



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:18 AM UTC

PDB ID : 9NO4 / pdb_00009no4
EMDB ID : EMD-49593
Title : Cryo-EM structure of Csm/AcrIIIA2/enolase 3:2 complex
Authors : Goswami, H.N.; Li, H.
Deposited on : 2025-03-07
Resolution : 2.67 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

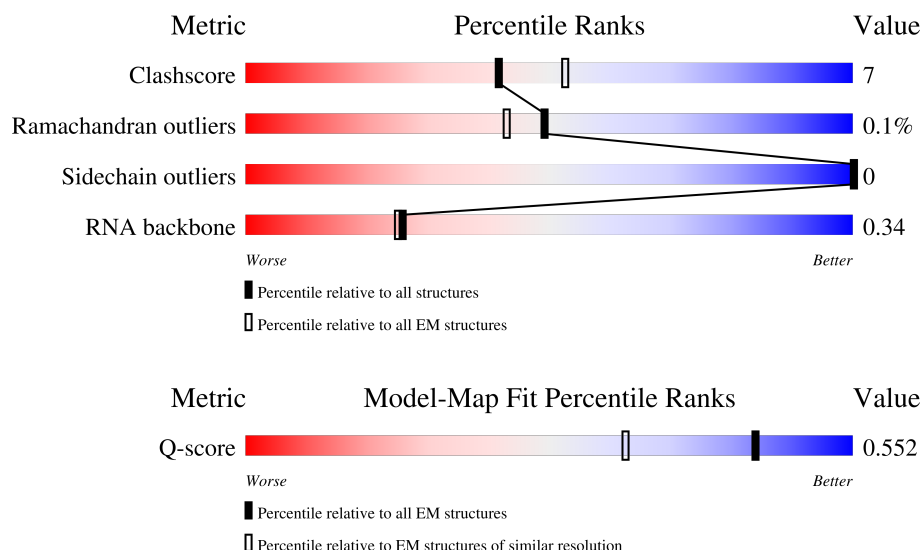
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

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	B	299	25% 73% 23% ••
2	E	220	8% 73% 26%
2	F	220	5% 81% 18% •

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Mol	Chain	Length	Quality of chain
3	G	220	 5% 80% 19% .
4	N	35	 57% 31% 11%
5	C	130	 9% 82% 15% .
5	D	130	 78% 17% . .
6	H	357	 80% 17% . .
7	I	434	 89% 10% .
7	J	434	 87% 12% .
7	K	434	 84% 15%
7	L	434	 86% 13% .
7	M	434	 87% 13%
7	O	434	 85% 14% .
7	P	434	 85% 14%
7	Q	434	 87% 12% .
8	R	105	 9% 86% 10% . .
9	A	758	 68% 80% 18% .

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 46513 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 CRISPR system Cms protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	297	Total	C	N	O	S	0	0
			2312	1482	383	442	5		

- Molecule 2 is a protein called CRISPR system Cms endoribonuclease Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	219	Total	C	N	O	S	0	0
			1692	1072	287	330	3		
2	F	220	Total	C	N	O	S	0	0
			1684	1066	287	328	3		

- Molecule 3 is a protein called CRISPR system Cms endoribonuclease Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	220	Total	C	N	O	S	0	0
			1697	1074	287	334	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	219	VAL	GLU	conflict	UNP A0AAN1ZZJ5

- Molecule 4 is a RNA chain called crRNA RNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	35	Total	C	N	O	P	0	0
			735	332	129	240	34		

- Molecule 5 is a protein called CRISPR system Cms protein Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	130	Total	C	N	O	S	0	0
			1080	686	187	203	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	130	Total	C	N	O	S	0	0
			1080	686	187	203	4		

- Molecule 6 is a protein called CRISPR system Cms protein Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	352	Total	C	N	O	S	0	0
			2863	1843	496	517	7		

- Molecule 7 is a protein called Enolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	J	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	K	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	L	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	M	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	O	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	P	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	Q	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	253	HIS	ARG	conflict	UNP Q03LI0
I	257	GLY	ASP	conflict	UNP Q03LI0
J	253	HIS	ARG	conflict	UNP Q03LI0
J	257	GLY	ASP	conflict	UNP Q03LI0
K	253	HIS	ARG	conflict	UNP Q03LI0
K	257	GLY	ASP	conflict	UNP Q03LI0
L	253	HIS	ARG	conflict	UNP Q03LI0
L	257	GLY	ASP	conflict	UNP Q03LI0
M	253	HIS	ARG	conflict	UNP Q03LI0
M	257	GLY	ASP	conflict	UNP Q03LI0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	253	HIS	ARG	conflict	UNP Q03LI0
O	257	GLY	ASP	conflict	UNP Q03LI0
P	253	HIS	ARG	conflict	UNP Q03LI0
P	257	GLY	ASP	conflict	UNP Q03LI0
Q	253	HIS	ARG	conflict	UNP Q03LI0
Q	257	GLY	ASP	conflict	UNP Q03LI0

- Molecule 8 is a protein called AcrIIIA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	104	Total	C	N	O	S	0	0
			785	493	147	143	2		

- Molecule 9 is a protein called CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	758	Total	C	N	O	S	0	0
			6137	3919	1026	1176	16		

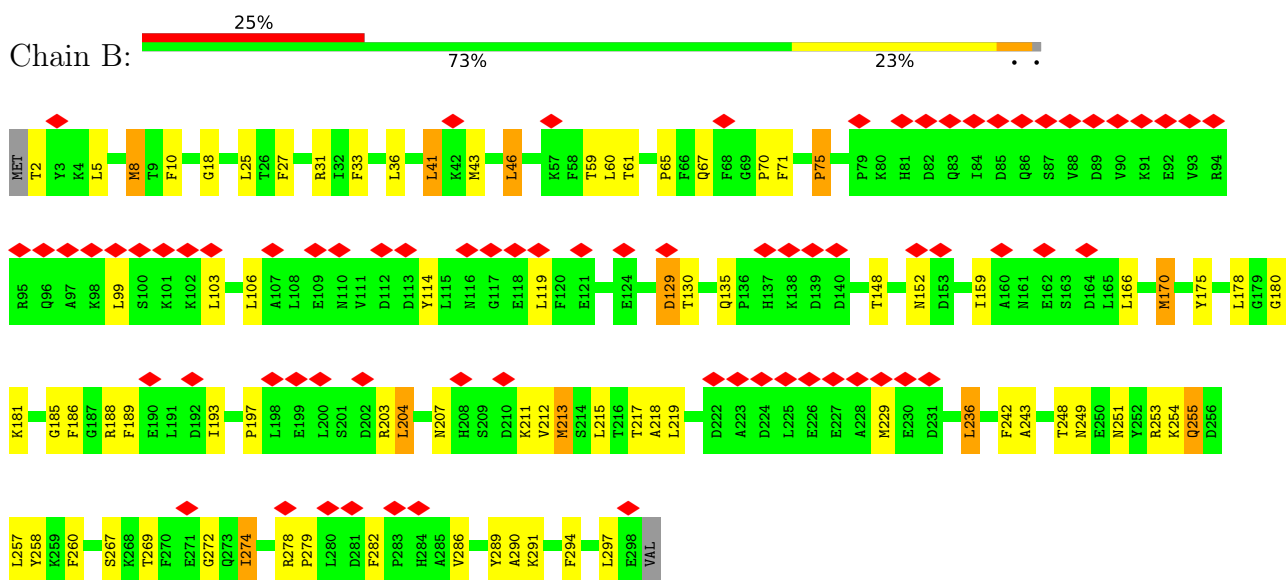
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	I	1	Total	Mg	0
			1	1	
10	J	1	Total	Mg	0
			1	1	
10	K	1	Total	Mg	0
			1	1	
10	L	1	Total	Mg	0
			1	1	
10	M	1	Total	Mg	0
			1	1	
10	O	1	Total	Mg	0
			1	1	
10	P	1	Total	Mg	0
			1	1	
10	Q	1	Total	Mg	0
			1	1	

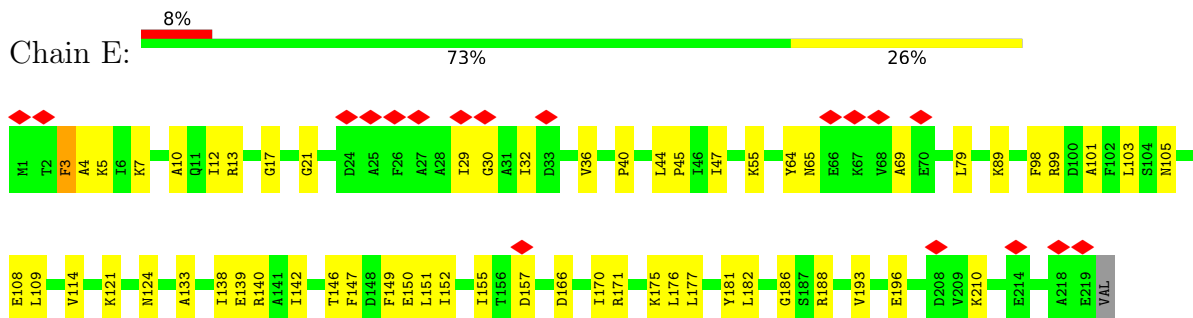
3 Residue-property plots

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.

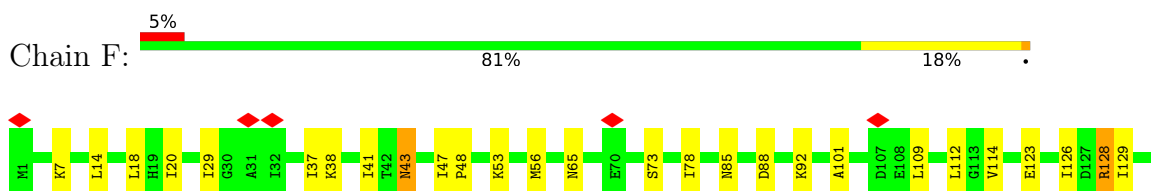
- Molecule 1: CRISPR system Cms protein Csm4



- Molecule 2: CRISPR system Cms endoribonuclease Csm3

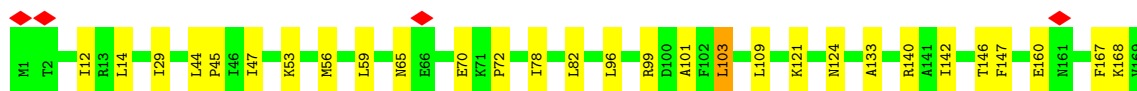
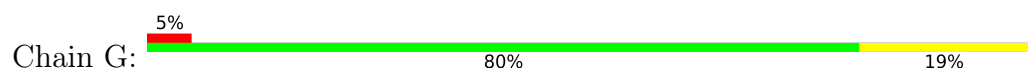


- Molecule 2: CRISPR system Cms endoribonuclease Csm3





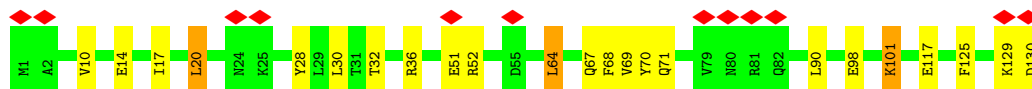
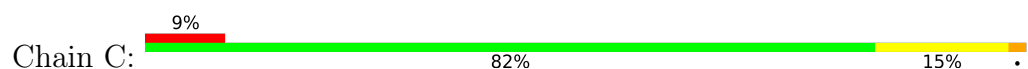
- Molecule 3: CRISPR system Cms endoribonuclease Csm3



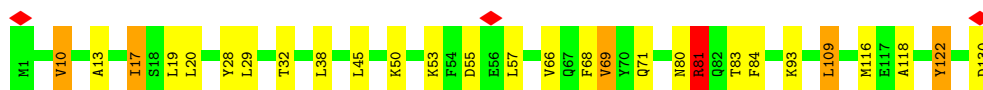
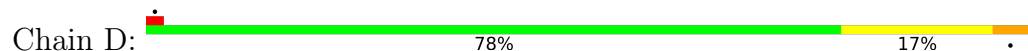
- Molecule 4: crRNA RNA (35-MER)



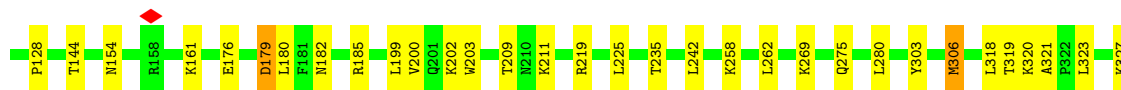
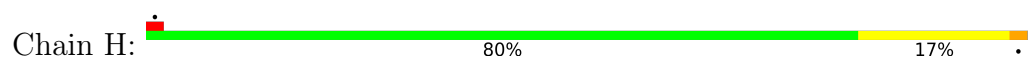
- Molecule 5: CRISPR system Cms protein Csm2

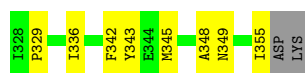


- Molecule 5: CRISPR system Cms protein Csm2



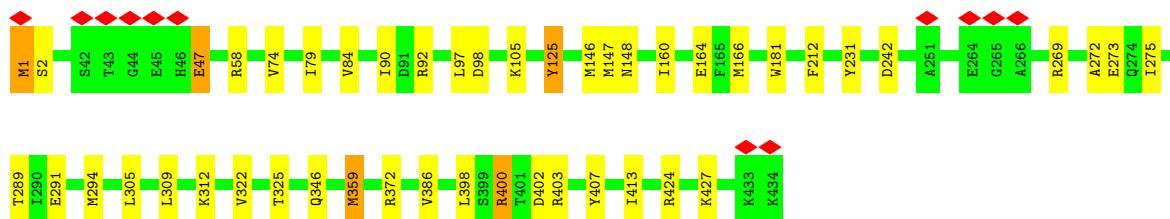
- Molecule 6: CRISPR system Cms protein Csm5





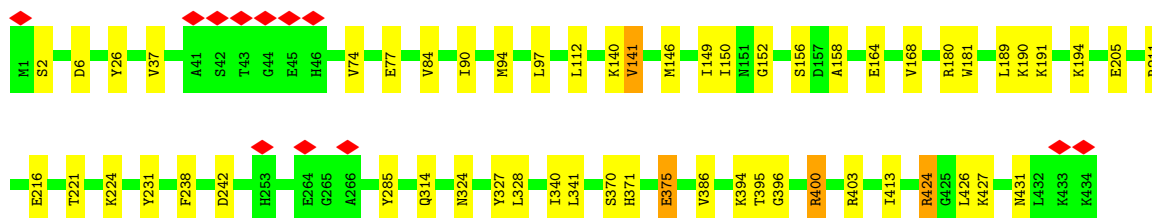
• Molecule 7: Enolase

Chain I: 89% 10%



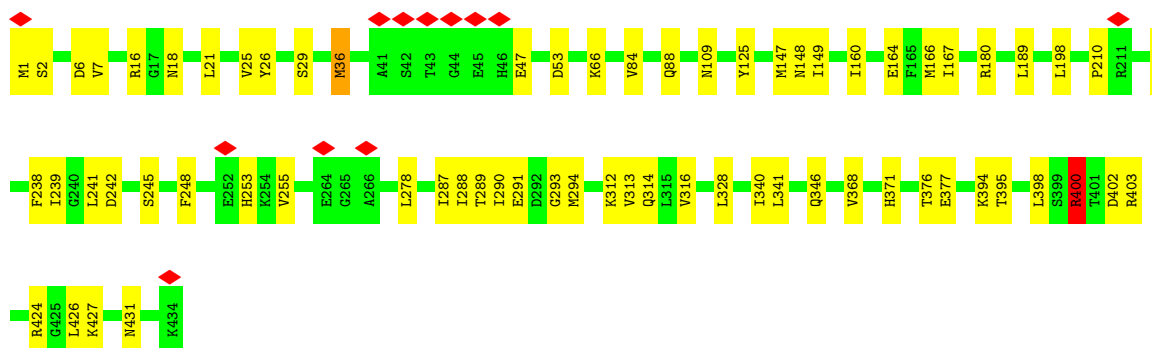
• Molecule 7: Enolase

Chain J: 87% 12%



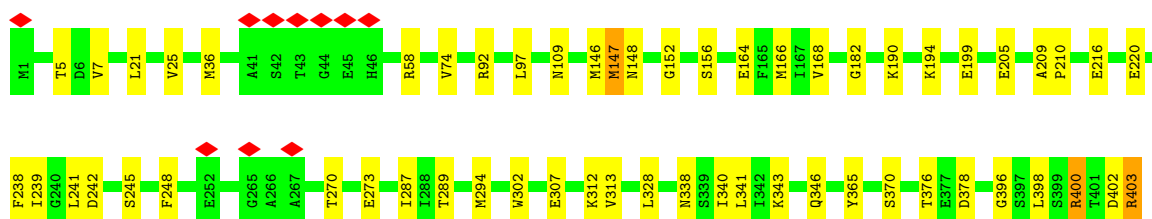
• Molecule 7: Enolase

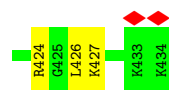
Chain K: 84% 15%



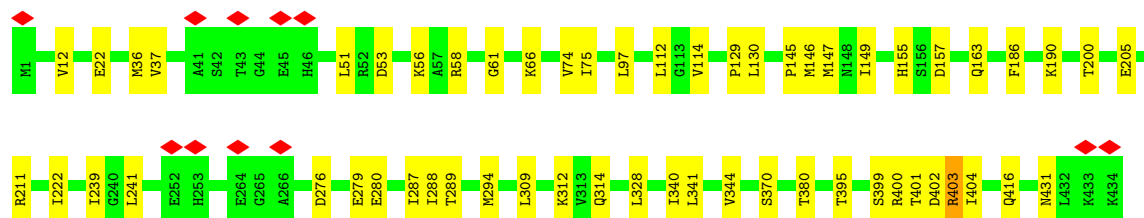
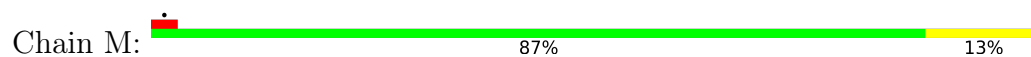
• Molecule 7: Enolase

Chain L: 86% 13%

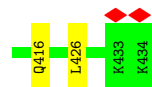
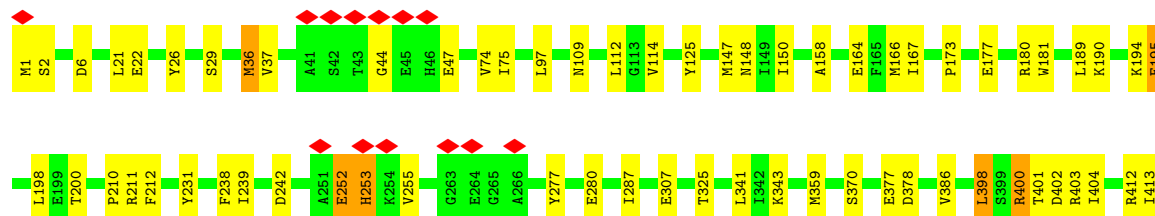
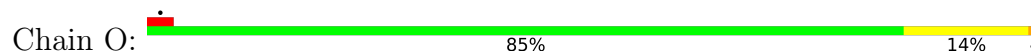




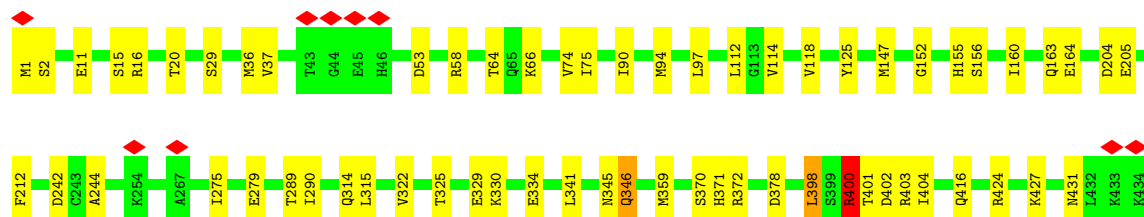
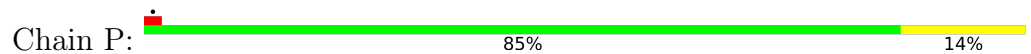
• Molecule 7: Enolase



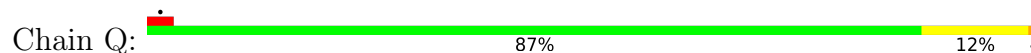
• Molecule 7: Enolase

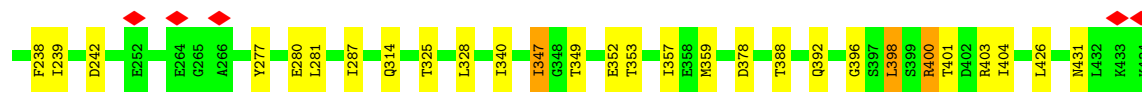


• Molecule 7: Enolase

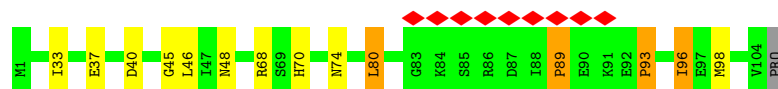
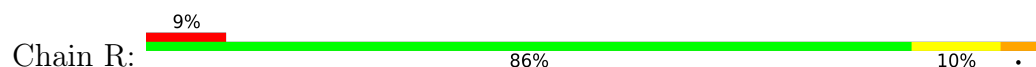


• Molecule 7: Enolase

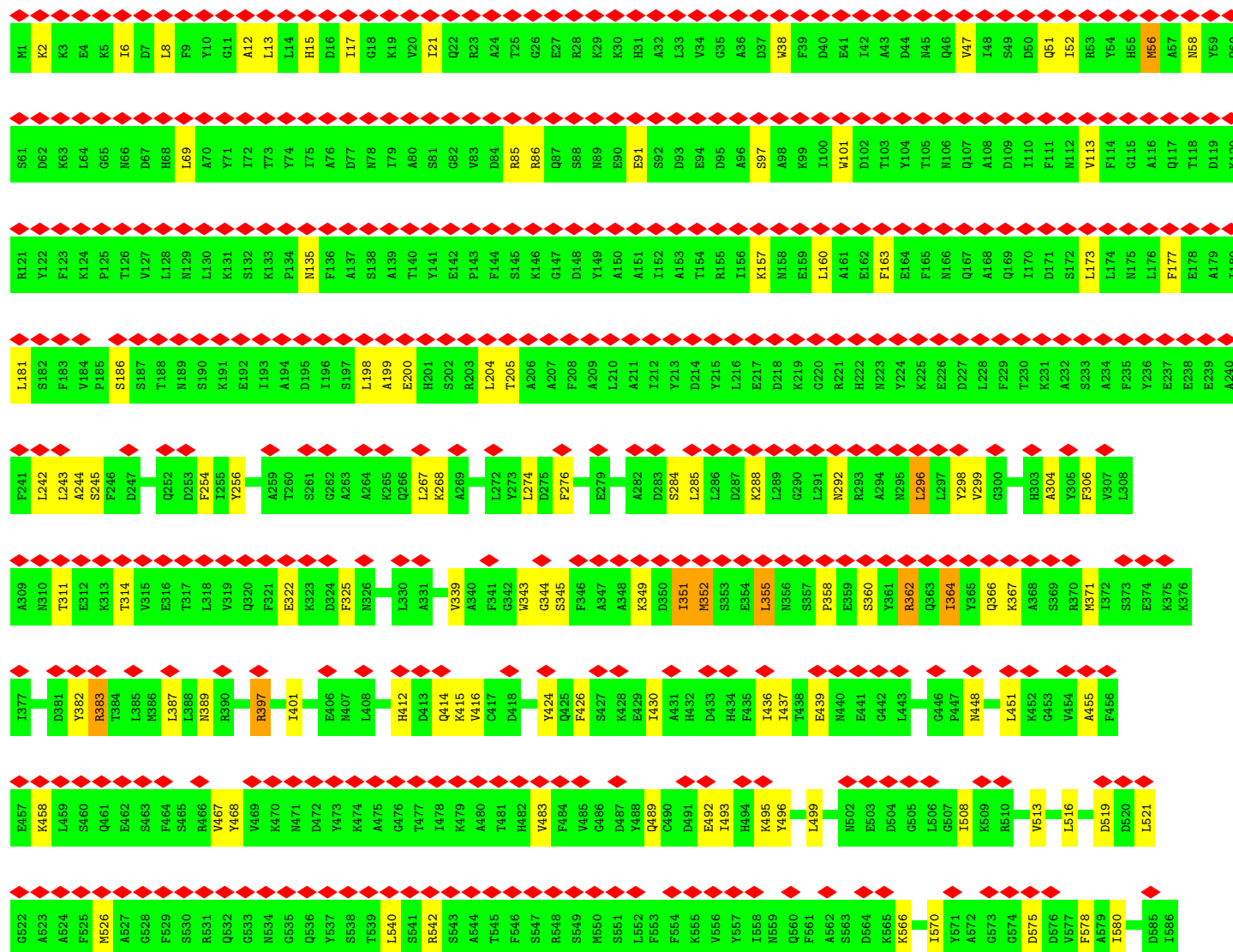
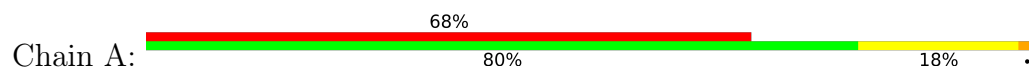


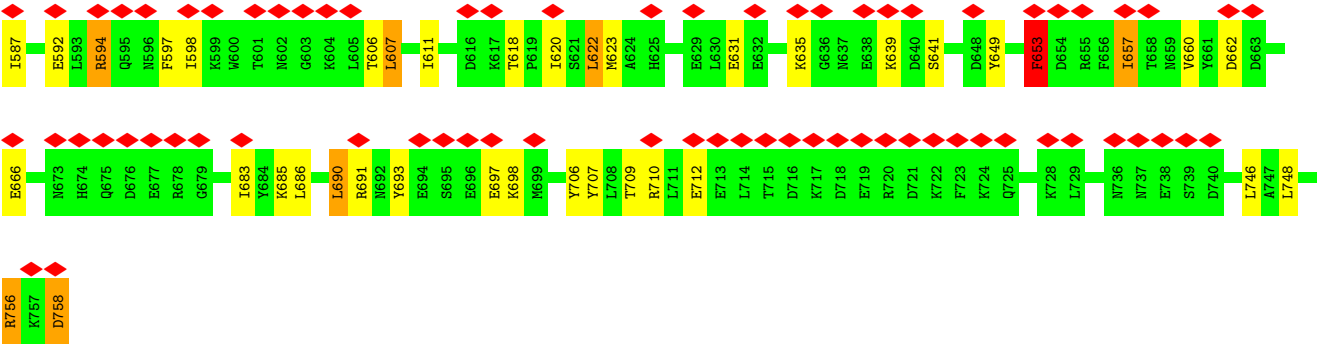


• Molecule 8: AcrIIIA2



• Molecule 9: CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	311708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.586	Depositor
Minimum map value	-0.565	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.216	Depositor
Map size ($\text{\AA}$)	463.68, 463.68, 463.68	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.96	16/2364 (0.7%)	0.88	7/3203 (0.2%)
2	E	0.76	4/1717 (0.2%)	0.77	1/2317 (0.0%)
2	F	0.63	1/1709 (0.1%)	0.77	2/2308 (0.1%)
3	G	0.60	2/1722 (0.1%)	0.70	2/2324 (0.1%)
4	N	0.37	0/821	0.45	0/1275
5	C	0.76	4/1095 (0.4%)	0.86	6/1465 (0.4%)
5	D	0.76	6/1095 (0.5%)	0.70	3/1465 (0.2%)
6	H	0.66	6/2930 (0.2%)	0.68	3/3940 (0.1%)
7	I	0.49	2/3362 (0.1%)	0.66	8/4548 (0.2%)
7	J	0.45	2/3362 (0.1%)	0.58	3/4548 (0.1%)
7	K	0.40	1/3362 (0.0%)	0.55	1/4548 (0.0%)
7	L	0.46	3/3362 (0.1%)	0.62	2/4548 (0.0%)
7	M	0.46	3/3362 (0.1%)	0.58	2/4548 (0.0%)
7	O	0.53	5/3362 (0.1%)	0.72	10/4548 (0.2%)
7	P	0.51	5/3362 (0.1%)	0.68	7/4548 (0.2%)
7	Q	0.48	4/3362 (0.1%)	0.56	3/4548 (0.1%)
8	R	0.64	2/804 (0.2%)	0.86	3/1087 (0.3%)
9	A	0.72	18/6264 (0.3%)	0.78	22/8436 (0.3%)
All	All	0.59	84/47417 (0.2%)	0.69	85/64204 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	F	0	2
3	G	0	1
5	D	0	1
7	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	J	0	2
7	K	0	1
7	L	0	1
7	M	0	1
7	O	0	3
7	P	0	3
9	A	0	5
All	All	0	23

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	MET	SD-CE	-18.20	1.34	1.79
9	A	623	MET	SD-CE	-17.97	1.34	1.79
7	I	125	TYR	CZ-OH	-15.07	1.06	1.38
9	A	618	THR	CB-OG1	-14.16	1.21	1.43
6	H	306	MET	SD-CE	-11.99	1.49	1.79
1	B	8	MET	SD-CE	-11.43	1.50	1.79
1	B	75	PRO	CA-C	11.42	1.68	1.52
1	B	215	LEU	CG-CD2	-10.85	1.16	1.52
5	D	10	VAL	CB-CG1	-10.71	1.17	1.52
9	A	657	ILE	CG1-CD1	-9.99	1.12	1.51
9	A	364	ILE	CG1-CD1	-9.92	1.13	1.51
5	C	20	LEU	CG-CD1	-9.42	1.21	1.52
7	Q	347	ILE	CG1-CD1	-7.78	1.21	1.51
1	B	255	GLN	CD-OE1	-7.65	1.09	1.23
2	E	210	LYS	C-O	-7.61	1.14	1.24
1	B	75	PRO	N-CD	7.54	1.58	1.47
7	L	403	ARG	CG-CD	-7.54	1.29	1.52
9	A	322	GLU	CD-OE1	-7.43	1.11	1.25
5	D	122	TYR	CZ-OH	-7.40	1.22	1.38
9	A	653	PHE	CE2-CZ	-7.39	1.16	1.38
7	O	252	GLU	CG-CD	-7.36	1.33	1.52
1	B	236	LEU	CG-CD2	-7.25	1.28	1.52
7	Q	398	LEU	CG-CD2	-7.06	1.29	1.52
1	B	274	ILE	CG1-CD1	-6.95	1.24	1.51
9	A	296	LEU	CG-CD1	-6.88	1.29	1.52
9	A	618	THR	CA-C	6.87	1.61	1.53
7	L	5	THR	CB-CG2	-6.69	1.30	1.52
7	P	279	GLU	CD-OE1	-6.68	1.12	1.25
9	A	351	ILE	CB-CG2	-6.55	1.30	1.52
9	A	756	ARG	CB-CG	-6.51	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	40	ASP	CG-OD1	-6.39	1.13	1.25
5	C	101	LYS	CE-NZ	-6.23	1.30	1.49
7	K	36	MET	SD-CE	-6.18	1.64	1.79
1	B	75	PRO	CA-CB	-6.18	1.45	1.53
7	L	307	GLU	CD-OE1	-6.15	1.13	1.25
1	B	193	ILE	CB-CG2	-6.14	1.32	1.52
1	B	204	LEU	CG-CD1	-6.13	1.32	1.52
1	B	255	GLN	CG-CD	-6.12	1.36	1.52
7	M	294	MET	SD-CE	-6.05	1.64	1.79
2	E	3	PHE	CE2-CZ	-6.02	1.20	1.38
9	A	587	ILE	CG1-CD1	-6.01	1.28	1.51
9	A	292	ASN	CG-ND2	-6.01	1.20	1.33
9	A	758	ASP	CG-OD1	-5.98	1.14	1.25
7	Q	205	GLU	CD-OE2	-5.98	1.14	1.25
9	A	592	GLU	CD-OE1	-5.96	1.14	1.25
6	H	179	ASP	CG-OD2	-5.95	1.14	1.25
9	A	607	LEU	CG-CD1	-5.91	1.33	1.52
5	C	98	GLU	CA-CB	5.87	1.63	1.53
9	A	611	ILE	CG1-CD1	-5.87	1.28	1.51
1	B	129	ASP	CG-OD1	-5.85	1.14	1.25
2	E	40	PRO	CB-CG	-5.85	1.20	1.49
7	O	252	GLU	CD-OE2	-5.79	1.14	1.25
7	O	195	GLU	CD-OE1	-5.76	1.14	1.25
7	P	346	GLN	CG-CD	-5.74	1.37	1.52
7	P	398	LEU	CG-CD2	-5.70	1.33	1.52
3	G	182	LEU	CG-CD2	-5.64	1.33	1.52
5	D	17	ILE	CG1-CD1	-5.55	1.30	1.51
7	J	216	GLU	CD-OE1	-5.45	1.15	1.25
2	F	43	ASN	CG-OD1	-5.42	1.13	1.23
5	D	122	TYR	CD2-CE2	-5.41	1.22	1.38
6	H	144	THR	CB-CG2	-5.40	1.34	1.52
3	G	103	LEU	CG-CD2	-5.35	1.34	1.52
7	I	125	TYR	CD2-CE2	-5.30	1.22	1.38
7	P	346	GLN	CD-NE2	-5.26	1.22	1.33
9	A	397	ARG	CG-CD	-5.26	1.36	1.52
7	O	195	GLU	CG-CD	-5.24	1.39	1.52
7	O	253	HIS	CA-CB	5.23	1.62	1.53
7	Q	349	THR	CB-CG2	-5.21	1.35	1.52
8	R	80	LEU	CG-CD1	-5.20	1.35	1.52
5	D	81	ARG	CB-CG	-5.15	1.36	1.52
2	E	157	ASP	CG-OD1	-5.15	1.15	1.25
5	D	109	LEU	CG-CD2	-5.14	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	622	LEU	CG-CD2	-5.14	1.35	1.52
6	H	66	THR	CB-CG2	-5.13	1.35	1.52
1	B	213	MET	CA-C	-5.08	1.46	1.52
6	H	49	LYS	CA-CB	-5.08	1.44	1.53
7	J	375	GLU	CD-OE2	-5.07	1.15	1.25
7	M	239	ILE	CG1-CD1	-5.07	1.31	1.51
1	B	178	LEU	CG-CD2	-5.06	1.35	1.52
6	H	13	LEU	CG-CD1	-5.04	1.35	1.52
7	P	334	GLU	CD-OE1	-5.03	1.15	1.25
7	M	51	LEU	CG-CD2	-5.02	1.35	1.52
5	C	101	LYS	CD-CE	-5.01	1.37	1.52
1	B	255	GLN	CD-NE2	-5.01	1.22	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	252	GLU	CG-CD-OE2	-18.20	76.53	118.40
7	I	1	MET	CG-SD-CE	-14.82	68.30	100.90
7	I	125	TYR	OH-CZ-CE2	-13.79	78.52	119.90
7	P	346	GLN	CG-CD-NE2	-11.88	98.58	116.40
9	A	352	MET	CG-SD-CE	-11.02	76.65	100.90
9	A	618	THR	CA-CB-OG1	10.64	125.55	109.60
7	O	252	GLU	OE1-CD-OE2	10.34	147.72	122.90
8	R	80	LEU	CD1-CG-CD2	-10.25	88.24	110.80
1	B	170	MET	CG-SD-CE	-10.23	78.40	100.90
1	B	213	MET	CG-SD-CE	-9.87	79.18	100.90
7	I	1	MET	CB-CG-SD	9.75	141.95	112.70
7	P	322	VAL	CA-CB-CG1	9.51	126.57	110.40
9	A	56	MET	CG-SD-CE	-9.34	80.36	100.90
1	B	46	LEU	CD1-CG-CD2	-8.88	91.26	110.80
5	C	101	LYS	CG-CD-CE	-8.66	91.39	111.30
5	C	101	LYS	CD-CE-NZ	8.56	139.28	111.90
9	A	657	ILE	CB-CG1-CD1	-8.44	96.07	113.80
7	I	1	MET	CB-CA-C	7.89	125.10	110.10
8	R	93	PRO	N-CA-CB	7.71	111.34	103.25
7	L	307	GLU	CG-CD-OE1	-7.25	101.73	118.40
7	P	275	ILE	CG1-CB-CG2	-7.22	89.05	110.70
8	R	89	PRO	N-CA-CB	6.95	110.55	103.25
9	A	618	THR	N-CA-C	-6.85	100.83	110.29
7	O	307	GLU	CG-CD-OE1	-6.64	103.12	118.40
9	A	592	GLU	CG-CD-OE1	-6.56	103.32	118.40
5	C	14	GLU	CB-CG-CD	-6.40	101.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	306	MET	CG-SD-CE	-6.34	86.95	100.90
1	B	129	ASP	OD1-CG-OD2	-6.32	107.73	122.90
9	A	292	ASN	CB-CG-ND2	-6.29	106.96	116.40
7	O	253	HIS	N-CA-CB	6.27	120.03	110.44
9	A	623	MET	CG-SD-CE	6.24	114.62	100.90
9	A	641	SER	CA-CB-OG	-6.22	98.66	111.10
7	O	36	MET	CG-SD-CE	-6.13	87.42	100.90
1	B	8	MET	CG-SD-CE	-6.12	87.42	100.90
9	A	397	ARG	CG-CD-NE	6.01	125.22	112.00
9	A	135	ASN	CB-CG-ND2	-6.00	107.39	116.40
9	A	383	ARG	CD-NE-CZ	5.93	132.70	124.40
5	D	10	VAL	N-CA-CB	-5.92	103.62	110.55
1	B	170	MET	CA-CB-CG	-5.91	102.28	114.10
7	J	141	VAL	CG1-CB-CG2	5.89	123.76	110.80
5	C	64	LEU	CB-CG-CD2	5.79	128.09	110.70
9	A	756	ARG	CB-CG-CD	5.77	124.56	111.30
7	P	11	GLU	CG-CD-OE1	-5.71	105.27	118.40
5	D	10	VAL	CG1-CB-CG2	-5.70	98.26	110.80
7	K	400	ARG	N-CA-CB	-5.67	101.63	109.97
6	H	49	LYS	CA-CB-CG	5.67	125.43	114.10
7	O	253	HIS	CA-CB-CG	5.63	119.43	113.80
5	C	14	GLU	OE1-CD-OE2	-5.62	109.40	122.90
1	B	41	LEU	CB-CG-CD1	5.58	127.43	110.70
7	I	359	MET	CG-SD-CE	-5.57	88.65	100.90
7	Q	400	ARG	N-CA-CB	-5.56	101.44	109.83
7	O	398	LEU	CA-C-N	-5.51	114.96	121.90
7	O	398	LEU	C-N-CA	-5.51	114.96	121.90
7	P	346	GLN	OE1-CD-NE2	-5.47	117.13	122.60
7	I	47	GLU	CG-CD-OE2	5.46	130.95	118.40
2	F	128	ARG	CD-NE-CZ	-5.40	116.83	124.40
7	I	47	GLU	OE1-CD-OE2	-5.40	109.94	122.90
7	J	77	GLU	CG-CD-OE2	-5.36	106.07	118.40
7	Q	147	MET	CG-SD-CE	5.35	112.68	100.90
9	A	690	LEU	CD1-CG-CD2	-5.34	99.05	110.80
9	A	594	ARG	CG-CD-NE	5.33	123.73	112.00
7	O	400	ARG	N-CA-CB	-5.32	102.51	110.17
7	P	322	VAL	CA-CB-CG2	5.30	119.42	110.40
7	O	343	LYS	CG-CD-CE	5.28	123.44	111.30
7	P	400	ARG	CA-CB-CG	5.27	124.65	114.10
9	A	594	ARG	CA-CB-CG	5.27	124.63	114.10
5	D	69	VAL	CA-CB-CG1	-5.25	101.48	110.40
7	J	285	TYR	CE1-CZ-OH	-5.25	104.15	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	653	PHE	CD1-CG-CD2	-5.24	110.74	118.60
9	A	618	THR	CB-CA-C	5.22	116.38	108.86
9	A	592	GLU	N-CA-CB	5.21	117.88	110.16
7	M	403	ARG	CB-CG-CD	5.20	123.26	111.30
9	A	592	GLU	CG-CD-OE2	5.19	130.35	118.40
9	A	355	LEU	N-CA-C	-5.19	108.21	114.75
2	E	210	LYS	CA-C-O	-5.19	114.24	120.10
6	H	60	GLU	CG-CD-OE1	-5.18	106.48	118.40
9	A	371	MET	CG-SD-CE	-5.16	89.55	100.90
7	M	294	MET	CG-SD-CE	-5.15	89.57	100.90
7	I	125	TYR	CE1-CZ-CE2	5.14	130.58	120.30
3	G	160	GLU	CA-C-N	5.13	131.34	121.54
3	G	160	GLU	C-N-CA	5.13	131.34	121.54
2	F	136	ARG	CD-NE-CZ	-5.08	117.28	124.40
5	C	98	GLU	CA-C-O	-5.08	114.12	119.97
7	L	147	MET	CG-SD-CE	-5.08	89.73	100.90
7	Q	205	GLU	CG-CD-OE1	5.05	130.01	118.40

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	352	MET	Mainchain
9	A	362	ARG	Sidechain
9	A	653	PHE	Sidechain
9	A	85	ARG	Sidechain
9	A	86	ARG	Sidechain
1	B	129	ASP	Sidechain
5	D	81	ARG	Sidechain
2	F	136	ARG	Sidechain
2	F	65	ASN	Sidechain
3	G	65	ASN	Sidechain
7	I	125	TYR	Sidechain
7	I	400	ARG	Sidechain
7	J	400	ARG	Sidechain
7	J	424	ARG	Sidechain
7	K	400	ARG	Sidechain
7	L	400	ARG	Sidechain
7	M	400	ARG	Sidechain
7	O	195	GLU	Sidechain
7	O	252	GLU	Sidechain
7	O	400	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	P	330	LYS	Mainchain
7	P	346	GLN	Sidechain
7	P	400	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2312	0	2216	63	0
2	E	1692	0	1674	47	0
2	F	1684	0	1641	34	0
3	G	1697	0	1667	33	0
4	N	735	0	377	13	0
5	C	1080	0	1099	17	0
5	D	1080	0	1099	24	0
6	H	2863	0	2898	48	0
7	I	3305	0	3240	30	0
7	J	3305	0	3241	36	0
7	K	3305	0	3241	43	0
7	L	3305	0	3241	39	0
7	M	3305	0	3241	34	0
7	O	3305	0	3241	38	0
7	P	3305	0	3241	36	0
7	Q	3305	0	3241	36	0
8	R	785	0	709	12	0
9	A	6137	0	5989	103	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
10	K	1	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
10	Q	1	0	0	0	0
All	All	46513	0	45296	623	0

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

All (623) 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)
7:K:36:MET:HE3	7:K:376:THR:HB	1.39	1.00
5:D:81:ARG:HH12	8:R:48:ASN:HB2	1.40	0.86
9:A:56:MET:HE1	9:A:91:GLU:HB3	1.61	0.82
3:G:44:LEU:HB3	3:G:103:LEU:HD12	1.63	0.80
7:Q:325:THR:HG23	7:Q:359:MET:HE1	1.63	0.79
7:O:36:MET:HE1	7:O:377:GLU:HG2	1.64	0.79
2:F:18:LEU:HD11	2:F:182:LEU:HD23	1.63	0.79
2:E:3:PHE:HZ	2:E:5:LYS:HZ2	1.32	0.78
7:I:148:ASN:HA	7:I:166:MET:HG2	1.64	0.78
7:L:205:GLU:HA	7:L:403:ARG:HE	1.49	0.78
6:H:303:TYR:HD1	6:H:306:MET:HE1	1.49	0.77
5:C:125:PHE:HA	9:A:709:THR:HG21	1.67	0.76
7:L:396:GLY:HA3	7:L:403:ARG:HD2	1.66	0.76
9:A:296:LEU:HD11	9:A:299:VAL:HG23	1.66	0.76
7:L:164:GLU:HB2	7:L:242:ASP:HB3	1.66	0.75
2:E:45:PRO:HD2	2:E:103:LEU:HD11	1.69	0.75
1:B:5:LEU:HD22	1:B:197:PRO:HD3	1.69	0.75
7:M:146:MET:HE2	7:M:289:THR:HG21	1.69	0.75
3:G:168:LYS:HG2	3:G:171:ARG:HH21	1.52	0.74
9:A:397:ARG:HD3	9:A:415:LYS:HG3	1.67	0.74
9:A:594:ARG:HD2	9:A:653:PHE:CE2	2.23	0.74
9:A:8:LEU:HD13	9:A:69:LEU:HB3	1.68	0.73
7:K:1:MET:HB2	7:K:29:SER:HB3	1.68	0.73
1:B:188:ARG:HD3	2:E:99:ARG:HG3	1.70	0.73
7:M:288:ILE:HG23	7:M:289:THR:HG23	1.70	0.72
6:H:219:ARG:HD2	6:H:345:MET:HE1	1.72	0.72
3:G:182:LEU:HD12	3:G:193:VAL:HG11	1.71	0.72
9:A:513:VAL:HG22	9:A:580:ILE:HG12	1.71	0.72
7:P:147:MET:SD	7:P:398:LEU:HD21	2.29	0.72
7:K:312:LYS:HG3	7:K:313:VAL:HG13	1.72	0.71
9:A:351:ILE:HD12	9:A:540:LEU:HD21	1.71	0.71
9:A:653:PHE:CE2	9:A:657:ILE:HD11	2.25	0.71
5:D:81:ARG:NH1	8:R:48:ASN:HB2	2.05	0.70
5:C:32:THR:HG22	5:C:130:ASP:HA	1.74	0.70
6:H:9:LYS:HD3	6:H:355:ILE:HD13	1.74	0.70
7:I:164:GLU:HB2	7:I:242:ASP:HB3	1.72	0.69
9:A:344:GLY:HA2	9:A:367:LYS:HD2	1.74	0.69
7:J:205:GLU:HG2	7:J:371:HIS:HE1	1.58	0.68
7:P:341:LEU:HD11	7:P:370:SER:HB2	1.75	0.68
7:O:36:MET:HE3	7:O:378:ASP:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:53:ASP:HA	7:K:66:LYS:HD2	1.76	0.68
2:F:38:LYS:HD3	2:F:43:ASN:OD1	1.94	0.68
7:L:341:LEU:HD11	7:L:370:SER:HB2	1.76	0.68
3:G:168:LYS:HG2	3:G:171:ARG:NH2	2.08	0.67
9:A:113:VAL:HG21	9:A:542:ARG:HH21	1.58	0.67
2:E:101:ALA:HB1	2:E:147:PHE:HB3	1.76	0.67
7:L:147:MET:SD	7:L:398:LEU:HD21	2.35	0.67
7:K:164:GLU:HB2	7:K:242:ASP:HB3	1.77	0.67
9:A:594:ARG:HD2	9:A:653:PHE:CD2	2.30	0.66
2:E:188:ARG:HH12	4:N:12:G:H5"	1.60	0.66
1:B:41:LEU:HB2	1:B:46:LEU:HD12	1.77	0.66
9:A:492:GLU:HB2	9:A:495:LYS:HD2	1.79	0.65
7:K:400:ARG:NE	7:L:400:ARG:HG2	2.12	0.65
7:I:146:MET:HE1	7:I:289:THR:HG21	1.77	0.65
7:Q:90:ILE:HG22	7:Q:94:MET:HE2	1.78	0.65
2:E:47:ILE:HB	2:E:101:ALA:HB3	1.79	0.64
7:J:341:LEU:HD11	7:J:370:SER:HB2	1.79	0.64
2:F:18:LEU:HD21	2:F:20:ILE:HG13	1.80	0.64
6:H:46:PHE:HA	6:H:89:PHE:CD2	2.33	0.64
7:M:309:LEU:HD23	7:M:312:LYS:HE3	1.80	0.64
7:M:341:LEU:HD11	7:M:370:SER:HB2	1.79	0.63
7:M:395:THR:O	7:M:403:ARG:HG3	1.98	0.63
2:F:29:ILE:HG21	5:C:117:GLU:HG2	1.81	0.63
7:O:37:VAL:HG13	7:O:112:LEU:HD23	1.80	0.63
7:K:288:ILE:HG23	7:K:289:THR:HG23	1.80	0.63
9:A:325:PHE:HD2	9:A:339:VAL:HG11	1.64	0.62
7:O:341:LEU:HD11	7:O:370:SER:HB2	1.79	0.62
1:B:243:ALA:HB2	1:B:254:LYS:HB3	1.81	0.62
9:A:519:ASP:HB2	9:A:639:LYS:HD3	1.80	0.62
9:A:397:ARG:CD	9:A:415:LYS:HG3	2.28	0.62
7:Q:347:ILE:HD12	7:Q:352:GLU:HB2	1.82	0.62
2:E:7:LYS:HD2	2:E:150:GLU:CD	2.25	0.62
7:K:147:MET:SD	7:K:398:LEU:HD21	2.39	0.61
7:J:190:LYS:HG2	7:J:194:LYS:HE2	1.82	0.61
7:Q:314:GLN:HG3	7:Q:431:ASN:HD21	1.65	0.61
9:A:311:THR:HG23	9:A:314:THR:H	1.66	0.61
2:E:177:LEU:HD11	2:E:182:LEU:HD13	1.83	0.61
7:P:90:ILE:HG22	7:P:94:MET:HE2	1.81	0.61
6:H:103:ARG:HD2	6:H:110:ALA:H	1.65	0.61
7:Q:164:GLU:HB2	7:Q:242:ASP:HB3	1.82	0.61
9:A:349:LYS:HG2	9:A:355:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:147:MET:SD	7:O:398:LEU:HD21	2.40	0.60
1:B:286:VAL:HG13	4:N:1:A:H3'	1.81	0.60
7:I:181:TRP:CD1	7:I:231:TYR:HH	2.19	0.60
7:J:164:GLU:HB2	7:J:242:ASP:HB3	1.82	0.60
7:M:112:LEU:HD11	7:M:344:VAL:HG22	1.84	0.60
9:A:38:TRP:CH2	9:A:157:LYS:HD2	2.37	0.60
9:A:285:LEU:HD23	9:A:306:PHE:CE2	2.37	0.60
8:R:74:ASN:ND2	7:P:416:GLN:HB3	2.17	0.60
9:A:439:GLU:OE2	9:A:448:ASN:HB3	2.01	0.59
6:H:185:ARG:HH21	6:H:235:THR:HG21	1.67	0.59
9:A:683:ILE:HG23	9:A:748:LEU:HD22	1.83	0.59
7:J:90:ILE:HG22	7:J:94:MET:HE2	1.84	0.59
9:A:8:LEU:HB2	9:A:69:LEU:HD13	1.83	0.59
7:K:160:ILE:HG23	7:K:215:THR:HG22	1.84	0.59
1:B:278:ARG:HD2	1:B:286:VAL:HG23	1.85	0.59
7:J:146:MET:HG2	7:J:168:VAL:HG22	1.85	0.59
9:A:516:LEU:HD11	9:A:607:LEU:HD23	1.84	0.59
7:P:400:ARG:HA	7:Q:400:ARG:HH21	1.68	0.58
7:Q:1:MET:HB2	7:Q:29:SER:HB3	1.85	0.58
3:G:47:ILE:HB	3:G:101:ALA:HB3	1.85	0.58
6:H:50:MET:HE1	6:H:78:PHE:CE2	2.39	0.58
7:L:190:LYS:HG2	7:L:194:LYS:HE2	1.86	0.58
5:D:66:VAL:HA	5:D:69:VAL:HG22	1.85	0.58
7:L:147:MET:HE1	7:L:182:GLY:HA3	1.86	0.58
2:F:137:GLN:NE2	5:C:36:ARG:HH21	2.01	0.58
9:A:521:LEU:HD22	9:A:575:ASP:HB3	1.84	0.58
2:F:37:ILE:HD11	2:F:48:PRO:HD3	1.86	0.58
7:J:424:ARG:HB3	7:J:427:LYS:HB2	1.85	0.58
7:J:181:TRP:CD1	7:J:231:TYR:HH	2.22	0.58
7:I:2:SER:HB2	7:I:84:VAL:HG12	1.85	0.58
7:I:400:ARG:NE	7:J:400:ARG:HG2	2.19	0.58
7:P:36:MET:HB2	7:P:378:ASP:HB2	1.85	0.58
5:C:69:VAL:HG11	5:D:122:TYR:CD1	2.38	0.58
6:H:18:ILE:HD11	6:H:348:ALA:HB2	1.85	0.58
7:J:37:VAL:HG13	7:J:112:LEU:HD23	1.84	0.58
7:M:37:VAL:HG13	7:M:112:LEU:HD23	1.86	0.58
7:M:401:THR:HA	7:M:404:ILE:HB	1.86	0.58
9:A:360:SER:O	9:A:364:ILE:HD12	2.03	0.58
1:B:75:PRO:HG2	1:B:114:TYR:HE2	1.69	0.57
7:I:147:MET:SD	7:I:398:LEU:HD21	2.44	0.57
1:B:61:THR:HG22	1:B:159:ILE:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:ILE:HD13	9:A:649:TYR:HE2	1.68	0.57
7:L:424:ARG:HB3	7:L:427:LYS:HB3	1.86	0.57
1:B:278:ARG:HE	1:B:279:PRO:HD2	1.67	0.57
1:B:130:THR:HG21	9:A:622:LEU:HD11	1.86	0.57
2:F:47:ILE:HB	2:F:101:ALA:HB3	1.87	0.57
6:H:50:MET:HE1	6:H:78:PHE:HE2	1.69	0.57
9:A:657:ILE:HD12	9:A:657:ILE:H	1.69	0.57
9:A:756:ARG:HG2	9:A:758:ASP:OD1	2.05	0.57
7:O:164:GLU:HB2	7:O:242:ASP:HB3	1.86	0.57
1:B:203:ARG:HH21	1:B:297:LEU:HA	1.70	0.57
7:J:141:VAL:HG21	7:J:424:ARG:HH12	1.70	0.57
1:B:175:TYR:HB3	2:E:152:ILE:HD13	1.86	0.56
3:G:56:MET:HE3	3:G:173:GLY:HA3	1.86	0.56
9:A:660:VAL:HG11	9:A:746:LEU:HD23	1.86	0.56
7:P:164:GLU:HB2	7:P:242:ASP:HB3	1.87	0.56
6:H:202:LYS:HB2	6:H:219:ARG:HH12	1.70	0.56
9:A:436:ILE:HG22	9:A:467:VAL:HG22	1.87	0.56
1:B:43:MET:HG3	2:E:3:PHE:HB2	1.88	0.56
2:E:3:PHE:HZ	2:E:5:LYS:NZ	2.03	0.56
7:J:74:VAL:HG12	7:J:97:LEU:HD21	1.87	0.56
7:P:400:ARG:HG2	7:Q:400:ARG:HG2	1.86	0.56
1:B:257:LEU:HD12	9:A:389:ASN:OD1	2.06	0.56
1:B:248:THR:HG23	1:B:282:PHE:CE1	2.41	0.56
6:H:55:LEU:HD23	6:H:82:ASN:HD22	1.70	0.56
7:K:400:ARG:HE	7:L:400:ARG:HG2	1.69	0.56
7:O:150:ILE:HD11	7:O:189:LEU:HD21	1.88	0.56
7:Q:155:HIS:CE1	7:Q:163:GLN:HE21	2.23	0.56
9:A:707:TYR:HD1	9:A:710:ARG:HD3	1.71	0.56
8:R:68:ARG:HB3	8:R:80:LEU:HD12	1.88	0.56
7:O:277:TYR:HD1	7:O:280:GLU:OE2	1.89	0.55
2:E:64:TYR:HB2	2:E:79:LEU:HD11	1.89	0.55
6:H:209:THR:HG22	6:H:211:LYS:HG2	1.87	0.55
9:A:285:LEU:HD23	9:A:306:PHE:HE2	1.71	0.55
5:D:80:ASN:HB3	8:R:46:LEU:HD22	1.87	0.55
7:L:205:GLU:HA	7:L:403:ARG:NE	2.20	0.55
9:A:47:VAL:HG12	9:A:51:GLN:HE21	1.72	0.55
7:L:148:ASN:HA	7:L:166:MET:HG3	1.88	0.55
1:B:2:THR:HA	1:B:204:LEU:HD22	1.89	0.55
7:Q:150:ILE:HD11	7:Q:189:LEU:HD21	1.88	0.55
2:E:188:ARG:HG3	2:E:188:ARG:HH11	1.72	0.55
9:A:296:LEU:HD13	9:A:306:PHE:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:150:ILE:HD11	7:J:189:LEU:HD21	1.89	0.54
1:B:255:GLN:HE22	1:B:279:PRO:HA	1.72	0.54
7:M:402:ASP:CG	7:M:403:ARG:HH11	2.15	0.54
9:A:657:ILE:HD12	9:A:657:ILE:N	2.21	0.54
7:P:37:VAL:HG13	7:P:112:LEU:HD23	1.90	0.54
9:A:351:ILE:HG23	9:A:540:LEU:HG	1.90	0.54
7:K:2:SER:HB2	7:K:84:VAL:HG12	1.89	0.54
3:G:59:LEU:HB3	3:G:176:LEU:HD23	1.89	0.54
1:B:25:LEU:HA	1:B:148:THR:HG21	1.90	0.54
1:B:70:PRO:HG2	1:B:197:PRO:HG2	1.90	0.54
2:E:124:ASN:HD22	2:E:133:ALA:HB1	1.73	0.54
2:F:129:ILE:HG13	3:G:70:GLU:OE1	2.08	0.54
7:L:199:GLU:CD	7:L:210:PRO:HA	2.32	0.54
7:M:129:PRO:HG3	7:M:416:GLN:HE22	1.72	0.54
7:O:74:VAL:HG12	7:O:97:LEU:HD21	1.90	0.54
7:L:36:MET:HE2	7:L:376:THR:HB	1.90	0.54
9:A:706:TYR:CE2	9:A:710:ARG:HD2	2.43	0.54
6:H:66:THR:HG22	6:H:67:ARG:HD2	1.90	0.53
7:L:152:GLY:HA2	7:L:156:SER:HB3	1.90	0.53
2:E:4:ALA:HB3	2:E:155:ILE:HB	1.89	0.53
7:K:314:GLN:HG3	7:K:431:ASN:HD21	1.73	0.53
7:M:155:HIS:HD2	7:M:163:GLN:HG3	1.73	0.53
7:O:181:TRP:CD1	7:O:231:TYR:HH	2.26	0.53
9:A:594:ARG:CZ	9:A:598:ILE:HG13	2.38	0.53
2:E:176:LEU:HD21	2:F:204:PHE:CE2	2.44	0.53
6:H:180:LEU:HD21	6:H:242:LEU:HD12	1.88	0.53
7:O:44:GLY:HA3	7:O:47:GLU:HG2	1.91	0.53
2:E:17:GLY:H	2:E:140:ARG:HH21	1.56	0.53
6:H:275:GLN:HB2	6:H:349:ASN:HB3	1.91	0.53
9:A:38:TRP:CZ2	9:A:157:LYS:HD2	2.44	0.53
9:A:693:TYR:CZ	9:A:697:GLU:HG3	2.43	0.53
6:H:154:ASN:HD22	6:H:161:LYS:NZ	2.06	0.53
7:J:6:ASP:HB3	7:J:26:TYR:HB2	1.91	0.53
3:G:185:SER:HB2	3:G:188:ARG:HH21	1.75	0.52
5:C:129:LYS:HG3	5:C:130:ASP:H	1.74	0.52
6:H:27:THR:HG23	6:H:29:ARG:H	1.74	0.52
7:M:22:GLU:HB3	7:M:36:MET:HG2	1.91	0.52
7:M:149:ILE:HD11	7:M:222:ILE:HG12	1.92	0.52
2:E:65:ASN:ND2	2:E:69:ALA:HB2	2.24	0.52
7:I:148:ASN:ND2	7:I:164:GLU:HG2	2.23	0.52
7:I:400:ARG:HE	7:J:400:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:74:VAL:HG12	7:L:97:LEU:HD21	1.91	0.52
7:M:276:ASP:O	7:M:280:GLU:HG3	2.08	0.52
7:P:1:MET:HB2	7:P:29:SER:HB3	1.91	0.52
6:H:49:LYS:HG3	6:H:89:PHE:CE1	2.45	0.52
5:D:53:LYS:NZ	5:D:55:ASP:HB2	2.25	0.52
7:M:328:LEU:HD13	7:M:340:ILE:HD12	1.90	0.52
7:Q:328:LEU:HD13	7:Q:340:ILE:HD12	1.92	0.52
7:O:147:MET:HB2	7:O:167:ILE:HG13	1.92	0.52
1:B:249:ASN:CG	2:E:89:LYS:HE3	2.34	0.52
9:A:97:SER:HG	9:A:101:TRP:CD1	2.28	0.52
2:F:128:ARG:HH22	3:G:72:PRO:HB3	1.75	0.51
7:O:6:ASP:HB3	7:O:26:TYR:HB2	1.91	0.51
7:M:58:ARG:HG3	7:O:180:ARG:HD2	1.92	0.51
6:H:24:GLU:HB3	6:H:116:LYS:HE3	1.92	0.51
2:F:73:SER:HA	2:F:85:ASN:ND2	2.25	0.51
7:P:289:THR:HG23	7:P:314:GLN:HE21	1.76	0.51
1:B:278:ARG:NE	1:B:279:PRO:HD2	2.25	0.51
5:D:10:VAL:HG13	5:D:122:TYR:OH	2.11	0.51
6:H:18:ILE:HD13	6:H:280:LEU:HB3	1.93	0.51
7:I:402:ASP:OD1	7:I:403:ARG:HG2	2.10	0.51
7:Q:152:GLY:HA2	7:Q:156:SER:HB3	1.93	0.51
1:B:166:LEU:O	1:B:170:MET:HG2	2.10	0.51
2:F:20:ILE:HD13	2:F:48:PRO:HD2	1.92	0.51
7:I:269:ARG:HB3	7:I:273:GLU:HB2	1.93	0.50
9:A:181:LEU:HB2	9:A:199:ALA:HB2	1.93	0.50
1:B:99:LEU:HD23	1:B:119:LEU:HD21	1.94	0.50
5:D:19:LEU:O	5:D:93:LYS:HE2	2.11	0.50
7:M:145:PRO:HG2	7:M:147:MET:HE3	1.93	0.50
7:O:238:PHE:CE1	7:O:426:LEU:HD21	2.46	0.50
1:B:103:LEU:HD21	1:B:106:LEU:HG	1.92	0.50
2:F:7:LYS:HZ2	2:F:150:GLU:HB3	1.76	0.50
7:L:328:LEU:HD13	7:L:340:ILE:HD12	1.92	0.50
9:A:163:PHE:CZ	9:A:173:LEU:HB2	2.47	0.50
7:L:36:MET:HB2	7:L:378:ASP:HB2	1.93	0.50
7:L:402:ASP:OD1	7:L:403:ARG:HG2	2.12	0.50
7:Q:6:ASP:HB2	7:Q:26:TYR:HB2	1.93	0.50
9:A:597:PHE:CD2	9:A:607:LEU:HD11	2.47	0.50
2:F:181:TYR:CG	2:F:186:GLY:HA3	2.47	0.50
6:H:329:PRO:HD3	8:R:98:MET:HA	1.92	0.50
7:J:238:PHE:CE1	7:J:426:LEU:HD21	2.47	0.50
1:B:159:ILE:HG21	1:B:204:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLY:HA3	1:B:291:LYS:HA	1.94	0.50
7:J:158:ALA:HB2	7:J:211:ARG:HA	1.93	0.50
7:M:205:GLU:CD	7:M:403:ARG:HH21	2.19	0.50
1:B:212:VAL:HB	1:B:294:PHE:HB3	1.94	0.50
5:D:38:LEU:HD21	5:D:71:GLN:HG3	1.94	0.50
7:M:157:ASP:HB2	7:M:211:ARG:CZ	2.42	0.50
9:A:499:LEU:HB3	9:A:566:LYS:HD2	1.92	0.50
2:E:98:PHE:CD1	2:E:151:LEU:HD13	2.47	0.49
7:M:56:LYS:HE2	7:M:61:GLY:HA3	1.95	0.49
7:O:148:ASN:ND2	7:O:164:GLU:HG2	2.27	0.49
7:P:325:THR:O	7:P:329:GLU:HG3	2.12	0.49
9:A:15:HIS:NE2	9:A:205:THR:HG21	2.27	0.49
2:F:112:LEU:O	5:D:50:LYS:HD3	2.12	0.49
6:H:29:ARG:HH21	6:H:68:PRO:HG3	1.76	0.49
7:I:98:ASP:O	7:I:105:LYS:HE2	2.12	0.49
1:B:8:MET:CE	1:B:170:MET:HE1	2.41	0.49
6:H:269:LYS:HE2	6:H:342:PHE:HD2	1.77	0.49
7:P:314:GLN:HG3	7:P:431:ASN:HD21	1.78	0.49
5:D:83:THR:HG23	6:H:67:ARG:NH2	2.27	0.49
7:O:148:ASN:HD21	7:O:164:GLU:HG2	1.77	0.49
7:K:328:LEU:HD13	7:K:340:ILE:HD12	1.93	0.49
6:H:320:LYS:HZ2	6:H:342:PHE:HE1	1.59	0.49
6:H:323:LEU:HD13	6:H:336:ILE:HG12	1.93	0.49
7:I:424:ARG:HB3	7:I:427:LYS:HB2	1.95	0.49
7:L:241:LEU:HD11	7:L:287:ILE:HD13	1.95	0.49
7:Q:204:ASP:HA	7:Q:400:ARG:NH1	2.27	0.49
9:A:416:VAL:HG11	9:A:424:TYR:CE2	2.48	0.49
2:F:53:LYS:NZ	4:N:12:G:H5'	2.26	0.49
7:O:239:ILE:O	7:O:287:ILE:HA	2.12	0.49
7:Q:160:ILE:HD11	7:Q:212:PHE:HB2	1.95	0.49
1:B:211:LYS:HD3	1:B:267:SER:HA	1.95	0.49
7:I:294:MET:HE3	7:I:305:LEU:HB2	1.93	0.49
2:E:142:ILE:HD12	2:F:41:ILE:HD11	1.94	0.49
2:E:181:TYR:CG	2:E:186:GLY:HA3	2.48	0.49
6:H:179:ASP:OD2	6:H:182:ASN:HB2	2.13	0.49
7:M:279:GLU:OE2	7:M:309:LEU:HG	2.13	0.49
7:P:401:THR:HA	7:P:404:ILE:HB	1.94	0.49
2:F:123:GLU:HB2	2:F:136:ARG:HE	1.77	0.49
5:D:45:LEU:HD12	5:D:57:LEU:HD11	1.95	0.49
5:D:69:VAL:HG11	6:H:60:GLU:OE1	2.13	0.49
7:Q:147:MET:SD	7:Q:398:LEU:HD21	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:238:PHE:CE1	7:Q:426:LEU:HD21	2.48	0.49
9:A:276:PHE:HD2	9:A:451:LEU:HD21	1.77	0.49
2:E:55:LYS:HE2	2:E:181:TYR:O	2.13	0.48
2:F:88:ASP:O	2:F:92:LYS:HG2	2.13	0.48
7:I:79:ILE:HD12	7:I:90:ILE:HG23	1.94	0.48
7:K:293:GLY:O	7:K:294:MET:HE2	2.13	0.48
7:O:412:ARG:O	7:O:416:GLN:HG3	2.13	0.48
1:B:289:TYR:CZ	1:B:291:LYS:HB2	2.49	0.48
5:C:20:LEU:HB2	5:C:28:TYR:HE1	1.78	0.48
7:J:152:GLY:HA2	7:J:156:SER:HB3	1.94	0.48
9:A:653:PHE:CD2	9:A:657:ILE:HD11	2.47	0.48
7:K:400:ARG:HG2	7:L:400:ARG:CZ	2.42	0.48
9:A:706:TYR:HE2	9:A:710:ARG:HH11	1.60	0.48
7:I:309:LEU:HD23	7:I:312:LYS:NZ	2.29	0.48
2:F:123:GLU:HA	4:N:21:G:H5"	1.95	0.48
7:K:2:SER:HB3	7:K:125:TYR:CZ	2.48	0.48
7:J:205:GLU:HG2	7:J:371:HIS:CE1	2.44	0.48
8:R:33:ILE:HB	8:R:37:GLU:HG3	1.96	0.48
9:A:358:PRO:O	9:A:362:ARG:HG3	2.13	0.48
5:D:17:ILE:HA	5:D:20:LEU:HG	1.96	0.48
7:I:47:GLU:OE2	7:I:322:VAL:HG21	2.13	0.48
7:J:371:HIS:HD2	7:J:394:LYS:O	1.97	0.48
9:A:351:ILE:CG2	9:A:540:LEU:HG	2.43	0.48
1:B:27:PHE:HB2	1:B:31:ARG:HD2	1.96	0.47
1:B:75:PRO:HG2	1:B:114:TYR:CE2	2.48	0.47
7:J:314:GLN:HG3	7:J:431:ASN:HD21	1.78	0.47
1:B:251:ASN:HD22	4:N:4:G:H1	1.60	0.47
2:F:78:ILE:HD13	2:F:165:GLU:OE2	2.14	0.47
6:H:200:VAL:HB	6:H:319:THR:OG1	2.14	0.47
5:D:32:THR:HB	5:D:130:ASP:HA	1.96	0.47
7:L:205:GLU:HA	7:L:403:ARG:HH21	1.80	0.47
7:P:325:THR:HB	7:P:359:MET:HE1	1.96	0.47
7:P:205:GLU:HG2	7:P:371:HIS:CE1	2.50	0.47
9:A:256:TYR:HD1	9:A:267:LEU:HD11	1.80	0.47
7:K:371:HIS:CD2	7:K:395:THR:HA	2.48	0.47
5:D:45:LEU:HD21	5:D:109:LEU:HD11	1.97	0.47
6:H:203:TRP:HB2	6:H:318:LEU:O	2.15	0.47
7:I:325:THR:HG23	7:I:359:MET:HE1	1.96	0.47
7:K:16:ARG:HD2	7:K:18:ASN:OD1	2.14	0.47
7:L:156:SER:HB2	7:L:209:ALA:HB1	1.95	0.47
7:O:148:ASN:HA	7:O:166:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:190:LYS:HG2	7:O:194:LYS:HE3	1.96	0.47
7:O:198:LEU:HD12	7:O:211:ARG:H	1.79	0.47
7:O:325:THR:HB	7:O:359:MET:HE1	1.96	0.47
6:H:103:ARG:HD2	6:H:110:ALA:N	2.30	0.47
7:K:278:LEU:HD22	7:K:290:ILE:HD13	1.97	0.47
7:M:75:ILE:HG21	7:M:114:VAL:HG21	1.96	0.47
7:M:241:LEU:HD11	7:M:287:ILE:HD13	1.97	0.47
3:G:101:ALA:HB1	3:G:147:PHE:HB3	1.96	0.46
7:K:239:ILE:O	7:K:287:ILE:HA	2.14	0.46
7:K:289:THR:HG22	7:K:314:GLN:HB3	1.97	0.46
7:P:424:ARG:HB3	7:P:427:LYS:HB2	1.98	0.46
7:Q:314:GLN:HE22	7:Q:392:GLN:HE22	1.63	0.46
2:F:129:ILE:HG23	6:H:176:GLU:OE1	2.15	0.46
5:D:68:PHE:HZ	5:D:116:MET:HE2	1.80	0.46
7:M:12:VAL:HG21	7:M:36:MET:HE3	1.96	0.46
2:F:192:LYS:HB2	3:G:99:ARG:NH1	2.31	0.46
7:J:371:HIS:CD2	7:J:395:THR:HA	2.50	0.46
7:L:216:GLU:O	7:L:220:GLU:HG2	2.16	0.46
7:O:158:ALA:HB2	7:O:211:ARG:HA	1.98	0.46
2:E:12:ILE:O	2:E:146:THR:HA	2.15	0.46
5:C:30:LEU:HD21	5:C:90:LEU:HD22	1.98	0.46
7:M:205:GLU:HA	7:M:403:ARG:NE	2.31	0.46
7:O:2:SER:HB3	7:O:125:TYR:CZ	2.50	0.46
7:Q:401:THR:HA	7:Q:404:ILE:HB	1.98	0.46
3:G:82:LEU:HD23	3:G:96:LEU:HD11	1.98	0.46
7:K:148:ASN:HA	7:K:166:MET:HG3	1.97	0.46
7:M:130:LEU:HD21	7:M:380:THR:HG23	1.98	0.46
2:E:109:LEU:HD13	2:E:142:ILE:HD11	1.96	0.46
3:G:186:GLY:HA2	3:G:190:TYR:H	1.81	0.46
7:K:6:ASP:OD1	7:K:26:TYR:HB2	2.16	0.46
7:K:47:GLU:HG3	7:K:346:GLN:HG2	1.98	0.46
1:B:274:ILE:HD11	1:B:289:TYR:CD1	2.51	0.46
7:I:160:ILE:HD11	7:I:212:PHE:HB2	1.98	0.46
7:K:238:PHE:CE1	7:K:426:LEU:HD21	2.51	0.46
7:Q:280:GLU:OE2	7:Q:281:LEU:HG	2.16	0.46
3:G:109:LEU:HD13	3:G:142:ILE:HD11	1.97	0.46
7:J:149:ILE:HG23	7:J:150:ILE:HG12	1.98	0.45
7:K:36:MET:HE1	7:K:377:GLU:CD	2.40	0.45
7:M:53:ASP:HA	7:M:66:LYS:HE3	1.98	0.45
9:A:707:TYR:HA	9:A:710:ARG:HG2	1.97	0.45
7:Q:74:VAL:HG12	7:Q:97:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:244:ALA:HA	9:A:343:TRP:HA	1.98	0.45
2:E:30:GLY:O	2:E:32:ILE:HG12	2.17	0.45
6:H:43:MET:HE1	6:H:59:PHE:HZ	1.81	0.45
7:J:396:GLY:HA3	7:J:403:ARG:HD2	1.97	0.45
9:A:243:LEU:HD22	9:A:364:ILE:HG22	1.97	0.45
2:E:10:ALA:HB3	2:E:149:PHE:HD2	1.81	0.45
2:E:21:GLY:HA2	2:E:36:VAL:HA	1.98	0.45
5:C:67:GLN:HE21	5:C:71:GLN:HE21	1.64	0.45
7:L:239:ILE:O	7:L:287:ILE:HA	2.16	0.45
7:O:253:HIS:HB2	7:O:255:VAL:HG22	1.99	0.45
6:H:306:MET:HB2	6:H:306:MET:HE3	1.86	0.45
7:I:148:ASN:CA	7:I:166:MET:HG2	2.41	0.45
7:J:2:SER:HB2	7:J:84:VAL:HG12	1.99	0.45
7:M:74:VAL:HG12	7:M:97:LEU:HD21	1.98	0.45
3:G:53:LYS:HE3	4:N:19:A:OP1	2.16	0.45
5:C:17:ILE:HA	5:C:20:LEU:HD13	1.98	0.45
7:I:74:VAL:HG12	7:I:97:LEU:HD21	1.99	0.45
2:F:53:LYS:HZ3	4:N:12:G:H5'	1.82	0.45
7:Q:149:ILE:HG13	7:Q:189:LEU:HD22	1.98	0.45
9:A:416:VAL:HG11	9:A:424:TYR:HE2	1.81	0.45
2:E:121:LYS:HD3	2:E:140:ARG:HH11	1.82	0.45
3:G:198:LEU:HG	3:G:216:LEU:HD13	1.99	0.45
7:K:198:LEU:HD13	7:K:210:PRO:HB2	1.99	0.45
7:J:140:LYS:HE2	7:K:88:GLN:OE1	2.16	0.45
7:K:149:ILE:HG12	7:K:189:LEU:HD23	1.99	0.45
7:L:294:MET:HB2	7:L:302:TRP:CD1	2.52	0.45
7:Q:357:ILE:HD13	7:Q:388:THR:HG21	1.98	0.45
1:B:67:GLN:HB3	1:B:71:PHE:HE1	1.82	0.45
9:A:200:GLU:O	9:A:204:LEU:HG	2.17	0.45
2:F:138:ILE:HD11	2:F:190:TYR:OH	2.16	0.44
6:H:185:ARG:NH2	6:H:235:THR:HG21	2.30	0.44
7:Q:163:GLN:HG2	7:Q:164:GLU:HG3	1.99	0.44
9:A:13:LEU:HG	9:A:177:PHE:HE2	1.82	0.44
9:A:493:ILE:HA	9:A:496:TYR:CD1	2.52	0.44
1:B:274:ILE:HD11	1:B:289:TYR:HD1	1.81	0.44
7:O:75:ILE:HG21	7:O:114:VAL:HG21	1.99	0.44
2:E:12:ILE:HG23	2:E:193:VAL:HB	2.00	0.44
2:F:109:LEU:O	2:F:114:VAL:HG12	2.17	0.44
7:I:272:ALA:HA	7:I:275:ILE:HD12	1.99	0.44
9:A:685:LYS:HD2	9:A:685:LYS:HA	1.81	0.44
1:B:36:LEU:HA	1:B:36:LEU:HD23	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD22	1:B:257:LEU:HD11	2.00	0.44
1:B:254:LYS:HD2	1:B:286:VAL:HG11	2.00	0.44
5:D:29:LEU:HD21	5:D:84:PHE:HB3	1.99	0.44
7:I:1:MET:HB2	7:I:1:MET:HE3	1.91	0.44
7:K:371:HIS:HD2	7:K:394:LYS:O	2.01	0.44
9:A:455:ALA:HB3	9:A:458:LYS:HE2	1.99	0.44
1:B:180:GLY:H	4:N:4:G:H5''	1.82	0.44
7:P:75:ILE:HG21	7:P:114:VAL:HG21	1.99	0.44
1:B:229:MET:HE1	9:A:382:TYR:HA	2.00	0.44
2:E:188:ARG:HG3	2:E:188:ARG:NH1	2.30	0.44
9:A:570:ILE:HB	9:A:578:PHE:HD1	1.82	0.44
2:E:138:ILE:HG21	2:E:138:ILE:HD13	1.72	0.44
7:L:7:VAL:HG22	7:L:25:VAL:HG22	1.99	0.44
7:P:53:ASP:HA	7:P:66:LYS:HD2	1.99	0.44
2:E:29:ILE:HG22	9:A:691:ARG:NH2	2.33	0.44
5:C:51:GLU:HG2	5:C:52:ARG:HG3	2.00	0.44
7:M:205:GLU:HA	7:M:403:ARG:CZ	2.48	0.44
7:O:402:ASP:OD1	7:O:403:ARG:HG2	2.18	0.44
9:A:349:LYS:HE2	9:A:355:LEU:O	2.17	0.43
1:B:170:MET:HB3	1:B:170:MET:HE3	1.35	0.43
6:H:114:VAL:HG22	6:H:199:LEU:HD11	2.00	0.43
6:H:154:ASN:HD22	6:H:161:LYS:HZ3	1.67	0.43
8:R:70:HIS:CD2	8:R:80:LEU:HD23	2.53	0.43
7:Q:277:TYR:O	7:Q:280:GLU:HG3	2.18	0.43
9:A:56:MET:HE1	9:A:91:GLU:CB	2.42	0.43
9:A:686:LEU:O	9:A:690:LEU:HD23	2.18	0.43
5:C:10:VAL:HG11	9:A:698:LYS:HB3	2.00	0.43
1:B:242:PHE:CE2	1:B:253:ARG:HD3	2.53	0.43
7:P:163:GLN:OE1	7:P:244:ALA:HB2	2.19	0.43
3:G:29:ILE:HG23	5:C:70:TYR:CD2	2.54	0.43
7:L:21:LEU:HD21	7:L:109:ASN:HB2	2.00	0.43
9:A:631:GLU:O	9:A:635:LYS:HG2	2.18	0.43
1:B:181:LYS:HB2	1:B:186:PHE:HD2	1.83	0.43
4:N:2:C:H2'	4:N:4:G:H4'	2.01	0.43
7:L:312:LYS:HG3	7:L:313:VAL:HG23	2.00	0.43
7:Q:347:ILE:HD11	7:Q:353:THR:OG1	2.19	0.43
9:A:12:ALA:O	9:A:15:HIS:CD2	2.72	0.43
1:B:213:MET:HB3	1:B:213:MET:HE2	1.72	0.43
1:B:249:ASN:HD21	2:E:89:LYS:HG2	1.82	0.43
2:F:14:LEU:HA	2:F:14:LEU:HD23	1.78	0.43
3:G:167:PHE:CE2	3:G:212:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:321:ALA:HB3	6:H:343:TYR:CD2	2.54	0.43
1:B:60:LEU:HB2	1:B:289:TYR:CE2	2.53	0.43
7:P:74:VAL:HG12	7:P:97:LEU:HD21	2.00	0.43
9:A:426:PHE:O	9:A:430:ILE:HG13	2.18	0.43
1:B:10:PHE:CD1	1:B:189:PHE:HB3	2.54	0.42
5:C:20:LEU:HD21	5:C:90:LEU:HD13	2.00	0.42
5:D:20:LEU:HB2	5:D:28:TYR:HE1	1.83	0.42
6:H:29:ARG:HD2	6:H:63:LEU:HD23	2.01	0.42
7:J:386:VAL:HG11	7:J:413:ILE:HG21	2.01	0.42
7:K:147:MET:HB2	7:K:167:ILE:HG13	2.00	0.42
7:K:424:ARG:HB3	7:K:427:LYS:HB2	2.01	0.42
7:P:2:SER:HB3	7:P:125:TYR:CZ	2.54	0.42
7:P:402:ASP:OD1	7:P:403:ARG:HG2	2.18	0.42
1:B:2:THR:N	1:B:59:THR:HG21	2.33	0.42
2:F:14:LEU:HD23	2:F:193:VAL:HG12	2.00	0.42
2:F:56:MET:HE3	2:F:173:GLY:HA3	2.02	0.42
2:F:101:ALA:HB1	2:F:147:PHE:HB3	2.02	0.42
3:G:45:PRO:HD2	3:G:103:LEU:HD11	2.01	0.42
8:R:33:ILE:HD13	8:R:33:ILE:HG21	1.81	0.42
7:M:190:LYS:HG3	7:M:200:THR:HG23	2.01	0.42
7:O:401:THR:HA	7:O:404:ILE:HB	2.00	0.42
9:A:362:ARG:O	9:A:366:GLN:HG2	2.19	0.42
1:B:217:THR:HA	1:B:260:PHE:O	2.19	0.42
7:O:194:LYS:HG3	7:O:200:THR:HG21	2.01	0.42
7:P:15:SER:HB3	7:Q:401:THR:HG23	2.00	0.42
9:A:662:ASP:HA	9:A:666:GLU:HG2	2.02	0.42
5:D:81:ARG:HD3	8:R:45:GLY:O	2.19	0.42
7:I:400:ARG:HG2	7:J:400:ARG:CZ	2.50	0.42
7:J:341:LEU:HA	7:J:341:LEU:HD12	1.72	0.42
9:A:15:HIS:HA	9:A:52:ILE:HG12	2.00	0.42
9:A:325:PHE:CD2	9:A:339:VAL:HG11	2.51	0.42
3:G:181:TYR:CG	3:G:186:GLY:HA3	2.55	0.42
5:D:20:LEU:HD23	5:D:93:LYS:HD2	2.02	0.42
7:K:341:LEU:HD12	7:K:368:VAL:HB	2.00	0.42
7:O:1:MET:HB2	7:O:29:SER:HB3	2.01	0.42
7:P:152:GLY:HA2	7:P:156:SER:HB3	2.01	0.42
7:K:253:HIS:HB2	7:K:255:VAL:HG12	2.01	0.42
2:E:171:ARG:O	2:E:175:LYS:HG2	2.20	0.42
9:A:242:LEU:HD23	9:A:345:SER:HA	2.01	0.42
3:G:12:ILE:O	3:G:146:THR:HA	2.20	0.42
5:D:13:ALA:O	5:D:17:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:46:PHE:CD1	6:H:89:PHE:HD2	2.38	0.42
7:Q:36:MET:HB2	7:Q:378:ASP:HB2	2.01	0.42
9:A:284:SER:O	9:A:288:LYS:HG2	2.20	0.42
9:A:298:TYR:O	9:A:304:ALA:HA	2.20	0.42
9:A:382:TYR:CE1	9:A:383:ARG:NE	2.88	0.42
9:A:709:THR:O	9:A:712:GLU:HB3	2.19	0.42
3:G:96:LEU:HD21	3:G:170:ILE:HD11	2.01	0.42
7:L:238:PHE:CE1	7:L:426:LEU:HD21	2.55	0.42
7:Q:347:ILE:HG21	7:Q:347:ILE:HD13	1.85	0.42
9:A:325:PHE:HD2	9:A:339:VAL:CG1	2.33	0.42
1:B:65:PRO:O	1:B:71:PHE:HB2	2.20	0.42
2:E:32:ILE:HG21	2:E:139:GLU:HG3	2.02	0.42
2:E:105:ASN:HB2	2:E:108:GLU:HB3	2.02	0.42
2:E:188:ARG:HH12	4:N:12:G:C5'	2.28	0.42
7:J:324:ASN:HB3	7:J:327:TYR:HB2	2.02	0.42
7:K:291:GLU:HG3	7:K:316:VAL:HB	2.02	0.42
7:L:400:ARG:HB2	7:L:402:ASP:OD1	2.19	0.42
7:O:22:GLU:HB3	7:O:36:MET:HG2	2.02	0.42
7:Q:1:MET:HE2	7:Q:125:TYR:CE1	2.55	0.42
1:B:33:PHE:CD2	1:B:289:TYR:HB2	2.55	0.41
6:H:48:ASN:O	6:H:52:GLU:HG2	2.20	0.41
7:J:191:LYS:HB3	7:J:191:LYS:HE3	1.83	0.41
7:M:314:GLN:HG3	7:M:431:ASN:HD21	1.85	0.41
7:Q:2:SER:HB2	7:Q:84:VAL:HG12	2.02	0.41
9:A:267:LEU:HD22	9:A:620:ILE:HG12	2.02	0.41
1:B:249:ASN:OD1	2:E:89:LYS:HE3	2.20	0.41
2:F:78:ILE:HG21	2:F:169:VAL:HG21	2.02	0.41
2:F:128:ARG:HH12	3:G:72:PRO:CA	2.32	0.41
7:I:58:ARG:HG3	7:J:180:ARG:HD2	2.00	0.41
8:R:33:ILE:HB	8:R:37:GLU:CG	2.50	0.41
7:O:210:PRO:HG2	7:O:212:PHE:CE2	2.54	0.41
7:P:1:MET:HE2	7:P:125:TYR:HE1	1.85	0.41
9:A:412:HIS:O	9:A:414:GLN:HG3	2.20	0.41
1:B:18:GLY:HA2	4:N:3:G:C8	2.56	0.41
1:B:185:GLY:HA2	2:E:99:ARG:HA	2.01	0.41
1:B:218:ALA:HA	1:B:290:ALA:HB1	2.02	0.41
2:E:166:ASP:O	2:E:170:ILE:HD12	2.19	0.41
7:Q:396:GLY:HA3	7:Q:403:ARG:HD2	2.01	0.41
9:A:2:LYS:O	9:A:6:ILE:HG12	2.20	0.41
9:A:245:SER:HA	9:A:304:ALA:O	2.20	0.41
1:B:274:ILE:HG23	1:B:274:ILE:HD12	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:GLY:HA3	2:E:140:ARG:HE	1.84	0.41
5:C:64:LEU:HG	5:C:68:PHE:HE2	1.84	0.41
6:H:258:LYS:HA	6:H:262:LEU:HB2	2.03	0.41
6:H:269:LYS:HE2	6:H:342:PHE:CD2	2.54	0.41
7:K:245:SER:HA	7:K:248:PHE:CE1	2.55	0.41
7:L:92:ARG:HA	7:L:92:ARG:HD3	1.85	0.41
7:P:341:LEU:HA	7:P:341:LEU:HD12	1.88	0.41
7:Q:220:GLU:O	7:Q:224:LYS:HG2	2.20	0.41
9:A:606:THR:C	9:A:607:LEU:HD12	2.44	0.41
2:F:128:ARG:HH12	3:G:72:PRO:N	2.18	0.41
6:H:13:LEU:HD11	6:H:225:LEU:HA	2.03	0.41
7:K:1:MET:HG3	7:K:125:TYR:HE1	1.85	0.41
7:L:343:LYS:HD2	7:L:346:GLN:NE2	2.36	0.41
7:M:146:MET:CE	7:M:289:THR:HG21	2.46	0.41
7:P:58:ARG:HG3	7:Q:180:ARG:HD2	2.02	0.41
9:A:508:ILE:HG21	9:A:508:ILE:HD13	1.84	0.41
3:G:78:ILE:O	3:G:82:LEU:HD13	2.20	0.41
5:D:69:VAL:HG12	6:H:64:ILE:HD11	2.02	0.41
7:M:186:PHE:CZ	7:M:399:SER:HB2	2.55	0.41
9:A:56:MET:HE3	9:A:58:ASN:HB2	2.01	0.41
2:F:126:ILE:HD11	4:N:20:C:C5	2.55	0.41
3:G:185:SER:HB2	3:G:188:ARG:NH2	2.34	0.41
5:C:101:LYS:HE2	5:C:101:LYS:HB3	1.62	0.41
7:L:146:MET:HG2	7:L:168:VAL:HG22	2.02	0.41
2:E:13:ARG:HE	2:E:196:GLU:CD	2.28	0.41
3:G:121:LYS:HD3	3:G:140:ARG:NH1	2.36	0.41
5:C:129:LYS:HG3	5:C:130:ASP:N	2.35	0.41
6:H:118:ILE:HD13	6:H:128:PRO:HG3	2.03	0.41
7:L:338:ASN:HA	7:L:365:TYR:CE1	2.56	0.41
7:P:155:HIS:CD2	7:P:163:GLN:HE21	2.39	0.41
9:A:366:GLN:OE1	9:A:526:MET:HE2	2.20	0.41
1:B:2:THR:HA	1:B:204:LEU:CD2	2.50	0.41
6:H:327:LYS:HB3	8:R:96:ILE:HA	2.02	0.41
7:J:221:THR:HA	7:J:224:LYS:HE3	2.03	0.41
7:J:375:GLU:HG3	7:J:403:ARG:HH12	1.84	0.41
7:J:375:GLU:HG3	7:J:403:ARG:NH1	2.36	0.41
7:M:341:LEU:HD12	7:M:341:LEU:HA	1.76	0.41
7:O:277:TYR:HA	7:O:280:GLU:HG2	2.03	0.41
7:P:16:ARG:HD3	7:P:204:ASP:OD1	2.21	0.41
7:P:290:ILE:HB	7:P:315:LEU:HD23	2.01	0.41
7:P:341:LEU:CD1	7:P:370:SER:HB2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:156:SER:HB2	7:Q:209:ALA:HB1	2.03	0.41
9:A:437:ILE:HD11	9:A:468:TYR:HE2	1.85	0.41
1:B:67:GLN:HE22	1:B:152:ASN:ND2	2.17	0.41
1:B:207:ASN:HA	1:B:269:THR:HG21	2.03	0.41
2:E:176:LEU:HA	2:E:176:LEU:HD23	1.76	0.41
3:G:177:LEU:HD21	3:G:182:LEU:HD21	2.02	0.41
7:P:160:ILE:HD11	7:P:212:PHE:HB2	2.03	0.41
7:P:345:ASN:HD21	7:P:372:ARG:HG3	1.86	0.41
9:A:17:ILE:O	9:A:21:ILE:HG12	2.21	0.41
2:E:109:LEU:O	2:E:114:VAL:HG22	2.21	0.40
7:I:242:ASP:HA	7:I:291:GLU:HB3	2.03	0.40
7:I:386:VAL:HG11	7:I:413:ILE:HG21	2.04	0.40
7:J:328:LEU:HD13	7:J:340:ILE:HD12	2.04	0.40
7:O:386:VAL:HG11	7:O:413:ILE:HG21	2.03	0.40
7:Q:239:ILE:O	7:Q:287:ILE:HA	2.20	0.40
9:A:160:LEU:HA	9:A:163:PHE:HB2	2.02	0.40
9:A:254:PHE:CD2	9:A:274:LEU:HD21	2.56	0.40
9:A:268:LYS:NZ	9:A:489:GLN:HB2	2.36	0.40
9:A:276:PHE:HE1	9:A:483:VAL:HG21	1.87	0.40
9:A:362:ARG:HG3	9:A:362:ARG:H	1.56	0.40
9:A:383:ARG:O	9:A:387:LEU:HD23	2.21	0.40
9:A:401:ILE:HD13	9:A:401:ILE:HG21	1.77	0.40
1:B:236:LEU:HD12	1:B:258:TYR:HB3	2.04	0.40
3:G:14:LEU:HD23	3:G:193:VAL:HG12	2.02	0.40
3:G:177:LEU:HD12	3:G:177:LEU:HA	1.72	0.40
7:I:147:MET:HG2	7:I:407:TYR:OH	2.21	0.40
7:K:180:ARG:HD2	7:L:58:ARG:HG3	2.03	0.40
7:O:21:LEU:HD21	7:O:109:ASN:HB2	2.03	0.40
7:P:20:THR:HA	7:P:64:THR:HG21	2.02	0.40
9:A:186:SER:HA	9:A:198:LEU:HD13	2.03	0.40
7:K:7:VAL:HG22	7:K:25:VAL:HG22	2.01	0.40
7:K:36:MET:HE1	7:K:377:GLU:HG2	2.04	0.40
7:K:241:LEU:HD11	7:K:287:ILE:HD13	2.02	0.40
7:L:245:SER:HA	7:L:248:PHE:CE2	2.56	0.40
7:O:341:LEU:HA	7:O:341:LEU:HD12	1.72	0.40
1:B:135:GLN:HB2	4:N:7:A:H1'	2.04	0.40
2:E:44:LEU:HB3	2:E:103:LEU:HD12	2.04	0.40
3:G:59:LEU:HD13	3:G:176:LEU:HB3	2.03	0.40
3:G:124:ASN:HD22	3:G:133:ALA:HB1	1.86	0.40
7:I:92:ARG:HD3	7:I:92:ARG:HA	1.84	0.40
7:I:346:GLN:HG3	7:I:372:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:21:LEU:HD21	7:K:109:ASN:HB2	2.02	0.40
7:L:146:MET:SD	7:L:289:THR:HG21	2.62	0.40
7:O:173:PRO:HG2	7:O:177:GLU:HG3	2.03	0.40
1:B:10:PHE:CE1	1:B:189:PHE:HB3	2.56	0.40
5:D:118:ALA:HB1	5:D:122:TYR:HE2	1.86	0.40
6:H:303:TYR:HA	6:H:306:MET:HE2	2.04	0.40
7:K:402:ASP:OD1	7:K:403:ARG:HG2	2.22	0.40
7:L:270:THR:H	7:L:273:GLU:HB2	1.87	0.40
7:P:90:ILE:HD13	7:P:118:VAL:HG11	2.03	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	B	295/299 (99%)	272 (92%)	23 (8%)	0	100	100
2	E	217/220 (99%)	203 (94%)	14 (6%)	0	100	100
2	F	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
3	G	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
5	C	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
5	D	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
6	H	350/357 (98%)	320 (91%)	30 (9%)	0	100	100
7	I	432/434 (100%)	420 (97%)	12 (3%)	0	100	100
7	J	432/434 (100%)	421 (98%)	11 (2%)	0	100	100
7	K	432/434 (100%)	421 (98%)	11 (2%)	0	100	100
7	L	432/434 (100%)	423 (98%)	9 (2%)	0	100	100
7	M	432/434 (100%)	417 (96%)	15 (4%)	0	100	100
7	O	432/434 (100%)	422 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	P	432/434 (100%)	422 (98%)	10 (2%)	0	100	100
7	Q	432/434 (100%)	416 (96%)	16 (4%)	0	100	100
8	R	102/105 (97%)	86 (84%)	13 (13%)	3 (3%)	3	8
9	A	756/758 (100%)	734 (97%)	22 (3%)	0	100	100
All	All	5868/5911 (99%)	5643 (96%)	222 (4%)	3 (0%)	49	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	R	89	PRO
8	R	93	PRO
8	R	96	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	B	244/263 (93%)	244 (100%)	0	100	100
2	E	178/188 (95%)	178 (100%)	0	100	100
2	F	173/188 (92%)	173 (100%)	0	100	100
3	G	178/188 (95%)	178 (100%)	0	100	100
5	C	119/119 (100%)	119 (100%)	0	100	100
5	D	119/119 (100%)	119 (100%)	0	100	100
6	H	306/312 (98%)	306 (100%)	0	100	100
7	I	338/338 (100%)	338 (100%)	0	100	100
7	J	338/338 (100%)	338 (100%)	0	100	100
7	K	338/338 (100%)	338 (100%)	0	100	100
7	L	338/338 (100%)	338 (100%)	0	100	100
7	M	338/338 (100%)	338 (100%)	0	100	100
7	O	338/338 (100%)	338 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	P	338/338 (100%)	338 (100%)	0	100	100
7	Q	338/338 (100%)	338 (100%)	0	100	100
8	R	72/94 (77%)	72 (100%)	0	100	100
9	A	649/649 (100%)	649 (100%)	0	100	100
All	All	4742/4824 (98%)	4742 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	HIS
1	B	125	HIS
1	B	152	ASN
1	B	207	ASN
1	B	208	HIS
1	B	249	ASN
1	B	251	ASN
1	B	273	GLN
2	E	124	ASN
2	F	134	ASN
2	F	137	GLN
3	G	65	ASN
3	G	206	ASN
5	C	34	GLN
5	C	75	ASN
5	D	75	ASN
5	D	95	GLN
5	D	110	GLN
6	H	82	ASN
6	H	115	ASN
6	H	154	ASN
6	H	182	ASN
6	H	251	GLN
7	I	65	GLN
7	I	213	ASN
7	I	371	HIS
7	J	18	ASN
7	J	65	GLN
7	J	346	GLN

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Mol	Chain	Res	Type
7	J	371	HIS
7	J	416	GLN
8	R	70	HIS
7	K	65	GLN
7	K	213	ASN
7	K	253	HIS
7	K	371	HIS
7	L	148	ASN
7	L	346	GLN
7	M	65	GLN
7	M	163	GLN
7	M	346	GLN
7	M	416	GLN
7	O	148	ASN
7	P	65	GLN
7	P	148	ASN
7	P	151	ASN
7	P	213	ASN
7	P	346	GLN
7	Q	65	GLN
7	Q	155	HIS
7	Q	213	ASN
7	Q	314	GLN
7	Q	431	ASN
9	A	363	GLN
9	A	595	GLN
9	A	725	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	N	34/35 (97%)	10 (29%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	N	2	C
4	N	3	G
4	N	8	C
4	N	10	U
4	N	12	G

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Mol	Chain	Res	Type
4	N	15	U
4	N	16	C
4	N	21	G
4	N	27	U
4	N	34	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

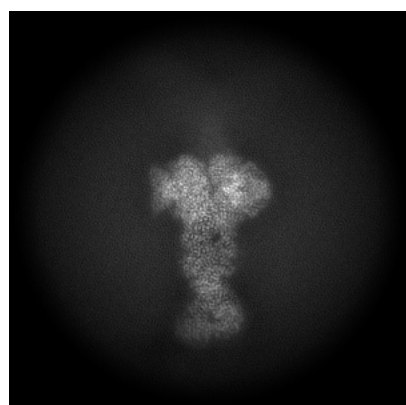
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49593. These allow visual inspection of the internal detail of the map and identification of artifacts.

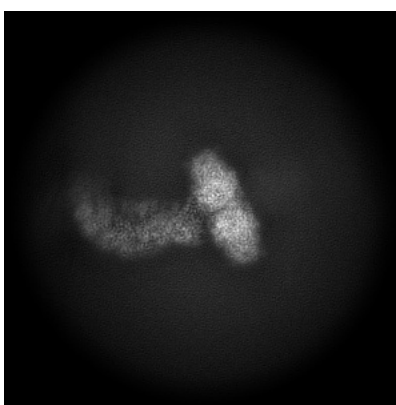
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

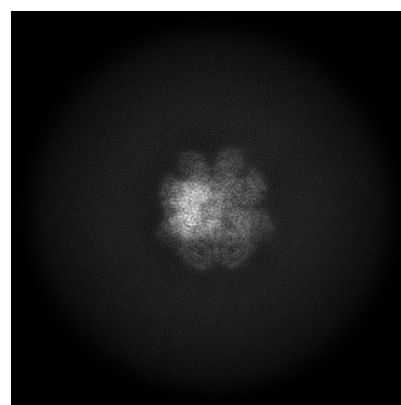
6.1.1 Primary map



X



Y

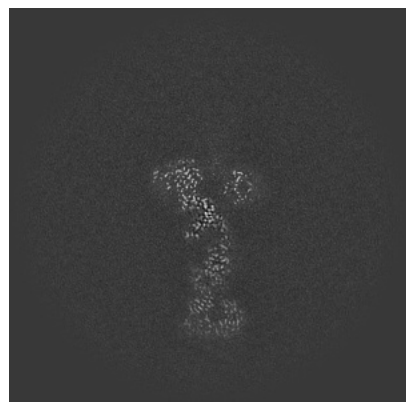


Z

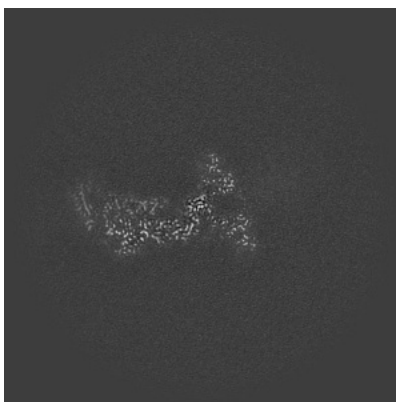
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

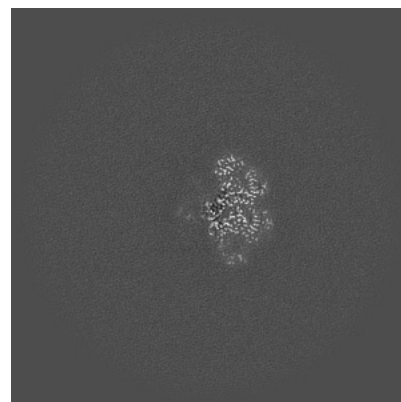
6.2.1 Primary map



X Index: 280



Y Index: 280

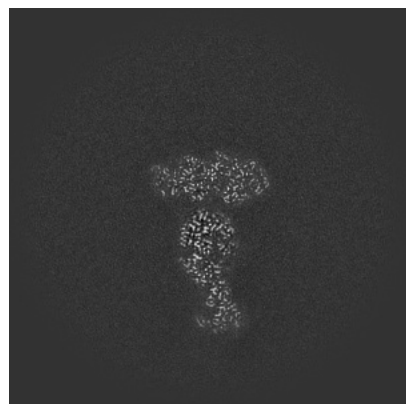


Z Index: 280

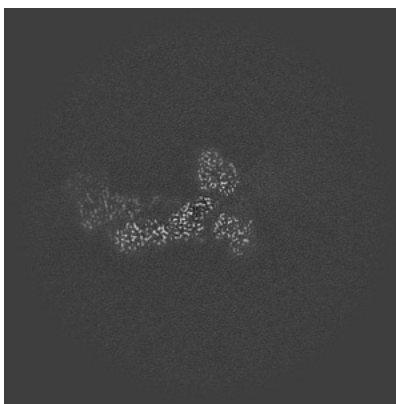
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

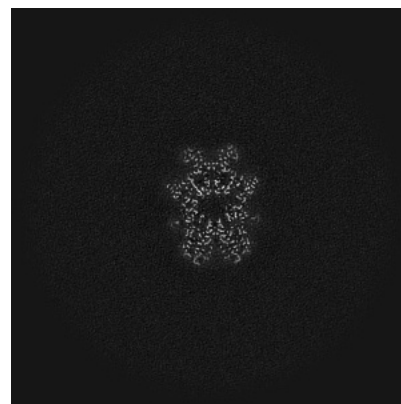
6.3.1 Primary map



X Index: 253



Y Index: 272

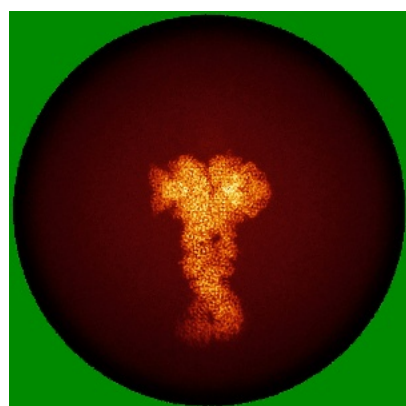


Z Index: 309

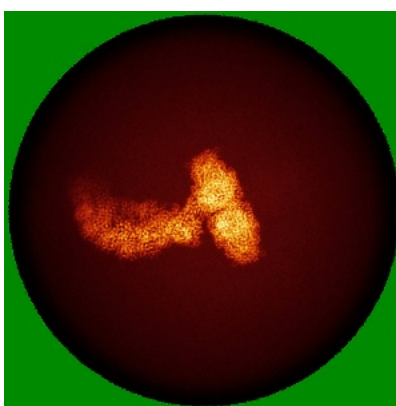
The images above show the largest variance slices of the map in three orthogonal directions.

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

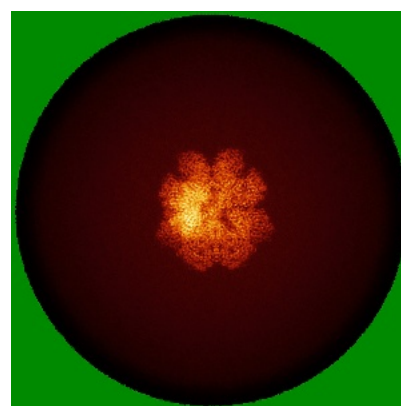
6.4.1 Primary map



X



Y

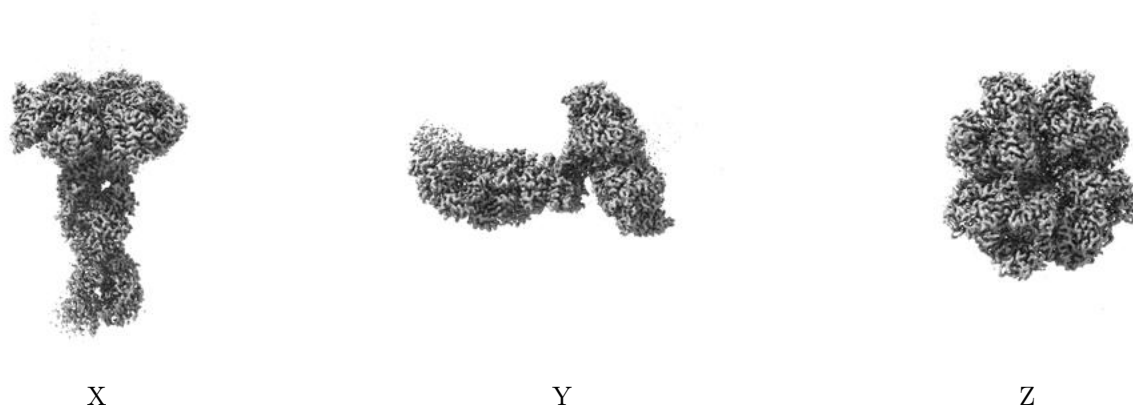


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

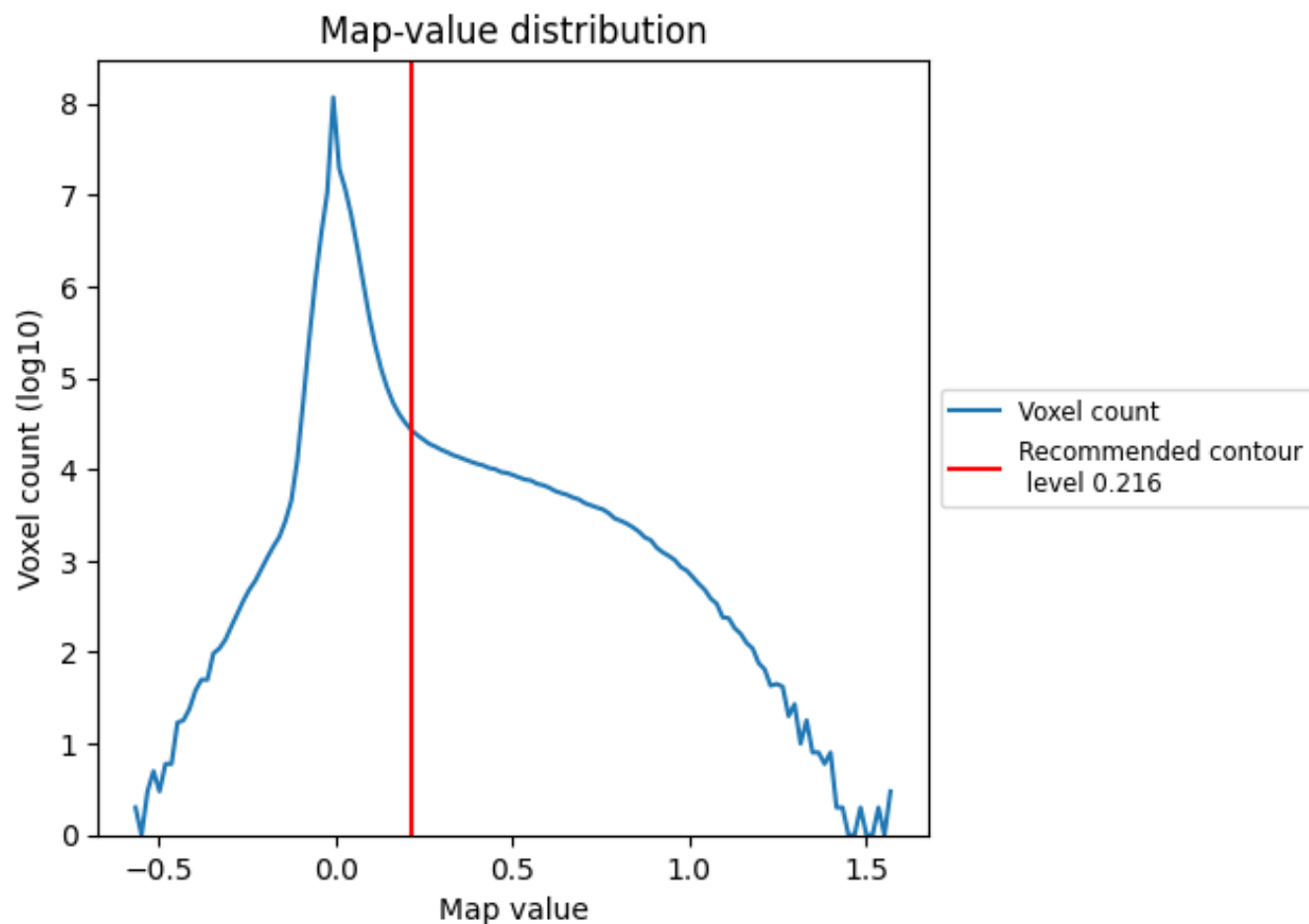
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

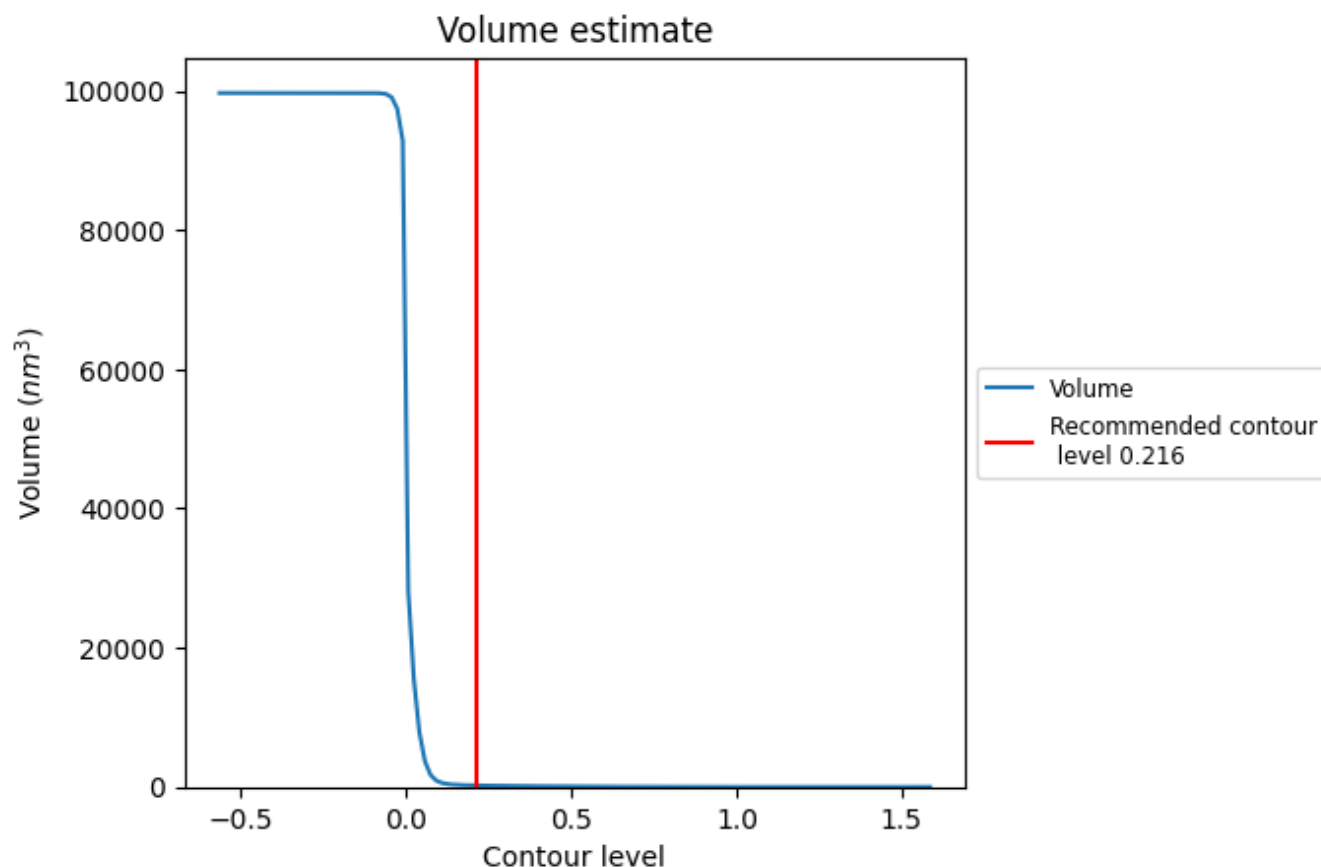
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

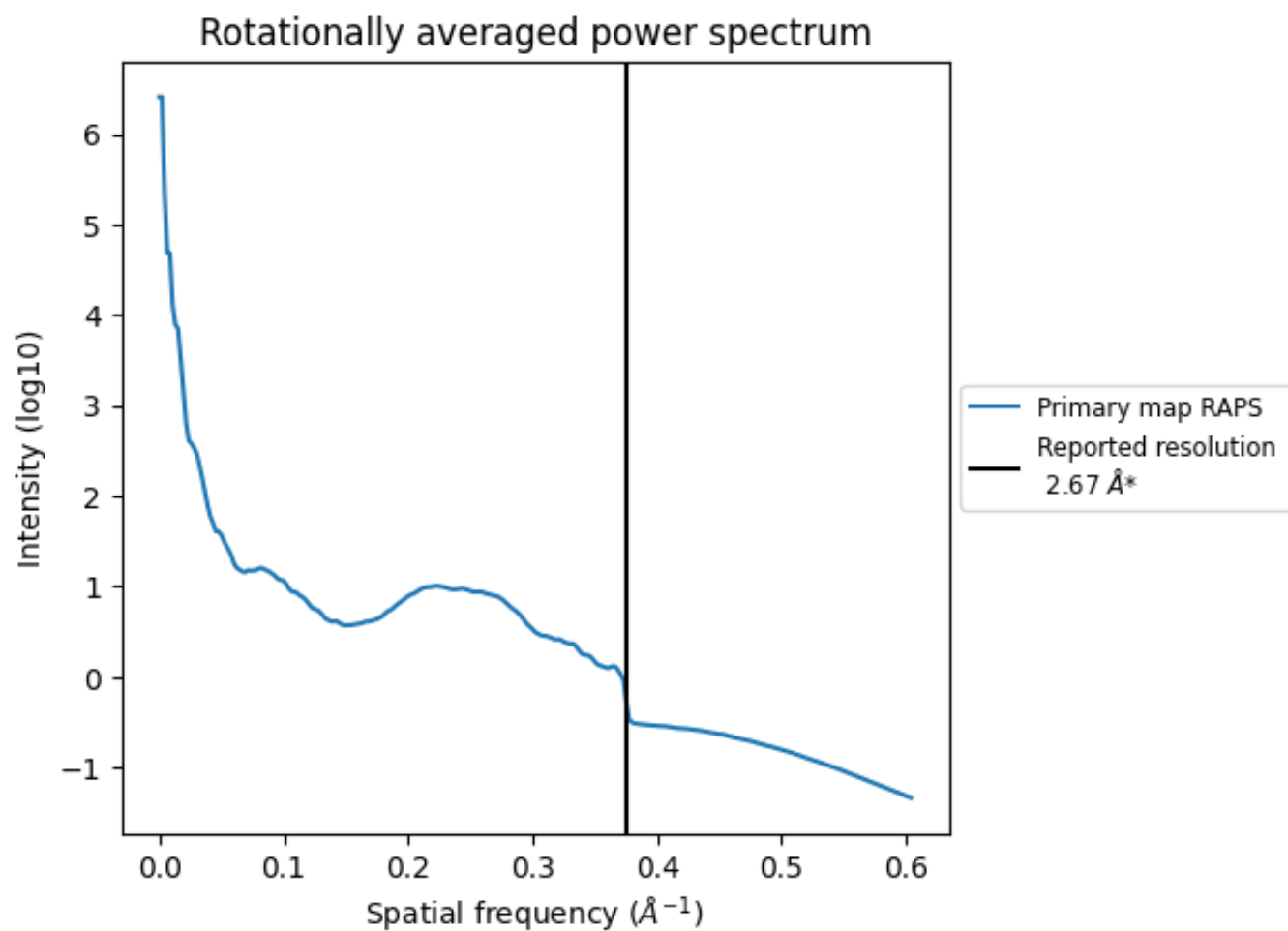
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 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 0.375 Å⁻¹

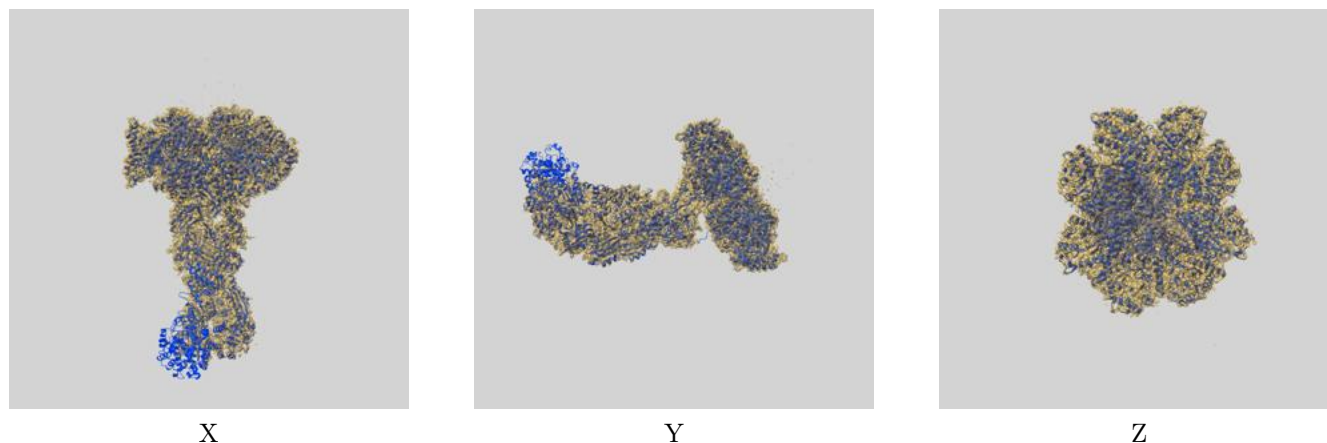
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

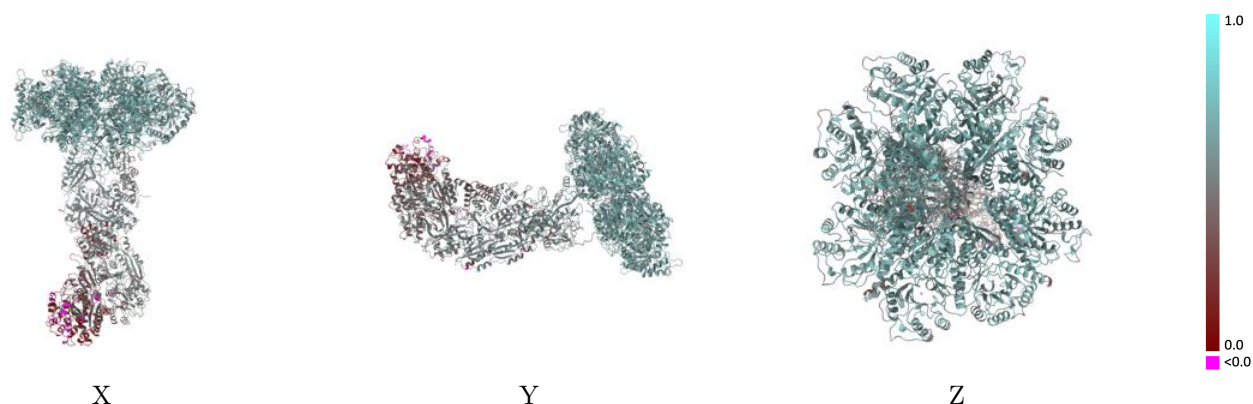
This section contains information regarding the fit between EMDB map EMD-49593 and PDB model 9NO4. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



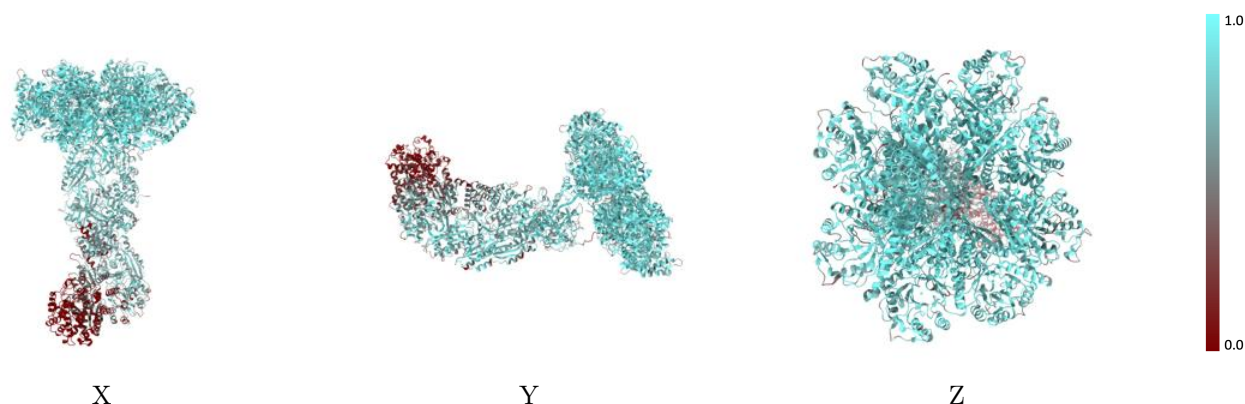
The images above show the 3D surface view of the map at the recommended contour level 0.216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



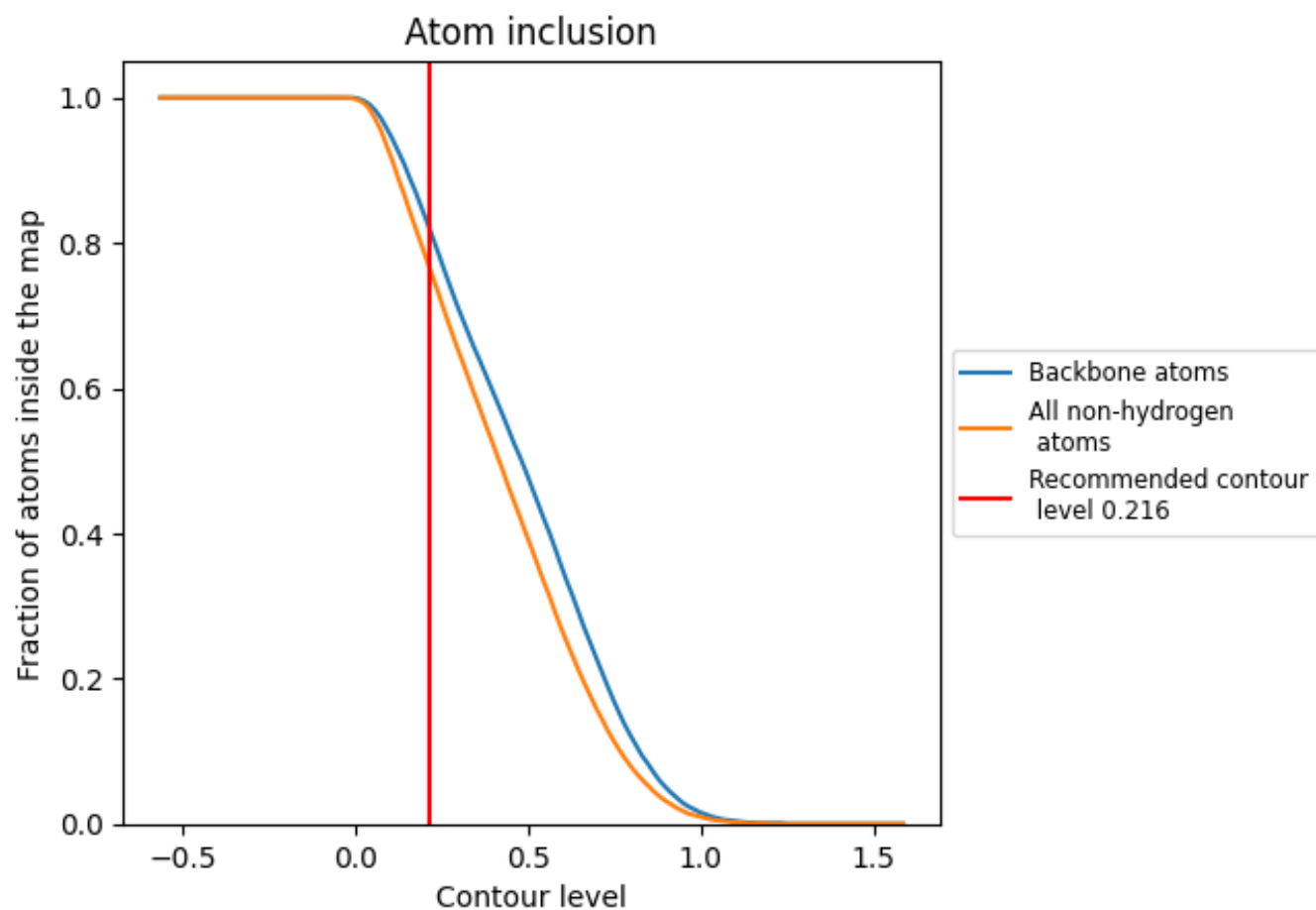
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.216).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.5520
A	 0.2690	 0.3250
B	 0.5810	 0.4520
C	 0.6970	 0.5000
D	 0.7640	 0.5140
E	 0.7270	 0.4950
F	 0.7790	 0.5170
G	 0.8010	 0.5320
H	 0.8180	 0.5330
I	 0.8920	 0.6310
J	 0.8880	 0.6250
K	 0.8810	 0.6280
L	 0.8870	 0.6230
M	 0.8810	 0.6250
N	 0.9260	 0.5460
O	 0.8800	 0.6250
P	 0.8780	 0.6270
Q	 0.8850	 0.6250
R	 0.8630	 0.5770

