



Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 03:57 PM EST

PDB ID : 8GAF
EMDB ID : EMD-29896
Title : Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3
for Genome Editing Applications
Authors : Hu, C.; Nam, K.H.; Ke, A.
Deposited on : 2023-02-22
Resolution : 3.64 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:

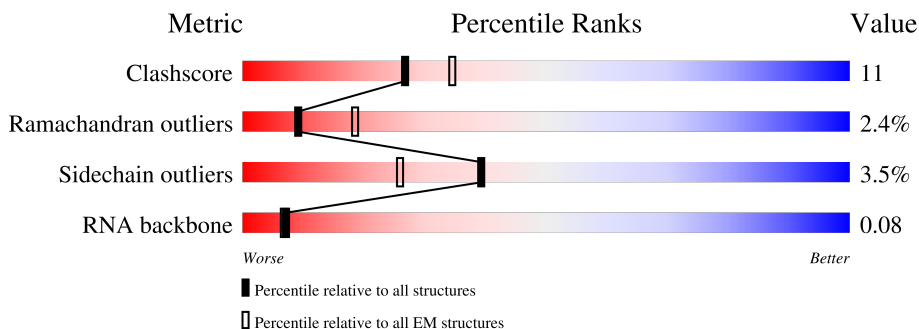
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



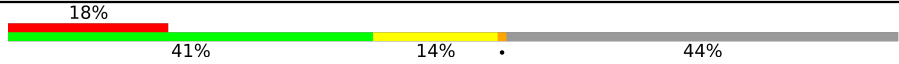



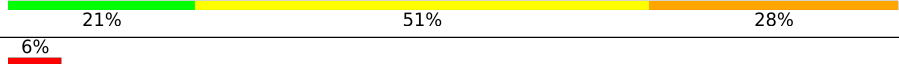
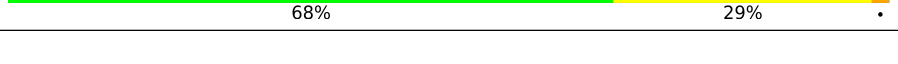
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	283	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9% 70% 29% •</p>
1	B	283	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 68% 30% •</p>
1	C	283	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 65% 32% •</p>
1	D	283	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 69% 29% •</p>
1	E	283	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">14% 70% 28% •</p>
1	F	283	<div style="display: flex; align-items: center;"> <div style="width: 29%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">29% 67% 26% • •</p>
1	M	283	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">• 65% 27% • 7%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	582	
2	H	582	
3	I	124	
3	J	124	
4	K	43	
5	N	205	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24582 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 Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	283	2261	1408	406	436	11	0	0
1	B	283	2261	1408	406	436	11	0	0
1	C	283	2261	1408	406	436	11	0	0
1	D	283	2261	1408	406	436	11	0	0
1	E	283	2261	1408	406	436	11	0	0
1	F	271	2173	1360	391	411	11	0	0
1	M	264	2110	1318	379	402	11	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLY	-	expression tag	UNP A0A378VEU0
B	284	GLY	-	expression tag	UNP A0A378VEU0
C	284	GLY	-	expression tag	UNP A0A378VEU0
D	284	GLY	-	expression tag	UNP A0A378VEU0
E	284	GLY	-	expression tag	UNP A0A378VEU0
F	284	GLY	-	expression tag	UNP A0A378VEU0
M	284	GLY	-	expression tag	UNP A0A378VEU0

- Molecule 2 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	325	2523	1601	438	475	9	0	0
2	H	233	1867	1189	335	336	7	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	190	ALA	VAL	conflict	UNP A0A1V0DVBX6
G	239	ALA	ILE	conflict	UNP A0A1V0DVBX6
G	242	ILE	VAL	conflict	UNP A0A1V0DVBX6
G	260	GLY	SER	conflict	UNP A0A1V0DVBX6
G	271	THR	ALA	conflict	UNP A0A1V0DVBX6
G	299	ALA	GLU	conflict	UNP A0A1V0DVBX6
G	306	ALA	THR	conflict	UNP A0A1V0DVBX6
G	317	CYS	GLN	conflict	UNP A0A1V0DVBX6
G	322	GLU	LYS	conflict	UNP A0A1V0DVBX6
G	323	ASP	GLU	conflict	UNP A0A1V0DVBX6
G	481	ILE	THR	conflict	UNP A0A1V0DVBX6
G	562	TYR	CYS	conflict	UNP A0A1V0DVBX6
H	190	ALA	VAL	conflict	UNP A0A1V0DVBX6
H	239	ALA	ILE	conflict	UNP A0A1V0DVBX6
H	242	ILE	VAL	conflict	UNP A0A1V0DVBX6
H	260	GLY	SER	conflict	UNP A0A1V0DVBX6
H	271	THR	ALA	conflict	UNP A0A1V0DVBX6
H	299	ALA	GLU	conflict	UNP A0A1V0DVBX6
H	306	ALA	THR	conflict	UNP A0A1V0DVBX6
H	317	CYS	GLN	conflict	UNP A0A1V0DVBX6
H	322	GLU	LYS	conflict	UNP A0A1V0DVBX6
H	323	ASP	GLU	conflict	UNP A0A1V0DVBX6
H	481	ILE	THR	conflict	UNP A0A1V0DVBX6
H	562	TYR	CYS	conflict	UNP A0A1V0DVBX6

- Molecule 3 is a protein called Cas11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
3	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

- Molecule 4 is a RNA chain called crRNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	43	Total	C	N	O	P	0	0
			916	408	161	304	43		

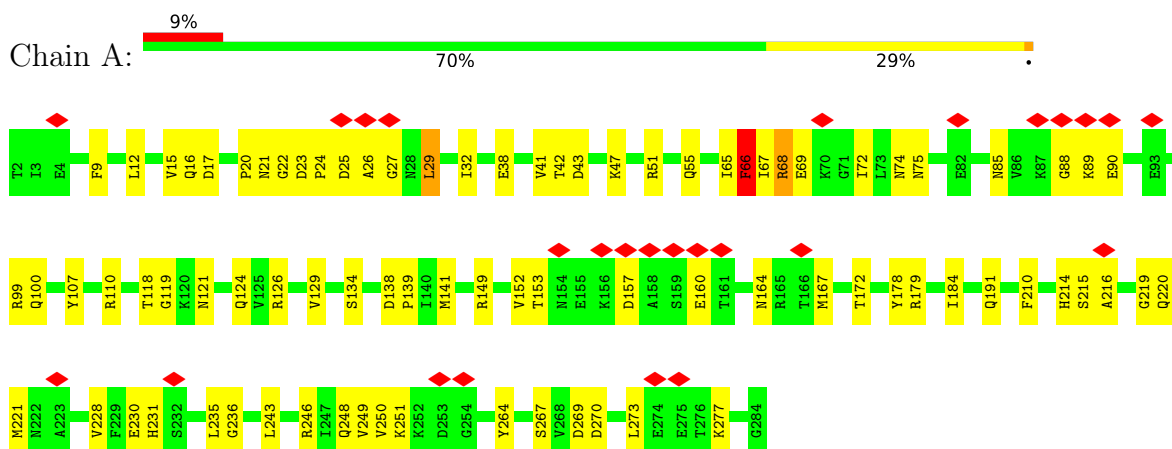
- Molecule 5 is a protein called Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	205	1674	1067	289	306	12	0	0

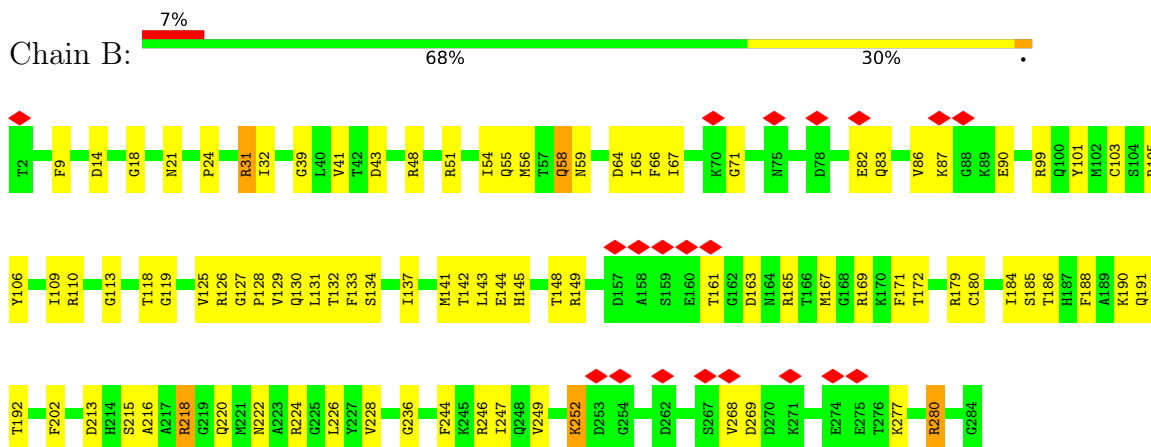
3 Residue-property plots

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

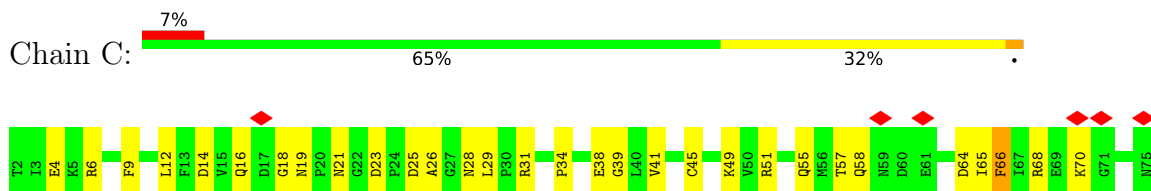
- Molecule 1: Cas7

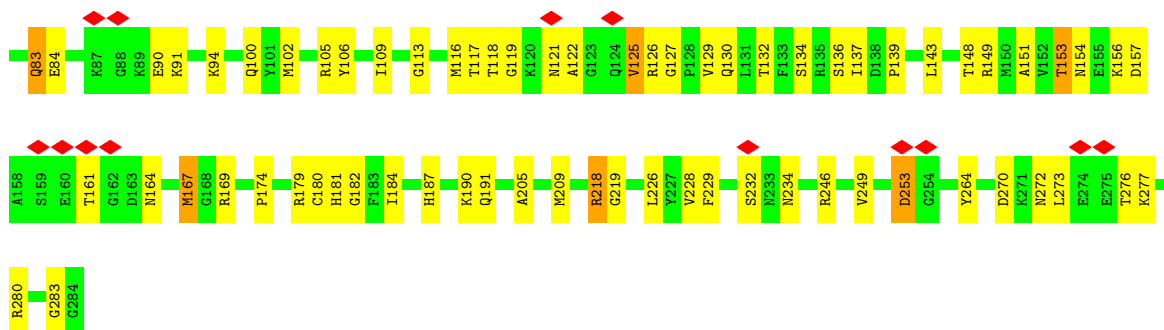


- Molecule 1: Cas7

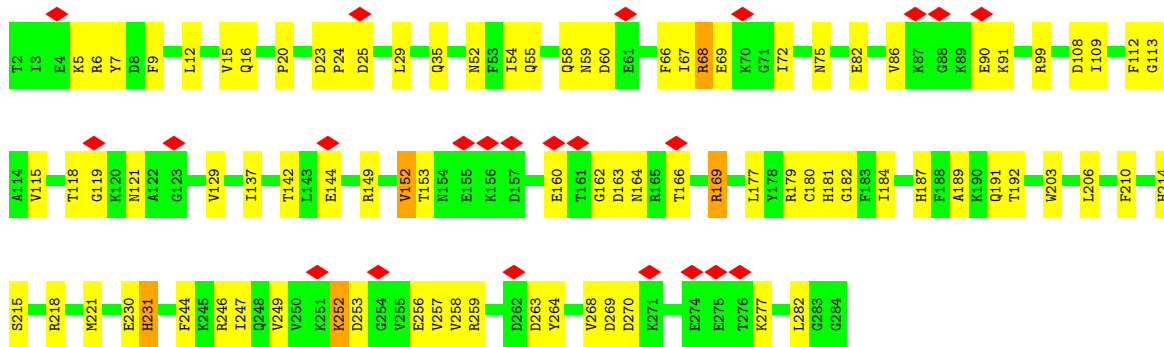


- Molecule 1: Cas7

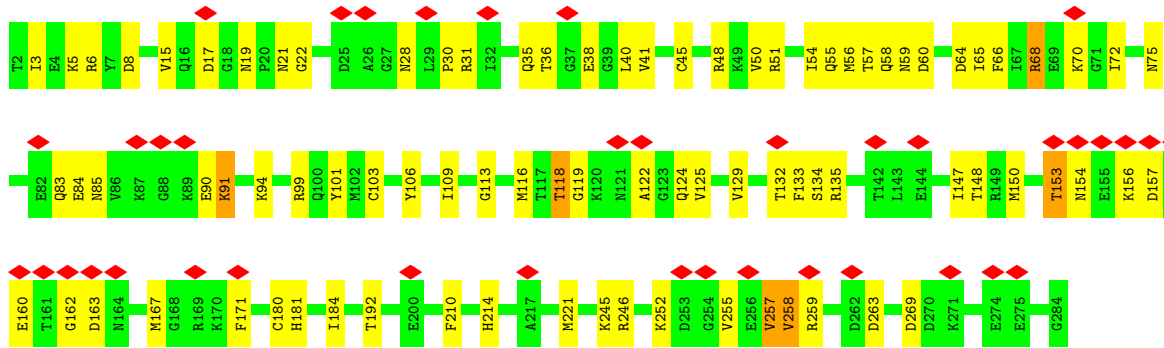




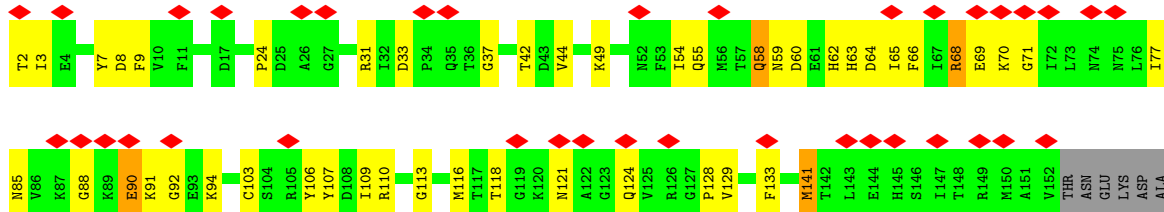
• Molecule 1: Cas7

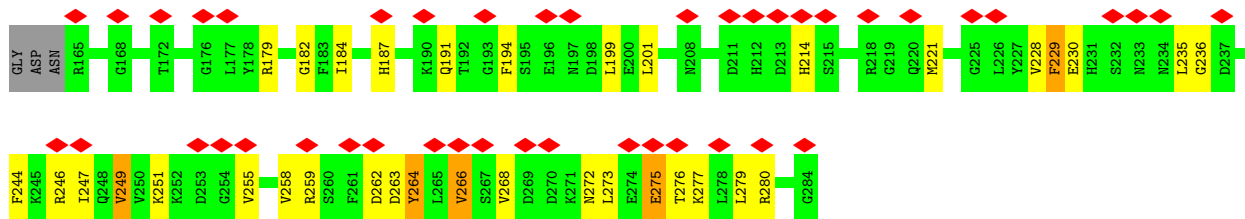


• Molecule 1: Cas7

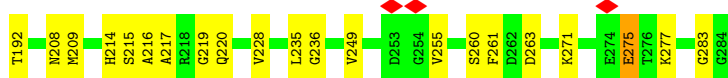


• Molecule 1: Cas7

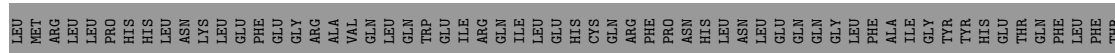
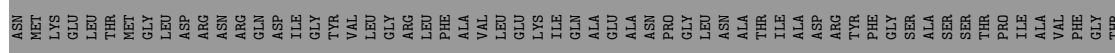
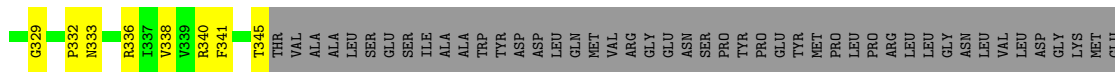
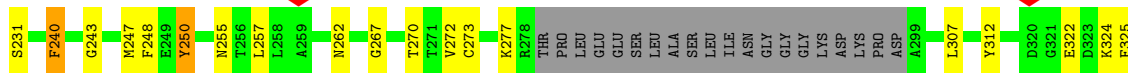
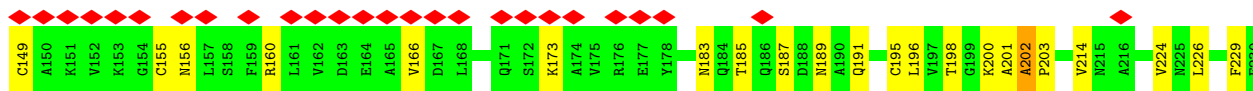
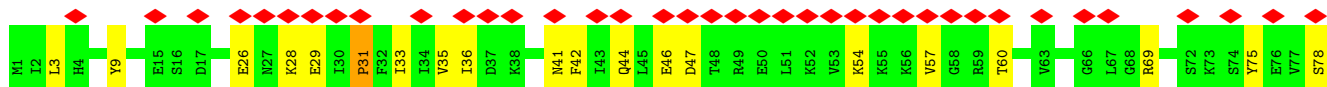




• Molecule 1: Cas7



• Molecule 2: Cas8



LYS
ASP
ALA
LEU
LEU
LYS
ASN
LEU
PHE
ASN
GLU
ALA

• Molecule 2: Cas8



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

ILE	ASP	ALA	VAL	LYS	ALA	TYR	LEU	LYS	TYR	ASN	GLY	GLN	CYS	TYR	THR	THR	THR	ALA	ALA	ASN	GLY	PRO
ASP	ALA	VAL	LYS	ALA	TYR	LYS	LEU	LYS	ASN	GLY	GLN	CYS	TYR	THR	THR	THR	THR	ALA	ALA	ASN	GLY	PRO
ASP	ALA	VAL	LYS	ALA	TYR	LYS	LEU	LYS	ASN	GLY	GLN	CYS	TYR	THR	THR	THR	THR	ALA	ALA	ASN	GLY	PRO
ASP	ALA	VAL	LYS	ALA	TYR	LYS	LEU	LYS	ASN	GLY	GLN	CYS	TYR	THR	THR	THR	THR	ALA	ALA	ASN	GLY	PRO
ASP	ALA	VAL	LYS	ALA	TYR	LYS	LEU	LYS	ASN	GLY	GLN	CYS	TYR	THR	THR	THR	THR	ALA	ALA	ASN	GLY	PRO

• Molecule 3: Cas11

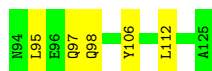


G2	D9	I10	G11	Y12	R16	L17	V20	L21	E22	E27	A28	N29	P30	G31	L32	N33	A34	A37	D38	R39	Y40	T47	A50	G53	M56	R57	L58	N64	K65	L66	F68	E69	L83	E84	H85	C86	Q87	R88	F89	P90	N91	H92	L93	N94	L95	Q98					
G89	L100	Q110	F111	L112	F113	T114	K115	M123	E124	A125																																									

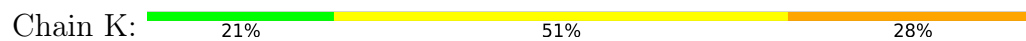
• Molecule 3: Cas11



G2	Q8	Y12	V13	R16	L17	V20	L21	T24	Q25	P30	G31	L32	N33	T35	A34	I36	A37	D38	R39	Y40	F41	G42	S45	A50	L55	M56	R57	L58	L59	P60	H61	H62	L63	N64	L75	Q76	W77	E78	I79	R80	Q81	I82	L83	E84	H85	C86	H92	L93
----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 4: crRNA (43-MER)



- Molecule 5: Cas5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103405	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.983	Depositor
Minimum map value	-0.427	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.119	Depositor
Map size (\AA)	393.59598, 393.59598, 393.59598	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4057, 1.4057, 1.4057	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	0.23	0/2303	0.40	0/3101
1	B	0.23	0/2303	0.39	0/3101
1	C	0.24	0/2303	0.40	0/3101
1	D	0.23	0/2303	0.39	0/3101
1	E	0.23	0/2303	0.39	0/3101
1	F	0.23	0/2214	0.39	0/2979
1	M	0.23	0/2150	0.40	0/2896
2	G	0.24	0/2572	0.38	0/3470
2	H	0.23	0/1903	0.37	0/2573
3	I	0.24	0/1030	0.35	0/1392
3	J	0.24	0/1030	0.36	0/1392
4	K	0.18	0/1022	0.77	0/1591
5	N	0.24	0/1712	0.40	0/2307
All	All	0.23	0/25148	0.41	0/34105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2261	0	2193	56	0
1	B	2261	0	2193	67	0
1	C	2261	0	2193	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2261	0	2193	54	0
1	E	2261	0	2193	54	0
1	F	2173	0	2120	50	0
1	M	2110	0	2050	54	0
2	G	2523	0	2507	57	0
2	H	1867	0	1891	50	0
3	I	1007	0	992	21	0
3	J	1007	0	992	32	0
4	K	916	0	464	32	0
5	N	1674	0	1663	44	0
All	All	24582	0	23644	530	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 11.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:HA3	3:J:58:LEU:HD11	1.70	0.74
1:B:133:PHE:HB2	1:M:17:ASP:HB3	1.69	0.73
1:E:55:GLN:HB2	1:E:65:ILE:HG21	1.73	0.71
1:C:34:PRO:HG2	2:H:511:THR:HG22	1.72	0.70
1:A:29:LEU:HD22	3:J:58:LEU:HD13	1.73	0.69
2:H:366:GLY:H	2:H:567:GLN:HE21	1.41	0.69
2:G:226:LEU:HD13	5:N:71:GLY:HA3	1.75	0.68
1:A:21:ASN:HD21	1:A:42:THR:HG23	1.59	0.68
1:B:228:VAL:HB	1:B:280:ARG:HG3	1.76	0.68
2:H:395:SER:HB2	1:M:26:ALA:HB2	1.75	0.67
1:C:125:VAL:O	4:K:17:C:O2'	2.13	0.66
3:I:38:ASP:HA	3:J:60:PRO:HB3	1.77	0.66
1:C:55:GLN:HB2	1:C:65:ILE:HG21	1.77	0.65
2:H:473:ARG:HH21	2:H:539:ILE:HG12	1.61	0.65
1:C:51:ARG:NH2	4:K:19:U:OP1	2.30	0.65
1:C:218:ARG:HH22	4:K:20:G:H1'	1.62	0.64
5:N:161:LEU:HD22	5:N:165:THR:HG21	1.80	0.64
1:B:247:ILE:HG23	1:B:268:VAL:HG12	1.79	0.64
1:D:152:VAL:HB	1:D:164:ASN:HB3	1.80	0.64
1:B:169:ARG:NH1	2:H:491:ALA:O	2.31	0.63
1:M:21:ASN:OD1	1:M:31:ARG:NE	2.31	0.63
2:H:428:LYS:O	2:H:433:ARG:NH1	2.31	0.63
1:E:70:LYS:NZ	1:F:92:GLY:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:473:ARG:HB3	2:H:539:ILE:HD13	1.82	0.62
4:K:9:A:H4'	4:K:10:G:OP1	1.99	0.61
1:E:51:ARG:NH2	4:K:37:C:OP1	2.33	0.61
1:B:24:PRO:HG2	1:M:147:ILE:HA	1.83	0.61
1:E:19:ASN:ND2	4:K:40:C:OP2	2.33	0.61
1:C:149:ARG:HB2	4:K:25:A:H1'	1.82	0.61
1:B:55:GLN:O	1:B:59:ASN:ND2	2.34	0.61
1:M:146:SER:HA	1:M:169:ARG:HA	1.81	0.61
1:B:55:GLN:HG3	1:B:65:ILE:HG13	1.82	0.60
3:I:20:VAL:HG12	3:I:112:LEU:HD11	1.83	0.60
3:J:24:ILE:HG12	3:J:75:LEU:HD23	1.82	0.60
4:K:32:A:N6	4:K:34:C:O2'	2.34	0.60
1:B:48:ARG:NH1	4:K:14:C:OP2	2.34	0.60
1:E:22:GLY:HA2	1:E:30:PRO:HA	1.82	0.60
1:E:116:MET:HB3	1:E:122:ALA:HB3	1.83	0.60
1:B:246:ARG:HG2	1:B:269:ASP:HB3	1.83	0.60
2:H:393:LEU:HB3	1:M:26:ALA:HB1	1.83	0.60
4:K:3:U:OP1	1:M:126:ARG:NH2	2.35	0.60
2:H:421:ARG:HD2	1:M:144:GLU:HB2	1.82	0.59
1:A:21:ASN:HB2	1:A:41:VAL:HG22	1.83	0.59
1:B:215:SER:OG	1:B:216:ALA:N	2.35	0.59
2:G:36:ILE:HG22	2:G:42:PHE:HA	1.84	0.59
2:H:503:SER:OG	2:H:504:THR:N	2.34	0.59
1:B:127:GLY:HA3	1:B:130:GLN:HE21	1.66	0.59
1:M:56:MET:O	1:M:59:ASN:ND2	2.35	0.59
1:B:24:PRO:HG3	4:K:15:A:H5'	1.84	0.59
1:B:51:ARG:NH1	4:K:13:U:OP1	2.36	0.59
2:H:354:ILE:HG13	2:H:406:LEU:HD22	1.84	0.59
3:I:95:LEU:HD11	3:J:50:ALA:HA	1.85	0.59
1:B:56:MET:HG2	1:C:187:HIS:HB3	1.85	0.58
1:F:141:MET:SD	1:F:141:MET:N	2.76	0.58
1:C:148:THR:HB	4:K:27:G:H5''	1.84	0.58
1:C:229:PHE:HB3	1:C:277:LYS:HD3	1.83	0.58
1:M:25:ASP:HA	5:N:66:ARG:HD3	1.84	0.58
1:A:15:VAL:HG11	1:A:20:PRO:HB3	1.86	0.58
1:B:32:ILE:HD11	2:H:500:SER:HB2	1.86	0.58
1:E:109:ILE:HA	1:E:113:GLY:HA2	1.85	0.58
2:H:481:ILE:HG12	2:H:532:LEU:HD13	1.86	0.58
1:F:33:ASP:HB3	1:F:37:GLY:H	1.68	0.58
1:C:64:ASP:HB2	1:C:106:TYR:HA	1.86	0.58
1:F:55:GLN:O	1:F:59:ASN:ND2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASP:HB2	1:B:106:TYR:HA	1.86	0.57
1:E:258:VAL:O	1:E:259:ARG:NH2	2.37	0.57
1:E:153:THR:OG1	1:E:154:ASN:N	2.36	0.57
1:A:17:ASP:OD1	1:A:172:THR:OG1	2.21	0.57
1:F:64:ASP:HB2	1:F:106:TYR:HA	1.85	0.57
2:G:35:VAL:HB	2:G:44:GLN:HG3	1.87	0.57
1:B:132:THR:HG21	1:M:220:GLN:HB2	1.87	0.57
1:D:7:TYR:HB2	1:D:184:ILE:HB	1.87	0.57
1:D:29:LEU:HD11	3:I:58:LEU:HB2	1.87	0.57
1:M:163:ASP:N	1:M:163:ASP:OD1	2.38	0.57
5:N:20:LYS:O	5:N:90:ARG:NH2	2.37	0.57
1:A:138:ASP:HB2	1:A:251:LYS:HD3	1.87	0.57
5:N:175:MET:HG2	5:N:189:GLU:HG3	1.87	0.56
1:C:226:LEU:HB3	1:C:283:GLY:H	1.70	0.56
1:C:18:GLY:HA3	1:C:219:GLY:HA3	1.87	0.56
1:C:41:VAL:HB	1:C:134:SER:HB2	1.87	0.56
5:N:22:GLU:HB3	5:N:91:ALA:HB3	1.87	0.56
1:C:253:ASP:N	1:C:253:ASP:OD1	2.39	0.56
2:H:501:ALA:HA	2:H:508:VAL:HG21	1.87	0.56
2:H:512:LEU:HD23	2:H:515:LEU:HD12	1.88	0.56
1:M:255:VAL:HG11	1:M:263:ASP:HB3	1.88	0.56
1:B:185:SER:OG	1:B:186:THR:N	2.33	0.56
1:D:35:GLN:HE22	3:I:50:ALA:HB2	1.70	0.56
1:M:150:MET:HA	1:M:165:ARG:HE	1.70	0.56
1:F:90:GLU:O	1:F:94:LYS:N	2.33	0.56
1:B:169:ARG:HD2	2:H:496:ARG:HB2	1.87	0.55
1:D:163:ASP:OD1	1:D:163:ASP:N	2.39	0.55
2:H:455:GLU:O	2:H:464:ARG:NH2	2.37	0.55
2:G:26:GLU:OE2	2:G:255:ASN:ND2	2.40	0.55
4:K:18:U:HO2'	4:K:19:U:H6	1.54	0.55
1:B:125:VAL:O	4:K:11:G:O2'	2.19	0.55
2:H:424:LYS:O	2:H:427:GLN:NE2	2.39	0.55
1:D:24:PRO:O	3:I:39:ARG:NH1	2.40	0.55
1:C:228:VAL:HB	1:C:280:ARG:HG3	1.89	0.55
5:N:53:LYS:HB3	5:N:103:HIS:HB2	1.89	0.55
1:C:4:GLU:O	1:C:234:ASN:ND2	2.40	0.54
2:G:75:TYR:HD2	2:G:99:GLN:HE21	1.55	0.54
1:M:114:ALA:H	1:M:125:VAL:HB	1.71	0.54
1:A:55:GLN:HB2	1:A:65:ILE:HG21	1.88	0.54
1:M:275:GLU:OE2	1:M:277:LYS:NZ	2.38	0.54
1:A:38:GLU:HA	1:A:139:PRO:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:CYS:O	1:B:110:ARG:NH2	2.40	0.54
1:E:3:ILE:HG13	1:E:5:LYS:H	1.72	0.54
2:G:121:ASP:O	2:G:123:GLY:N	2.40	0.54
1:M:120:LYS:HB3	5:N:183:ARG:HG2	1.88	0.54
5:N:66:ARG:NH2	5:N:89:GLN:OE1	2.40	0.54
1:E:91:LYS:HA	1:E:94:LYS:HB3	1.88	0.54
1:C:25:ASP:OD2	2:H:496:ARG:NH2	2.39	0.54
1:C:118:THR:OG1	1:C:119:GLY:N	2.40	0.54
1:D:23:ASP:OD2	3:I:40:TYR:OH	2.25	0.54
2:G:78:SER:O	2:G:110:LYS:NZ	2.41	0.54
2:G:322:GLU:HG2	2:H:351:SER:HB3	1.89	0.54
1:M:49:LYS:HB3	1:M:209:MET:HB2	1.89	0.54
1:A:41:VAL:HB	1:A:134:SER:HB2	1.89	0.54
1:B:9:PHE:HB2	1:B:226:LEU:HD11	1.90	0.54
1:B:21:ASN:HB2	1:B:41:VAL:HG13	1.88	0.54
1:B:144:GLU:O	2:H:496:ARG:NH1	2.41	0.54
1:D:246:ARG:HB3	1:D:269:ASP:HB2	1.90	0.54
1:B:163:ASP:OD1	1:B:163:ASP:N	2.38	0.54
1:M:117:THR:OG1	5:N:75:SER:OG	2.25	0.54
1:E:38:GLU:OE1	1:E:135:ARG:NH1	2.41	0.54
1:E:118:THR:OG1	1:E:119:GLY:N	2.39	0.53
1:D:149:ARG:NH2	1:D:153:THR:OG1	2.41	0.53
1:E:210:PHE:O	1:E:214:HIS:NE2	2.41	0.53
1:A:22:GLY:HA3	4:K:27:G:H3'	1.90	0.53
1:E:36:THR:HG23	1:E:38:GLU:H	1.73	0.53
1:F:55:GLN:HB2	1:F:65:ILE:HG21	1.89	0.53
2:G:185:THR:O	2:G:189:ASN:ND2	2.42	0.53
2:H:478:LEU:HD23	2:H:516:LEU:HD13	1.91	0.53
1:C:91:LYS:HA	1:C:94:LYS:HB3	1.91	0.53
1:D:179:ARG:NH1	1:D:244:PHE:O	2.42	0.53
1:E:163:ASP:OD2	1:E:163:ASP:N	2.42	0.53
1:M:44:VAL:HA	1:M:47:LYS:HE3	1.90	0.53
1:C:126:ARG:HH12	4:K:14:C:H42	1.57	0.53
1:C:270:ASP:HA	1:C:273:LEU:HD21	1.91	0.52
1:A:248:GLN:HG3	1:A:267:SER:HB2	1.91	0.52
1:E:132:THR:HB	1:E:181:HIS:H	1.74	0.52
2:G:202:ALA:HB1	2:G:243:GLY:HA3	1.92	0.52
1:M:30:PRO:HD3	1:M:171:PHE:HB3	1.91	0.52
1:B:31:ARG:HH11	1:M:145:HIS:HB3	1.75	0.52
1:B:32:ILE:HA	1:B:39:GLY:HA2	1.90	0.52
1:F:276:THR:HG23	1:F:277:LYS:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:ASN:ND2	1:M:42:THR:OG1	2.42	0.52
1:M:215:SER:OG	1:M:216:ALA:N	2.42	0.52
1:C:45:CYS:SG	1:C:49:LYS:NZ	2.82	0.52
1:A:210:PHE:HB3	1:A:221:MET:HB3	1.92	0.52
1:A:124:GLN:OE1	4:K:23:G:N2	2.43	0.52
1:B:82:GLU:HA	1:B:86:VAL:HG12	1.91	0.52
2:G:47:ASP:N	2:G:47:ASP:OD1	2.41	0.52
2:H:414:SER:HB3	1:M:32:ILE:HD11	1.92	0.52
1:M:260:SER:OG	1:M:261:PHE:N	2.43	0.52
1:A:107:TYR:HD1	1:A:110:ARG:HH11	1.57	0.52
1:D:179:ARG:HE	1:D:181:HIS:CE1	2.28	0.52
1:F:77:ILE:HD11	1:F:116:MET:HB3	1.92	0.52
1:A:24:PRO:O	1:A:26:ALA:N	2.42	0.51
1:B:215:SER:HB3	1:B:218:ARG:HH11	1.76	0.51
2:G:262:ASN:HB3	2:G:272:VAL:HG23	1.92	0.51
1:D:169:ARG:HH22	3:I:65:LYS:HB2	1.75	0.51
2:H:550:LEU:HD13	2:H:554:GLN:HB3	1.92	0.51
1:C:12:LEU:HG	1:C:179:ARG:HB2	1.91	0.51
1:B:186:THR:HG22	1:B:190:LYS:HE3	1.92	0.51
1:A:74:ASN:HD21	1:A:119:GLY:H	1.58	0.51
1:A:231:HIS:HA	1:A:277:LYS:HG3	1.92	0.51
1:C:26:ALA:HB2	2:H:515:LEU:HD23	1.93	0.51
1:E:129:VAL:HG22	1:E:184:ILE:HG12	1.92	0.51
2:G:195:CYS:SG	2:G:196:LEU:N	2.83	0.51
1:B:213:ASP:OD2	4:K:14:C:N4	2.42	0.51
1:E:246:ARG:HE	1:E:269:ASP:HB2	1.75	0.51
1:F:228:VAL:HG13	1:F:280:ARG:HG3	1.92	0.51
1:D:215:SER:HB3	1:D:218:ARG:HG2	1.93	0.51
1:C:21:ASN:OD1	1:C:31:ARG:NE	2.44	0.51
1:D:52:ASN:OD1	1:D:68:ARG:NH2	2.40	0.51
1:F:62:HIS:O	1:F:63:HIS:ND1	2.44	0.51
3:J:21:LEU:HD22	3:J:55:LEU:HB3	1.91	0.51
1:D:259:ARG:HB3	1:E:135:ARG:HH12	1.76	0.51
1:E:41:VAL:HB	1:E:134:SER:HB2	1.93	0.51
1:D:257:VAL:HG21	1:E:35:GLN:HB3	1.92	0.51
1:E:72:ILE:HB	1:E:75:ASN:HB2	1.92	0.51
1:F:54:ILE:HG13	1:F:65:ILE:HG23	1.94	0.50
1:F:179:ARG:NH1	1:F:244:PHE:O	2.43	0.50
2:G:83:ASP:O	2:G:156:ASN:ND2	2.44	0.50
2:G:345:THR:OG1	2:H:409:ARG:NH1	2.45	0.50
5:N:44:LYS:HG3	5:N:45:PRO:HD2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:22:GLU:HG3	3:I:37:ALA:HB2	1.93	0.50
3:J:17:LEU:HD22	3:J:83:LEU:HD21	1.94	0.50
1:A:230:GLU:O	1:A:277:LYS:HA	2.10	0.50
2:H:386:LEU:HB2	1:M:169:ARG:HH11	1.77	0.50
3:J:34:ALA:O	3:J:39:ARG:NH2	2.45	0.50
1:M:36:THR:HG23	1:M:38:GLU:H	1.75	0.50
1:M:110:ARG:HA	1:M:192:THR:HB	1.92	0.50
1:C:153:THR:OG1	1:C:154:ASN:N	2.41	0.50
1:F:103:CYS:O	1:F:110:ARG:NH2	2.39	0.50
5:N:31:PRO:HB3	5:N:51:VAL:HG11	1.94	0.50
1:D:230:GLU:O	1:D:277:LYS:HA	2.11	0.50
2:G:257:LEU:HB3	2:G:272:VAL:HG21	1.93	0.50
1:D:55:GLN:O	1:D:59:ASN:ND2	2.44	0.49
2:G:33:ILE:HG23	2:G:46:GLU:HB3	1.94	0.49
1:A:100:GLN:NE2	1:A:191:GLN:O	2.43	0.49
1:B:148:THR:HG22	1:B:167:MET:HG2	1.94	0.49
1:C:180:CYS:SG	1:C:181:HIS:N	2.86	0.49
1:D:25:ASP:HA	3:I:39:ARG:HD3	1.94	0.49
1:C:232:SER:OG	1:C:276:THR:OG1	2.27	0.49
1:D:149:ARG:NH2	1:D:166:THR:OG1	2.44	0.49
1:F:8:ASP:OD1	1:F:8:ASP:N	2.45	0.49
1:F:109:ILE:HA	1:F:113:GLY:HA2	1.93	0.49
1:A:270:ASP:OD1	1:A:270:ASP:N	2.46	0.49
1:C:169:ARG:HD2	3:J:39:ARG:HG2	1.94	0.49
1:D:160:GLU:HG2	1:D:162:GLY:H	1.77	0.49
1:C:148:THR:N	4:K:27:G:OP2	2.44	0.49
1:D:258:VAL:HG13	1:D:263:ASP:HB2	1.94	0.49
2:G:108:THR:HA	2:G:111:VAL:HG22	1.95	0.49
5:N:13:CYS:HA	5:N:25:SER:HB2	1.94	0.49
1:C:143:LEU:HG	1:C:174:PRO:HD3	1.95	0.49
1:F:262:ASP:OD1	1:F:262:ASP:N	2.41	0.49
1:M:41:VAL:HB	1:M:134:SER:HB2	1.94	0.49
1:B:188:PHE:HA	1:B:191:GLN:HG2	1.93	0.49
1:C:167:MET:HG2	4:K:27:G:H22	1.78	0.49
3:J:93:LEU:HG	3:J:97:GLN:HB3	1.95	0.49
1:C:102:MET:HB3	1:C:109:ILE:HD13	1.94	0.49
2:G:333:ASN:OD1	5:N:66:ARG:NH2	2.46	0.49
3:J:13:VAL:HG11	3:J:86:CYS:HB2	1.94	0.49
1:F:58:GLN:HE21	1:F:60:ASP:HB2	1.78	0.48
3:I:38:ASP:O	3:J:64:ASN:ND2	2.34	0.48
1:A:243:LEU:HD21	1:A:277:LYS:HE3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:VAL:O	1:D:259:ARG:NH2	2.46	0.48
5:N:60:ILE:HD12	5:N:62:TRP:HE1	1.78	0.48
1:D:108:ASP:O	1:D:112:PHE:N	2.45	0.48
2:G:33:ILE:HD11	2:G:160:ARG:HB2	1.95	0.48
2:G:214:VAL:HG12	2:G:270:THR:HB	1.95	0.48
1:A:69:GLU:O	1:C:164:ASN:ND2	2.42	0.48
1:B:215:SER:OG	4:K:17:C:OP1	2.31	0.48
1:D:109:ILE:HA	1:D:113:GLY:HA2	1.94	0.48
2:G:191:GLN:H	2:G:203:PRO:HB3	1.77	0.48
2:G:198:THR:O	2:G:200:LYS:NZ	2.43	0.48
2:H:543:CYS:SG	2:H:544:GLN:N	2.86	0.48
1:M:70:LYS:HE3	5:N:84:GLU:HB2	1.95	0.48
1:D:129:VAL:HG22	1:D:184:ILE:HG12	1.96	0.48
1:B:43:ASP:OD2	1:B:43:ASP:N	2.44	0.48
2:H:550:LEU:HD22	2:H:554:GLN:HG2	1.95	0.48
3:J:24:ILE:HD12	3:J:59:LEU:HD21	1.94	0.48
1:D:247:ILE:HG23	1:D:268:VAL:HG12	1.96	0.48
3:I:2:GLY:N	3:J:84:GLU:OE1	2.47	0.48
5:N:96:LYS:NZ	5:N:97:ASP:OD2	2.39	0.48
1:D:118:THR:OG1	1:D:119:GLY:N	2.47	0.48
1:E:99:ARG:HH21	1:E:125:VAL:HG22	1.78	0.48
3:J:21:LEU:HD23	3:J:59:LEU:HD13	1.96	0.48
1:E:64:ASP:HB2	1:E:106:TYR:HA	1.96	0.48
2:G:333:ASN:ND2	5:N:89:GLN:O	2.46	0.47
5:N:117:ASN:HD22	5:N:120:LYS:HD3	1.79	0.47
3:I:29:ASN:N	3:I:29:ASN:OD1	2.46	0.47
1:D:214:HIS:HE1	1:D:221:MET:H	1.62	0.47
1:F:214:HIS:HE1	1:F:221:MET:H	1.62	0.47
1:M:214:HIS:ND1	1:M:219:GLY:O	2.36	0.47
1:A:121:ASN:ND2	1:B:161:THR:O	2.41	0.47
2:G:111:VAL:HG21	2:G:131:LEU:HD12	1.96	0.47
5:N:69:GLU:OE1	5:N:90:ARG:NH1	2.46	0.47
2:G:224:VAL:HG23	2:G:240:PHE:HE1	1.80	0.47
2:G:267:GLY:HA2	2:H:389:LYS:HE2	1.97	0.47
1:B:137:ILE:HG13	1:B:249:VAL:HG23	1.95	0.47
2:G:183:ASN:O	2:G:187:SER:OG	2.33	0.47
1:A:68:ARG:HB3	1:A:69:GLU:H	1.54	0.47
1:A:214:HIS:ND1	1:A:219:GLY:O	2.45	0.47
1:B:277:LYS:HE2	1:B:277:LYS:HB2	1.77	0.47
1:D:68:ARG:HB3	1:D:69:GLU:H	1.51	0.47
1:D:169:ARG:HH12	3:I:65:LYS:HD3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ALA:HA	1:D:192:THR:HG22	1.97	0.47
1:F:246:ARG:HH12	1:F:272:ASN:HB2	1.78	0.47
5:N:12:ALA:HB2	5:N:98:VAL:HG21	1.97	0.47
1:E:40:LEU:HD21	1:E:133:PHE:HD2	1.80	0.47
3:I:94:ASN:O	3:I:98:GLN:N	2.42	0.47
1:M:70:LYS:O	1:M:74:ASN:ND2	2.48	0.47
1:A:126:ARG:HH12	4:K:20:G:H22	1.62	0.47
1:C:39:GLY:N	1:C:136:SER:OG	2.42	0.47
1:F:249:VAL:HB	1:F:266:VAL:HG12	1.96	0.47
1:A:16:GLN:HB2	1:A:220:GLN:HB3	1.96	0.47
1:C:23:ASP:HB3	1:C:26:ALA:HB3	1.96	0.47
1:C:109:ILE:HA	1:C:113:GLY:HA2	1.97	0.47
1:C:116:MET:HG3	1:C:122:ALA:HB3	1.97	0.47
1:A:12:LEU:HG	1:A:179:ARG:HB2	1.97	0.46
1:B:118:THR:O	1:M:154:ASN:ND2	2.46	0.46
1:C:83:GLN:HB3	1:C:84:GLU:H	1.53	0.46
1:D:214:HIS:CE1	1:D:221:MET:H	2.33	0.46
1:E:17:ASP:HB3	1:F:133:PHE:HB2	1.97	0.46
1:F:2:THR:OG1	1:F:3:ILE:N	2.48	0.46
1:F:230:GLU:OE2	1:F:280:ARG:NE	2.45	0.46
2:G:108:THR:O	2:G:112:ASN:ND2	2.49	0.46
1:M:23:ASP:N	1:M:29:LEU:O	2.45	0.46
1:C:129:VAL:HG22	1:C:184:ILE:HD12	1.96	0.46
1:C:127:GLY:O	1:C:130:GLN:NE2	2.46	0.46
1:F:229:PHE:CD1	1:F:279:LEU:HD13	2.50	0.46
1:F:258:VAL:O	1:F:259:ARG:NH2	2.48	0.46
2:G:340:ARG:NH2	2:H:395:SER:OG	2.48	0.46
3:I:17:LEU:HD22	3:I:83:LEU:HD21	1.96	0.46
3:J:45:SER:HB3	3:J:98:GLN:HE22	1.80	0.46
1:C:21:ASN:ND2	4:K:20:G:O2'	2.48	0.46
1:E:5:LYS:HE2	1:E:5:LYS:HB2	1.82	0.46
1:E:255:VAL:HG21	1:E:263:ASP:HB3	1.97	0.46
2:G:97:GLN:O	2:G:99:GLN:N	2.49	0.46
3:J:20:VAL:HG12	3:J:112:LEU:HD11	1.97	0.46
1:A:23:ASP:H	4:K:27:G:H2'	1.80	0.46
3:I:95:LEU:HD21	3:J:50:ALA:HB2	1.97	0.46
1:A:43:ASP:OD1	1:A:43:ASP:N	2.49	0.46
1:A:141:MET:HA	3:I:47:THR:HG21	1.97	0.46
1:B:215:SER:HB3	1:B:218:ARG:HD2	1.98	0.46
2:G:224:VAL:HG13	2:G:229:PHE:HD2	1.81	0.46
1:M:6:ARG:NH2	1:M:235:LEU:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:HB3	1:B:180:CYS:HB2	1.98	0.46
2:G:85:TYR:HB3	2:G:155:CYS:HB3	1.96	0.46
3:J:16:ARG:HB3	3:J:82:ILE:HD13	1.97	0.46
1:M:39:GLY:HA3	1:M:178:TYR:HE1	1.81	0.46
1:B:148:THR:HA	1:B:167:MET:HA	1.98	0.45
1:A:51:ARG:HB3	1:A:65:ILE:HG23	1.97	0.45
1:A:129:VAL:HG22	1:A:184:ILE:HG12	1.98	0.45
1:C:12:LEU:HD21	1:C:249:VAL:HG21	1.98	0.45
1:E:85:ASN:OD1	1:E:85:ASN:N	2.50	0.45
1:E:124:GLN:HE22	4:K:32:A:H61	1.64	0.45
1:A:149:ARG:HH12	1:A:153:THR:HG23	1.81	0.45
1:A:235:LEU:HG	1:C:57:THR:HG22	1.97	0.45
1:E:6:ARG:NH1	1:E:8:ASP:OD1	2.49	0.45
1:F:91:LYS:HA	1:F:94:LYS:HB3	1.97	0.45
1:B:129:VAL:HG13	1:B:184:ILE:HG12	1.99	0.45
5:N:16:ARG:NH2	5:N:18:GLU:OE2	2.49	0.45
1:C:117:THR:HA	1:C:121:ASN:HA	1.98	0.45
5:N:164:ILE:HG12	5:N:198:VAL:HG12	1.98	0.45
1:D:54:ILE:O	1:D:58:GLN:HB2	2.17	0.45
1:D:82:GLU:HA	1:D:86:VAL:HG22	1.97	0.45
1:F:235:LEU:HB3	1:F:236:GLY:H	1.56	0.45
1:A:12:LEU:HD21	1:A:249:VAL:HG21	1.97	0.45
1:B:48:ARG:HG2	4:K:14:C:C2	2.52	0.45
1:B:169:ARG:HA	1:B:169:ARG:HD3	1.85	0.45
2:G:31:PRO:HD2	2:G:156:ASN:HB3	1.98	0.45
1:B:143:LEU:HB3	1:B:145:HIS:CD2	2.52	0.45
1:B:220:GLN:HE21	1:B:222:ASN:HD21	1.63	0.45
1:E:147:ILE:HA	1:F:31:ARG:HH22	1.82	0.45
2:H:463:ASN:O	2:H:465:GLN:N	2.43	0.45
1:C:246:ARG:NH1	1:C:272:ASN:O	2.50	0.45
1:D:162:GLY:HA2	1:F:121:ASN:HB2	1.98	0.45
2:H:359:ASP:OD1	2:H:360:ASP:N	2.50	0.45
2:H:506:ILE:HD12	3:J:95:LEU:HD23	1.99	0.45
3:I:110:GLN:HB2	3:J:80:ARG:HB3	1.99	0.45
5:N:205:PRO:HA	5:N:206:PRO:HD3	1.89	0.45
1:B:83:GLN:HG3	1:B:101:TYR:CZ	2.52	0.44
1:B:179:ARG:NH1	1:B:244:PHE:O	2.50	0.44
1:E:21:ASN:ND2	1:E:45:CYS:SG	2.90	0.44
1:F:85:ASN:HB2	1:F:94:LYS:HD3	1.99	0.44
1:A:270:ASP:HA	1:A:273:LEU:HD21	1.99	0.44
1:D:252:LYS:HB3	1:D:253:ASP:H	1.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLU:HG2	1:E:162:GLY:H	1.81	0.44
2:G:262:ASN:ND2	2:G:273:CYS:O	2.51	0.44
3:J:20:VAL:HG21	3:J:79:ILE:HG12	1.98	0.44
1:B:252:LYS:HD3	1:B:252:LYS:HA	1.81	0.44
1:D:6:ARG:HB3	1:D:231:HIS:HD2	1.82	0.44
1:D:142:THR:HG22	1:D:144:GLU:H	1.82	0.44
1:E:68:ARG:NH1	1:F:124:GLN:OE1	2.48	0.44
1:F:187:HIS:O	1:F:191:GLN:NE2	2.50	0.44
4:K:9:A:N6	1:M:24:PRO:HB3	2.33	0.44
3:J:60:PRO:O	3:J:64:ASN:ND2	2.50	0.44
5:N:21:VAL:HG23	5:N:22:GLU:HG2	1.99	0.44
2:G:195:CYS:HB2	2:G:202:ALA:HB3	2.00	0.44
1:A:246:ARG:HB3	1:A:269:ASP:HB2	1.99	0.44
1:E:31:ARG:HH21	4:K:39:U:H5'	1.83	0.44
2:G:336:ARG:HH12	5:N:88:GLN:HB3	1.82	0.44
1:M:9:PHE:HB3	1:M:228:VAL:HG13	2.00	0.44
1:B:14:ASP:N	1:B:14:ASP:OD1	2.50	0.43
1:D:58:GLN:NE2	1:D:60:ASP:OD1	2.50	0.43
1:D:210:PHE:O	1:D:214:HIS:NE2	2.51	0.43
1:E:103:CYS:HB3	1:E:192:THR:HA	1.99	0.43
1:E:156:LYS:HB3	1:E:157:ASP:H	1.65	0.43
2:G:28:LYS:HA	2:G:28:LYS:HD3	1.74	0.43
1:A:235:LEU:HB3	1:A:236:GLY:H	1.61	0.43
1:C:137:ILE:HG13	1:C:249:VAL:HB	2.00	0.43
1:E:257:VAL:HB	1:E:258:VAL:H	1.68	0.43
1:F:68:ARG:O	1:F:70:LYS:N	2.51	0.43
2:G:139:LYS:HA	2:G:139:LYS:HD2	1.85	0.43
1:D:15:VAL:HG21	1:D:20:PRO:HG3	2.01	0.43
1:E:83:GLN:HG3	1:E:101:TYR:CZ	2.53	0.43
2:H:461:ASP:O	2:H:473:ARG:NH1	2.51	0.43
4:K:5:A:H5'	5:N:143:ARG:HD3	2.00	0.43
1:A:65:ILE:O	1:A:66:PHE:HB2	2.18	0.43
1:B:65:ILE:HD13	1:B:65:ILE:HA	1.91	0.43
1:C:84:GLU:H	1:C:84:GLU:HG3	1.69	0.43
1:E:150:MET:HE3	1:F:68:ARG:HB2	2.00	0.43
2:H:397:LEU:HD13	2:H:415:LEU:HD22	1.99	0.43
2:G:29:GLU:HG3	2:G:60:THR:HG22	2.01	0.43
1:M:43:ASP:HA	1:M:46:LEU:HD23	2.00	0.43
1:A:65:ILE:HD13	1:A:65:ILE:HA	1.88	0.43
1:A:215:SER:OG	1:A:216:ALA:N	2.52	0.43
1:B:126:ARG:HD3	1:B:188:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:THR:HB	1:F:44:VAL:HG22	2.00	0.43
1:A:152:VAL:HB	1:A:164:ASN:HB3	2.01	0.43
1:F:251:LYS:HG2	1:F:264:TYR:HE1	1.84	0.43
2:G:329:GLY:HA3	2:G:341:PHE:HD2	1.83	0.43
3:J:25:GLN:HG3	3:J:36:ILE:HG23	2.00	0.43
5:N:70:VAL:HB	5:N:83:ILE:HG22	1.99	0.43
5:N:184:ASP:OD2	5:N:187:ASN:ND2	2.52	0.43
5:N:186:ASN:OD1	5:N:186:ASN:N	2.51	0.43
1:B:109:ILE:HA	1:B:113:GLY:HA2	2.01	0.43
1:C:25:ASP:HB3	2:H:515:LEU:HB3	2.01	0.43
2:G:229:PHE:HZ	5:N:88:GLN:HG3	1.82	0.43
3:J:20:VAL:O	3:J:24:ILE:HG13	2.18	0.43
4:K:21:C:H1'	4:K:22:C:C2	2.53	0.43
5:N:48:ARG:HD2	5:N:48:ARG:HA	1.81	0.43
5:N:105:ASP:OD1	5:N:105:ASP:N	2.50	0.43
1:A:99:ARG:HH22	1:A:191:GLN:HB3	1.84	0.43
1:D:187:HIS:O	1:D:191:GLN:NE2	2.42	0.43
1:F:255:VAL:HG11	1:F:263:ASP:HB3	2.01	0.43
2:G:118:LEU:HD23	2:G:118:LEU:HA	1.82	0.43
1:B:131:LEU:HD11	1:B:202:PHE:HZ	1.83	0.42
1:C:149:ARG:HG2	1:C:151:ALA:H	1.84	0.42
2:H:524:GLU:H	2:H:524:GLU:HG3	1.67	0.42
2:H:412:PRO:HD2	2:H:415:LEU:HD23	2.01	0.42
3:I:115:LYS:HE3	3:I:115:LYS:HB2	1.79	0.42
1:M:41:VAL:O	1:M:134:SER:N	2.52	0.42
1:B:191:GLN:HG3	1:B:192:THR:HG23	2.00	0.42
1:D:180:CYS:SG	1:D:181:HIS:N	2.93	0.42
1:F:258:VAL:HG11	1:F:264:TYR:CZ	2.55	0.42
2:G:324:LYS:HB3	2:G:325:PHE:H	1.58	0.42
5:N:14:PHE:HB2	5:N:26:TYR:HB2	2.01	0.42
1:A:72:ILE:HD12	1:A:75:ASN:HD22	1.83	0.42
1:A:124:GLN:H	1:A:124:GLN:HG2	1.72	0.42
1:D:203:TRP:HB3	1:D:282:LEU:HD22	2.02	0.42
1:E:85:ASN:HB2	1:E:94:LYS:HG3	2.02	0.42
1:F:9:PHE:CZ	1:F:182:GLY:HA3	2.55	0.42
2:G:121:ASP:HB2	2:G:124:VAL:HG22	2.02	0.42
3:J:37:ALA:O	3:J:41:PHE:HB2	2.19	0.42
1:M:30:PRO:HD2	1:M:142:THR:HB	2.01	0.42
1:A:89:LYS:HE3	1:A:89:LYS:HB3	1.87	0.42
1:A:157:ASP:OD1	1:A:157:ASP:N	2.52	0.42
1:B:64:ASP:OD2	1:B:105:ARG:NE	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:THR:HG22	1:F:235:LEU:HG	2.00	0.42
1:M:23:ASP:OD1	1:M:31:ARG:HG2	2.19	0.42
5:N:129:ALA:HA	5:N:149:PHE:HE2	1.85	0.42
1:A:47:LYS:HB3	1:A:51:ARG:HH21	1.84	0.42
1:B:236:GLY:O	1:M:208:ASN:ND2	2.53	0.42
1:D:72:ILE:HG22	1:D:75:ASN:H	1.84	0.42
2:G:247:MET:HA	2:G:250:TYR:CD1	2.55	0.42
2:H:350:LEU:O	2:H:353:SER:OG	2.35	0.42
2:H:423:ASN:HB3	2:H:498:PHE:HE1	1.84	0.42
2:H:471:LEU:HG	2:H:509:PHE:HE2	1.84	0.42
3:I:110:GLN:HG2	3:J:84:GLU:HG2	2.01	0.42
1:B:99:ARG:HH21	1:B:125:VAL:HA	1.85	0.42
1:D:206:LEU:HD23	1:D:206:LEU:HA	1.87	0.42
1:E:150:MET:HB3	1:F:68:ARG:HG3	2.02	0.42
1:F:7:TYR:CZ	1:F:230:GLU:HG2	2.55	0.42
1:B:18:GLY:HA2	1:B:172:THR:HG22	2.00	0.41
1:C:100:GLN:NE2	1:C:191:GLN:O	2.41	0.41
1:D:270:ASP:OD1	1:D:270:ASP:N	2.39	0.41
1:F:107:TYR:CZ	1:F:201:LEU:HD23	2.55	0.41
2:G:173:LYS:HA	2:G:173:LYS:HD2	1.82	0.41
5:N:19:LEU:HD12	5:N:19:LEU:HA	1.92	0.41
1:A:134:SER:HB3	1:A:178:TYR:HB3	2.01	0.41
1:E:246:ARG:HB3	1:E:269:ASP:HB2	2.02	0.41
2:G:3:LEU:HD12	5:N:18:GLU:HB2	2.02	0.41
1:M:12:LEU:HD12	1:M:179:ARG:HB2	2.02	0.41
1:A:277:LYS:HB2	1:A:277:LYS:HE2	1.85	0.41
1:E:55:GLN:HA	1:E:59:ASN:HB2	2.03	0.41
1:F:275:GLU:H	1:F:275:GLU:HG3	1.56	0.41
2:G:139:LYS:NZ	2:G:142:GLN:O	2.54	0.41
2:H:557:LEU:HD23	2:H:557:LEU:HA	1.95	0.41
1:M:65:ILE:O	1:M:67:ILE:N	2.53	0.41
1:C:19:ASN:ND2	1:C:28:ASN:O	2.53	0.41
1:F:247:ILE:HG12	1:F:268:VAL:HG12	2.03	0.41
2:G:338:VAL:HG23	5:N:91:ALA:HB2	2.03	0.41
1:C:64:ASP:OD2	1:C:105:ARG:NH1	2.52	0.41
2:G:307:LEU:HG	2:H:378:PRO:HD3	2.03	0.41
1:B:149:ARG:HB2	4:K:19:U:H1'	2.03	0.41
1:B:224:ARG:HD3	1:B:224:ARG:HA	1.88	0.41
1:C:273:LEU:HB2	1:C:277:LYS:HE3	2.02	0.41
1:E:59:ASN:HD22	1:E:65:ILE:HG13	1.84	0.41
2:H:482:GLN:NE2	2:H:493:ILE:HG23	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:5:LEU:O	5:N:101:ARG:HA	2.20	0.41
1:B:67:ILE:HD12	1:B:71:GLY:HA3	2.03	0.41
1:C:23:ASP:N	1:C:29:LEU:O	2.41	0.41
1:E:50:VAL:O	1:E:54:ILE:HG12	2.20	0.41
1:F:129:VAL:HG22	1:F:184:ILE:HD12	2.03	0.41
2:G:97:GLN:HB3	2:G:98:GLU:H	1.62	0.41
2:H:509:PHE:O	2:H:513:MET:HG2	2.21	0.41
1:M:275:GLU:H	1:M:275:GLU:HG3	1.55	0.41
5:N:44:LYS:O	5:N:46:ALA:N	2.48	0.41
1:C:9:PHE:CZ	1:C:182:GLY:HA3	2.56	0.41
1:E:28:ASN:HB3	1:E:171:PHE:HE2	1.85	0.41
2:G:54:LYS:HB3	2:G:54:LYS:HE2	1.76	0.41
2:H:404:ALA:HB1	2:H:411:LEU:HD12	2.03	0.41
1:A:9:PHE:HB3	1:A:228:VAL:HG13	2.02	0.41
1:B:118:THR:HG21	1:M:153:THR:HB	2.03	0.41
1:B:141:MET:HG3	3:J:95:LEU:HD22	2.02	0.41
1:B:220:GLN:HB2	1:C:132:THR:HG21	2.02	0.41
1:C:38:GLU:HA	1:C:139:PRO:HA	2.02	0.41
1:C:161:THR:HB	1:D:121:ASN:HD22	1.86	0.41
1:C:187:HIS:HA	1:C:190:LYS:HE2	2.03	0.41
1:C:205:ALA:O	1:C:209:MET:HB3	2.21	0.41
1:D:9:PHE:CZ	1:D:182:GLY:HA3	2.55	0.41
1:D:277:LYS:HB2	1:D:277:LYS:HE2	1.72	0.41
2:G:195:CYS:SG	2:G:198:THR:OG1	2.66	0.41
2:H:474:LEU:HD12	2:H:536:ILE:HD11	2.02	0.41
3:J:83:LEU:HD23	3:J:83:LEU:HA	1.90	0.41
5:N:68:ASN:HD22	5:N:89:GLN:HG2	1.86	0.41
5:N:131:LYS:HD3	5:N:131:LYS:HA	1.89	0.41
1:C:6:ARG:HA	1:C:184:ILE:O	2.21	0.41
1:E:245:LYS:HA	1:E:245:LYS:HD3	1.76	0.41
2:H:417:GLN:HG2	1:M:141:MET:HG3	2.03	0.41
3:J:77:TRP:HA	3:J:80:ARG:HH21	1.86	0.41
1:A:118:THR:OG1	1:A:119:GLY:N	2.54	0.40
3:J:25:GLN:HG2	3:J:62:HIS:CE1	2.56	0.40
1:M:45:CYS:O	1:M:49:LYS:HG2	2.20	0.40
1:M:99:ARG:NH2	1:M:191:GLN:O	2.55	0.40
1:M:150:MET:HG2	1:M:165:ARG:HH21	1.86	0.40
1:D:137:ILE:HG13	1:D:249:VAL:HB	2.04	0.40
1:E:15:VAL:HG23	1:E:221:MET:HG2	2.02	0.40
1:F:49:LYS:HB2	1:F:49:LYS:HE2	1.84	0.40
2:H:469:TYR:HE1	2:H:560:ILE:HG22	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:ARG:NH2	1:M:236:GLY:HA3	2.36	0.40
1:A:32:ILE:HD13	3:J:57:ARG:NH1	2.35	0.40
1:A:243:LEU:HD13	1:A:243:LEU:HA	1.94	0.40
1:B:54:ILE:O	1:B:58:GLN:N	2.50	0.40
1:F:194:PHE:HE2	1:F:199:LEU:HD13	1.86	0.40
2:G:214:VAL:HB	2:G:332:PRO:HD3	2.03	0.40
1:M:19:ASN:N	1:M:217:ALA:O	2.43	0.40
5:N:58:LYS:HD3	5:N:97:ASP:HB3	2.02	0.40
1:D:256:GLU:HG3	1:D:257:VAL:HG22	2.03	0.40
2:G:247:MET:HA	2:G:250:TYR:HD1	1.86	0.40
2:G:340:ARG:HH12	5:N:66:ARG:NH1	2.20	0.40
1:C:14:ASP:OD1	1:C:14:ASP:N	2.53	0.40
1:D:177:LEU:HD23	1:D:249:VAL:HG11	2.02	0.40
1:E:56:MET:HG3	1:F:187:HIS:HB2	2.03	0.40
1:E:84:GLU:H	1:E:84:GLU:HG3	1.74	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	281/283 (99%)	227 (81%)	47 (17%)	7 (2%)	5	35
1	B	281/283 (99%)	230 (82%)	44 (16%)	7 (2%)	5	35
1	C	281/283 (99%)	223 (79%)	49 (17%)	9 (3%)	4	31
1	D	281/283 (99%)	238 (85%)	38 (14%)	5 (2%)	8	42
1	E	281/283 (99%)	228 (81%)	45 (16%)	8 (3%)	5	33
1	F	267/283 (94%)	206 (77%)	53 (20%)	8 (3%)	4	32
1	M	260/283 (92%)	219 (84%)	39 (15%)	2 (1%)	19	58
2	G	321/582 (55%)	249 (78%)	62 (19%)	10 (3%)	4	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	231/582 (40%)	191 (83%)	34 (15%)	6 (3%)	5	34
3	I	122/124 (98%)	111 (91%)	10 (8%)	1 (1%)	19	58
3	J	122/124 (98%)	114 (93%)	7 (6%)	1 (1%)	19	58
5	N	203/205 (99%)	174 (86%)	24 (12%)	5 (2%)	5	35
All	All	2931/3598 (82%)	2410 (82%)	452 (15%)	69 (2%)	9	36

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	68	ARG
2	G	31	PRO
1	C	253	ASP
1	D	16	GLN
1	D	231	HIS
1	D	252	LYS
2	G	98	GLU
2	G	201	ALA
2	H	487	PRO
3	J	30	PRO
1	A	68	ARG
1	A	90	GLU
1	A	167	MET
1	B	119	GLY
1	B	128	PRO
1	C	16	GLN
1	C	58	GLN
1	C	90	GLU
1	D	90	GLU
1	E	90	GLU
1	E	118	THR
1	F	71	GLY
1	F	90	GLU
2	G	80	LEU
2	G	83	ASP
2	G	166	VAL
2	G	277	LYS
2	H	432	GLY
2	H	450	LEU
2	H	571	THR
1	M	66	PHE
1	M	283	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	N	194	GLN
5	N	195	CYS
5	N	199	ASN
1	A	25	ASP
1	A	67	ILE
1	B	58	GLN
1	B	66	PHE
1	B	87	LYS
1	B	90	GLU
1	C	66	PHE
1	C	68	ARG
1	C	70	LYS
1	E	58	GLN
1	F	58	GLN
1	F	69	GLU
2	G	41	ASN
2	G	231	SER
2	H	365	ARG
2	H	395	SER
5	N	46	ALA
5	N	82	TYR
1	A	66	PHE
1	B	31	ARG
1	C	83	GLN
1	C	153	THR
1	D	67	ILE
1	E	66	PHE
1	E	153	THR
1	E	167	MET
1	F	118	THR
1	F	128	PRO
2	G	202	ALA
1	A	88	GLY
1	F	88	GLY
1	E	257	VAL
3	I	30	PRO
1	F	24	PRO

5.3.2 Protein sidechains [i](#)

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	245/245 (100%)	239 (98%)	6 (2%)	49	74
1	B	245/245 (100%)	239 (98%)	6 (2%)	49	74
1	C	245/245 (100%)	238 (97%)	7 (3%)	42	71
1	D	245/245 (100%)	235 (96%)	10 (4%)	30	63
1	E	245/245 (100%)	238 (97%)	7 (3%)	42	71
1	F	235/245 (96%)	226 (96%)	9 (4%)	33	65
1	M	229/245 (94%)	222 (97%)	7 (3%)	40	70
2	G	261/475 (55%)	253 (97%)	8 (3%)	40	70
2	H	196/475 (41%)	186 (95%)	10 (5%)	24	58
3	I	104/104 (100%)	98 (94%)	6 (6%)	20	54
3	J	104/104 (100%)	99 (95%)	5 (5%)	25	59
5	N	182/182 (100%)	175 (96%)	7 (4%)	33	65
All	All	2536/3055 (83%)	2448 (96%)	88 (4%)	39	67

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	66	PHE
1	A	85	ASN
1	A	160	GLU
1	A	250	VAL
1	A	264	TYR
1	B	142	THR
1	B	165	ARG
1	B	171	PHE
1	B	218	ARG
1	B	252	LYS
1	B	280	ARG
1	C	66	PHE
1	C	125	VAL
1	C	156	LYS
1	C	157	ASP
1	C	167	MET
1	C	218	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	264	TYR
1	D	5	LYS
1	D	12	LEU
1	D	66	PHE
1	D	68	ARG
1	D	91	LYS
1	D	99	ARG
1	D	115	VAL
1	D	152	VAL
1	D	169	ARG
1	D	264	TYR
1	E	48	ARG
1	E	60	ASP
1	E	91	LYS
1	E	148	THR
1	E	180	CYS
1	E	252	LYS
1	E	258	VAL
1	F	66	PHE
1	F	68	ARG
1	F	141	MET
1	F	229	PHE
1	F	249	VAL
1	F	264	TYR
1	F	266	VAL
1	F	273	LEU
1	F	275	GLU
2	G	9	TYR
2	G	57	VAL
2	G	69	ARG
2	G	149	CYS
2	G	240	PHE
2	G	248	PHE
2	G	250	TYR
2	G	312	TYR
2	H	363	MET
2	H	374	TYR
2	H	396	ASP
2	H	431	TYR
2	H	438	LYS
2	H	449	ARG
2	H	466	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	498	PHE
2	H	514	ARG
2	H	515	LEU
3	I	12	TYR
3	I	21	LEU
3	I	92	HIS
3	I	98	GLN
3	I	113	PHE
3	I	114	THR
3	J	12	TYR
3	J	38	ASP
3	J	41	PHE
3	J	92	HIS
3	J	106	TYR
1	M	115	VAL
1	M	156	LYS
1	M	163	ASP
1	M	165	ARG
1	M	249	VAL
1	M	271	LYS
1	M	275	GLU
5	N	20	LYS
5	N	30	THR
5	N	44	LYS
5	N	101	ARG
5	N	130	LYS
5	N	131	LYS
5	N	145	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	75	ASN
1	A	130	GLN
1	A	145	HIS
1	B	16	GLN
1	B	81	HIS
1	B	130	GLN
1	B	181	HIS
1	B	222	ASN
1	C	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	85	ASN
1	C	124	GLN
1	D	181	HIS
1	D	212	HIS
1	D	231	HIS
1	E	19	ASN
1	E	59	ASN
1	E	181	HIS
1	F	52	ASN
1	F	58	GLN
1	F	191	GLN
2	G	99	GLN
2	G	104	HIS
2	G	181	GLN
2	G	189	ASN
2	H	518	HIS
2	H	567	GLN
3	J	61	HIS
1	M	220	GLN
5	N	68	ASN
5	N	88	GLN
5	N	117	ASN
5	N	136	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	K	42/43 (97%)	24 (57%)	2 (4%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	K	2	U
4	K	3	U
4	K	4	G
4	K	5	A
4	K	6	A
4	K	7	A
4	K	8	C
4	K	9	A
4	K	10	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	13	U
4	K	15	A
4	K	16	G
4	K	19	U
4	K	21	C
4	K	23	G
4	K	24	U
4	K	27	G
4	K	29	G
4	K	31	C
4	K	33	U
4	K	35	G
4	K	37	C
4	K	39	U
4	K	43	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	K	4	G
4	K	9	A

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 monosaccharides 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

There are no chain breaks in this entry.

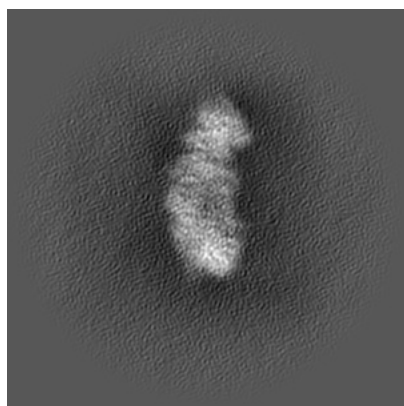
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29896. These allow visual inspection of the internal detail of the map and identification of artifacts.

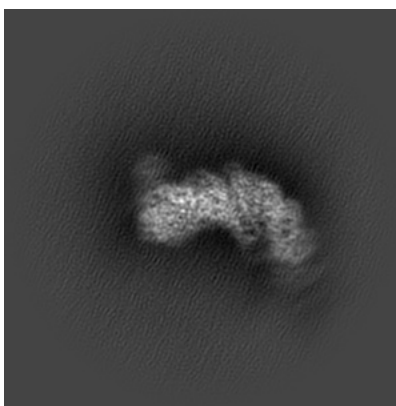
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

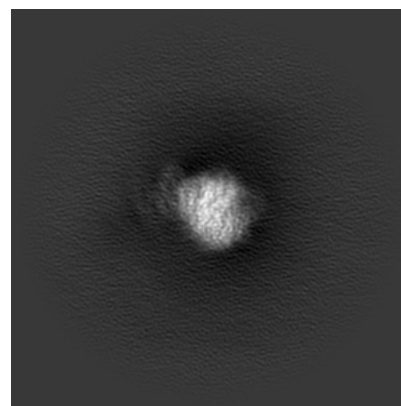
6.1.1 Primary map



X

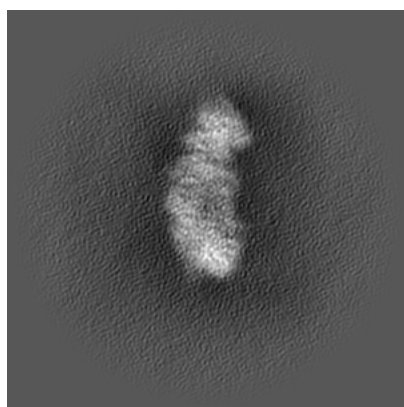


Y

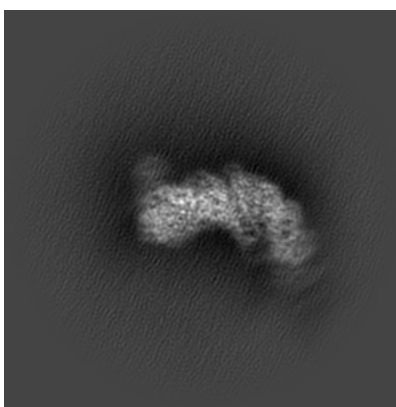


Z

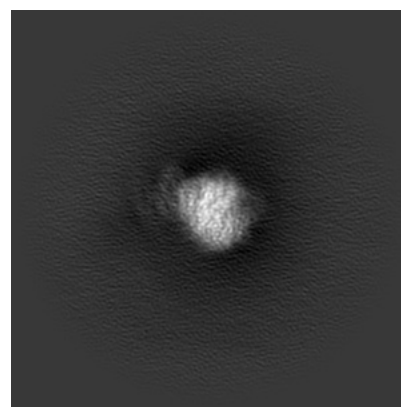
6.1.2 Raw map



X



Y

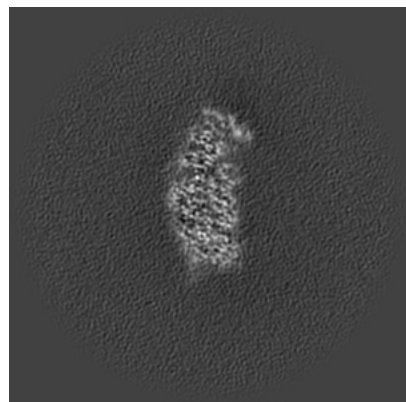


Z

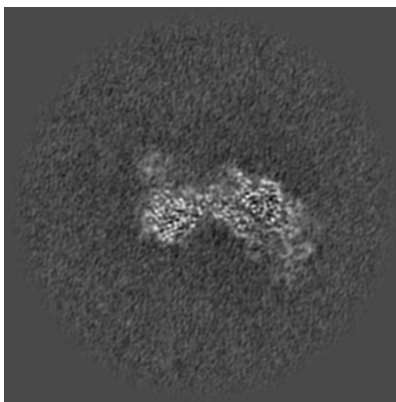
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

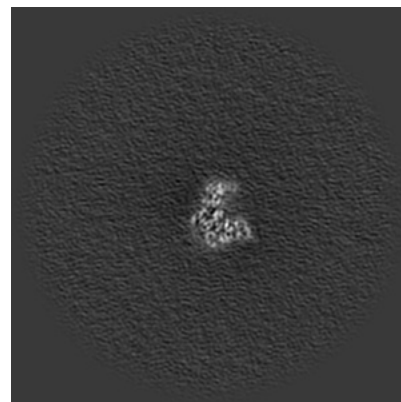
6.2.1 Primary map



X Index: 140

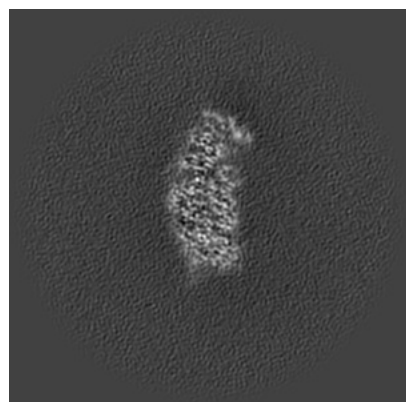


Y Index: 140

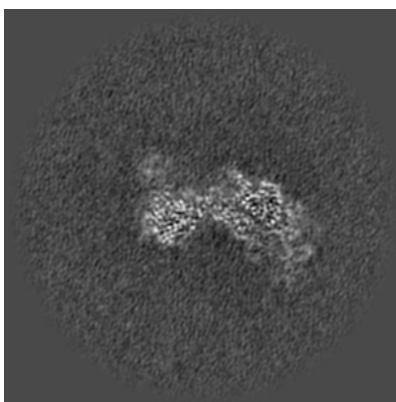


Z Index: 140

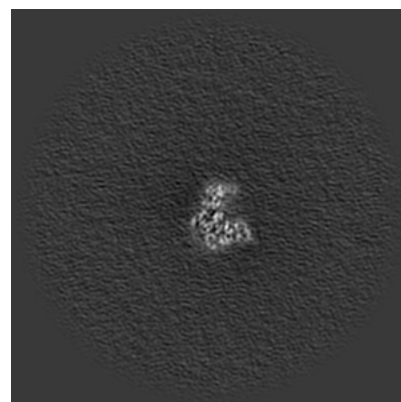
6.2.2 Raw map



X Index: 140



Y Index: 140

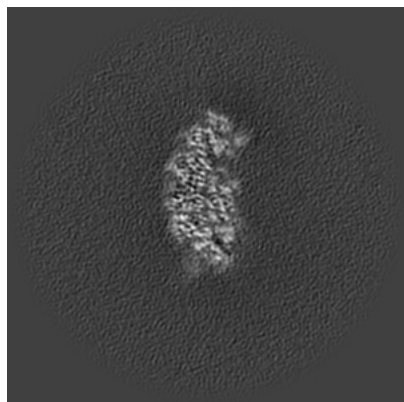


Z Index: 140

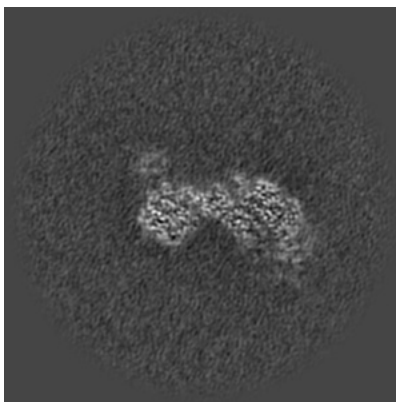
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

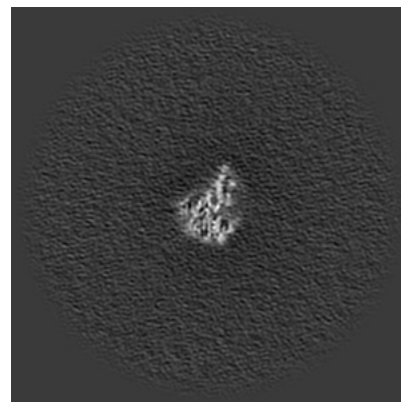
6.3.1 Primary map



X Index: 144

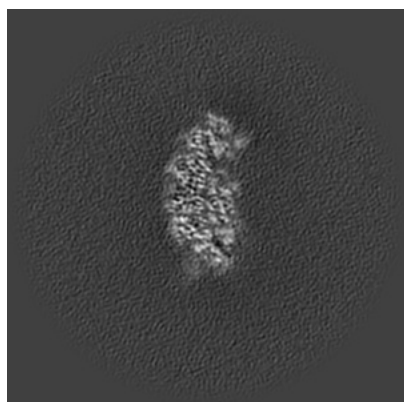


Y Index: 143

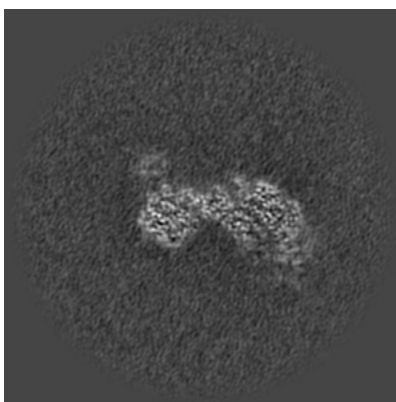


Z Index: 124

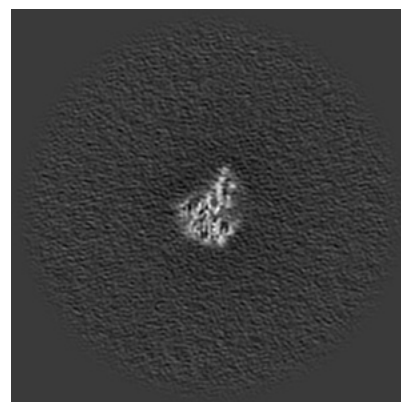
6.3.2 Raw map



X Index: 144



Y Index: 143

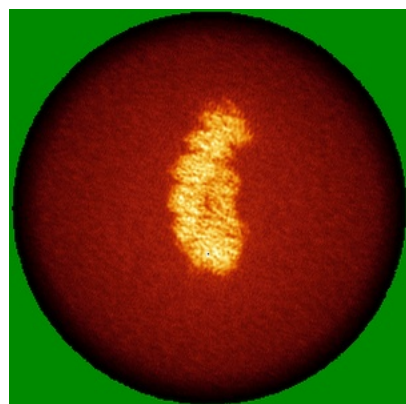


Z Index: 124

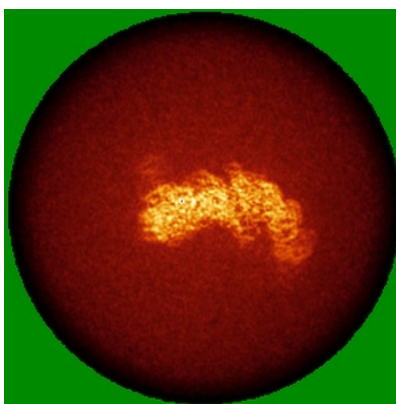
The images above show the largest variance slices of the map in three orthogonal directions.

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

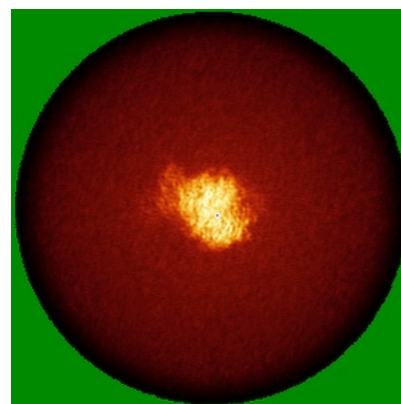
6.4.1 Primary map



X

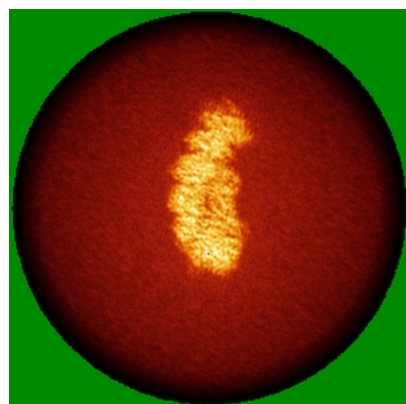


Y

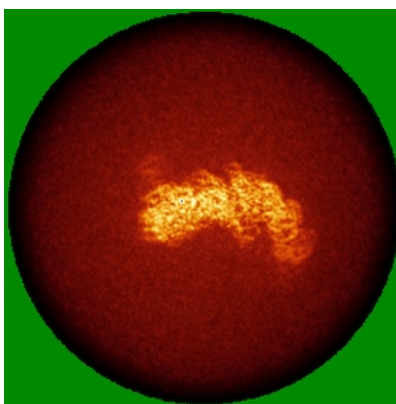


Z

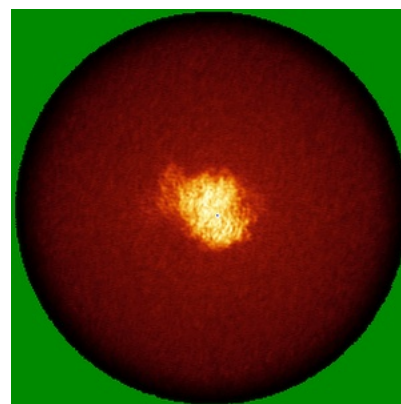
6.4.2 Raw map



X



Y

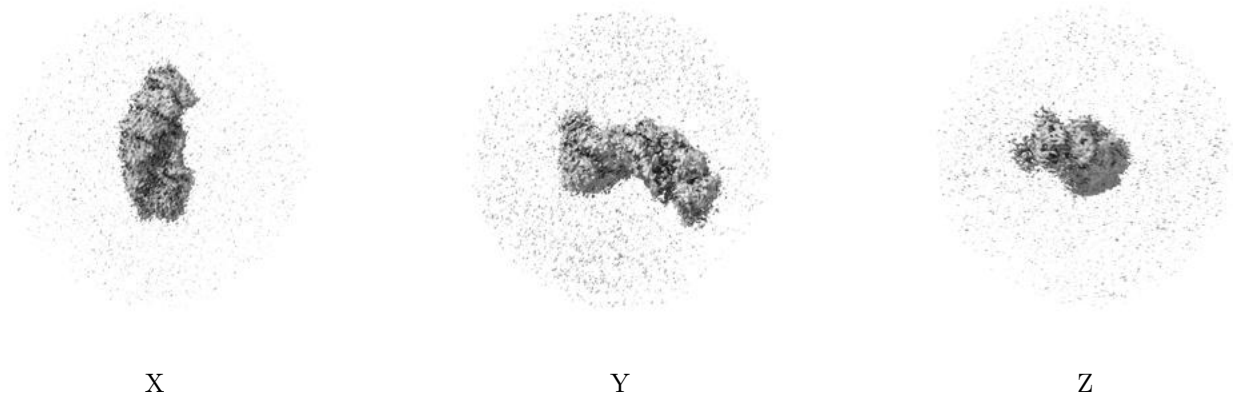


Z

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.

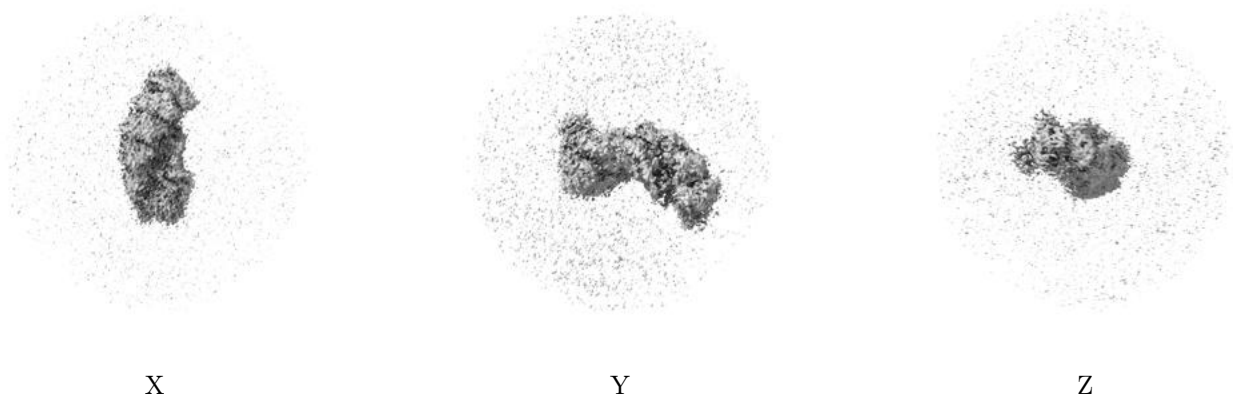
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.119. 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.

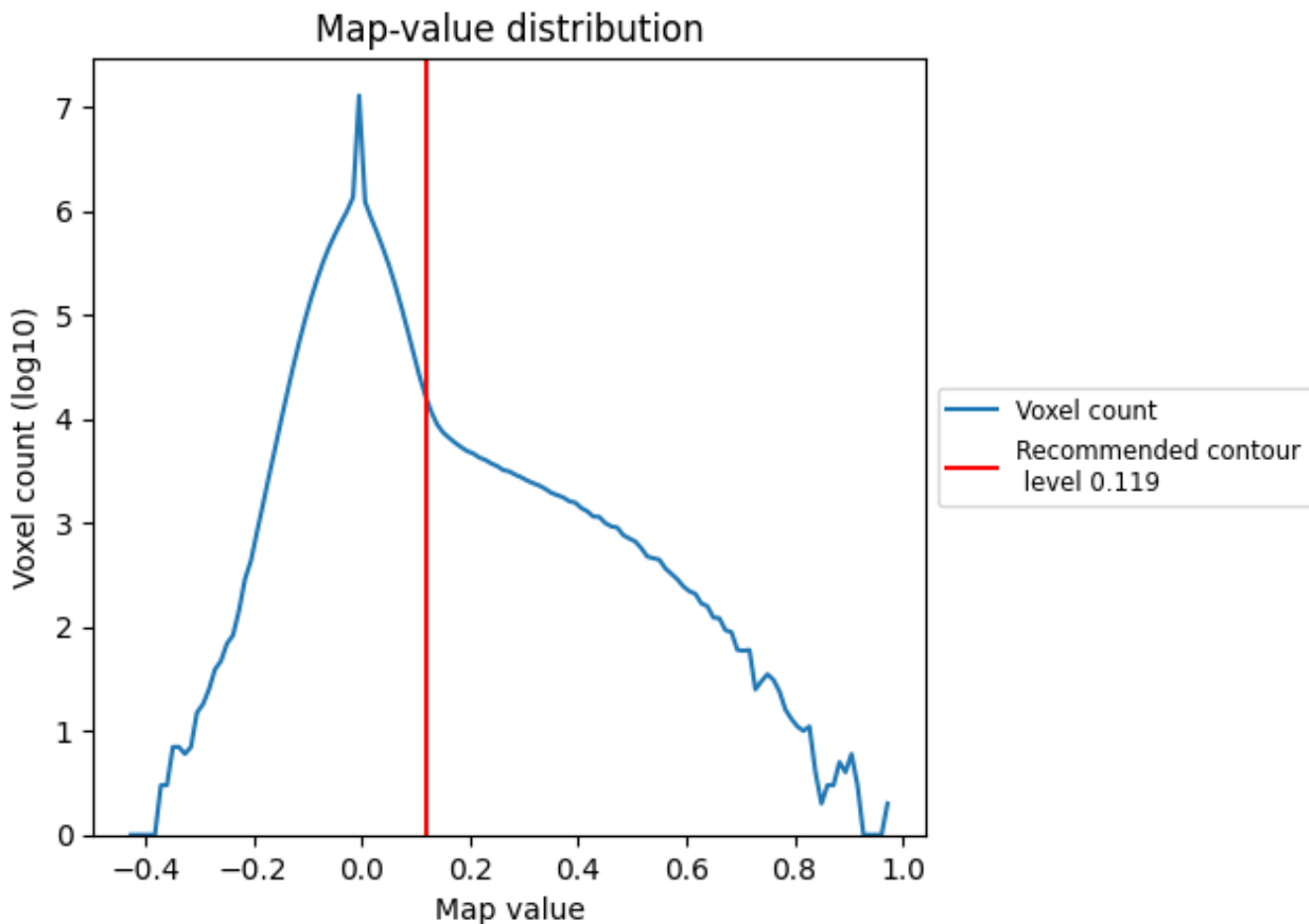
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

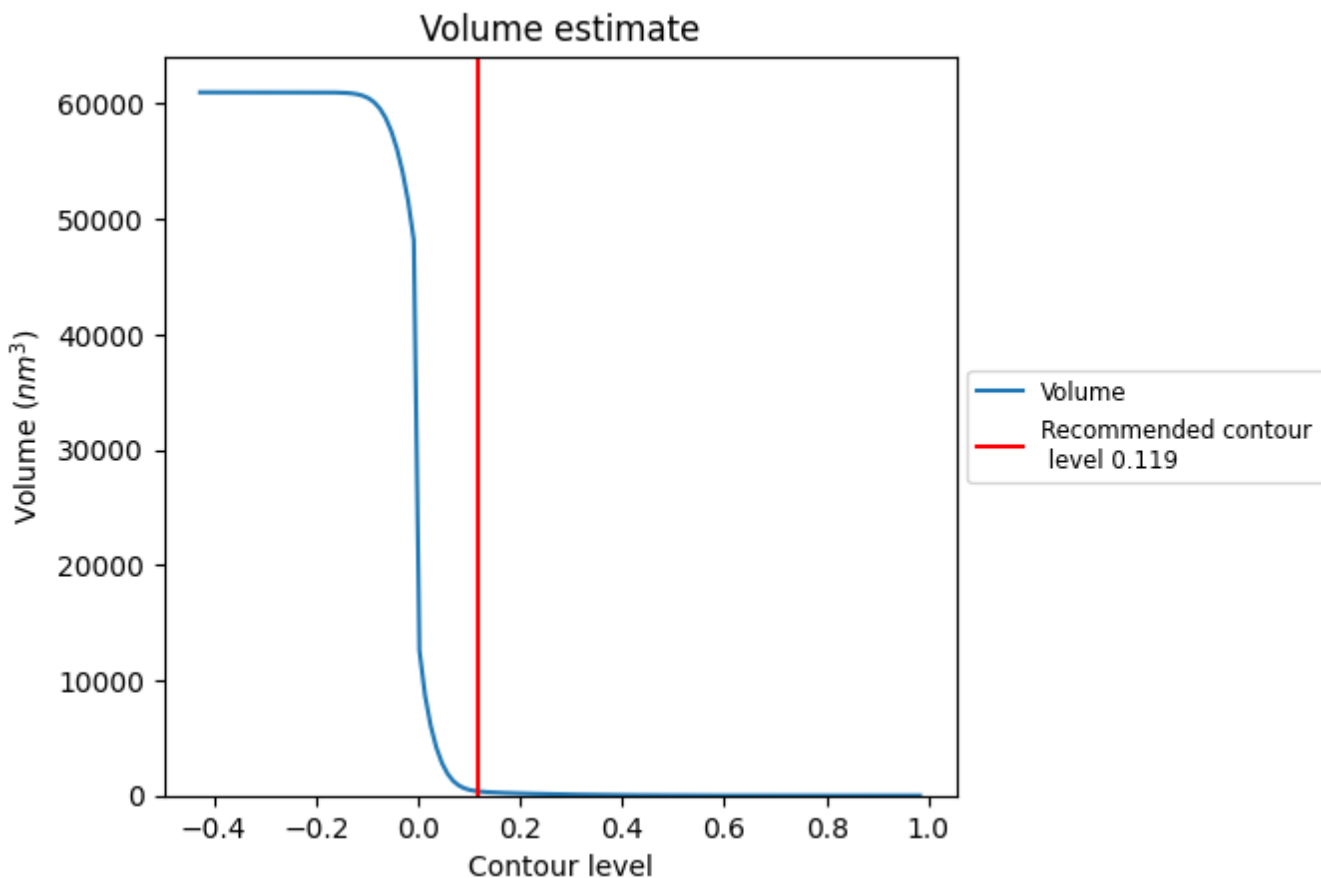
This section contains the results of statistical analysis of the map.

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.

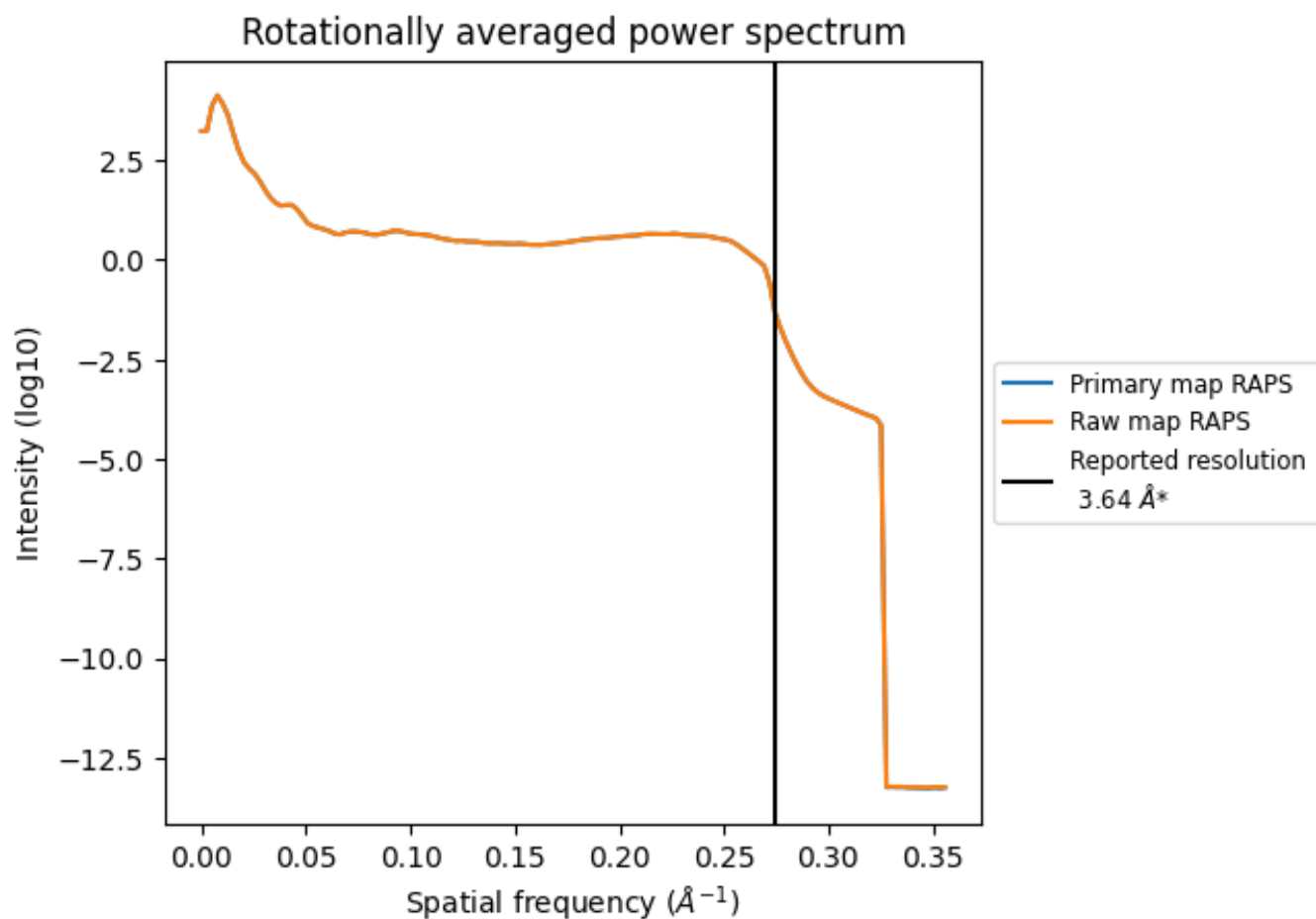
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm³; this corresponds to an approximate mass of 327 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 [i](#)

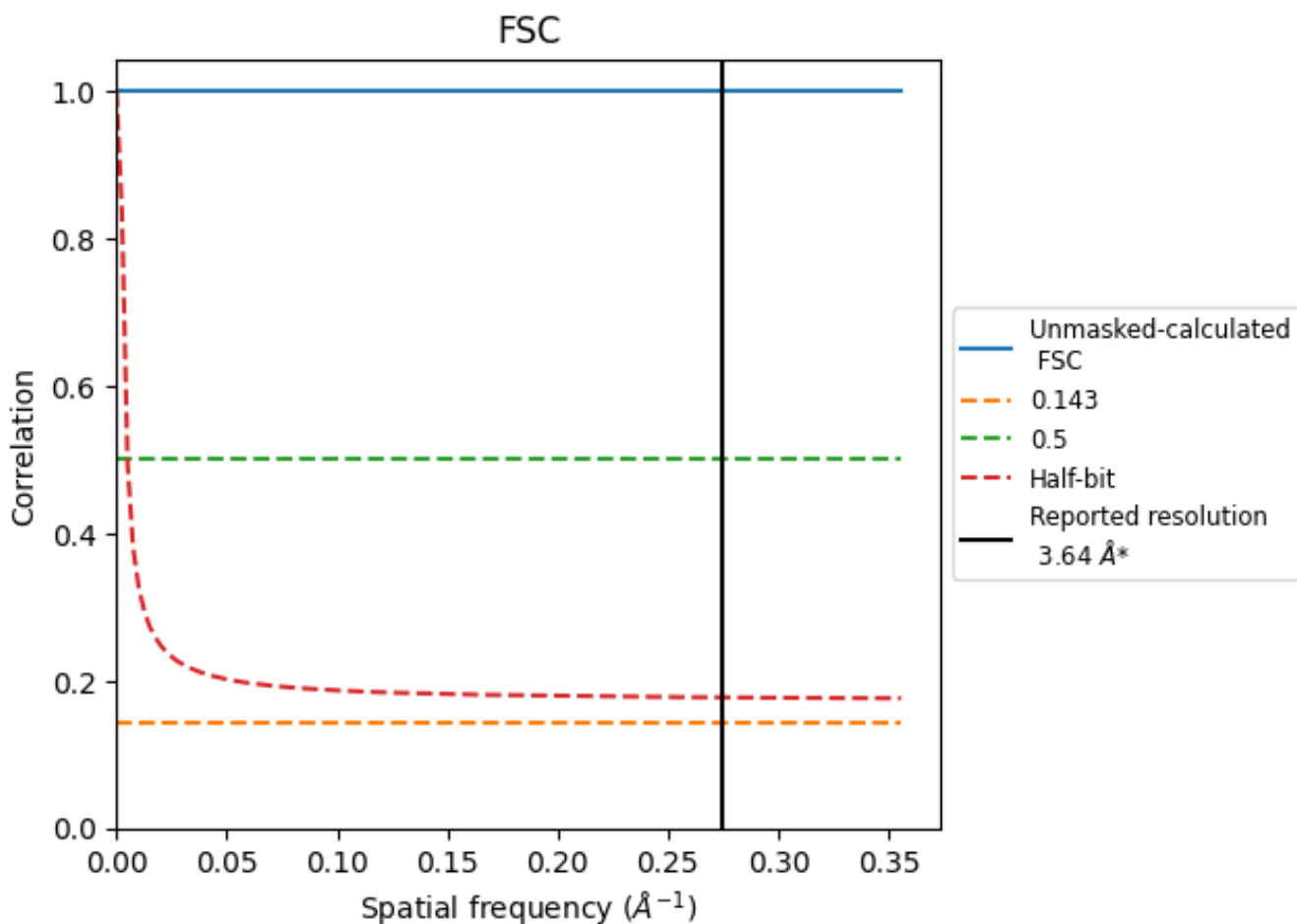


*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

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 0.275 Å⁻¹

8.2 Resolution estimates [i](#)

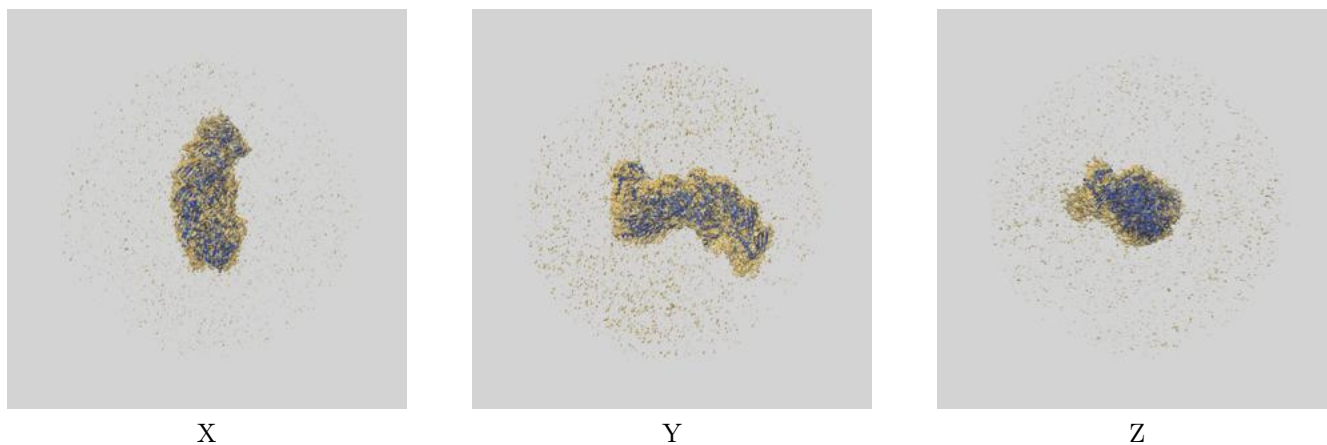
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

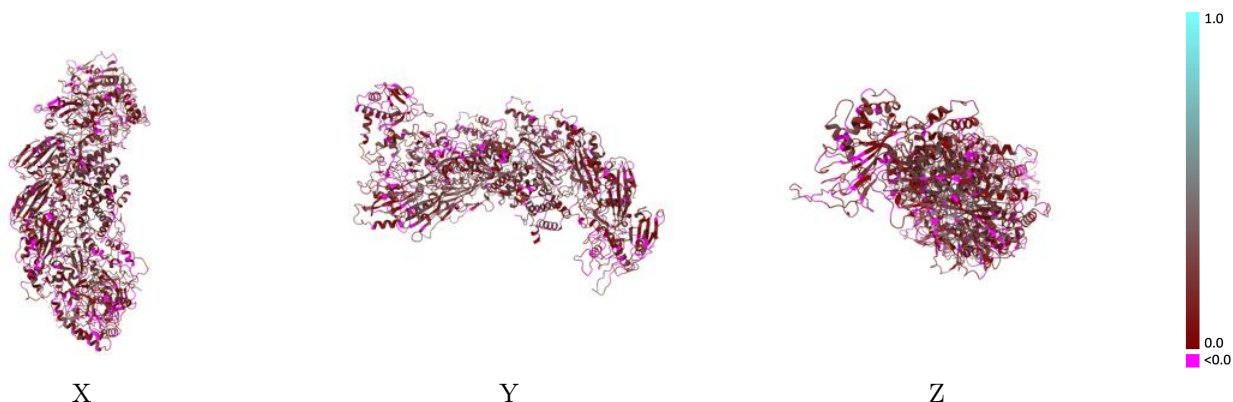
This section contains information regarding the fit between EMDB map EMD-29896 and PDB model 8GAF. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



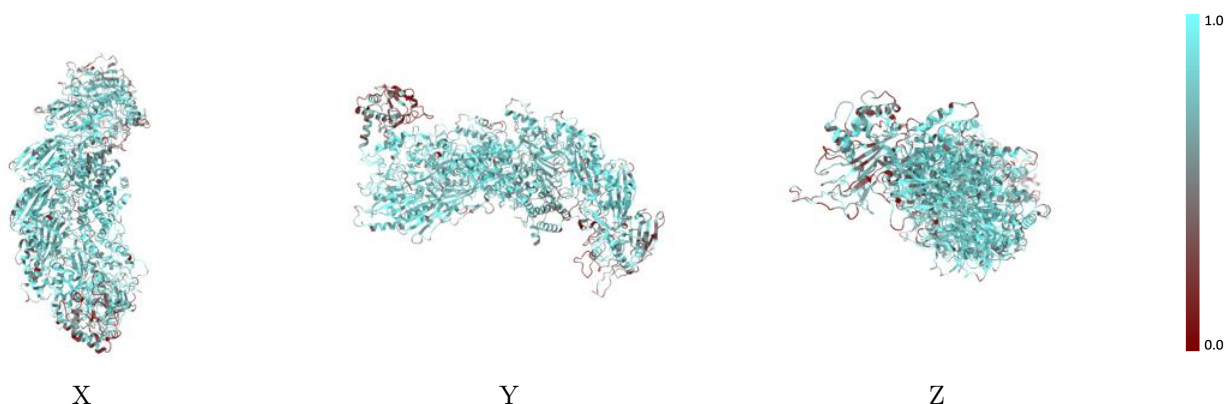
The images above show the 3D surface view of the map at the recommended contour level 0.119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



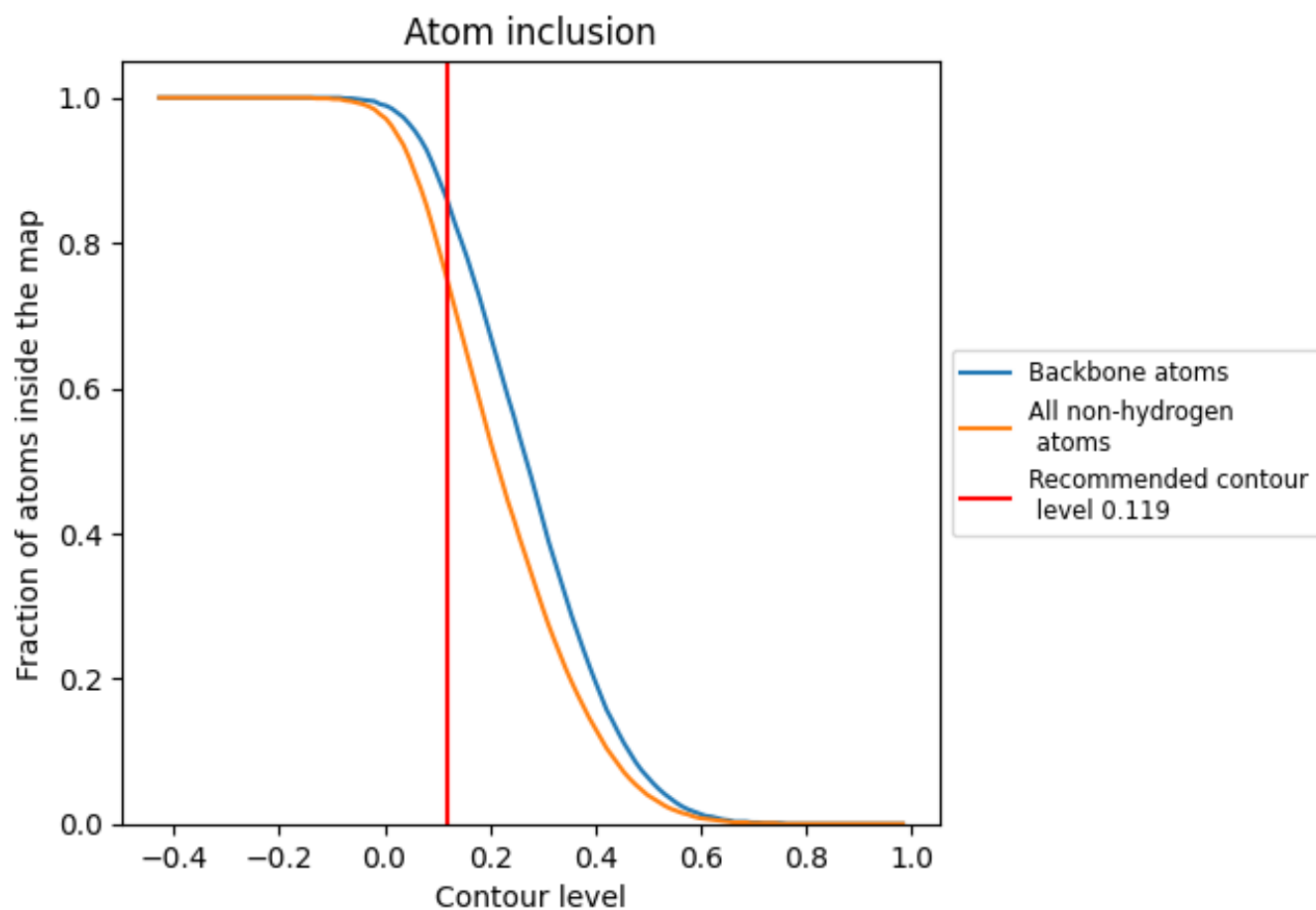
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.119).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7510	 0.1590
A	 0.7870	 0.1750
B	 0.7800	 0.1580
C	 0.7900	 0.1880
D	 0.7760	 0.1680
E	 0.7240	 0.1400
F	 0.5830	 0.1300
G	 0.5770	 0.1310
H	 0.8620	 0.1550
I	 0.6510	 0.1730
J	 0.8200	 0.2190
K	 0.8820	 0.1730
M	 0.8440	 0.1680
N	 0.7930	 0.1380

