0.19	0/4223	0.30	0/5744
1	H	0.18	0/4223	0.28	0/5744
1	I	0.19	0/4223	0.31	1/5744 (0.0%)
1	J	0.19	0/4223	0.29	0/5744
1	K	0.19	0/4223	0.29	0/5744
1	L	0.19	0/4223	0.29	0/5744
2	M	0.21	0/6466	0.30	0/8830
2	N	0.21	0/6466	0.30	0/8830
2	O	0.21	0/6466	0.31	0/8830
2	P	0.21	0/6466	0.31	0/8830
2	Q	0.21	0/6466	0.30	0/8830
2	R	0.21	0/6466	0.30	0/8830
3	AE	0.21	0/1347	0.28	0/1837
3	AF	0.20	0/1347	0.27	0/1837
3	AG	0.21	0/1347	0.28	0/1837
3	AN	0.21	0/1347	0.29	0/1837
3	AO	0.20	0/1347	0.27	0/1837
3	AP	0.21	0/1347	0.31	0/1837
3	AW	0.21	0/1347	0.29	0/1837
3	AX	0.20	0/1347	0.27	0/1837
3	AY	0.21	0/1347	0.28	0/1837
3	BF	0.22	0/1347	0.29	0/1837
3	BG	0.20	0/1347	0.27	0/1837
3	BH	0.21	0/1347	0.29	0/1837
3	BO	0.21	0/1347	0.29	0/1837
3	BP	0.20	0/1347	0.27	0/1837
3	BQ	0.21	0/1347	0.29	0/1837
3	BX	0.21	0/1347	0.28	0/1837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BY	0.20	0/1347	0.27	0/1837
3	BZ	0.21	0/1347	0.28	0/1837
4	AA	0.22	0/1561	0.32	0/2127
4	AB	0.22	0/1561	0.32	0/2127
4	AC	0.22	0/1561	0.32	0/2127
4	AD	0.23	0/1561	0.35	0/2127
4	S	0.22	0/1561	0.30	0/2127
4	T	0.22	0/1561	0.32	0/2127
4	U	0.22	0/1561	0.31	0/2127
4	V	0.22	0/1561	0.33	0/2127
4	W	0.23	0/1561	0.33	0/2127
4	X	0.22	0/1561	0.32	0/2127
4	Y	0.22	0/1561	0.31	0/2127
4	Z	0.22	0/1561	0.34	0/2127
All	All	0.20	0/132450	0.30	2/180498 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	LEU	N-CA-C	-5.04	106.47	113.18
1	I	368	LEU	N-CA-C	-5.02	106.50	113.18

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	4128	0	4062	29	0
1	B	4128	0	4062	28	0
1	C	4128	0	4062	31	0
1	D	4128	0	4062	27	0
1	E	4128	0	4062	27	0
1	F	4128	0	4062	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4128	0	4062	28	0
1	H	4128	0	4062	25	0
1	I	4128	0	4062	31	0
1	J	4128	0	4062	22	0
1	K	4128	0	4062	25	0
1	L	4128	0	4062	25	0
2	M	6330	0	6142	24	0
2	N	6330	0	6142	29	0
2	O	6330	0	6142	27	0
2	P	6330	0	6142	23	0
2	Q	6330	0	6142	30	0
2	R	6330	0	6142	23	0
3	AE	1320	0	1285	2	0
3	AF	1320	0	1285	5	0
3	AG	1320	0	1285	4	0
3	AN	1320	0	1285	5	0
3	AO	1320	0	1285	6	0
3	AP	1320	0	1285	6	0
3	AW	1320	0	1285	4	0
3	AX	1320	0	1285	8	0
3	AY	1320	0	1285	6	0
3	BF	1320	0	1285	5	0
3	BG	1320	0	1285	6	0
3	BH	1320	0	1285	6	0
3	BO	1320	0	1285	2	0
3	BP	1320	0	1285	5	0
3	BQ	1320	0	1285	4	0
3	BX	1320	0	1285	3	0
3	BY	1320	0	1285	4	0
3	BZ	1320	0	1285	3	0
4	AA	1525	0	1526	7	0
4	AB	1525	0	1526	8	0
4	AC	1525	0	1526	8	0
4	AD	1525	0	1526	12	0
4	S	1525	0	1526	4	0
4	T	1525	0	1526	9	0
4	U	1525	0	1526	6	0
4	V	1525	0	1526	10	0
4	W	1525	0	1526	7	0
4	X	1525	0	1526	14	0
4	Y	1525	0	1526	5	0
4	Z	1525	0	1526	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	129576	0	127038	542	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 2.

All (542) 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)
4:V:99:ASN:HB3	4:V:185:ARG:HE	1.44	0.83
4:Z:99:ASN:HB3	4:Z:185:ARG:HE	1.51	0.76
1:I:397:THR:HB	1:J:396:ALA:HA	1.67	0.76
1:B:394:ARG:HH21	1:B:402:ARG:HH12	1.38	0.71
3:BZ:37:LEU:HD13	4:Z:1:MET:HE2	1.73	0.71
4:AA:132:PRO:HG2	4:AB:91:ILE:HG13	1.73	0.71
4:AC:132:PRO:HG2	4:AD:91:ILE:HG13	1.73	0.69
1:B:397:THR:HG21	1:C:396:ALA:HB2	1.75	0.69
4:X:91:ILE:HG13	4:W:132:PRO:HG2	1.73	0.68
4:U:132:PRO:HG2	4:V:91:ILE:HG13	1.73	0.68
4:T:91:ILE:HG13	4:S:132:PRO:HG2	1.74	0.68
4:Y:132:PRO:HG2	4:Z:91:ILE:HG13	1.74	0.68
4:Z:93:VAL:HG13	4:Z:119:LEU:HD11	1.76	0.68
2:M:133:HIS:HD2	2:N:326:GLN:H	1.40	0.67
2:P:133:HIS:HD2	2:Q:326:GLN:H	1.40	0.67
4:T:93:VAL:HG13	4:T:119:LEU:HD11	1.77	0.67
2:Q:214:ARG:HH12	2:Q:310:LEU:HD21	1.60	0.66
4:AD:93:VAL:HG13	4:AD:119:LEU:HD11	1.78	0.66
1:C:394:ARG:HH21	1:C:402:ARG:HH21	1.42	0.65
2:M:3:ILE:HD11	2:M:814:ASN:HB3	1.78	0.65
2:M:214:ARG:HH12	2:M:310:LEU:HD21	1.60	0.65
4:X:93:VAL:HG13	4:X:119:LEU:HD11	1.79	0.65
2:P:214:ARG:HH12	2:P:310:LEU:HD21	1.61	0.65
2:N:214:ARG:HH12	2:N:310:LEU:HD21	1.60	0.65
1:B:193:GLN:HB3	1:B:202:ALA:HB3	1.79	0.64
1:H:193:GLN:HB3	1:H:202:ALA:HB3	1.79	0.64
3:AW:149:PRO:HG3	3:AW:167:GLU:HA	1.80	0.64
1:J:193:GLN:HB3	1:J:202:ALA:HB3	1.80	0.63
1:L:193:GLN:HB3	1:L:202:ALA:HB3	1.80	0.63
2:R:764:MET:HE3	3:AY:100:LEU:HD23	1.80	0.63
1:E:193:GLN:HB3	1:E:202:ALA:HB3	1.80	0.62
1:K:193:GLN:HB3	1:K:202:ALA:HB3	1.80	0.62
2:O:764:MET:HE3	3:BH:100:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BF:149:PRO:HG3	3:BF:167:GLU:HA	1.80	0.62
1:D:193:GLN:HB3	1:D:202:ALA:HB3	1.80	0.62
1:F:193:GLN:HB3	1:F:202:ALA:HB3	1.80	0.61
2:O:775:VAL:HG22	3:BG:98:SER:HB2	1.82	0.61
4:V:93:VAL:HG13	4:V:119:LEU:HD11	1.83	0.61
3:AN:149:PRO:HG3	3:AN:167:GLU:HA	1.82	0.61
3:BO:149:PRO:HG3	3:BO:167:GLU:HA	1.83	0.61
1:G:193:GLN:HB3	1:G:202:ALA:HB3	1.83	0.61
2:Q:775:VAL:HG22	3:BP:98:SER:HB2	1.83	0.60
1:I:193:GLN:HB3	1:I:202:ALA:HB3	1.84	0.60
4:AB:93:VAL:HG13	4:AB:119:LEU:HD11	1.83	0.60
1:A:193:GLN:HB3	1:A:202:ALA:HB3	1.83	0.60
1:H:66:GLU:HG2	1:H:80:TYR:CE1	2.37	0.59
3:BF:4:ILE:HG22	3:BF:6:ILE:HG12	1.85	0.59
2:O:516:PHE:HD1	2:O:524:SER:HB3	1.67	0.59
3:AX:101:THR:HG23	3:AX:104:ASP:H	1.68	0.59
1:B:66:GLU:HG2	1:B:80:TYR:CE1	2.37	0.59
1:C:193:GLN:HB3	1:C:202:ALA:HB3	1.84	0.58
3:BX:149:PRO:HG3	3:BX:167:GLU:HA	1.85	0.58
1:E:66:GLU:HG2	1:E:80:TYR:CE1	2.39	0.58
3:AE:149:PRO:HG3	3:AE:167:GLU:HA	1.86	0.58
2:N:764:MET:HE3	3:AP:100:LEU:HD23	1.87	0.57
1:C:394:ARG:HB3	1:D:393:THR:HG23	1.85	0.57
1:D:66:GLU:HG2	1:D:80:TYR:CE1	2.40	0.57
2:R:516:PHE:HD1	2:R:524:SER:HB3	1.70	0.57
4:AD:132:PRO:HG2	4:S:91:ILE:HG13	1.87	0.57
1:I:480:LEU:HA	1:J:515:ILE:HD11	1.87	0.56
1:K:66:GLU:HG2	1:K:80:TYR:CE1	2.39	0.56
1:C:480:LEU:HA	1:D:515:ILE:HD11	1.86	0.56
1:F:66:GLU:HG2	1:F:80:TYR:CE1	2.40	0.56
1:A:66:GLU:HG2	1:A:80:TYR:CE1	2.41	0.56
1:E:333:GLN:HG3	4:AA:95:TYR:CD1	2.40	0.56
2:N:516:PHE:HD1	2:N:524:SER:HB3	1.71	0.56
1:K:333:GLN:HG3	4:U:95:TYR:CD1	2.40	0.56
1:G:391:SER:HB2	1:G:394:ARG:HH22	1.70	0.56
1:J:66:GLU:HG2	1:J:80:TYR:CE1	2.40	0.56
1:C:333:GLN:HG3	4:Y:95:TYR:CD1	2.41	0.55
1:G:66:GLU:HG2	1:G:80:TYR:CE1	2.41	0.55
1:L:66:GLU:HG2	1:L:80:TYR:CE1	2.40	0.55
2:Q:764:MET:HE3	3:BQ:100:LEU:HD23	1.87	0.55
1:I:333:GLN:HG3	4:S:95:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:516:PHE:HD1	2:M:524:SER:HB3	1.71	0.55
1:A:333:GLN:HG3	4:W:95:TYR:CD1	2.42	0.55
1:I:66:GLU:HG2	1:I:80:TYR:CE1	2.42	0.55
1:C:66:GLU:HG2	1:C:80:TYR:CE1	2.42	0.55
4:V:132:PRO:HG2	4:W:91:ILE:HG13	1.88	0.55
3:BQ:96:THR:HB	4:AD:39:ILE:HD13	1.89	0.55
2:Q:516:PHE:HD1	2:Q:524:SER:HB3	1.71	0.54
3:AW:5:LYS:HG2	3:AW:9:VAL:HG21	1.89	0.54
3:BH:90:THR:HG21	3:BH:111:ARG:HD3	1.88	0.54
4:AC:91:ILE:HG13	4:AB:132:PRO:HG2	1.89	0.54
4:AD:96:LEU:HD23	4:AD:100:ILE:HD11	1.89	0.54
1:E:394:ARG:HB3	1:E:398:GLU:HG2	1.88	0.54
1:G:333:GLN:HG3	4:AC:95:TYR:CD1	2.42	0.54
1:G:480:LEU:HA	1:H:515:ILE:HD11	1.89	0.54
4:X:132:PRO:HG2	4:Y:91:ILE:HG13	1.88	0.54
4:X:96:LEU:HD23	4:X:100:ILE:HD11	1.90	0.54
1:B:296:ALA:HB2	1:B:380:LEU:HD23	1.89	0.54
4:Z:132:PRO:HG2	4:AA:91:ILE:HG13	1.90	0.53
1:H:398:GLU:HG3	1:I:386:LEU:HD23	1.89	0.53
2:M:52:THR:HG22	2:M:645:GLN:HG2	1.90	0.53
1:H:296:ALA:HB2	1:H:380:LEU:HD23	1.89	0.53
4:X:99:ASN:HB2	4:X:185:ARG:HD2	1.90	0.53
1:A:480:LEU:HA	1:B:515:ILE:HD11	1.89	0.53
2:R:381:ASN:HB2	2:R:453:GLN:HE21	1.74	0.53
2:N:775:VAL:HG12	3:AO:98:SER:O	2.09	0.53
2:N:353:GLU:HG2	2:O:352:VAL:HG22	1.89	0.53
2:N:52:THR:HG22	2:N:645:GLN:HG2	1.91	0.52
2:P:52:THR:HG22	2:P:645:GLN:HG2	1.90	0.52
3:BF:4:ILE:HG23	3:BF:29:PRO:HG3	1.91	0.52
4:T:132:PRO:HG2	4:U:91:ILE:HG13	1.90	0.52
1:E:296:ALA:HB2	1:E:380:LEU:HD23	1.91	0.52
1:K:296:ALA:HB2	1:K:380:LEU:HD23	1.91	0.52
2:Q:309:ASP:HB2	2:Q:314:VAL:HG11	1.92	0.51
4:AD:99:ASN:HB2	4:AD:185:ARG:HD2	1.91	0.51
1:G:394:ARG:HB3	1:G:398:GLU:HB3	1.91	0.51
1:C:296:ALA:HB2	1:C:380:LEU:HD23	1.92	0.51
2:Q:52:THR:HG22	2:Q:645:GLN:HG2	1.91	0.51
2:R:309:ASP:HB2	2:R:314:VAL:HG11	1.92	0.51
1:I:296:ALA:HB2	1:I:380:LEU:HD23	1.92	0.51
1:H:397:THR:HG21	1:I:396:ALA:HB2	1.93	0.51
2:P:309:ASP:HB2	2:P:314:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:205:THR:HA	2:R:264:PRO:HG2	1.92	0.51
2:R:775:VAL:HG12	3:AX:98:SER:O	2.10	0.51
1:E:258:MET:HE2	1:E:262:LYS:HA	1.93	0.51
1:A:386:LEU:HD13	1:L:398:GLU:HG3	1.93	0.51
2:O:205:THR:HA	2:O:264:PRO:HG2	1.92	0.51
2:O:309:ASP:HB2	2:O:314:VAL:HG11	1.93	0.50
2:R:52:THR:HG22	2:R:645:GLN:HG2	1.92	0.50
2:N:205:THR:HA	2:N:264:PRO:HG2	1.94	0.50
2:N:309:ASP:HB2	2:N:314:VAL:HG11	1.92	0.50
2:P:205:THR:HA	2:P:264:PRO:HG2	1.93	0.50
1:K:258:MET:HE2	1:K:262:LYS:HA	1.93	0.50
1:D:490:LEU:HD21	1:E:481:LEU:HD23	1.93	0.50
2:M:205:THR:HA	2:M:264:PRO:HG2	1.92	0.50
2:M:309:ASP:HB2	2:M:314:VAL:HG11	1.92	0.50
2:N:11:ASN:HB3	2:N:44:GLY:HA2	1.94	0.50
1:I:439:GLU:CD	1:I:439:GLU:H	2.20	0.50
1:J:490:LEU:HD21	1:K:481:LEU:HD23	1.94	0.50
4:V:100:ILE:HG22	4:V:101:GLN:H	1.77	0.50
2:O:21:ALA:HA	2:O:731:LEU:HD21	1.94	0.50
1:L:323:MET:HG3	1:L:357:PHE:HA	1.93	0.50
2:N:372:THR:HG23	2:N:374:ILE:H	1.77	0.49
2:O:52:THR:HG22	2:O:645:GLN:HG2	1.92	0.49
2:M:519:SER:HB3	2:M:523:THR:OG1	2.12	0.49
1:I:490:LEU:HD12	1:J:509:LEU:HD11	1.93	0.49
2:Q:205:THR:HA	2:Q:264:PRO:HG2	1.94	0.49
1:F:323:MET:HG3	1:F:357:PHE:HA	1.93	0.49
3:AX:131:ALA:HB3	3:AX:134:LEU:HG	1.95	0.49
1:K:394:ARG:HE	1:K:402:ARG:HH21	1.61	0.49
1:B:323:MET:HG3	1:B:357:PHE:HA	1.94	0.49
1:D:86:ASP:HB2	1:D:307:LEU:HD12	1.94	0.49
2:Q:21:ALA:HA	2:Q:731:LEU:HD21	1.94	0.49
1:C:490:LEU:HD12	1:D:509:LEU:HD11	1.94	0.49
2:O:270:GLY:HA3	2:O:288:LEU:HB3	1.94	0.49
4:AD:2:ILE:HG21	4:S:88:ALA:HB3	1.95	0.49
2:Q:763:ASN:O	2:Q:775:VAL:HG21	2.12	0.49
2:R:372:THR:HG23	2:R:374:ILE:H	1.78	0.49
1:C:396:ALA:O	1:C:400:GLU:HB3	2.13	0.49
1:J:323:MET:HG3	1:J:357:PHE:HA	1.95	0.49
1:J:398:GLU:HG2	1:K:386:LEU:HD23	1.94	0.49
2:N:21:ALA:HA	2:N:731:LEU:HD21	1.95	0.48
1:C:545:GLY:HA3	1:D:543:GLN:HE22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:372:THR:HG23	2:Q:374:ILE:H	1.77	0.48
2:R:21:ALA:HA	2:R:731:LEU:HD21	1.93	0.48
3:AX:26:ILE:HD11	3:AX:67:ILE:HG12	1.95	0.48
3:BG:26:ILE:HD11	3:BG:67:ILE:HG12	1.94	0.48
1:F:86:ASP:HB2	1:F:307:LEU:HD12	1.96	0.48
2:N:488:ASN:HB2	2:N:673:GLY:HA3	1.96	0.48
3:AO:131:ALA:HB3	3:AO:134:LEU:HG	1.94	0.48
3:BG:131:ALA:HB3	3:BG:134:LEU:HG	1.95	0.48
3:BP:131:ALA:HB3	3:BP:134:LEU:HG	1.95	0.48
1:H:323:MET:HG3	1:H:357:PHE:HA	1.94	0.48
1:A:249:GLU:CD	1:A:249:GLU:H	2.21	0.48
2:R:270:GLY:HA3	2:R:288:LEU:HB3	1.94	0.48
1:G:258:MET:HE2	1:G:262:LYS:HA	1.96	0.48
1:I:150:ASN:H	1:I:178:ARG:HH22	1.59	0.48
1:J:86:ASP:HB2	1:J:307:LEU:HD12	1.94	0.48
1:G:394:ARG:HE	1:G:402:ARG:HH21	1.61	0.48
1:H:490:LEU:HD21	1:I:481:LEU:HD23	1.96	0.48
1:A:296:ALA:HB2	1:A:380:LEU:HD23	1.95	0.48
2:Q:455:GLN:HG3	2:R:412:MET:HE1	1.95	0.48
2:Q:488:ASN:HB2	2:Q:673:GLY:HA3	1.96	0.48
1:G:249:GLU:H	1:G:249:GLU:CD	2.21	0.48
4:AB:100:ILE:HG22	4:AB:101:GLN:H	1.78	0.48
1:L:86:ASP:HB2	1:L:307:LEU:HD12	1.95	0.48
2:N:133:HIS:CE1	2:O:325:GLU:HG3	2.49	0.48
2:Q:133:HIS:CE1	2:R:325:GLU:HG3	2.48	0.48
3:AY:96:THR:HG22	4:T:32:ASP:HA	1.95	0.48
1:B:480:LEU:HD13	1:C:515:ILE:HD11	1.96	0.48
1:C:249:GLU:CD	1:C:249:GLU:H	2.22	0.48
1:L:296:ALA:HB2	1:L:380:LEU:HD23	1.96	0.48
2:M:325:GLU:HG3	2:R:133:HIS:CE1	2.49	0.48
1:B:490:LEU:HD21	1:C:481:LEU:HD23	1.96	0.48
1:G:439:GLU:CD	1:G:439:GLU:H	2.21	0.48
1:K:439:GLU:CD	1:K:439:GLU:H	2.21	0.48
1:E:439:GLU:H	1:E:439:GLU:CD	2.21	0.48
1:F:124:GLY:O	1:F:523:ARG:HD2	2.14	0.48
2:O:519:SER:HB3	2:O:523:THR:OG1	2.13	0.47
1:B:40:ALA:HB1	1:B:191:MET:HB3	1.96	0.47
1:B:70:LEU:HD13	1:B:74:LEU:HD13	1.95	0.47
1:A:258:MET:HE2	1:A:262:LYS:HA	1.95	0.47
2:O:372:THR:HG23	2:O:374:ILE:H	1.79	0.47
1:E:394:ARG:HB2	1:E:399:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:ALA:HA	2:M:731:LEU:HD21	1.96	0.47
1:G:296:ALA:HB2	1:G:380:LEU:HD23	1.95	0.47
1:L:124:GLY:O	1:L:523:ARG:HD2	2.14	0.47
1:I:249:GLU:H	1:I:249:GLU:CD	2.22	0.47
3:AY:131:ALA:HB3	3:AY:134:LEU:HG	1.96	0.47
1:E:249:GLU:CD	1:E:249:GLU:H	2.22	0.47
1:H:40:ALA:HB1	1:H:191:MET:HB3	1.97	0.47
2:R:214:ARG:HH12	2:R:310:LEU:HD21	1.79	0.47
2:P:372:THR:HG23	2:P:374:ILE:H	1.80	0.47
2:P:488:ASN:HB2	2:P:673:GLY:HA3	1.96	0.47
3:AP:131:ALA:HB3	3:AP:134:LEU:HG	1.97	0.47
1:D:323:MET:HG3	1:D:357:PHE:HA	1.95	0.47
1:F:40:ALA:HB1	1:F:191:MET:HB3	1.97	0.47
1:K:249:GLU:CD	1:K:249:GLU:H	2.22	0.47
2:P:21:ALA:HA	2:P:731:LEU:HD21	1.95	0.47
3:AF:131:ALA:HB3	3:AF:134:LEU:HG	1.97	0.47
3:AW:131:ALA:HB3	3:AW:134:LEU:HG	1.97	0.47
1:H:480:LEU:HD13	1:I:515:ILE:HD11	1.96	0.47
1:A:398:GLU:HG2	1:B:386:LEU:HD13	1.97	0.47
2:M:132:ALA:HB2	2:M:277:PHE:CE1	2.50	0.47
2:M:372:THR:HG23	2:M:374:ILE:H	1.80	0.47
3:BY:131:ALA:HB3	3:BY:134:LEU:HG	1.97	0.47
1:D:124:GLY:O	1:D:523:ARG:HD2	2.15	0.47
1:F:296:ALA:HB2	1:F:380:LEU:HD23	1.96	0.47
1:I:545:GLY:HA3	1:J:543:GLN:HE22	1.80	0.47
3:BF:131:ALA:HB3	3:BF:134:LEU:HG	1.97	0.47
3:BQ:131:ALA:HB3	3:BQ:134:LEU:HG	1.97	0.47
1:A:439:GLU:CD	1:A:439:GLU:H	2.21	0.46
3:BH:131:ALA:HB3	3:BH:134:LEU:HG	1.96	0.46
3:BY:120:GLN:HA	3:BY:123:GLN:HG2	1.97	0.46
4:T:99:ASN:HB2	4:T:185:ARG:HD2	1.97	0.46
2:O:133:HIS:CE1	2:P:325:GLU:HG3	2.51	0.46
1:C:439:GLU:CD	1:C:439:GLU:H	2.21	0.46
1:D:40:ALA:HB1	1:D:191:MET:HB3	1.97	0.46
1:J:445:PRO:HB2	1:J:448:ILE:HG23	1.97	0.46
1:L:40:ALA:HB1	1:L:191:MET:HB3	1.97	0.46
2:Q:503:SER:HB3	2:Q:535:TYR:HB2	1.98	0.46
1:B:394:ARG:HH22	1:C:389:VAL:HG13	1.81	0.46
1:J:70:LEU:HG	1:J:74:LEU:HD23	1.97	0.46
1:K:394:ARG:HE	1:K:402:ARG:NH2	2.14	0.46
2:O:132:ALA:HB2	2:O:277:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:132:ALA:HB2	2:R:277:PHE:CE1	2.51	0.46
2:R:299:ALA:HB3	2:R:313:LEU:HB3	1.97	0.46
3:AF:120:GLN:HA	3:AF:123:GLN:HG2	1.98	0.46
3:BF:5:LYS:HG2	3:BF:9:VAL:HG21	1.96	0.46
1:J:124:GLY:O	1:J:523:ARG:HD2	2.15	0.46
1:A:86:ASP:HB2	1:A:307:LEU:HD12	1.98	0.46
1:A:545:GLY:HA3	1:B:543:GLN:HE22	1.81	0.46
2:O:763:ASN:O	2:O:775:VAL:HG21	2.15	0.46
1:D:445:PRO:HB2	1:D:448:ILE:HG23	1.97	0.46
2:P:132:ALA:HB2	2:P:277:PHE:CE1	2.50	0.46
3:AF:105:LEU:HD23	3:AF:105:LEU:HA	1.82	0.46
4:U:174:ALA:HB2	4:V:55:SER:HA	1.97	0.46
1:A:515:ILE:HD11	1:L:480:LEU:HA	1.98	0.46
1:I:331:ASN:HD22	4:AD:177:GLN:HG2	1.81	0.46
1:J:66:GLU:HG2	1:J:80:TYR:HE1	1.81	0.46
2:M:488:ASN:HB2	2:M:673:GLY:HA3	1.96	0.46
3:BH:2:SER:HB3	3:BH:107:GLY:HA2	1.98	0.46
1:J:40:ALA:HB1	1:J:191:MET:HB3	1.97	0.46
4:AD:54:GLY:HA2	4:AD:91:ILE:HG23	1.97	0.46
4:V:95:TYR:CZ	4:V:120:ILE:HG13	2.51	0.46
2:N:270:GLY:HA3	2:N:288:LEU:HB3	1.97	0.46
1:D:296:ALA:HB2	1:D:380:LEU:HD23	1.98	0.46
4:Z:54:GLY:HA2	4:Z:91:ILE:HG23	1.98	0.46
4:AB:95:TYR:CZ	4:AB:120:ILE:HG13	2.51	0.45
4:T:54:GLY:HA2	4:T:91:ILE:HG23	1.98	0.45
4:X:54:GLY:HA2	4:X:91:ILE:HG23	1.97	0.45
4:X:95:TYR:CZ	4:X:120:ILE:HG13	2.52	0.45
2:N:455:GLN:HG3	2:O:412:MET:HE1	1.98	0.45
1:C:331:ASN:HD22	4:X:177:GLN:HG2	1.81	0.45
1:G:86:ASP:HB2	1:G:307:LEU:HD12	1.98	0.45
2:O:9:THR:HG21	2:P:22:ARG:HD3	1.98	0.45
2:O:299:ALA:HB3	2:O:313:LEU:HB3	1.97	0.45
1:D:70:LEU:HG	1:D:74:LEU:HD23	1.98	0.45
1:G:207:TRP:HB2	1:G:237:ILE:HB	1.97	0.45
1:J:296:ALA:HB2	1:J:380:LEU:HD23	1.98	0.45
4:AA:174:ALA:HB2	4:AB:55:SER:HA	1.97	0.45
2:Q:270:GLY:HA3	2:Q:288:LEU:HB3	1.97	0.45
2:R:503:SER:HB3	2:R:535:TYR:HB2	1.99	0.45
2:O:344:LYS:HD2	2:O:365:PRO:HB3	1.99	0.45
3:AX:120:GLN:HA	3:AX:123:GLN:HG2	1.99	0.45
1:C:40:ALA:HB1	1:C:191:MET:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:GLU:CD	1:E:122:GLU:H	2.25	0.45
4:X:55:SER:HA	4:W:174:ALA:HB2	1.98	0.45
2:N:503:SER:HB3	2:N:535:TYR:HB2	1.98	0.45
1:E:394:ARG:HA	1:F:393:THR:HG21	1.98	0.45
1:K:37:ARG:HG3	1:K:204:PHE:CD1	2.52	0.45
1:K:122:GLU:CD	1:K:122:GLU:H	2.25	0.45
1:A:207:TRP:HB2	1:A:237:ILE:HB	1.97	0.45
2:N:132:ALA:HB2	2:N:277:PHE:CE1	2.52	0.45
1:D:250:LYS:HB3	1:D:250:LYS:HE2	1.80	0.44
4:AC:174:ALA:HB2	4:AD:55:SER:HA	1.99	0.44
1:A:122:GLU:H	1:A:122:GLU:CD	2.26	0.44
3:AY:2:SER:HB3	3:AY:107:GLY:HA2	1.99	0.44
1:C:207:TRP:HB2	1:C:237:ILE:HB	1.99	0.44
1:D:249:GLU:CD	1:D:249:GLU:H	2.24	0.44
1:E:40:ALA:HB1	1:E:191:MET:HB3	1.99	0.44
1:E:331:ASN:HD22	4:Z:177:GLN:HG2	1.82	0.44
1:F:480:LEU:HA	1:G:515:ILE:HD11	1.98	0.44
1:G:122:GLU:CD	1:G:122:GLU:H	2.25	0.44
1:I:207:TRP:HB2	1:I:237:ILE:HB	1.99	0.44
1:K:331:ASN:HD22	4:T:177:GLN:HG2	1.82	0.44
4:AD:95:TYR:CZ	4:AD:120:ILE:HG13	2.51	0.44
4:X:2:ILE:HG21	4:Y:88:ALA:HB3	1.98	0.44
4:Z:100:ILE:HD13	4:Z:100:ILE:H	1.81	0.44
2:M:270:GLY:HA3	2:M:288:LEU:HB3	1.99	0.44
3:AN:131:ALA:HB3	3:AN:134:LEU:HG	2.00	0.44
3:BG:120:GLN:HA	3:BG:123:GLN:HG2	1.99	0.44
1:C:122:GLU:H	1:C:122:GLU:CD	2.26	0.44
1:G:331:ASN:HD22	4:AB:177:GLN:HG2	1.81	0.44
2:Q:132:ALA:HB2	2:Q:277:PHE:CE1	2.53	0.44
1:H:124:GLY:O	1:H:523:ARG:HD2	2.17	0.44
2:O:503:SER:HB3	2:O:535:TYR:HB2	1.99	0.44
2:P:353:GLU:HG3	2:Q:352:VAL:HG22	1.98	0.44
1:B:207:TRP:HB2	1:B:237:ILE:HB	2.00	0.44
1:F:395:THR:H	1:G:393:THR:HG23	1.83	0.44
2:N:763:ASN:O	2:N:775:VAL:HG11	2.17	0.44
1:E:37:ARG:HG3	1:E:204:PHE:CD1	2.52	0.44
1:A:37:ARG:HG3	1:A:204:PHE:CD1	2.53	0.44
2:P:355:PRO:HG3	2:Q:362:TYR:HE1	1.82	0.44
1:B:124:GLY:O	1:B:523:ARG:HD2	2.18	0.44
1:L:445:PRO:HB2	1:L:448:ILE:HG23	2.00	0.44
1:A:323:MET:HG3	1:A:357:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:HD22	4:V:177:GLN:HG2	1.83	0.44
1:I:40:ALA:HB1	1:I:191:MET:HB3	1.99	0.44
1:L:207:TRP:HB2	1:L:237:ILE:HB	2.00	0.44
1:L:250:LYS:HE2	1:L:250:LYS:HB3	1.77	0.44
1:G:37:ARG:HG3	1:G:204:PHE:CD1	2.53	0.43
1:J:493:PRO:C	1:J:495:ALA:H	2.26	0.43
1:A:389:VAL:HA	1:L:402:ARG:NH1	2.34	0.43
1:A:493:PRO:C	1:A:495:ALA:H	2.26	0.43
2:N:349:SER:O	2:N:352:VAL:HG22	2.19	0.43
1:B:86:ASP:HB2	1:B:307:LEU:HD12	2.01	0.43
1:C:493:PRO:C	1:C:495:ALA:H	2.26	0.43
1:D:66:GLU:HG2	1:D:80:TYR:HE1	1.81	0.43
1:H:493:PRO:C	1:H:495:ALA:H	2.26	0.43
1:I:258:MET:HE2	1:I:262:LYS:HA	2.00	0.43
1:I:394:ARG:HE	1:I:402:ARG:HH21	1.64	0.43
4:X:174:ALA:HB2	4:Y:55:SER:HA	2.00	0.43
1:D:493:PRO:C	1:D:495:ALA:H	2.26	0.43
1:K:40:ALA:HB1	1:K:191:MET:HB3	1.99	0.43
4:T:100:ILE:HG22	4:T:101:GLN:H	1.83	0.43
2:P:353:GLU:CD	2:P:353:GLU:H	2.27	0.43
3:AW:101:THR:HG22	3:AW:103:SER:H	1.83	0.43
3:BP:120:GLN:HA	3:BP:123:GLN:HG2	2.01	0.43
1:B:66:GLU:HG2	1:B:80:TYR:HE1	1.81	0.43
1:I:122:GLU:CD	1:I:122:GLU:H	2.26	0.43
1:F:70:LEU:HG	1:F:74:LEU:HD23	2.01	0.43
1:L:70:LEU:HG	1:L:74:LEU:HD23	2.01	0.43
2:M:9:THR:HG21	2:N:22:ARG:HD2	2.01	0.43
2:R:488:ASN:HB2	2:R:673:GLY:HA3	2.00	0.43
3:AP:90:THR:HG21	3:AP:111:ARG:HD3	2.00	0.43
1:C:258:MET:HE2	1:C:262:LYS:HA	2.00	0.43
1:G:323:MET:HG3	1:G:357:PHE:HA	2.00	0.43
1:A:32:ARG:HH22	1:A:242:TRP:NE1	2.17	0.43
1:A:100:MET:HB3	1:A:104:MET:HE2	1.99	0.43
3:BO:131:ALA:HB3	3:BO:134:LEU:HG	2.00	0.43
1:G:394:ARG:HA	1:H:393:THR:HG23	2.01	0.43
1:H:37:ARG:HG3	1:H:204:PHE:CD1	2.54	0.43
4:W:93:VAL:HG13	4:W:119:LEU:HD11	2.00	0.43
2:Q:519:SER:HB3	2:Q:523:THR:HB	2.01	0.43
2:R:751:GLN:HG3	2:R:799:THR:HG23	2.01	0.43
3:AN:7:ASN:H	3:AN:7:ASN:ND2	2.17	0.43
1:F:490:LEU:HD21	1:G:481:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:344:LYS:HD2	2:M:365:PRO:HB3	2.00	0.43
2:N:519:SER:HB3	2:N:523:THR:HB	2.01	0.43
2:P:9:THR:HG21	2:Q:22:ARG:HD2	2.00	0.43
1:G:493:PRO:C	1:G:495:ALA:H	2.26	0.43
1:K:338:ARG:HG3	1:K:339:PRO:HD2	2.01	0.43
2:M:20:PHE:CZ	2:M:33:ARG:HG3	2.54	0.43
1:B:445:PRO:HB2	1:B:448:ILE:HG23	2.01	0.43
1:F:445:PRO:HB2	1:F:448:ILE:HG23	2.00	0.43
1:G:490:LEU:HD12	1:H:509:LEU:HD11	2.01	0.43
4:AC:54:GLY:HA2	4:AC:91:ILE:HG23	2.01	0.43
4:X:100:ILE:HG12	4:X:117:PHE:HE1	1.83	0.43
2:Q:299:ALA:HB3	2:Q:313:LEU:HB3	2.01	0.42
1:B:493:PRO:C	1:B:495:ALA:H	2.27	0.42
2:O:488:ASN:HB2	2:O:673:GLY:HA3	2.00	0.42
3:AO:120:GLN:HA	3:AO:123:GLN:HG2	2.00	0.42
1:E:86:ASP:HB2	1:E:307:LEU:HD12	2.01	0.42
1:E:338:ARG:HG3	1:E:339:PRO:HD2	2.01	0.42
1:E:493:PRO:C	1:E:495:ALA:H	2.27	0.42
1:H:86:ASP:HB2	1:H:307:LEU:HD12	2.01	0.42
1:H:207:TRP:HB2	1:H:237:ILE:HB	2.00	0.42
4:T:174:ALA:HB2	4:U:55:SER:HA	2.01	0.42
1:A:481:LEU:HD23	1:L:490:LEU:HD21	2.01	0.42
1:B:37:ARG:HG3	1:B:204:PHE:CD1	2.54	0.42
1:H:401:ILE:HD13	1:H:401:ILE:HA	1.91	0.42
2:N:379:ILE:O	2:N:382:GLN:HG2	2.19	0.42
2:P:270:GLY:HA3	2:P:288:LEU:HB3	2.00	0.42
3:AG:131:ALA:HB3	3:AG:134:LEU:HG	2.02	0.42
1:K:330:PHE:CE2	1:L:342:ILE:HD11	2.55	0.42
2:O:429:PRO:HG2	2:O:432:ILE:HB	2.01	0.42
3:AE:108:ASP:HB3	3:AF:109:PHE:CE1	2.55	0.42
1:G:32:ARG:HH22	1:G:242:TRP:NE1	2.17	0.42
1:G:100:MET:HB3	1:G:104:MET:HE2	2.00	0.42
1:J:207:TRP:HB2	1:J:237:ILE:HB	2.01	0.42
2:P:503:SER:HB3	2:P:535:TYR:HB2	2.01	0.42
3:BZ:131:ALA:HB3	3:BZ:134:LEU:HG	2.01	0.42
1:B:330:PHE:CE2	1:C:342:ILE:HD11	2.55	0.42
1:F:493:PRO:C	1:F:495:ALA:H	2.27	0.42
1:I:493:PRO:C	1:I:495:ALA:H	2.26	0.42
1:L:524:GLU:CD	1:L:524:GLU:H	2.27	0.42
4:Z:75:PRO:HG3	4:Z:83:GLU:HG2	2.02	0.42
4:Z:174:ALA:HB2	4:AA:55:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:429:PRO:HG2	2:Q:432:ILE:HB	2.02	0.42
2:R:429:PRO:HG2	2:R:432:ILE:HB	2.02	0.42
3:AP:85:MET:HE3	3:AP:115:MET:HG3	2.02	0.42
1:H:330:PHE:CE2	1:I:342:ILE:HD11	2.55	0.42
1:F:207:TRP:HB2	1:F:237:ILE:HB	2.00	0.42
1:J:297:TYR:CD2	1:J:298:PRO:HD3	2.55	0.42
2:M:503:SER:HB3	2:M:535:TYR:HB2	2.01	0.42
2:N:429:PRO:HG2	2:N:432:ILE:HB	2.02	0.42
2:R:4:ARG:HD2	2:R:725:THR:HG22	2.01	0.42
1:K:186:PRO:HA	1:K:187:PRO:HD3	1.93	0.42
1:K:493:PRO:C	1:K:495:ALA:H	2.27	0.42
2:M:611:GLN:HB2	2:M:613:TRP:CE2	2.55	0.42
2:O:751:GLN:HG3	2:O:799:THR:HG23	2.01	0.42
1:D:297:TYR:CD2	1:D:298:PRO:HD3	2.55	0.42
1:E:241:ALA:HB3	1:E:275:TRP:HZ3	1.85	0.42
1:E:330:PHE:CE2	1:F:342:ILE:HD11	2.54	0.42
1:F:336:THR:HG22	1:F:338:ARG:HG2	2.01	0.42
1:F:397:THR:HG21	1:G:396:ALA:HB2	2.02	0.42
1:K:86:ASP:HB2	1:K:307:LEU:HD12	2.01	0.42
4:AC:93:VAL:HG13	4:AC:119:LEU:HD11	2.01	0.42
1:A:40:ALA:HB1	1:A:191:MET:HB3	2.02	0.41
3:AP:39:TRP:HZ2	4:V:1:MET:HG2	1.84	0.41
3:AX:88:ASP:HB2	3:AY:6:ILE:O	2.20	0.41
1:C:353:PRO:HG2	1:C:355:LYS:HZ1	1.85	0.41
3:BY:88:ASP:HB2	3:BZ:6:ILE:O	2.20	0.41
1:D:186:PRO:HA	1:D:187:PRO:HD3	1.94	0.41
1:F:524:GLU:H	1:F:524:GLU:CD	2.27	0.41
4:AB:162:GLN:H	4:AB:162:GLN:HG2	1.49	0.41
2:Q:379:ILE:O	2:Q:382:GLN:HG2	2.20	0.41
4:AD:67:ILE:HG22	4:AD:84:CYS:HB2	2.03	0.41
2:P:611:GLN:HB2	2:P:613:TRP:CE2	2.55	0.41
3:AO:26:ILE:HD11	3:AO:67:ILE:HG12	2.02	0.41
1:H:66:GLU:HG2	1:H:80:TYR:HE1	1.81	0.41
1:H:445:PRO:HB2	1:H:448:ILE:HG23	2.01	0.41
1:I:32:ARG:HH22	1:I:242:TRP:NE1	2.18	0.41
1:I:353:PRO:HG2	1:I:355:LYS:HZ1	1.86	0.41
4:V:99:ASN:HB3	4:V:185:ARG:NE	2.22	0.41
4:W:11:LYS:HE3	4:W:45:TYR:CD1	2.56	0.41
2:N:299:ALA:HB3	2:N:313:LEU:HB3	2.01	0.41
2:R:20:PHE:CZ	2:R:33:ARG:HG3	2.55	0.41
3:AN:7:ASN:OD1	4:W:126:PRO:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BX:94:SER:H	3:BX:98:SER:HB2	1.85	0.41
3:BX:108:ASP:HB3	3:BY:109:PHE:CE1	2.55	0.41
1:C:124:GLY:O	1:C:523:ARG:HD2	2.21	0.41
1:G:40:ALA:HB1	1:G:191:MET:HB3	2.02	0.41
1:J:402:ARG:NH2	1:K:389:VAL:HA	2.36	0.41
4:AC:11:LYS:HE3	4:AC:45:TYR:CD1	2.55	0.41
2:M:379:ILE:O	2:M:382:GLN:HG2	2.21	0.41
2:P:419:ASP:CG	2:P:420:TYR:H	2.29	0.41
1:D:207:TRP:HB2	1:D:237:ILE:HB	2.01	0.41
1:E:490:LEU:HD21	1:F:481:LEU:HD23	2.03	0.41
1:I:394:ARG:HE	1:I:402:ARG:NH2	2.18	0.41
1:J:524:GLU:CD	1:J:524:GLU:H	2.28	0.41
1:K:323:MET:HG3	1:K:357:PHE:HA	2.03	0.41
1:A:490:LEU:HD12	1:B:509:LEU:HD11	2.01	0.41
2:P:302:TYR:CD2	2:Q:174:VAL:HG12	2.55	0.41
2:Q:283:ILE:HG13	2:Q:296:LEU:HG	2.02	0.41
3:AX:94:SER:O	3:AY:102:GLY:HA3	2.21	0.41
1:E:209:GLN:HB3	1:E:234:LYS:HG2	2.03	0.41
1:E:323:MET:HG3	1:E:357:PHE:HA	2.03	0.41
1:H:439:GLU:CD	1:H:439:GLU:H	2.29	0.41
1:A:342:ILE:HD11	1:L:330:PHE:CE2	2.56	0.41
2:Q:67:VAL:HG12	2:Q:69:GLN:HG3	2.03	0.41
2:Q:558:ASP:OD1	2:Q:583:GLY:HA3	2.21	0.41
1:B:186:PRO:HA	1:B:187:PRO:HD3	1.94	0.41
1:B:250:LYS:HE2	1:B:250:LYS:HB3	1.78	0.41
1:D:524:GLU:CD	1:D:524:GLU:H	2.28	0.41
1:A:396:ALA:HA	1:A:399:ALA:HB3	2.02	0.41
2:M:133:HIS:CD2	2:N:326:GLN:H	2.30	0.41
2:M:558:ASP:OD1	2:M:583:GLY:HA3	2.20	0.41
2:O:20:PHE:CZ	2:O:33:ARG:HG3	2.55	0.41
3:AO:94:SER:O	3:AP:102:GLY:HA3	2.21	0.41
3:BG:88:ASP:HB2	3:BH:6:ILE:O	2.20	0.41
1:C:32:ARG:HH22	1:C:242:TRP:NE1	2.18	0.41
1:C:209:GLN:HB3	1:C:234:LYS:HG2	2.03	0.41
1:E:499:SER:O	1:F:520:ILE:HG13	2.21	0.41
1:G:499:SER:O	1:H:520:ILE:HG13	2.21	0.41
1:H:250:LYS:HE2	1:H:250:LYS:HB3	1.78	0.41
1:H:430:LEU:HD23	1:H:430:LEU:HA	1.91	0.41
1:I:186:PRO:HA	1:I:187:PRO:HD3	1.94	0.41
1:L:66:GLU:HG2	1:L:80:TYR:HE1	1.86	0.41
1:L:122:GLU:CD	1:L:122:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:439:GLU:CD	1:L:439:GLU:H	2.29	0.41
1:L:493:PRO:C	1:L:495:ALA:H	2.27	0.41
4:AC:131:PRO:HA	4:AC:132:PRO:HD3	1.99	0.41
1:A:124:GLY:O	1:A:523:ARG:HD2	2.22	0.41
2:M:302:TYR:CD2	2:N:174:VAL:HG12	2.55	0.41
2:N:67:VAL:HG12	2:N:69:GLN:HG3	2.03	0.41
2:O:547:LEU:HD23	2:O:634:ILE:HG22	2.03	0.41
3:AF:88:ASP:HB2	3:AG:6:ILE:O	2.20	0.41
3:BP:26:ILE:HD11	3:BP:67:ILE:HG12	2.03	0.41
1:B:122:GLU:CD	1:B:122:GLU:H	2.29	0.41
1:I:241:ALA:HA	1:I:254:GLN:O	2.21	0.41
1:K:490:LEU:HD21	1:L:481:LEU:HD23	2.03	0.41
4:U:70:ILE:HG22	4:U:82:TYR:HB3	2.03	0.41
1:A:499:SER:O	1:B:520:ILE:HG13	2.21	0.40
2:O:4:ARG:HD2	2:O:725:THR:HG22	2.03	0.40
2:P:379:ILE:O	2:P:382:GLN:HG2	2.21	0.40
2:R:412:MET:HE3	2:R:412:MET:HB2	1.99	0.40
1:C:297:TYR:CD2	1:C:298:PRO:HD3	2.57	0.40
1:D:122:GLU:H	1:D:122:GLU:CD	2.30	0.40
1:F:297:TYR:CD2	1:F:298:PRO:HD3	2.56	0.40
1:F:401:ILE:HD13	1:F:401:ILE:HA	1.93	0.40
4:AA:54:GLY:HA2	4:AA:91:ILE:HG23	2.03	0.40
2:M:419:ASP:CG	2:M:420:TYR:H	2.29	0.40
3:AG:85:MET:HE3	3:AG:115:MET:HG3	2.03	0.40
3:AN:26:ILE:HD11	3:AN:67:ILE:HG12	2.03	0.40
3:AX:149:PRO:HG3	3:AX:167:GLU:HA	2.03	0.40
1:C:37:ARG:HG3	1:C:204:PHE:CD1	2.56	0.40
1:I:37:ARG:HG3	1:I:204:PHE:CD1	2.56	0.40
1:K:209:GLN:HB3	1:K:234:LYS:HG2	2.04	0.40
1:L:297:TYR:CD2	1:L:298:PRO:HD3	2.56	0.40
2:Q:285:GLY:HA3	2:Q:294:VAL:HG12	2.03	0.40
2:Q:419:ASP:CG	2:Q:420:TYR:H	2.29	0.40
3:BG:116:MET:HG3	3:BH:116:MET:SD	2.62	0.40
1:B:439:GLU:CD	1:B:439:GLU:H	2.30	0.40
1:E:159:LEU:O	1:E:162:VAL:HG12	2.22	0.40
1:E:186:PRO:HA	1:E:187:PRO:HD3	1.93	0.40
1:F:430:LEU:HD23	1:F:430:LEU:HA	1.93	0.40
1:K:499:SER:O	1:L:520:ILE:HG13	2.21	0.40
4:X:27:THR:OG1	4:X:30:THR:HG22	2.22	0.40
2:N:285:GLY:HA3	2:N:294:VAL:HG12	2.03	0.40
2:P:344:LYS:HD2	2:P:365:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP:149:PRO:HG3	3:BP:167:GLU:HA	2.02	0.40
1:C:250:LYS:HG3	1:C:251:GLU:HG2	2.03	0.40
1:D:397:THR:HG21	1:E:396:ALA:HA	2.04	0.40
1:F:439:GLU:CD	1:F:439:GLU:H	2.29	0.40
1:I:124:GLY:O	1:I:523:ARG:HD2	2.21	0.40
1:J:250:LYS:HB3	1:J:250:LYS:HE2	1.81	0.40
4:AA:159:ARG:HD2	4:AA:159:ARG:HA	1.88	0.40
2:O:666:THR:HG22	2:O:696:GLU:HG2	2.04	0.40
2:P:547:LEU:HD23	2:P:634:ILE:HG22	2.02	0.40
3:AG:90:THR:HG21	3:AG:111:ARG:HD3	2.03	0.40
3:AO:149:PRO:HG3	3:AO:167:GLU:HA	2.03	0.40
3:BQ:2:SER:HB3	3:BQ:107:GLY:HA2	2.03	0.40
1:C:499:SER:O	1:D:520:ILE:HG13	2.22	0.40
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.94	0.40
1:D:439:GLU:CD	1:D:439:GLU:H	2.28	0.40
1:I:297:TYR:CD2	1:I:298:PRO:HD3	2.57	0.40
4:X:100:ILE:HG12	4:X:117:PHE:CE1	2.57	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	517/554 (93%)	498 (96%)	19 (4%)	0	100	100
1	B	517/554 (93%)	494 (96%)	23 (4%)	0	100	100
1	C	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	D	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	E	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	F	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	G	517/554 (93%)	493 (95%)	24 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	517/554 (93%)	496 (96%)	21 (4%)	0	100	100
1	I	517/554 (93%)	496 (96%)	21 (4%)	0	100	100
1	J	517/554 (93%)	494 (96%)	23 (4%)	0	100	100
1	K	517/554 (93%)	497 (96%)	20 (4%)	0	100	100
1	L	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
2	M	815/818 (100%)	790 (97%)	24 (3%)	1 (0%)	48	40
2	N	815/818 (100%)	791 (97%)	24 (3%)	0	100	100
2	O	815/818 (100%)	788 (97%)	27 (3%)	0	100	100
2	P	815/818 (100%)	791 (97%)	23 (3%)	1 (0%)	48	40
2	Q	815/818 (100%)	792 (97%)	23 (3%)	0	100	100
2	R	815/818 (100%)	790 (97%)	25 (3%)	0	100	100
3	AE	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AF	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	AG	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AN	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AO	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AP	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AW	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AX	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AY	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BF	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BG	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BH	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BO	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BP	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BQ	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BX	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BY	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BZ	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
4	AA	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	AB	191/201 (95%)	188 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AC	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	AD	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	S	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	T	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	U	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	V	191/201 (95%)	188 (98%)	3 (2%)	0	100	100
4	W	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	X	191/201 (95%)	189 (99%)	2 (1%)	0	100	100
4	Y	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	Z	191/201 (95%)	189 (99%)	2 (1%)	0	100	100
All	All	16446/25812 (64%)	15967 (97%)	477 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	337	ILE
2	P	337	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	440/473 (93%)	417 (95%)	23 (5%)	21	13
1	B	440/473 (93%)	424 (96%)	16 (4%)	31	23
1	C	440/473 (93%)	413 (94%)	27 (6%)	17	9
1	D	440/473 (93%)	419 (95%)	21 (5%)	23	15
1	E	440/473 (93%)	417 (95%)	23 (5%)	21	13
1	F	440/473 (93%)	419 (95%)	21 (5%)	23	15
1	G	440/473 (93%)	418 (95%)	22 (5%)	22	14
1	H	440/473 (93%)	421 (96%)	19 (4%)	26	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	440/473 (93%)	415 (94%)	25 (6%)	18	11
1	J	440/473 (93%)	418 (95%)	22 (5%)	22	14
1	K	440/473 (93%)	418 (95%)	22 (5%)	22	14
1	L	440/473 (93%)	421 (96%)	19 (4%)	26	18
2	M	694/695 (100%)	681 (98%)	13 (2%)	50	47
2	N	694/695 (100%)	682 (98%)	12 (2%)	53	52
2	O	694/695 (100%)	685 (99%)	9 (1%)	61	61
2	P	694/695 (100%)	680 (98%)	14 (2%)	48	46
2	Q	694/695 (100%)	682 (98%)	12 (2%)	53	52
2	R	694/695 (100%)	681 (98%)	13 (2%)	50	47
3	AE	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	AF	144/532 (27%)	141 (98%)	3 (2%)	47	44
3	AG	144/532 (27%)	143 (99%)	1 (1%)	76	78
3	AN	144/532 (27%)	141 (98%)	3 (2%)	47	44
3	AO	144/532 (27%)	141 (98%)	3 (2%)	47	44
3	AP	144/532 (27%)	143 (99%)	1 (1%)	76	78
3	AW	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	AX	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	AY	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	BF	144/532 (27%)	139 (96%)	5 (4%)	32	24
3	BG	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	BH	144/532 (27%)	141 (98%)	3 (2%)	47	44
3	BO	144/532 (27%)	140 (97%)	4 (3%)	38	32
3	BP	144/532 (27%)	141 (98%)	3 (2%)	47	44
3	BQ	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	BX	144/532 (27%)	143 (99%)	1 (1%)	76	78
3	BY	144/532 (27%)	142 (99%)	2 (1%)	59	59
3	BZ	144/532 (27%)	140 (97%)	4 (3%)	38	32
4	AA	169/176 (96%)	163 (96%)	6 (4%)	31	23
4	AB	169/176 (96%)	162 (96%)	7 (4%)	27	19
4	AC	169/176 (96%)	165 (98%)	4 (2%)	43	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	169/176 (96%)	162 (96%)	7 (4%)	27	19
4	S	169/176 (96%)	162 (96%)	7 (4%)	27	19
4	T	169/176 (96%)	164 (97%)	5 (3%)	36	30
4	U	169/176 (96%)	163 (96%)	6 (4%)	31	23
4	V	169/176 (96%)	165 (98%)	4 (2%)	43	38
4	W	169/176 (96%)	163 (96%)	6 (4%)	31	23
4	X	169/176 (96%)	165 (98%)	4 (2%)	43	38
4	Y	169/176 (96%)	163 (96%)	6 (4%)	31	23
4	Z	169/176 (96%)	159 (94%)	10 (6%)	18	10
All	All	14064/21534 (65%)	13614 (97%)	450 (3%)	35	27

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	127	LEU
1	A	129	GLN
1	A	146	ILE
1	A	190	VAL
1	A	212	ILE
1	A	214	ASN
1	A	224	VAL
1	A	249	GLU
1	A	254	GLN
1	A	262	LYS
1	A	338	ARG
1	A	394	ARG
1	A	397	THR
1	A	405	GLU
1	A	408	GLU
1	A	439	GLU
1	A	448	ILE
1	A	494	GLU
1	A	500	LEU
1	A	506	LEU
1	A	515	ILE
1	A	529	LEU
2	M	3	ILE
2	M	12	ARG

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Mol	Chain	Res	Type
2	M	67	VAL
2	M	257	ASN
2	M	361	VAL
2	M	526	ILE
2	M	598	LEU
2	M	623	VAL
2	M	721	LEU
2	M	763	ASN
2	M	770	THR
2	M	775	VAL
2	M	783	ARG
2	N	12	ARG
2	N	67	VAL
2	N	353	GLU
2	N	361	VAL
2	N	408	LEU
2	N	526	ILE
2	N	598	LEU
2	N	726	GLN
2	N	763	ASN
2	N	770	THR
2	N	775	VAL
2	N	783	ARG
2	O	9	THR
2	O	12	ARG
2	O	67	VAL
2	O	353	GLU
2	O	526	ILE
2	O	598	LEU
2	O	763	ASN
2	O	770	THR
2	O	775	VAL
2	P	12	ARG
2	P	67	VAL
2	P	257	ASN
2	P	353	GLU
2	P	452	LEU
2	P	526	ILE
2	P	598	LEU
2	P	622	THR
2	P	721	LEU
2	P	763	ASN

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Mol	Chain	Res	Type
2	P	766	LEU
2	P	770	THR
2	P	775	VAL
2	P	783	ARG
2	Q	67	VAL
2	Q	353	GLU
2	Q	361	VAL
2	Q	397	MET
2	Q	408	LEU
2	Q	435	ARG
2	Q	452	LEU
2	Q	526	ILE
2	Q	598	LEU
2	Q	622	THR
2	Q	763	ASN
2	Q	770	THR
2	R	12	ARG
2	R	67	VAL
2	R	353	GLU
2	R	361	VAL
2	R	435	ARG
2	R	453	GLN
2	R	526	ILE
2	R	598	LEU
2	R	622	THR
2	R	763	ASN
2	R	770	THR
2	R	775	VAL
2	R	783	ARG
3	AE	98	SER
3	AE	136	VAL
3	AF	105	LEU
3	AF	136	VAL
3	AF	146	ARG
3	AG	34	GLU
3	AN	98	SER
3	AN	136	VAL
3	AN	146	ARG
3	AO	136	VAL
3	AO	146	ARG
3	AO	172	ASP
3	AP	34	GLU

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Mol	Chain	Res	Type
3	AW	98	SER
3	AW	136	VAL
3	AX	136	VAL
3	AX	146	ARG
3	AY	34	GLU
3	AY	171	ILE
3	BF	4	ILE
3	BF	98	SER
3	BF	111	ARG
3	BF	136	VAL
3	BF	146	ARG
3	BG	136	VAL
3	BG	172	ASP
3	BH	34	GLU
3	BH	171	ILE
3	BH	173	GLU
3	BO	98	SER
3	BO	136	VAL
3	BO	146	ARG
3	BO	172	ASP
3	BP	136	VAL
3	BP	146	ARG
3	BP	172	ASP
3	BQ	34	GLU
3	BQ	136	VAL
3	BX	136	VAL
3	BY	136	VAL
3	BY	146	ARG
3	BZ	34	GLU
3	BZ	92	ILE
3	BZ	136	VAL
3	BZ	173	GLU
1	B	190	VAL
1	B	249	GLU
1	B	262	LYS
1	B	368	LEU
1	B	402	ARG
1	B	408	GLU
1	B	439	GLU
1	B	448	ILE
1	B	494	GLU
1	B	500	LEU

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Mol	Chain	Res	Type
1	B	506	LEU
1	B	515	ILE
1	B	524	GLU
1	B	529	LEU
1	B	531	GLN
1	B	546	VAL
1	C	70	LEU
1	C	127	LEU
1	C	129	GLN
1	C	146	ILE
1	C	190	VAL
1	C	205	ARG
1	C	212	ILE
1	C	214	ASN
1	C	224	VAL
1	C	249	GLU
1	C	254	GLN
1	C	262	LYS
1	C	338	ARG
1	C	386	LEU
1	C	394	ARG
1	C	395	THR
1	C	397	THR
1	C	407	LEU
1	C	408	GLU
1	C	439	GLU
1	C	448	ILE
1	C	494	GLU
1	C	500	LEU
1	C	506	LEU
1	C	515	ILE
1	C	529	LEU
1	C	548	ILE
1	D	70	LEU
1	D	122	GLU
1	D	127	LEU
1	D	146	ILE
1	D	190	VAL
1	D	249	GLU
1	D	262	LYS
1	D	338	ARG
1	D	368	LEU

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Mol	Chain	Res	Type
1	D	398	GLU
1	D	408	GLU
1	D	439	GLU
1	D	448	ILE
1	D	494	GLU
1	D	500	LEU
1	D	506	LEU
1	D	515	ILE
1	D	524	GLU
1	D	527	GLU
1	D	529	LEU
1	D	546	VAL
1	E	66	GLU
1	E	70	LEU
1	E	127	LEU
1	E	129	GLN
1	E	146	ILE
1	E	190	VAL
1	E	212	ILE
1	E	214	ASN
1	E	224	VAL
1	E	254	GLN
1	E	262	LYS
1	E	338	ARG
1	E	386	LEU
1	E	398	GLU
1	E	407	LEU
1	E	408	GLU
1	E	439	GLU
1	E	448	ILE
1	E	494	GLU
1	E	500	LEU
1	E	506	LEU
1	E	515	ILE
1	E	529	LEU
1	F	70	LEU
1	F	122	GLU
1	F	127	LEU
1	F	146	ILE
1	F	190	VAL
1	F	249	GLU
1	F	262	LYS

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Mol	Chain	Res	Type
1	F	368	LEU
1	F	389	VAL
1	F	394	ARG
1	F	398	GLU
1	F	408	GLU
1	F	439	GLU
1	F	448	ILE
1	F	494	GLU
1	F	500	LEU
1	F	506	LEU
1	F	515	ILE
1	F	524	GLU
1	F	527	GLU
1	F	529	LEU
1	G	66	GLU
1	G	127	LEU
1	G	129	GLN
1	G	146	ILE
1	G	190	VAL
1	G	212	ILE
1	G	214	ASN
1	G	224	VAL
1	G	249	GLU
1	G	254	GLN
1	G	262	LYS
1	G	338	ARG
1	G	386	LEU
1	G	397	THR
1	G	408	GLU
1	G	439	GLU
1	G	448	ILE
1	G	494	GLU
1	G	500	LEU
1	G	506	LEU
1	G	515	ILE
1	G	529	LEU
1	H	70	LEU
1	H	127	LEU
1	H	146	ILE
1	H	190	VAL
1	H	249	GLU
1	H	262	LYS

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Mol	Chain	Res	Type
1	H	338	ARG
1	H	368	LEU
1	H	389	VAL
1	H	393	THR
1	H	408	GLU
1	H	439	GLU
1	H	448	ILE
1	H	494	GLU
1	H	500	LEU
1	H	506	LEU
1	H	515	ILE
1	H	524	GLU
1	H	529	LEU
1	I	70	LEU
1	I	127	LEU
1	I	129	GLN
1	I	146	ILE
1	I	190	VAL
1	I	205	ARG
1	I	212	ILE
1	I	214	ASN
1	I	224	VAL
1	I	249	GLU
1	I	254	GLN
1	I	262	LYS
1	I	338	ARG
1	I	394	ARG
1	I	395	THR
1	I	397	THR
1	I	407	LEU
1	I	408	GLU
1	I	439	GLU
1	I	448	ILE
1	I	494	GLU
1	I	500	LEU
1	I	506	LEU
1	I	515	ILE
1	I	529	LEU
1	J	70	LEU
1	J	122	GLU
1	J	127	LEU
1	J	146	ILE

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Mol	Chain	Res	Type
1	J	190	VAL
1	J	249	GLU
1	J	262	LYS
1	J	338	ARG
1	J	368	LEU
1	J	394	ARG
1	J	408	GLU
1	J	439	GLU
1	J	448	ILE
1	J	494	GLU
1	J	500	LEU
1	J	506	LEU
1	J	515	ILE
1	J	524	GLU
1	J	527	GLU
1	J	529	LEU
1	J	531	GLN
1	J	546	VAL
1	K	66	GLU
1	K	70	LEU
1	K	127	LEU
1	K	129	GLN
1	K	146	ILE
1	K	190	VAL
1	K	212	ILE
1	K	214	ASN
1	K	224	VAL
1	K	254	GLN
1	K	262	LYS
1	K	338	ARG
1	K	402	ARG
1	K	407	LEU
1	K	408	GLU
1	K	439	GLU
1	K	448	ILE
1	K	494	GLU
1	K	500	LEU
1	K	506	LEU
1	K	515	ILE
1	K	529	LEU
1	L	70	LEU
1	L	127	LEU

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Mol	Chain	Res	Type
1	L	146	ILE
1	L	190	VAL
1	L	249	GLU
1	L	262	LYS
1	L	368	LEU
1	L	394	ARG
1	L	407	LEU
1	L	408	GLU
1	L	439	GLU
1	L	448	ILE
1	L	494	GLU
1	L	500	LEU
1	L	506	LEU
1	L	515	ILE
1	L	524	GLU
1	L	529	LEU
1	L	531	GLN
4	T	4	LEU
4	T	55	SER
4	T	91	ILE
4	T	170	ARG
4	T	177	GLN
4	AC	73	LEU
4	AC	91	ILE
4	AC	155	ARG
4	AC	157	LEU
4	AD	4	LEU
4	AD	42	GLU
4	AD	91	ILE
4	AD	100	ILE
4	AD	170	ARG
4	AD	177	GLN
4	AD	180	VAL
4	S	22	VAL
4	S	39	ILE
4	S	73	LEU
4	S	91	ILE
4	S	115	GLN
4	S	155	ARG
4	S	157	LEU
4	X	91	ILE
4	X	100	ILE

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Mol	Chain	Res	Type
4	X	177	GLN
4	X	180	VAL
4	U	22	VAL
4	U	73	LEU
4	U	91	ILE
4	U	155	ARG
4	U	157	LEU
4	U	159	ARG
4	V	76	THR
4	V	91	ILE
4	V	170	ARG
4	V	177	GLN
4	W	22	VAL
4	W	57	ARG
4	W	73	LEU
4	W	91	ILE
4	W	155	ARG
4	W	157	LEU
4	Y	22	VAL
4	Y	52	GLU
4	Y	73	LEU
4	Y	91	ILE
4	Y	155	ARG
4	Y	157	LEU
4	Z	42	GLU
4	Z	52	GLU
4	Z	55	SER
4	Z	69	ILE
4	Z	76	THR
4	Z	91	ILE
4	Z	99	ASN
4	Z	100	ILE
4	Z	170	ARG
4	Z	177	GLN
4	AA	22	VAL
4	AA	39	ILE
4	AA	73	LEU
4	AA	91	ILE
4	AA	157	LEU
4	AA	159	ARG
4	AB	4	LEU
4	AB	91	ILE

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Mol	Chain	Res	Type
4	AB	99	ASN
4	AB	162	GLN
4	AB	170	ARG
4	AB	177	GLN
4	AB	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	79	GLN
1	A	110	GLN
1	A	129	GLN
1	A	141	HIS
1	A	193	GLN
1	A	349	GLN
2	M	63	ASN
2	M	133	HIS
2	M	359	ASN
2	M	480	HIS
2	M	580	ASN
2	N	63	ASN
2	N	182	GLN
2	N	359	ASN
2	N	360	ASN
2	N	480	HIS
2	N	703	ASN
2	O	63	ASN
2	O	348	GLN
2	O	480	HIS
2	O	580	ASN
2	O	604	GLN
2	O	703	ASN
2	O	778	GLN
2	P	63	ASN
2	P	133	HIS
2	P	348	GLN
2	P	480	HIS
2	P	580	ASN
2	Q	63	ASN
2	Q	147	GLN
2	Q	182	GLN

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Mol	Chain	Res	Type
2	Q	343	ASN
2	Q	348	GLN
2	Q	368	GLN
2	Q	480	HIS
2	Q	580	ASN
2	Q	703	ASN
2	R	63	ASN
2	R	206	HIS
2	R	480	HIS
2	R	580	ASN
2	R	599	ASN
2	R	604	GLN
2	R	703	ASN
3	AE	11	GLN
3	AE	123	GLN
3	AE	129	GLN
3	AF	129	GLN
3	AG	129	GLN
3	AN	7	ASN
3	AN	11	GLN
3	AN	129	GLN
3	AO	99	ASN
3	AO	129	GLN
3	AP	123	GLN
3	AP	129	GLN
3	AW	129	GLN
3	AX	129	GLN
3	AY	129	GLN
3	BF	11	GLN
3	BF	129	GLN
3	BG	129	GLN
3	BH	129	GLN
3	BO	11	GLN
3	BO	82	GLN
3	BO	129	GLN
3	BP	129	GLN
3	BQ	129	GLN
3	BX	11	GLN
3	BX	123	GLN
3	BX	129	GLN
3	BY	129	GLN
3	BZ	129	GLN

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Mol	Chain	Res	Type
1	B	79	GLN
1	B	141	HIS
1	B	193	GLN
1	B	349	GLN
1	B	450	ASN
1	B	543	GLN
1	C	67	ASN
1	C	79	GLN
1	C	107	GLN
1	C	110	GLN
1	C	129	GLN
1	C	141	HIS
1	C	193	GLN
1	C	254	GLN
1	C	349	GLN
1	D	79	GLN
1	D	103	ASN
1	D	193	GLN
1	D	349	GLN
1	D	419	ASN
1	D	450	ASN
1	D	531	GLN
1	D	535	GLN
1	D	543	GLN
1	E	67	ASN
1	E	79	GLN
1	E	110	GLN
1	E	129	GLN
1	E	141	HIS
1	E	193	GLN
1	E	349	GLN
1	F	67	ASN
1	F	78	GLN
1	F	79	GLN
1	F	103	ASN
1	F	141	HIS
1	F	349	GLN
1	F	450	ASN
1	F	531	GLN
1	F	535	GLN
1	G	67	ASN
1	G	79	GLN

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Mol	Chain	Res	Type
1	G	110	GLN
1	G	129	GLN
1	G	141	HIS
1	G	193	GLN
1	G	349	GLN
1	H	79	GLN
1	H	141	HIS
1	H	193	GLN
1	H	349	GLN
1	H	531	GLN
1	H	535	GLN
1	I	67	ASN
1	I	79	GLN
1	I	107	GLN
1	I	110	GLN
1	I	129	GLN
1	I	141	HIS
1	I	193	GLN
1	I	254	GLN
1	I	349	GLN
1	J	79	GLN
1	J	103	ASN
1	J	193	GLN
1	J	349	GLN
1	J	418	GLN
1	J	450	ASN
1	J	543	GLN
1	K	67	ASN
1	K	110	GLN
1	K	129	GLN
1	K	141	HIS
1	K	193	GLN
1	K	349	GLN
1	L	67	ASN
1	L	78	GLN
1	L	79	GLN
1	L	103	ASN
1	L	141	HIS
1	L	333	GLN
1	L	349	GLN
1	L	450	ASN
1	L	543	GLN

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Mol	Chain	Res	Type
4	T	99	ASN
4	T	101	GLN
4	T	186	HIS
4	AC	62	GLN
4	AC	94	GLN
4	AD	99	ASN
4	AD	101	GLN
4	S	62	GLN
4	S	94	GLN
4	X	99	ASN
4	X	101	GLN
4	X	186	HIS
4	U	62	GLN
4	U	94	GLN
4	W	62	GLN
4	W	94	GLN
4	W	186	HIS
4	Y	62	GLN
4	Y	94	GLN
4	Z	101	GLN
4	AA	62	GLN
4	AA	94	GLN
4	AA	186	HIS
4	AB	62	GLN
4	AB	94	GLN
4	AB	186	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

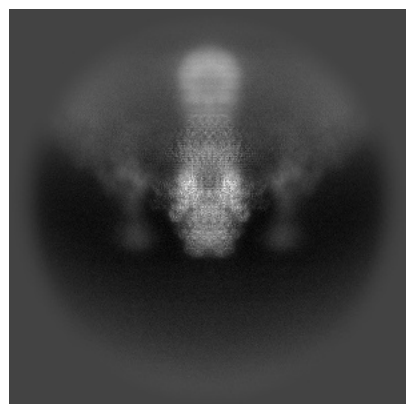
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47975. These allow visual inspection of the internal detail of the map and identification of artifacts.

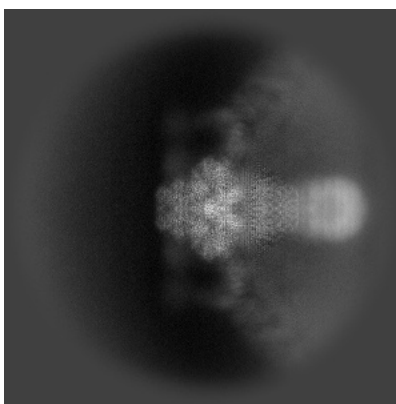
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

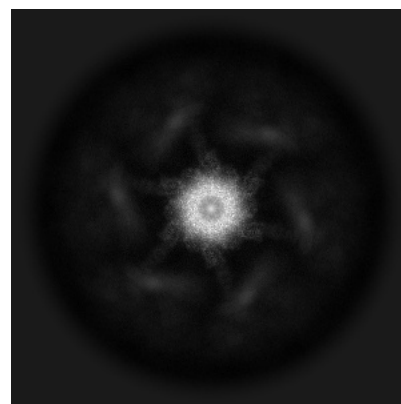
6.1.1 Primary map



X

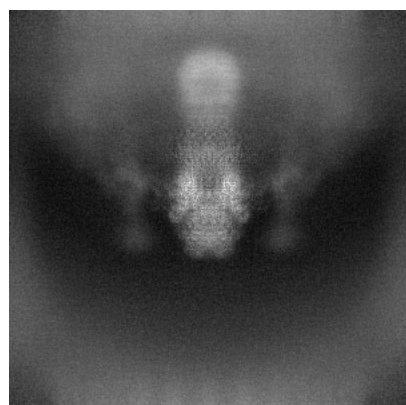


Y

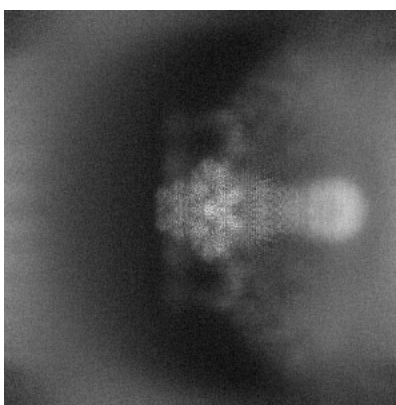


Z

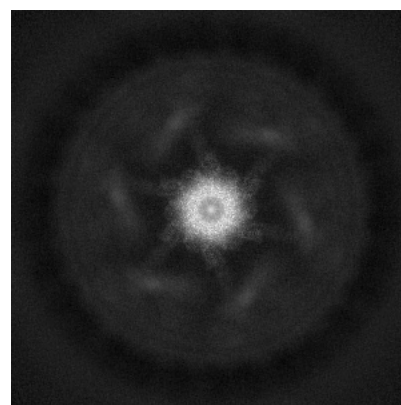
6.1.2 Raw map



X



Y

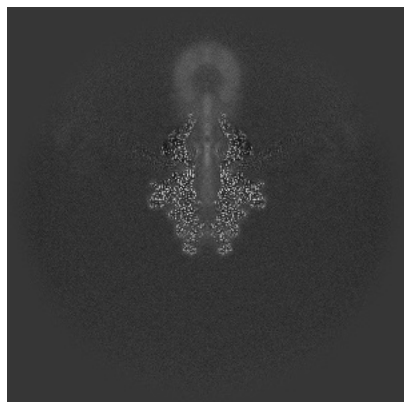


Z

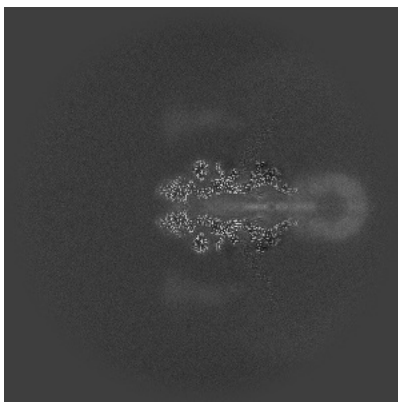
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

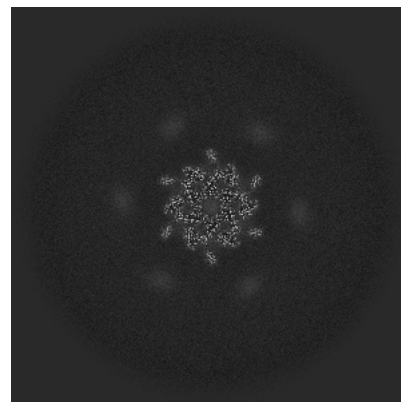
6.2.1 Primary map



X Index: 400

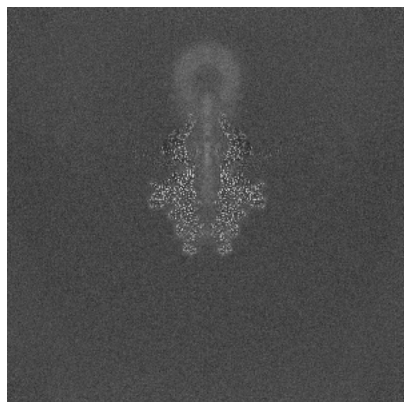


Y Index: 400

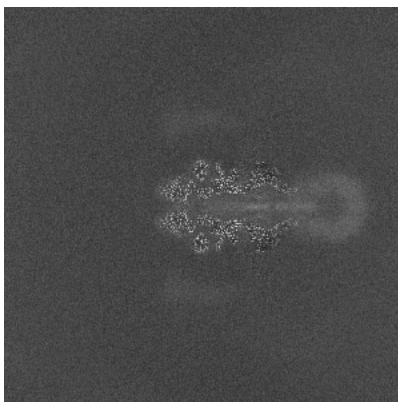


Z Index: 400

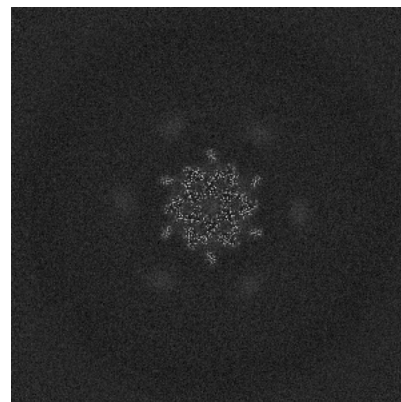
6.2.2 Raw map



X Index: 400



Y Index: 400

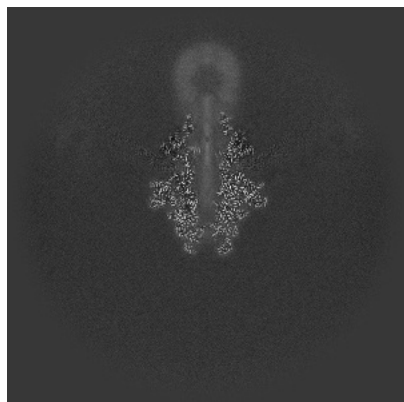


Z Index: 400

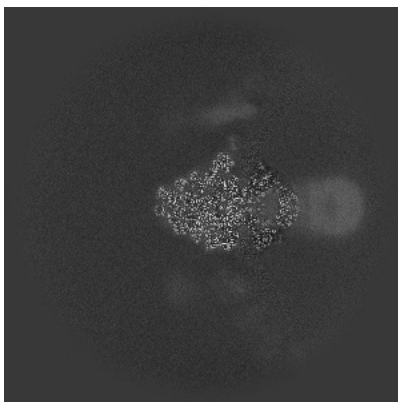
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

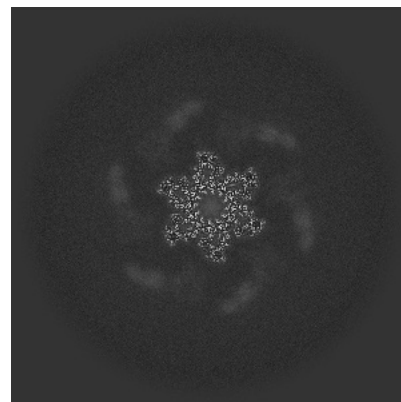
6.3.1 Primary map



X Index: 403

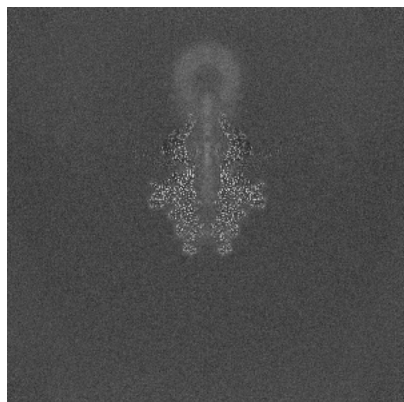


Y Index: 370

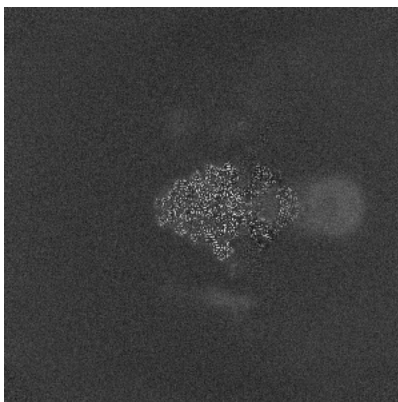


Z Index: 436

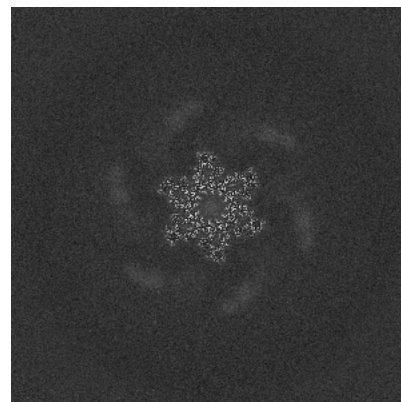
6.3.2 Raw map



X Index: 400



Y Index: 430

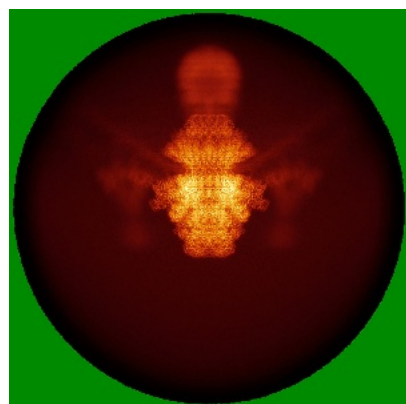


Z Index: 436

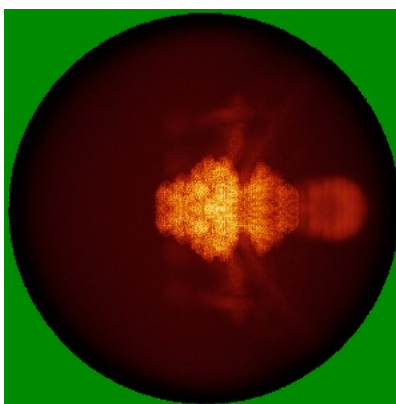
The images above show the largest variance slices of the map in three orthogonal directions.

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

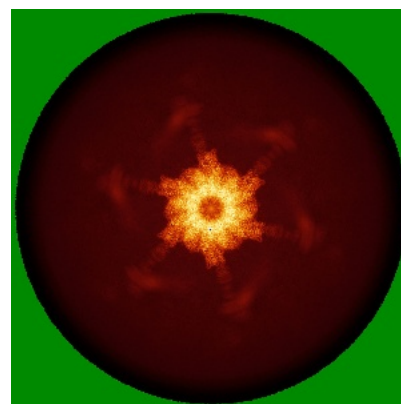
6.4.1 Primary map



X

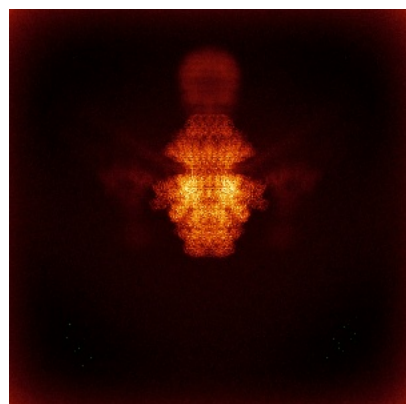


Y

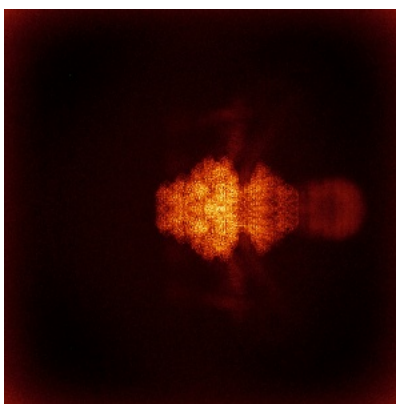


Z

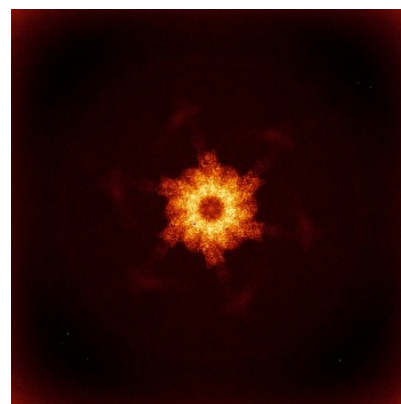
6.4.2 Raw map



X



Y

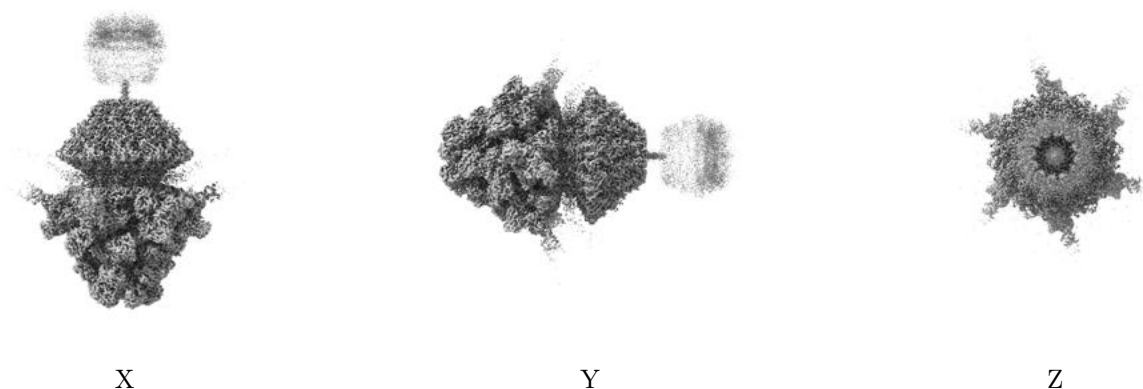


Z

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

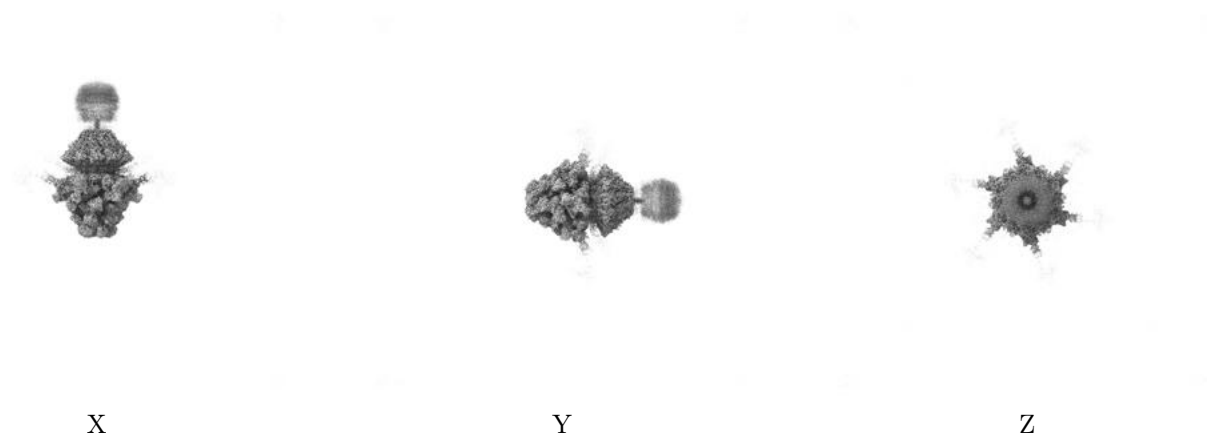
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

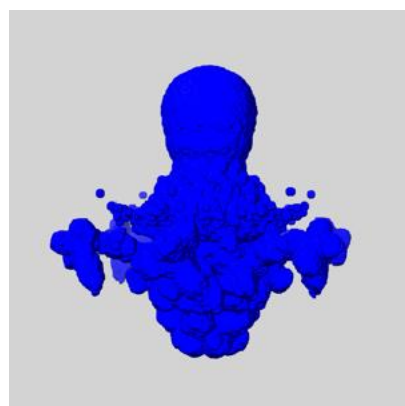
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

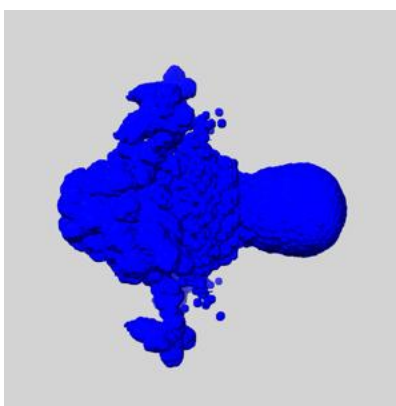
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

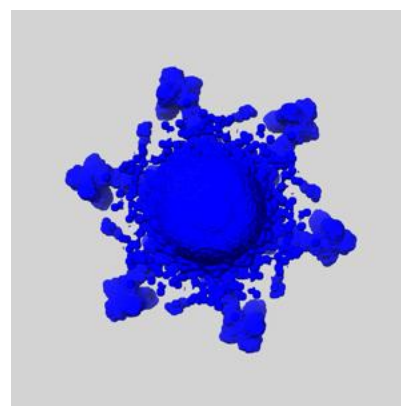
6.6.1 emd_47975_msk_1.map [i](#)



X



Y

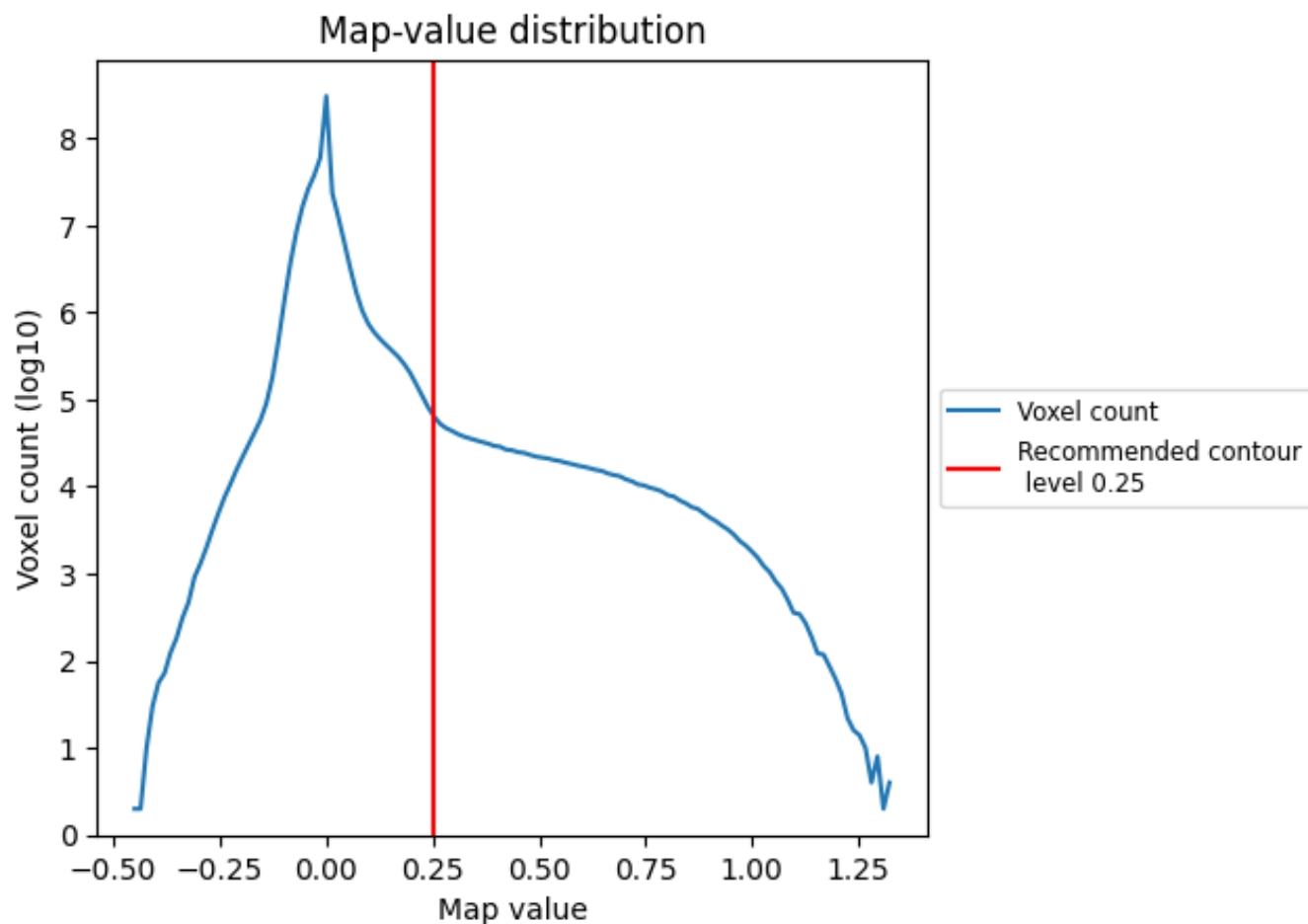


Z

7 Map analysis [i](#)

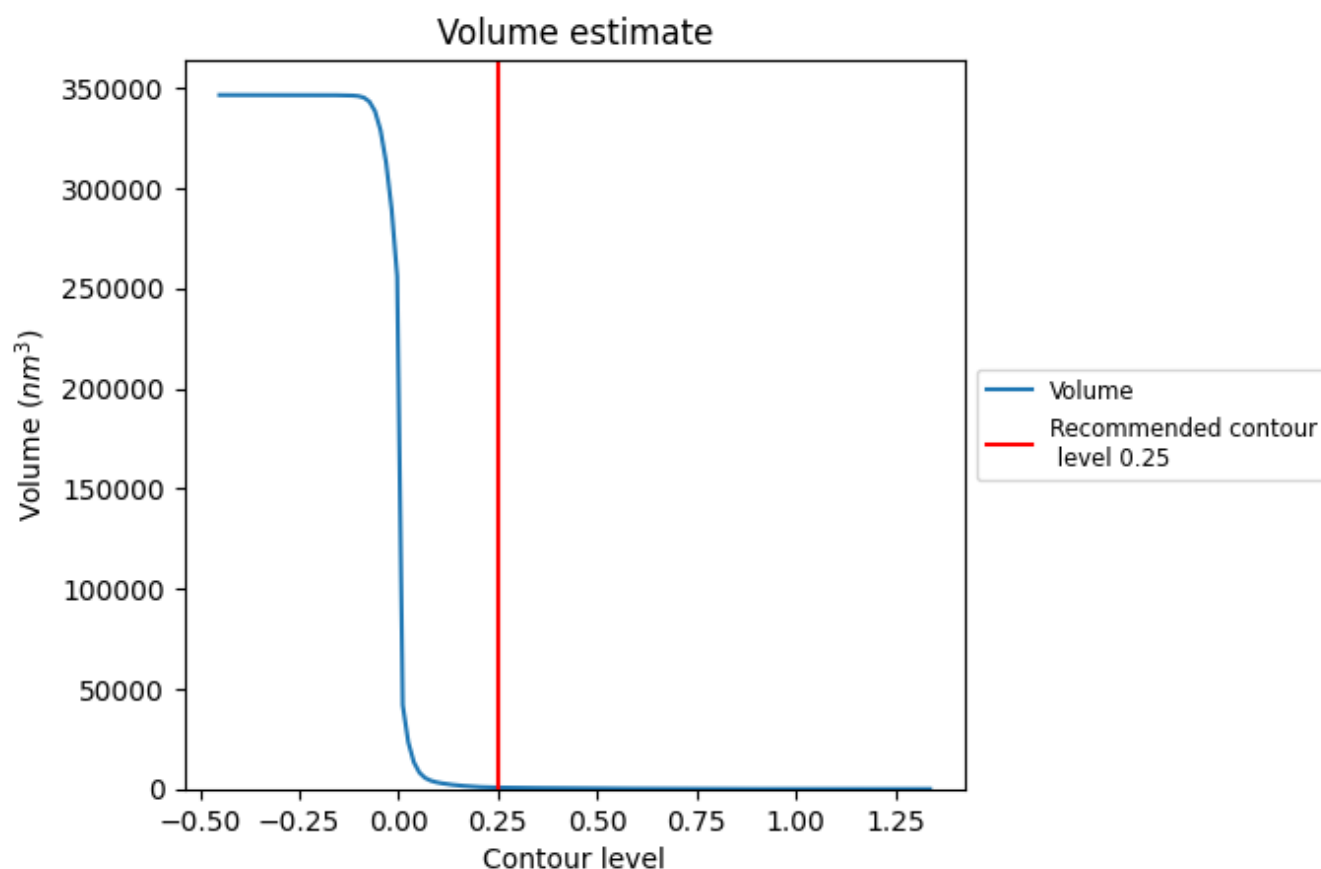
This section contains the results of statistical analysis of the map.

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.

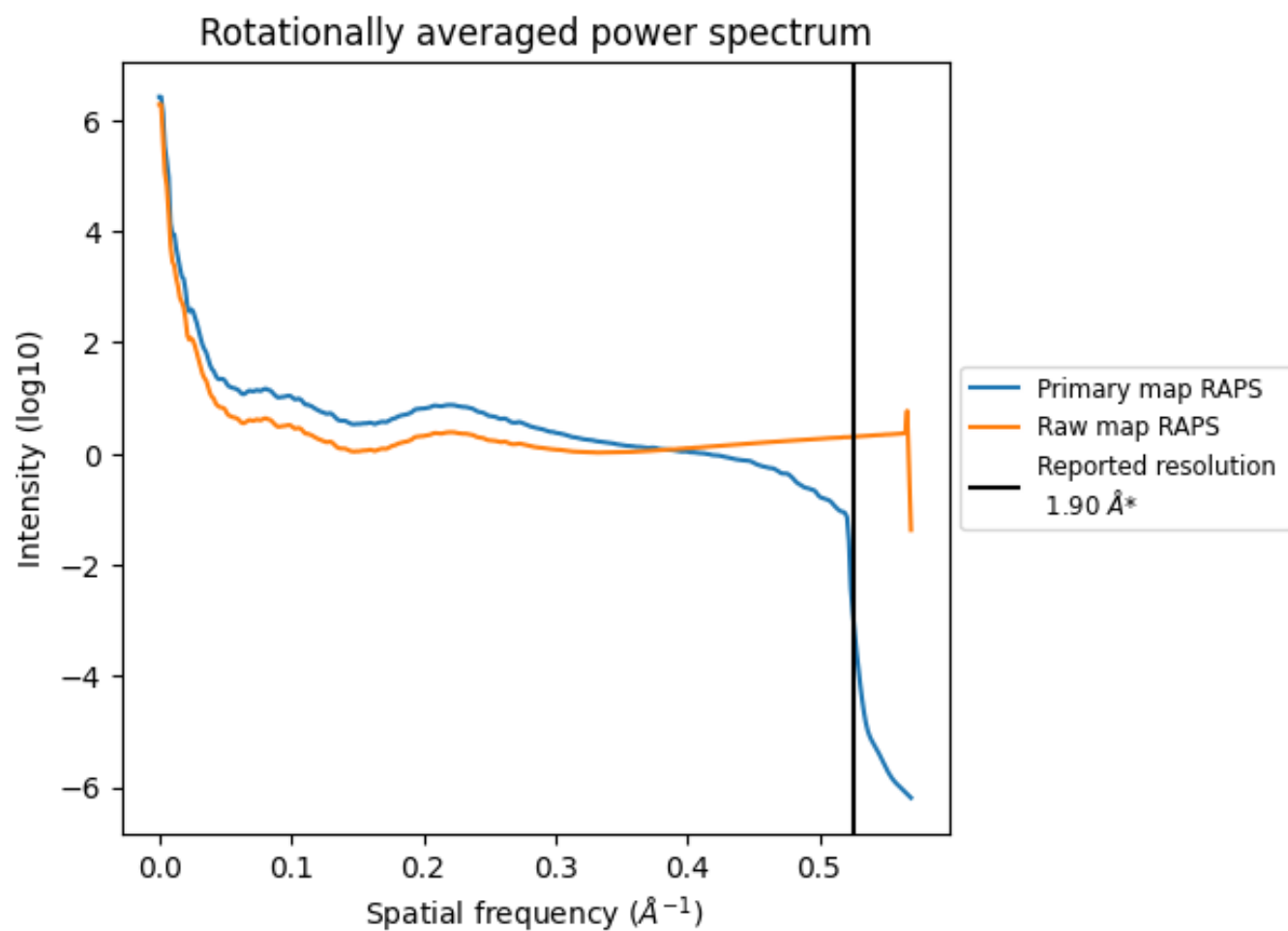
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm^3 ; this corresponds to an approximate mass of 631 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 ⓘ

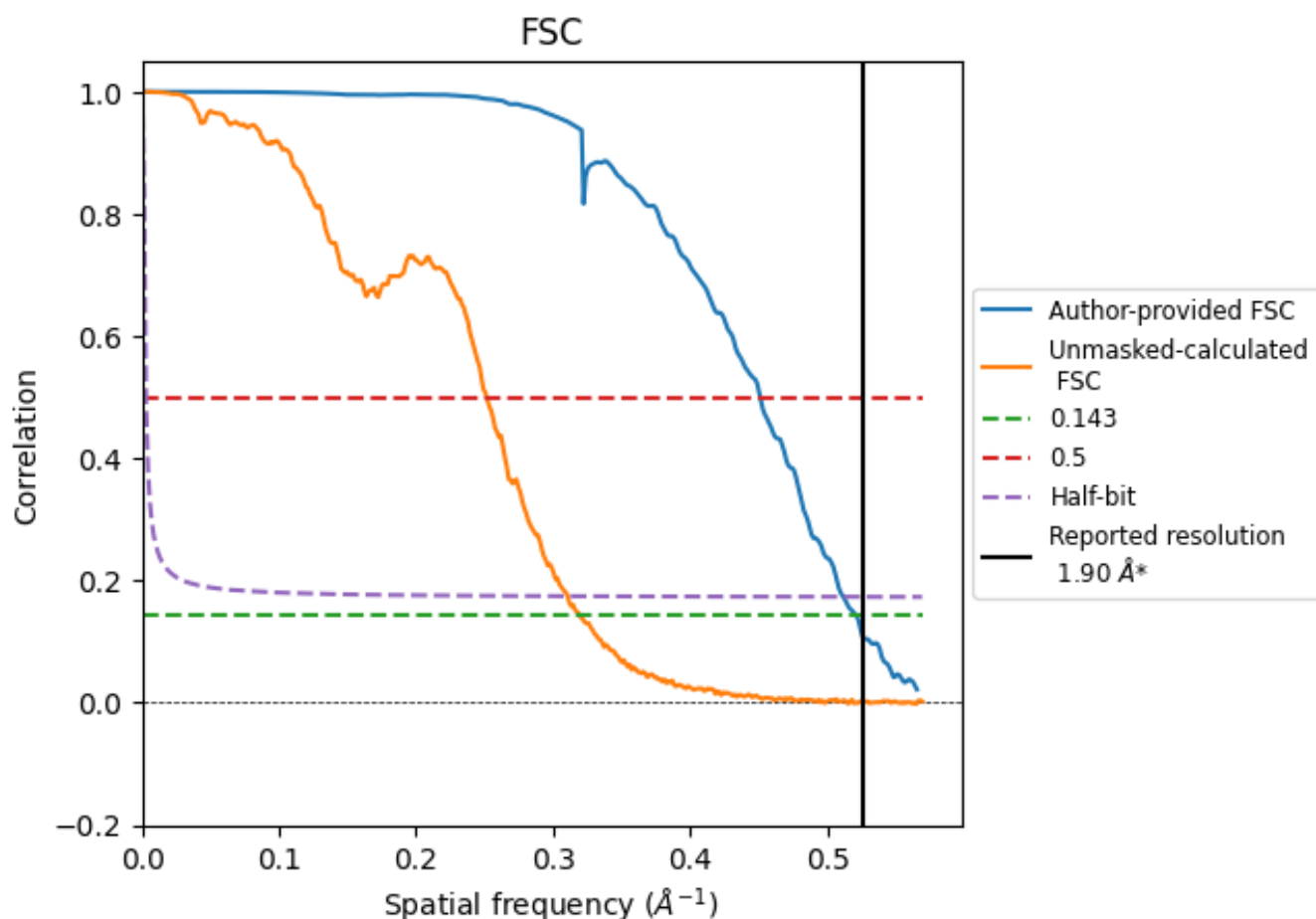


*Reported resolution corresponds to spatial frequency of 0.526 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.526 Å⁻¹

8.2 Resolution estimates [i](#)

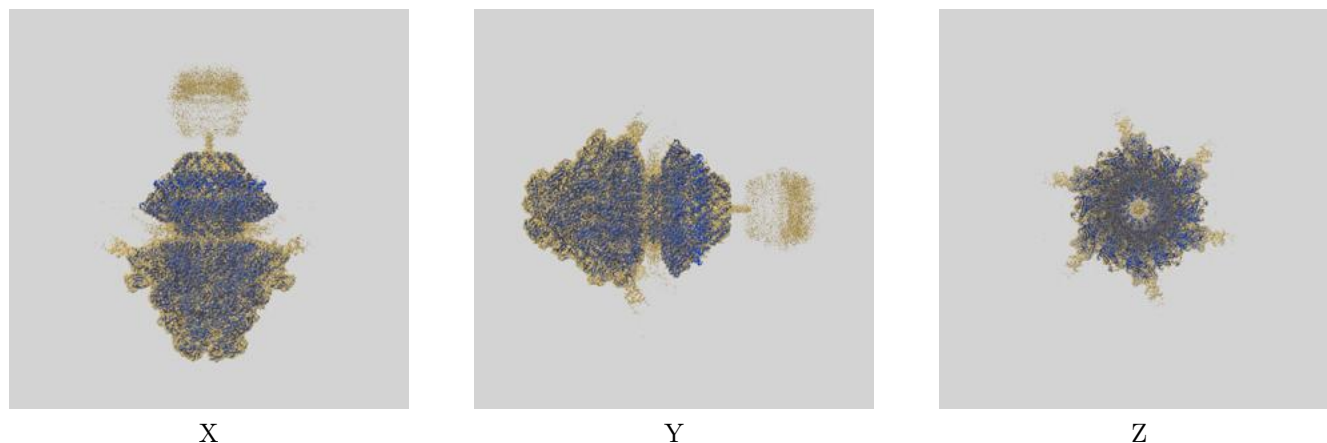
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.92	2.22	1.95
Unmasked-calculated*	3.13	3.97	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 1.9 by more than 10 %

9 Map-model fit [i](#)

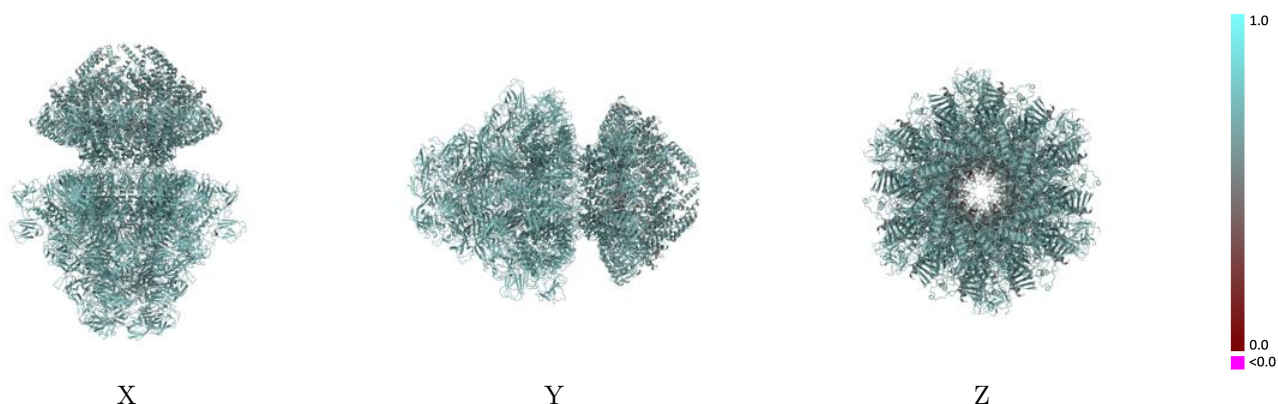
This section contains information regarding the fit between EMDB map EMD-47975 and PDB model 9EFK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



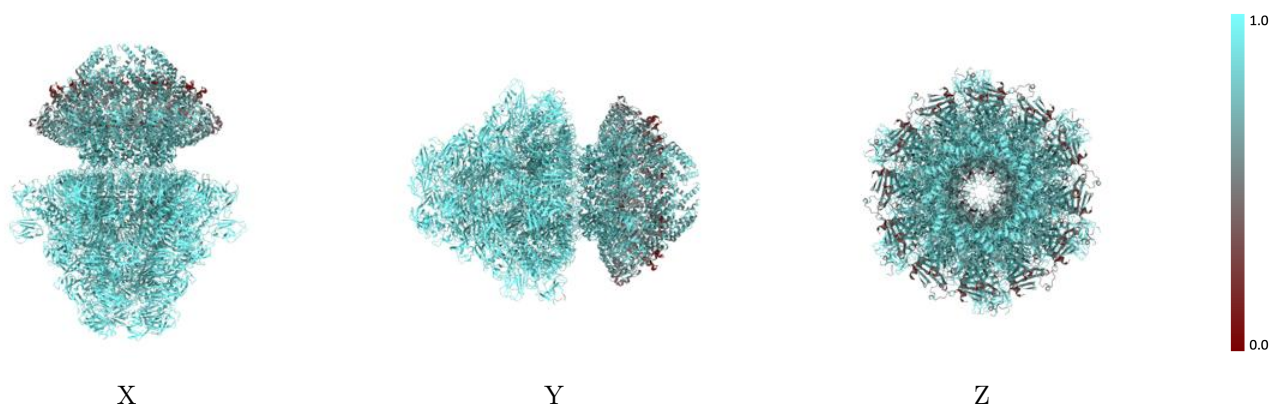
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



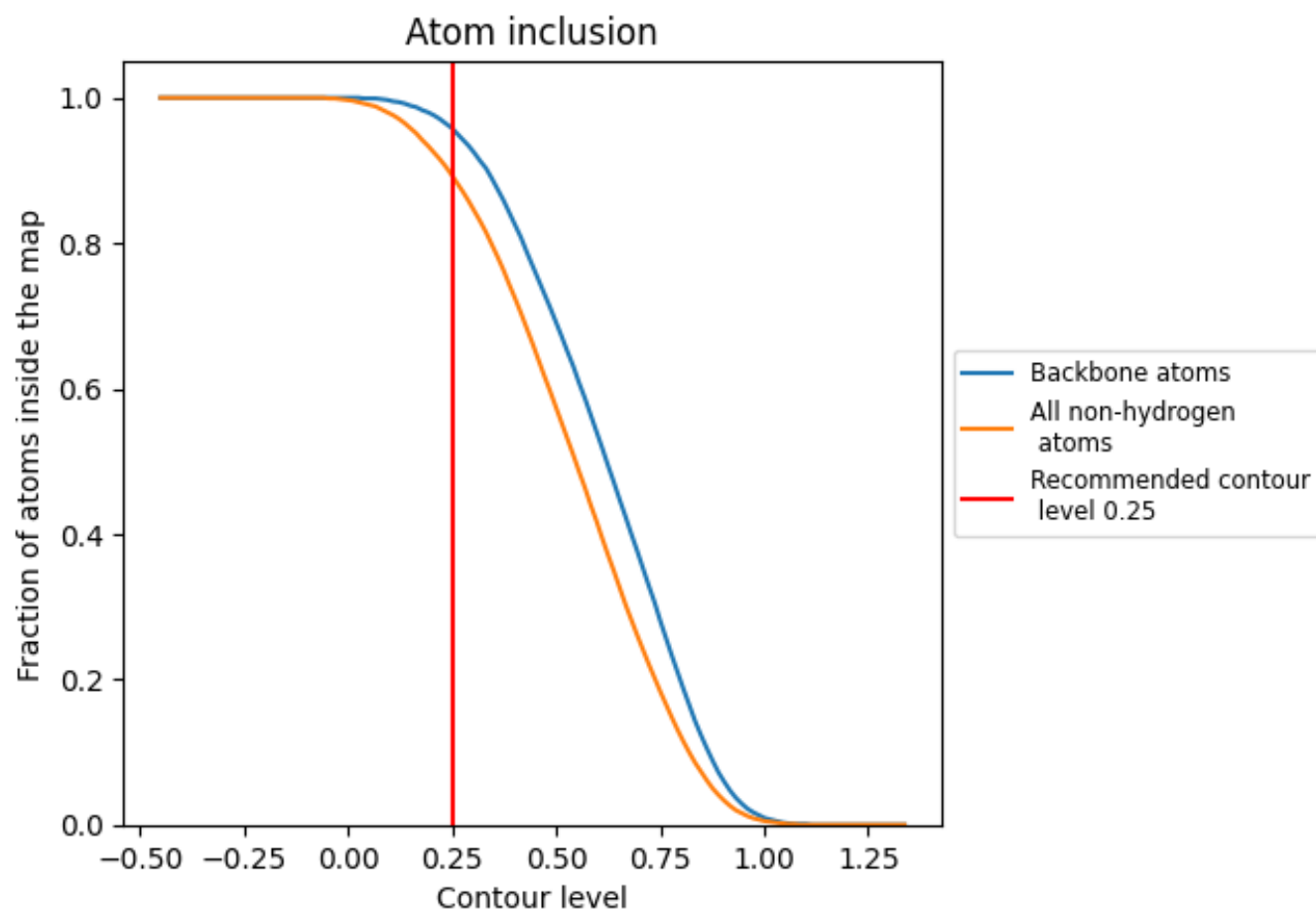
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.6700
A	 0.7890	 0.6500
AA	 0.9660	 0.7020
AB	 0.9600	 0.6950
AC	 0.9650	 0.7000
AD	 0.9550	 0.6940
AE	 0.9630	 0.6890
AF	 0.9570	 0.6770
AG	 0.9620	 0.6910
AN	 0.9600	 0.6920
AO	 0.9580	 0.6780
AP	 0.9590	 0.6940
AW	 0.9610	 0.6850
AX	 0.9530	 0.6740
AY	 0.9580	 0.6860
B	 0.7760	 0.6440
BF	 0.9640	 0.6930
BG	 0.9580	 0.6820
BH	 0.9580	 0.6910
BO	 0.9650	 0.6860
BP	 0.9530	 0.6760
BQ	 0.9590	 0.6880
BX	 0.9650	 0.6910
BY	 0.9550	 0.6820
BZ	 0.9590	 0.6920
C	 0.7860	 0.6470
D	 0.7710	 0.6410
E	 0.7870	 0.6460
F	 0.7740	 0.6410
G	 0.7870	 0.6430
H	 0.7750	 0.6390
I	 0.7850	 0.6420
J	 0.7760	 0.6400
K	 0.7860	 0.6450
L	 0.7730	 0.6430



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Chain	Atom inclusion	Q-score
M	 0.9670	 0.6810
N	 0.9650	 0.6830
O	 0.9640	 0.6830
P	 0.9660	 0.6820
Q	 0.9660	 0.6810
R	 0.9660	 0.6790
S	 0.9680	 0.7010
T	 0.9580	 0.6970
U	 0.9670	 0.7010
V	 0.9570	 0.6950
W	 0.9670	 0.7030
X	 0.9650	 0.7010
Y	 0.9670	 0.7040
Z	 0.9590	 0.6950