



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:30 PM UTC

PDB ID : 8K22 / pdb_00008k22
EMDB ID : EMD-36825
Title : ICP1 Csy-dsDNA-Cas1-Cas2/3 complex (half form)
Authors : Zhang, L.X.; Feng, Y.
Deposited on : 2023-07-12
Resolution : 2.92 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

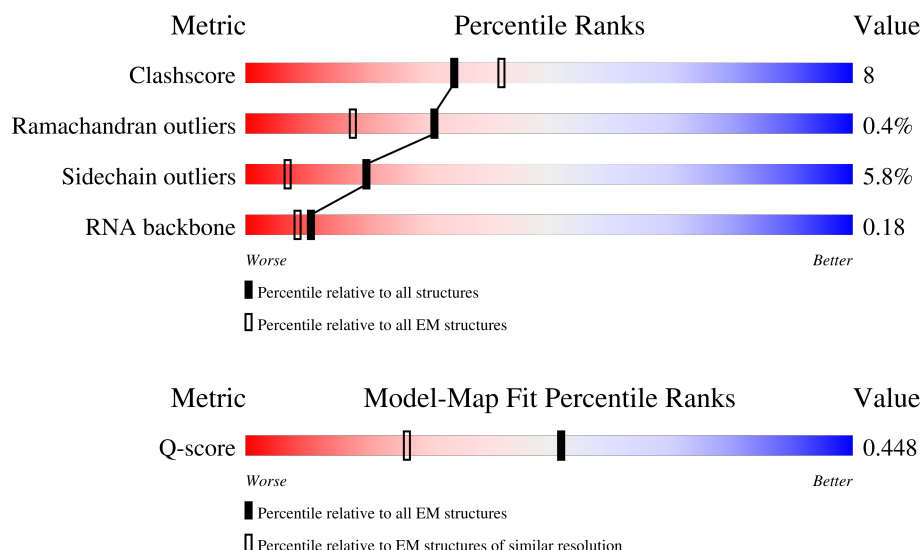
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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	178	80%19%..
2	C	248	79%18%. .
3	D	295	10%77%18%. .

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Mol	Chain	Length	Quality of chain
3	E	295	
3	d	295	
3	e	295	
4	G	306	
4	I	306	
4	J	306	
4	K	306	
4	L	306	
4	M	306	
5	H	168	
6	P	60	
7	Q	43	
7	U	43	
8	R	31	
9	A	930	
9	a	930	
10	V	21	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 39285 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 Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	177	Total	C	N	O	S	0	0
			1415	896	235	274	10		

- Molecule 2 is a protein called Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	247	Total	C	N	O	S	0	0
			1903	1214	320	355	14		

- Molecule 3 is a protein called Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	295	Total	C	N	O	S	2	0
			2323	1484	398	429	12		
3	E	295	Total	C	N	O	S	0	0
			2329	1491	394	431	13		
3	d	295	Total	C	N	O	S	2	0
			2337	1492	401	431	13		
3	e	295	Total	C	N	O	S	0	0
			2324	1489	393	429	13		

- Molecule 4 is a protein called Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	302	Total	C	N	O	S	0	0
			2314	1456	392	459	7		
4	I	302	Total	C	N	O	S	0	0
			2298	1447	389	455	7		
4	J	302	Total	C	N	O	S	0	0
			2318	1459	393	459	7		
4	K	302	Total	C	N	O	S	0	0
			2318	1459	393	459	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	302	Total	C	N	O	S	0	0
			2307	1450	391	459	7		
4	M	302	Total	C	N	O	S	0	0
			2314	1456	392	459	7		

- Molecule 5 is a protein called Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	165	Total	C	N	O	S	0	0
			1290	818	221	245	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	51	ILE	VAL	conflict	UNP F1D5V5

- Molecule 6 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	60	Total	C	N	O	P	0	0
			1260	565	210	425	60		

- Molecule 7 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	43	Total	C	N	O	P	0	0
			898	425	184	246	43		
7	U	21	Total	C	N	O	P	0	0
			439	209	88	121	21		

- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	31	Total	C	N	O	P	0	0
			620	299	94	196	31		

- Molecule 9 is a protein called HD Cas3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	75	Total	C	N	O	S	0	0
			579	370	101	104	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	929	Total	C	N	O	S	0	0
			7278	4632	1245	1367	34		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	834	LYS	ARG	conflict	UNP F1D5V9
A	834	LYS	ARG	conflict	UNP F1D5V9

- Molecule 10 is a DNA chain called DNA (5'-D(*AP*TP*CP*TP*TP*CP*CP*CP*TP*AP*TP*TP*TP*AP*AP*AP*TP*TP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	21	Total	C	N	O	P	0	0
			419	205	65	129	20		

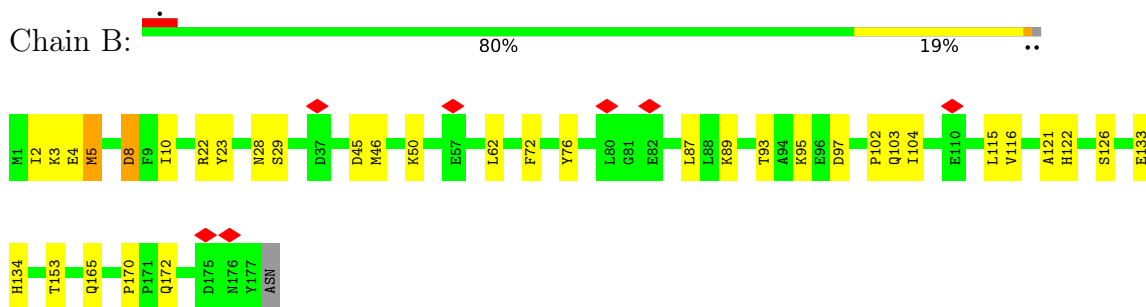
- Molecule 11 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	2	Total	Mn	0
			2	2	

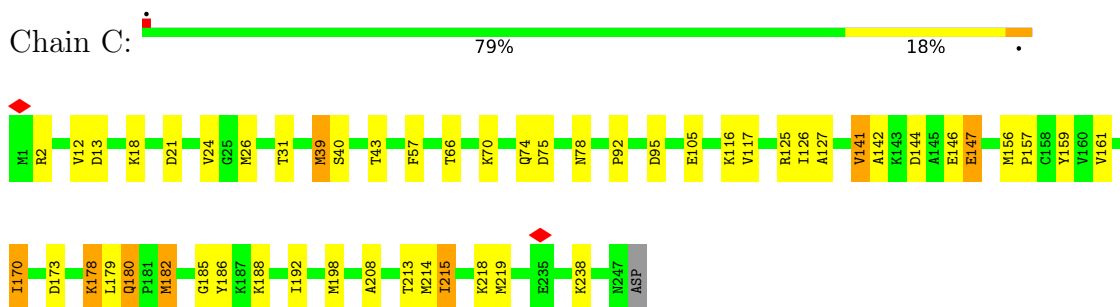
3 Residue-property plots [i](#)

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.

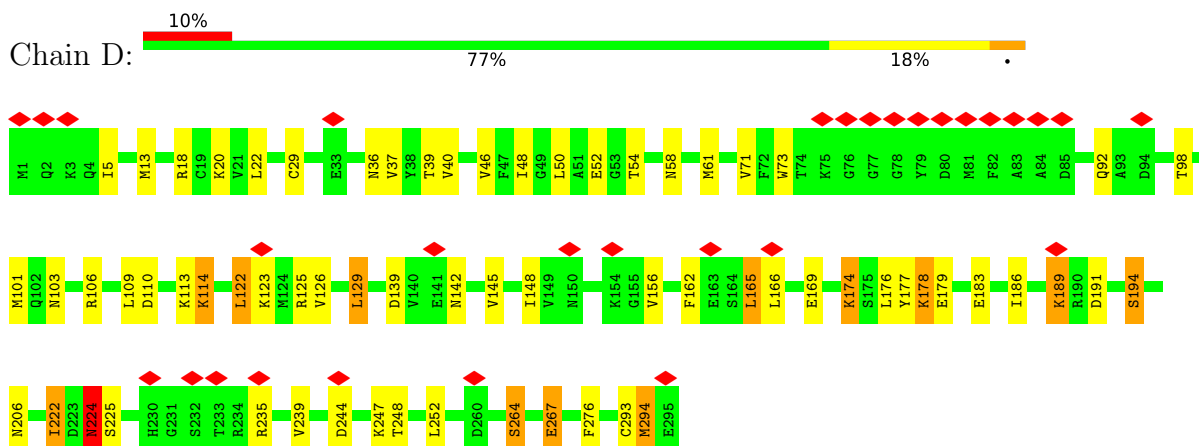
• Molecule 1: Csy1



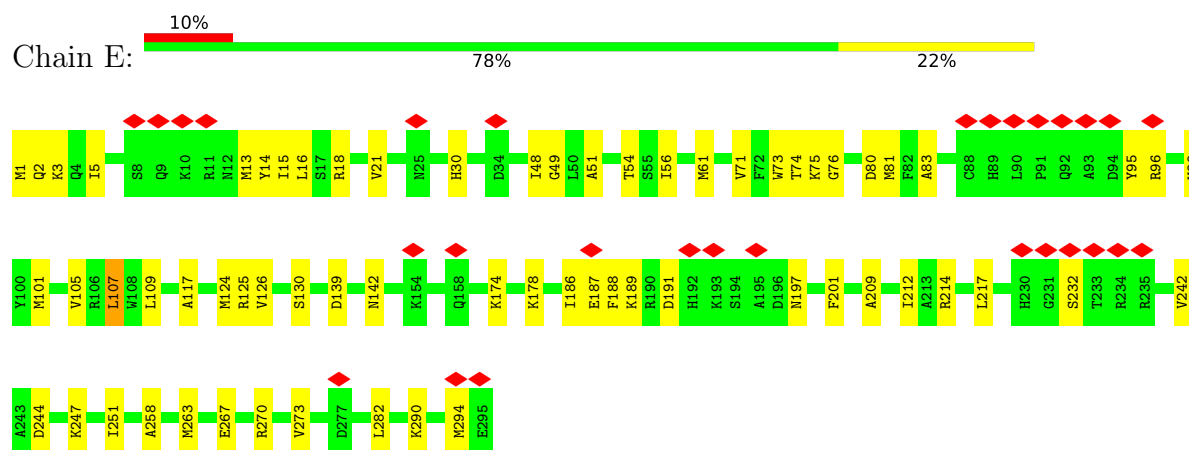
• Molecule 2: Csy2



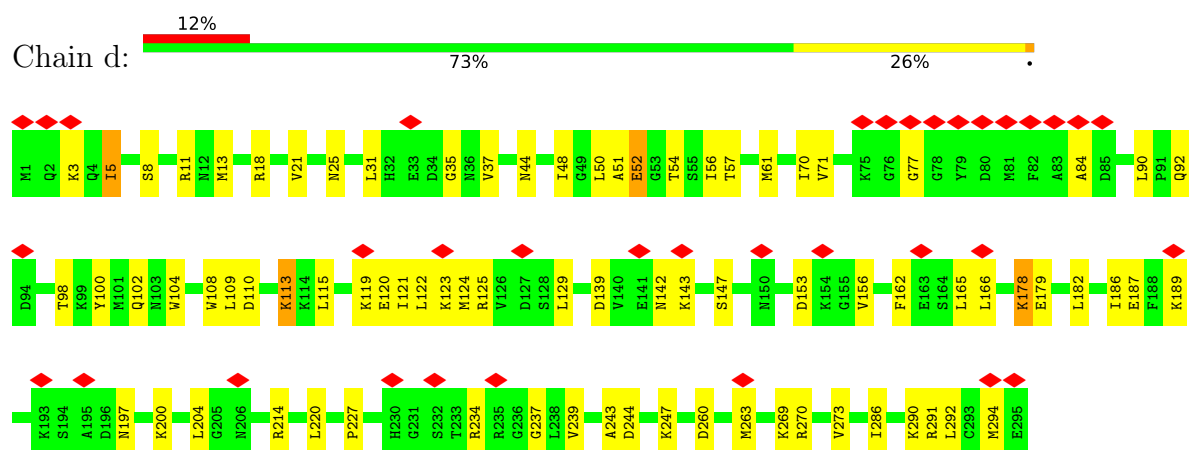
• Molecule 3: Cas1



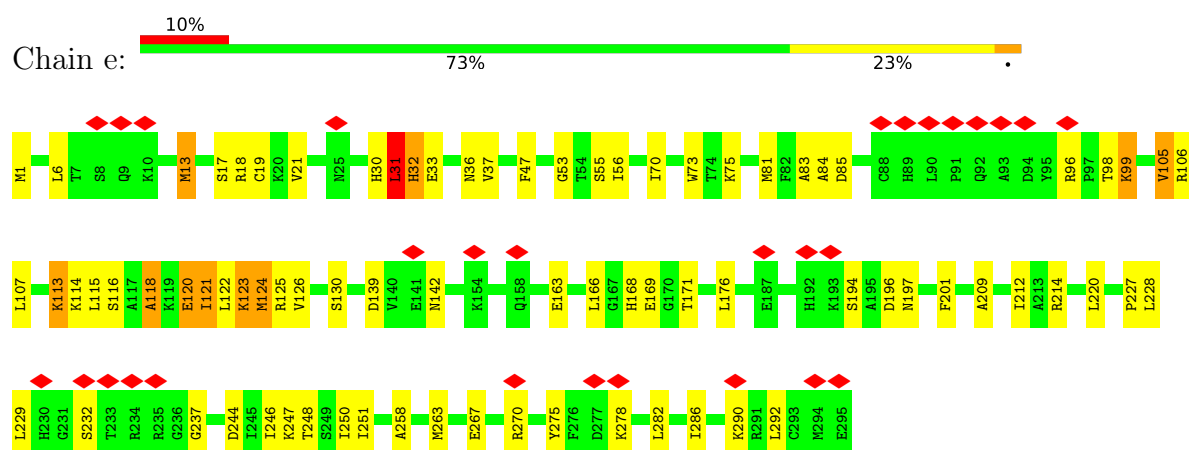
- Molecule 3: Cas1



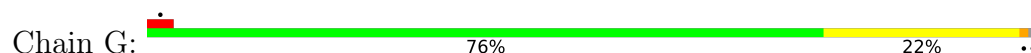
- Molecule 3: Cas1

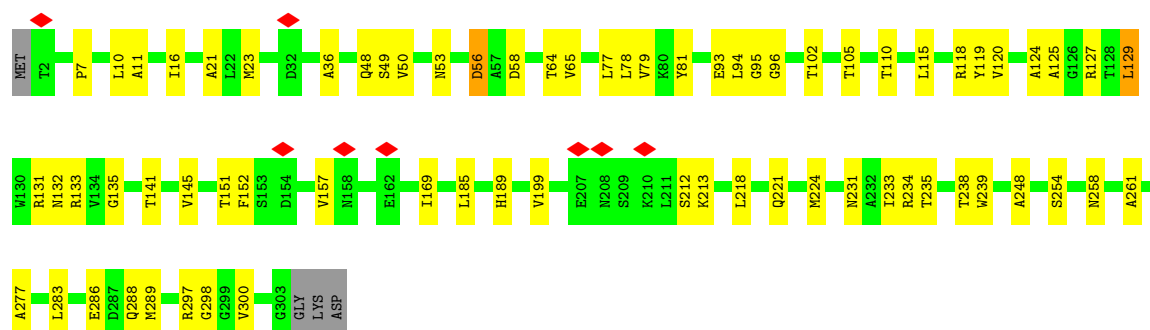


- Molecule 3: Cas1



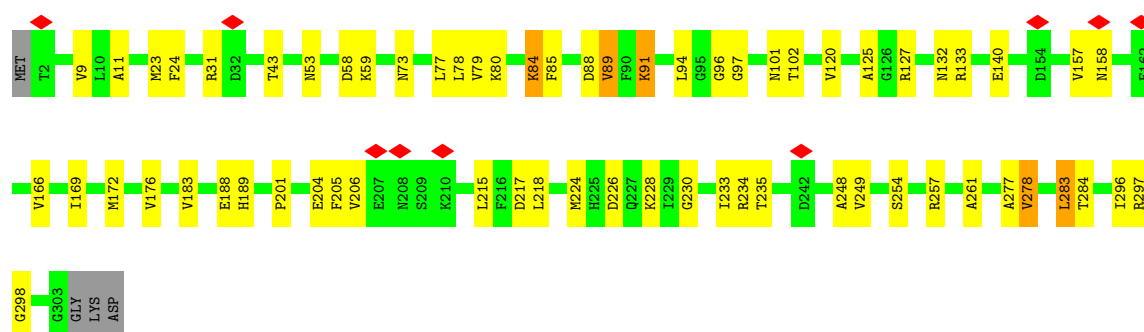
- Molecule 4: Csy3





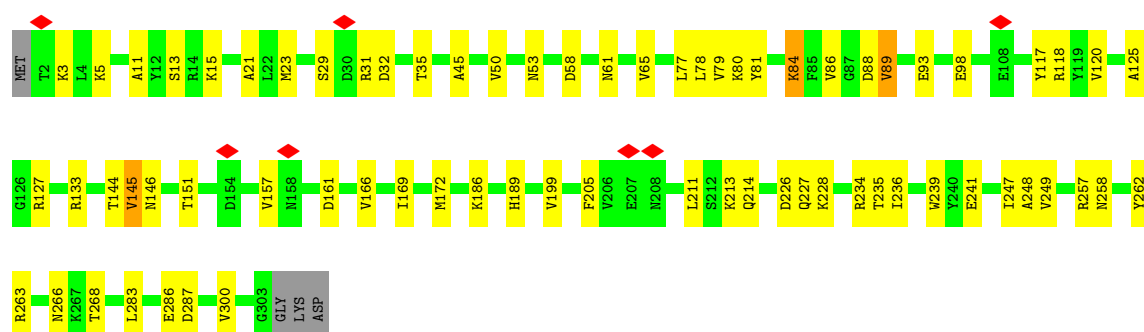
• Molecule 4: Csy3

Chain I: 77% 20% ..



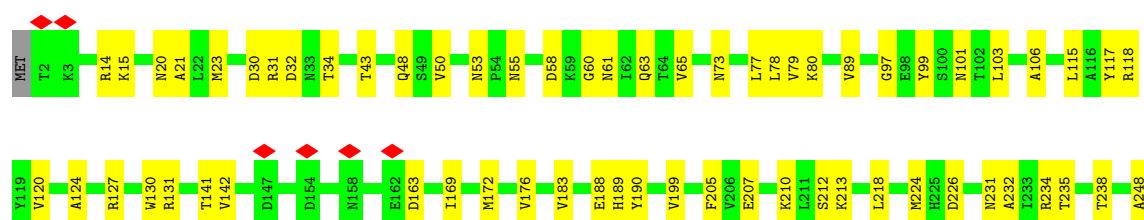
• Molecule 4: Csy3

Chain J: 75% 22% ..



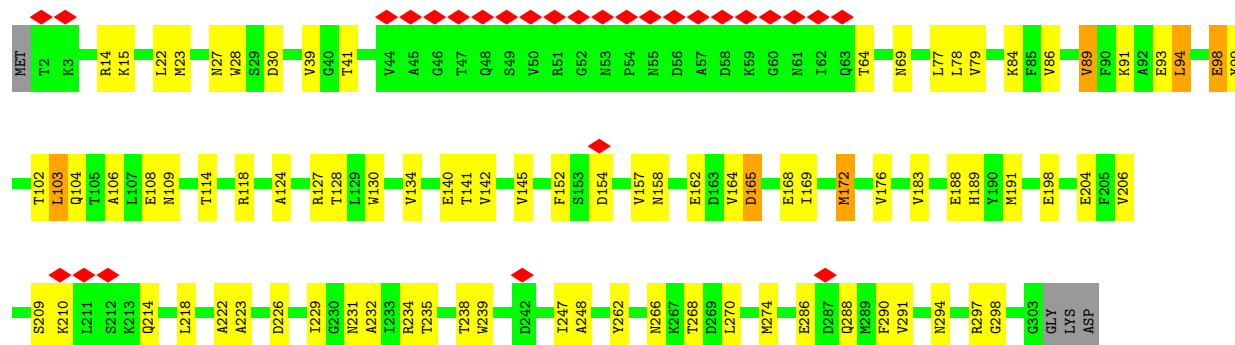
• Molecule 4: Csy3

Chain K: 74% 25% .

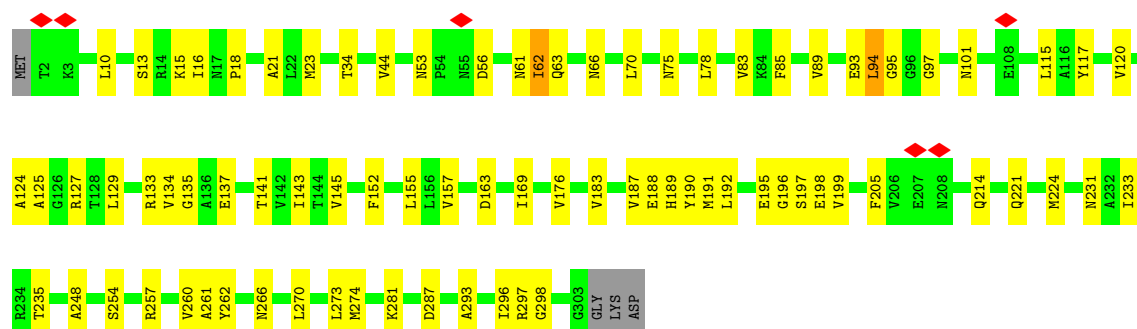




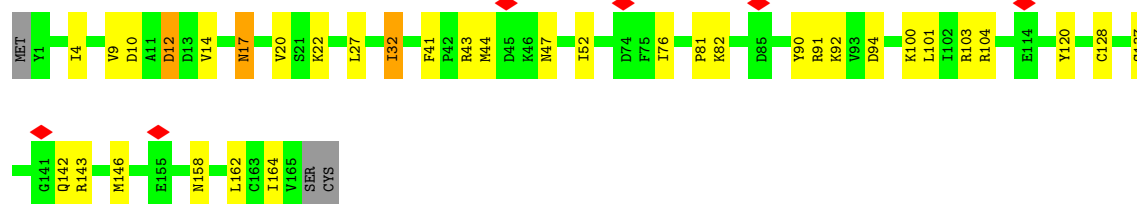
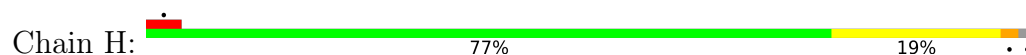
• Molecule 4: Csy3



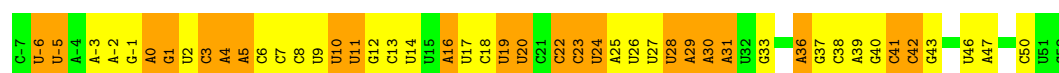
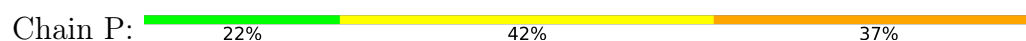
• Molecule 4: Csy3



• Molecule 5: Csy4



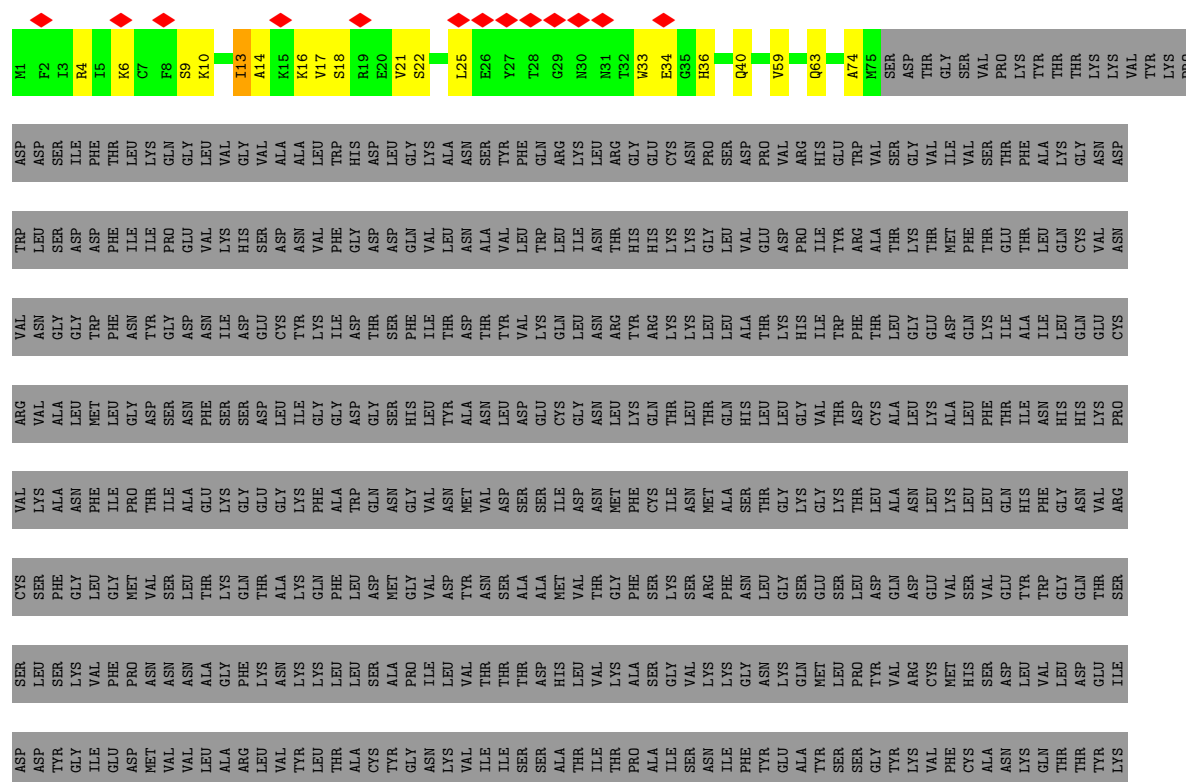
• Molecule 6: RNA (60-MER)



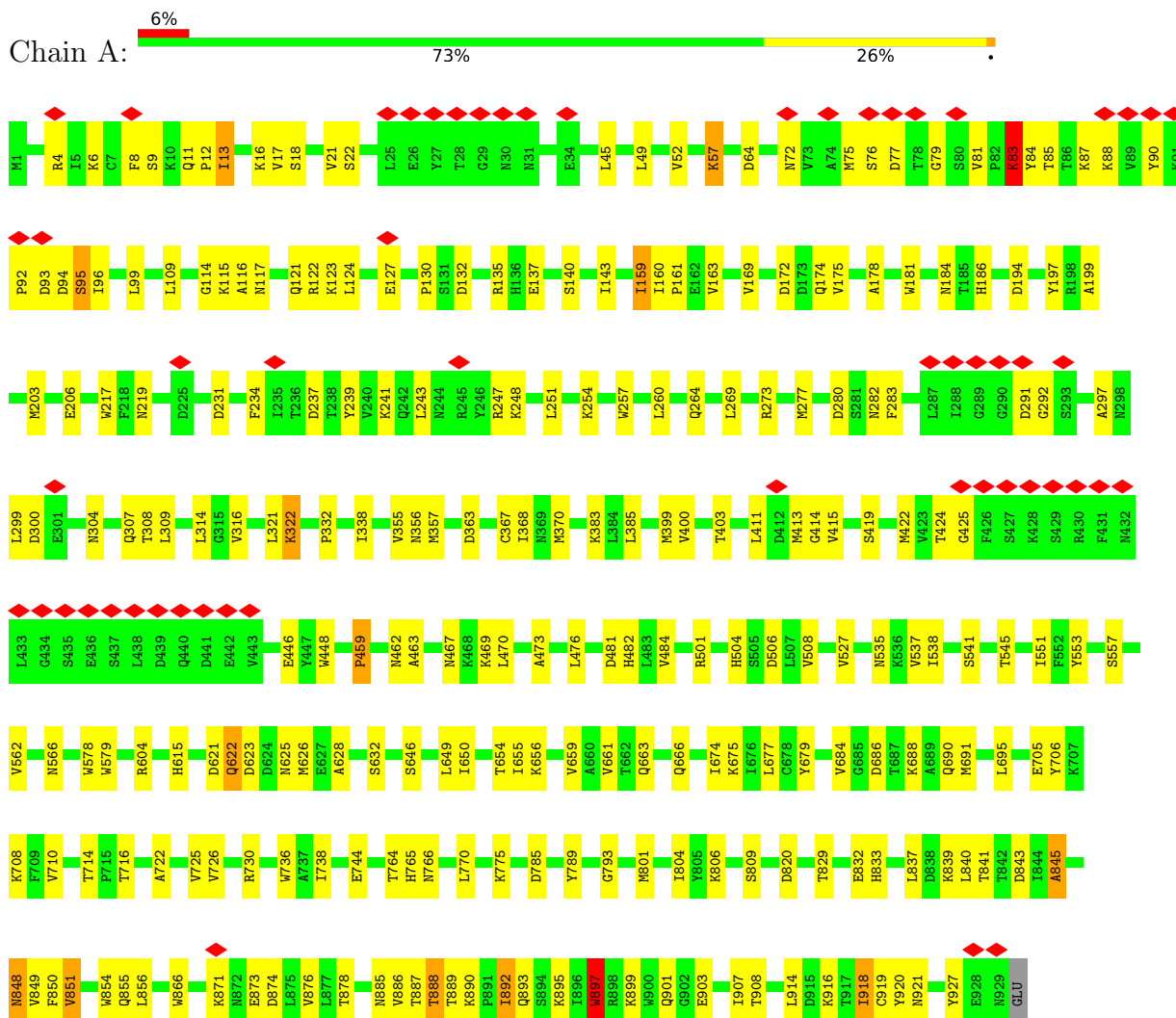
A1	G2	C3	A4	A5	A10	T21	DA	DA	DG	DC	DC	DA	DA	DG	DG	DG	DT	DT	DG	DA	DC	DG	DA	DA	DA	DC	DC	DC
----	----	----	----	----	-----	-----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

Chain R: 19% 81% 19%

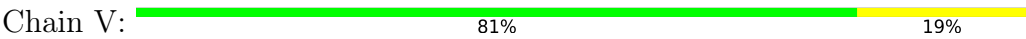
Chain a: 6% 92%



- Molecule 9: HD Cas3-type domain-containing protein



● Molecule 10: DNA (5'-D(*AP*TP*CP*TP*TP*CP*CP*CP*TP*AP*TP*TP*TP*AP*AP*AP*TP*TP*GP*CP*T)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	235177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.640	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/1448	0.61	2/1956 (0.1%)
2	C	0.32	0/1940	0.67	4/2625 (0.2%)
3	D	0.48	0/2377	0.76	2/3215 (0.1%)
3	E	0.26	0/2377	0.62	3/3210 (0.1%)
3	d	0.34	0/2391	0.74	0/3231
3	e	0.51	2/2373 (0.1%)	0.75	6/3208 (0.2%)
4	G	0.34	0/2354	0.60	1/3198 (0.0%)
4	I	0.36	0/2338	0.65	2/3180 (0.1%)
4	J	0.35	0/2358	0.67	2/3202 (0.1%)
4	K	0.36	0/2358	0.64	0/3202
4	L	0.42	0/2347	0.78	5/3190 (0.2%)
4	M	0.28	0/2354	0.63	2/3198 (0.1%)
5	H	0.37	0/1308	0.77	1/1757 (0.1%)
6	P	0.34	0/1404	0.62	2/2181 (0.1%)
7	Q	0.31	0/1014	0.53	1/1565 (0.1%)
7	U	0.31	0/495	0.48	0/763
8	R	0.28	0/688	0.53	0/1057
9	A	0.37	1/7432 (0.0%)	0.72	14/10072 (0.1%)
9	a	0.34	0/588	0.79	0/791
10	V	0.54	0/466	0.80	1/716 (0.1%)
All	All	0.37	3/40410 (0.0%)	0.68	48/55517 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	31	LEU	CA-C	-6.96	1.44	1.53
9	A	83	LYS	CA-C	-6.25	1.44	1.52
3	e	96	ARG	C-N	5.02	1.39	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	98	GLU	N-CA-C	-10.38	100.69	113.97
4	J	53	ASN	CB-CA-C	10.11	118.38	111.20
9	A	13	ILE	N-CA-C	-9.93	103.36	112.90
9	A	77	ASP	N-CA-C	-9.79	101.21	113.55
5	H	12	ASP	N-CA-C	-8.65	102.53	113.43
9	A	892	ILE	N-CA-C	-8.22	98.03	109.21
3	e	32	HIS	N-CA-C	-6.70	99.98	109.96
6	P	41	C	C4'-C3'-O3'	6.58	119.27	109.40
3	e	118	ALA	N-CA-C	-6.54	104.07	111.07
3	D	177	TYR	N-CA-C	-6.42	104.21	111.07
1	B	8	ASP	N-CA-C	-6.21	104.59	111.36
3	D	224	ASN	N-CA-C	-6.13	106.78	114.56
3	e	96	ARG	CA-C-N	-6.06	114.03	120.03
3	e	96	ARG	C-N-CA	-6.06	114.03	120.03
3	E	96	ARG	CA-C-N	-5.97	113.82	119.85
3	E	96	ARG	C-N-CA	-5.97	113.82	119.85
4	J	53	ASN	N-CA-CB	-5.96	105.05	111.66
4	I	53	ASN	CA-CB-CG	5.95	118.55	112.60
9	A	897	TRP	N-CA-CB	5.93	119.39	110.14
1	B	3	LYS	N-CA-C	-5.76	104.97	112.23
9	A	76	SER	N-CA-C	5.69	117.67	108.34
9	A	159	ILE	CA-CB-CG1	5.65	120.01	110.40
7	Q	52	DA	C2'-C3'-O3'	5.58	119.87	111.50
3	e	33	GLU	N-CA-C	-5.54	106.36	113.01
9	A	448	TRP	CA-C-N	5.48	132.15	121.41
9	A	448	TRP	C-N-CA	5.48	132.15	121.41
9	A	57	LYS	CB-CG-CD	5.47	123.89	111.30
9	A	545	THR	N-CA-C	-5.44	102.80	110.31
2	C	213	THR	N-CA-C	-5.38	101.58	109.81
4	L	106	ALA	N-CA-C	-5.36	107.75	114.56
3	e	107	LEU	N-CA-C	-5.35	105.53	111.36
9	A	855	GLN	N-CA-C	-5.32	105.65	111.82
6	P	41	C	C2'-C3'-O3'	5.24	117.35	109.50
4	L	162	GLU	N-CA-C	5.23	117.28	108.96
4	G	56	ASP	N-CA-C	-5.19	106.90	113.18
2	C	180	GLN	CA-C-N	-5.17	113.27	120.25
2	C	180	GLN	C-N-CA	-5.17	113.27	120.25
4	L	268	THR	N-CA-C	-5.14	105.02	113.50
9	A	79	GLY	N-CA-C	-5.13	104.74	112.60
4	M	61	ASN	CA-C-N	5.09	131.14	121.97
4	M	61	ASN	C-N-CA	5.09	131.14	121.97
10	V	2	DT	C4'-C3'-O3'	-5.09	102.36	110.00
4	I	88	ASP	N-CA-C	-5.06	104.45	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	210	LYS	CB-CA-C	-5.06	110.72	116.54
9	A	459	PRO	CA-C-N	5.03	129.55	122.46
9	A	459	PRO	C-N-CA	5.03	129.55	122.46
3	E	178	LYS	CA-CB-CG	5.00	124.11	114.10
2	C	170	ILE	N-CA-C	5.00	115.67	110.82

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	B	1415	0	1353	17	0
2	C	1903	0	1916	34	0
3	D	2323	0	2294	40	0
3	E	2329	0	2300	39	0
3	d	2337	0	2318	46	0
3	e	2324	0	2296	40	0
4	G	2314	0	2249	38	0
4	I	2298	0	2216	37	0
4	J	2318	0	2260	37	0
4	K	2318	0	2260	46	0
4	L	2307	0	2229	46	0
4	M	2314	0	2249	47	0
5	H	1290	0	1336	26	0
6	P	1260	0	641	36	0
7	Q	898	0	481	9	0
7	U	439	0	237	5	0
8	R	620	0	355	5	0
9	A	7278	0	7186	129	0
9	a	579	0	595	14	0
10	V	419	0	243	4	0
11	A	2	0	0	0	0
All	All	39285	0	37014	609	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 8.

All (609) 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)
9:A:663:GLN:HG2	9:A:892:ILE:HD11	1.49	0.94
4:K:21:ALA:HA	4:K:80:LYS:O	1.83	0.79
3:D:224:ASN:HD21	3:D:239:VAL:HG12	1.52	0.73
5:H:10:ASP:CG	4:L:158:ASN:HD21	1.96	0.73
9:A:174:GLN:HB3	9:A:257:TRP:HE1	1.56	0.71
4:L:84:LYS:HD3	4:M:135:GLY:HA3	1.72	0.71
5:H:10:ASP:OD2	4:L:158:ASN:ND2	2.23	0.71
4:M:78:LEU:HA	4:M:189:HIS:O	1.90	0.70
4:K:79:VAL:HB	4:K:189:HIS:HB2	1.73	0.70
6:P:43:G:H21	6:P:47:A:H62	1.39	0.69
4:G:78:LEU:HA	4:G:189:HIS:O	1.93	0.68
3:D:191:ASP:HB3	3:D:194:SER:HB2	1.76	0.67
4:M:89:VAL:HB	4:M:296:ILE:HG22	1.77	0.67
4:M:97:GLY:O	4:M:101:ASN:ND2	2.27	0.67
3:D:103:ASN:HB2	3:D:293:CYS:HB2	1.77	0.67
3:D:109:LEU:HD11	3:E:105:VAL:HG12	1.77	0.66
2:C:2:ARG:HB2	2:C:142:ALA:HB3	1.78	0.66
4:M:44:VAL:O	4:M:62:ILE:HA	1.96	0.65
6:P:10:U:H5	7:Q:41:DG:H1	1.45	0.65
3:d:13:MET:HB3	3:d:273:VAL:HG22	1.79	0.64
5:H:143:ARG:HH12	6:P:36:A:H4'	1.63	0.64
2:C:156:MET:HE3	2:C:157:PRO:HA	1.81	0.63
4:L:94:LEU:HD23	4:M:257:ARG:HG3	1.80	0.63
3:E:75:LYS:HB3	3:E:80:ASP:HB3	1.81	0.62
4:J:21:ALA:HA	4:J:80:LYS:O	1.98	0.62
4:K:78:LEU:HA	4:K:189:HIS:O	2.00	0.62
3:E:197:ASN:O	3:E:201:PHE:HB2	2.00	0.61
3:e:139:ASP:O	3:e:142:ASN:ND2	2.33	0.61
4:I:201:PRO:HG2	4:I:215:LEU:HD13	1.82	0.61
4:L:15:LYS:HE2	4:L:89:VAL:HA	1.83	0.61
9:A:194:ASP:HB3	9:A:197:TYR:HB2	1.82	0.61
1:B:5:MET:HB3	1:B:62:LEU:HD13	1.83	0.61
9:a:9:SER:OG	9:a:10:LYS:N	2.34	0.61
3:d:197:ASN:HA	3:d:200:LYS:HE3	1.83	0.60
4:G:7:PRO:HG2	4:G:10:LEU:HB2	1.83	0.60
9:A:744:GLU:HG3	9:A:829:THR:HG22	1.83	0.60
3:e:70:ILE:HD11	3:e:85:ASP:HB2	1.84	0.59
3:D:36:ASN:ND2	9:a:74:ALA:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:GLN:NE2	3:E:81:MET:SD	2.76	0.59
4:J:78:LEU:HA	4:J:189:HIS:O	2.01	0.59
3:d:139:ASP:O	3:d:142:ASN:ND2	2.36	0.59
4:I:78:LEU:HA	4:I:189:HIS:O	2.03	0.59
9:A:273:ARG:HG2	9:A:277:MET:HE2	1.85	0.59
3:e:122:LEU:HD21	3:e:229:LEU:HD11	1.86	0.58
9:A:99:LEU:HD21	9:A:257:TRP:HE3	1.68	0.58
4:K:127:ARG:HD3	4:K:235:THR:HB	1.84	0.58
9:A:481:ASP:HB3	9:A:866:TRP:HE1	1.69	0.58
3:D:139:ASP:O	3:D:142:ASN:ND2	2.35	0.58
9:A:677:LEU:HB2	9:A:897:TRP:HE1	1.67	0.58
4:G:127:ARG:NH2	4:G:157:VAL:O	2.36	0.58
4:M:13:SER:OG	4:M:15:LYS:NZ	2.37	0.58
9:a:10:LYS:O	9:a:14:ALA:N	2.32	0.58
4:I:125:ALA:O	4:I:133:ARG:NH2	2.37	0.58
2:C:39:MET:HE1	2:C:117:VAL:HG22	1.85	0.57
3:D:110:ASP:HB3	3:D:113:LYS:HB2	1.86	0.57
3:d:18:ARG:HH22	3:d:52:GLU:HB2	1.69	0.57
9:A:675:LYS:HB3	9:A:897:TRP:HB3	1.86	0.57
7:U:10:DA:H61	10:V:12:DT:H3	1.51	0.57
1:B:170:PRO:HD3	2:C:26:MET:HB2	1.86	0.57
3:E:267:GLU:HA	3:E:270:ARG:HG2	1.87	0.57
4:L:41:THR:HG22	4:L:64:THR:HG22	1.86	0.57
7:U:2:DG:N2	10:V:21:DT:O2	2.38	0.57
5:H:20:VAL:HG13	5:H:52:ILE:HD11	1.84	0.57
4:L:290:PHE:O	4:L:294:ASN:ND2	2.37	0.57
3:D:139:ASP:OD1	3:D:139:ASP:N	2.38	0.57
3:E:81:MET:O	3:E:214:ARG:NH1	2.36	0.57
5:H:158:ASN:HD21	5:H:162:LEU:HB2	1.70	0.57
3:d:37:VAL:HB	9:A:83:LYS:HB2	1.86	0.57
9:A:237:ASP:O	9:A:241:LYS:NZ	2.38	0.57
3:d:21:VAL:HB	3:d:56:ILE:HG13	1.86	0.57
4:K:270:LEU:O	4:K:274:MET:HB2	2.04	0.57
1:B:28:ASN:ND2	1:B:97:ASP:OD1	2.38	0.56
1:B:133:GLU:HG2	1:B:134:HIS:HD2	1.70	0.56
9:A:115:LYS:O	9:A:121:GLN:NE2	2.38	0.56
9:A:677:LEU:HB2	9:A:897:TRP:NE1	2.20	0.56
9:A:473:ALA:O	9:A:501:ARG:NH1	2.37	0.56
4:L:14:ARG:NH2	6:P:28:U:OP1	2.39	0.56
4:K:118:ARG:NH2	4:K:238:THR:OG1	2.38	0.56
3:D:39:THR:HG21	9:A:22:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:36:HIS:HB3	3:d:11:ARG:HD3	1.86	0.56
9:A:203:MET:HB2	9:A:206:GLU:HB3	1.87	0.56
4:K:142:VAL:HB	4:K:188:GLU:HB2	1.88	0.56
4:M:231:ASN:ND2	6:P:24:U:OP2	2.39	0.56
9:A:292:GLY:H	9:A:308:THR:HG21	1.71	0.56
3:d:56:ILE:HD13	3:d:61:MET:HG2	1.87	0.55
4:G:118:ARG:NH2	4:G:238:THR:OG1	2.39	0.55
4:L:152:PHE:CE1	4:L:165:ASP:HB3	2.41	0.55
3:d:90:LEU:HD21	3:d:214:ARG:HH22	1.72	0.55
4:M:16:ILE:HG21	4:M:233:ILE:HG21	1.88	0.55
4:L:297:ARG:NH1	4:L:298:GLY:O	2.39	0.55
3:e:220:LEU:HD13	3:e:290:LYS:HZ3	1.71	0.55
8:R:41:DT:OP1	9:A:656:LYS:NZ	2.35	0.55
3:d:291:ARG:HA	3:d:294:MET:HE2	1.87	0.55
4:I:102:THR:HG23	4:I:278:VAL:HG22	1.89	0.55
4:L:206:VAL:O	6:P:31:A:N6	2.40	0.55
4:M:10:LEU:HD12	4:M:95:GLY:HA3	1.90	0.55
3:d:3:LYS:HD2	3:d:5:ILE:H	1.72	0.55
5:H:137:SER:OG	5:H:142:GLN:O	2.25	0.54
4:J:78:LEU:HD21	4:J:80:LYS:HZ1	1.72	0.54
4:M:270:LEU:O	4:M:274:MET:HB2	2.07	0.54
4:G:102:THR:HA	4:G:105:THR:HG22	1.88	0.54
4:M:133:ARG:HH12	4:M:157:VAL:HG21	1.72	0.54
3:E:189:LYS:NZ	3:E:191:ASP:OD2	2.41	0.54
1:B:29:SER:O	1:B:95:LYS:NZ	2.41	0.54
4:M:176:VAL:HG21	4:M:183:VAL:HB	1.90	0.54
3:d:57:THR:HG22	3:e:55:SER:HB3	1.89	0.54
9:A:64:ASP:OD1	9:A:64:ASP:N	2.39	0.54
5:H:94:ASP:OD2	6:P:50:C:N4	2.39	0.54
3:d:25:ASN:N	7:U:3:DC:OP2	2.40	0.54
3:e:121:ILE:HG13	3:e:292:LEU:HD11	1.90	0.54
2:C:125:ARG:NH1	6:P:-3:A:OP1	2.41	0.54
3:D:40:VAL:HG11	3:D:48:ILE:HD11	1.90	0.54
9:A:90:TYR:HD1	9:A:92:PRO:HD3	1.73	0.54
9:A:890:LYS:C	9:A:921:ASN:HD21	2.16	0.54
2:C:95:ASP:OD2	4:K:20:ASN:ND2	2.41	0.54
4:L:124:ALA:HA	4:L:141:THR:HG21	1.90	0.54
2:C:75:ASP:HB2	2:C:78:ASN:HD21	1.72	0.53
4:L:231:ASN:HB2	6:P:30:A:H5'	1.88	0.53
4:I:297:ARG:NH1	4:I:298:GLY:O	2.41	0.53
4:K:235:THR:HA	4:K:248:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:152:PHE:HE1	4:L:165:ASP:HB3	1.73	0.53
9:A:551:ILE:HG21	9:A:840:LEU:HB3	1.90	0.53
9:A:283:PHE:O	9:A:307:GLN:NE2	2.39	0.53
3:E:51:ALA:HB1	3:E:76:GLY:HA2	1.90	0.53
3:e:81:MET:O	3:e:214:ARG:NH1	2.39	0.53
3:E:48:ILE:HG23	3:E:71:VAL:HG13	1.90	0.53
5:H:17:ASN:ND2	5:H:47:ASN:OD1	2.42	0.53
9:A:123:LYS:HG3	9:A:130:PRO:HA	1.91	0.53
4:M:137:GLU:HB2	4:M:192:LEU:HB3	1.91	0.52
4:K:15:LYS:HG3	4:K:89:VAL:HG12	1.91	0.52
9:A:140:SER:HA	9:A:143:ILE:HD12	1.91	0.52
3:E:212:ILE:HG13	3:E:282:LEU:HD12	1.91	0.52
4:G:235:THR:HA	4:G:248:ALA:HA	1.91	0.52
4:I:58:ASP:OD1	4:I:58:ASP:N	2.41	0.52
4:J:125:ALA:O	4:J:133:ARG:NH2	2.40	0.52
6:P:4:A:N1	7:Q:47:DG:O6	2.42	0.52
3:D:103:ASN:ND2	3:D:294:MET:O	2.43	0.52
4:G:10:LEU:HA	4:G:95:GLY:HA2	1.91	0.52
4:K:65:VAL:HG22	4:K:213:LYS:HB3	1.91	0.52
3:d:260:ASP:O	9:A:356:ASN:ND2	2.42	0.52
3:e:114:LYS:HD2	3:e:228:LEU:HD23	1.91	0.52
4:G:11:ALA:HB3	4:G:94:LEU:HB3	1.92	0.52
4:K:21:ALA:HB1	4:K:79:VAL:HG13	1.92	0.52
4:K:124:ALA:HA	4:K:141:THR:HG21	1.89	0.52
5:H:143:ARG:HH22	6:P:36:A:H5'	1.74	0.52
3:E:21:VAL:HB	3:E:56:ILE:HG13	1.91	0.52
9:A:666:GLN:HA	9:A:895:LYS:HD2	1.92	0.52
9:A:851:VAL:HG13	9:A:854:TRP:HB2	1.90	0.52
1:B:72:PHE:O	1:B:76:TYR:HB2	2.09	0.52
9:A:801:MET:HA	9:A:804:ILE:HG12	1.92	0.52
4:M:273:LEU:HD13	4:M:287:ASP:HB2	1.92	0.52
3:e:73:TRP:HB2	3:e:83:ALA:HB3	1.91	0.52
2:C:141:VAL:HG21	9:A:199:ALA:HB2	1.92	0.52
4:M:18:PRO:HB3	4:M:83:VAL:HG22	1.91	0.52
9:A:845:ALA:HB3	9:A:848:ASN:HB2	1.92	0.52
4:G:135:GLY:HA3	4:I:84:LYS:HD3	1.92	0.51
4:M:56:ASP:OD1	4:M:56:ASP:N	2.36	0.51
3:e:120:GLU:HG2	3:e:123:LYS:HE2	1.93	0.51
2:C:43:THR:O	2:C:116:LYS:NZ	2.43	0.51
4:L:127:ARG:NH2	4:L:157:VAL:O	2.43	0.51
4:I:120:VAL:HG11	4:I:169:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:15:LYS:HG3	4:J:89:VAL:HG12	1.93	0.51
4:J:117:TYR:OH	4:J:161:ASP:O	2.28	0.51
4:L:142:VAL:HB	4:L:188:GLU:HG2	1.92	0.51
4:M:117:TYR:OH	4:M:163:ASP:N	2.43	0.51
4:I:31:ARG:NH2	4:I:140:GLU:OE2	2.42	0.51
4:J:13:SER:OG	4:K:131:ARG:NH1	2.44	0.51
4:L:22:LEU:HD21	4:L:218:LEU:HD22	1.91	0.51
6:P:22:C:O2'	6:P:23:C:O4'	2.26	0.51
4:J:263:ARG:NH1	4:J:268:THR:O	2.41	0.51
4:K:23:MET:HB3	4:K:77:LEU:HD11	1.94	0.51
4:J:205:PHE:HB3	4:K:43:THR:HB	1.93	0.50
4:L:128:THR:HB	4:L:229:ILE:HD12	1.93	0.50
9:A:632:SER:HB3	9:A:738:ILE:HD12	1.92	0.50
4:L:22:LEU:HD13	4:L:223:ALA:HB2	1.92	0.50
3:d:48:ILE:HG12	3:d:71:VAL:HG22	1.93	0.50
3:e:194:SER:OG	3:e:196:ASP:OD1	2.29	0.50
4:I:176:VAL:HG21	4:I:183:VAL:HB	1.92	0.50
4:M:23:MET:O	4:M:221:GLN:NE2	2.39	0.50
9:a:18:SER:O	9:a:22:SER:HB3	2.11	0.50
9:A:527:VAL:HG13	9:A:537:VAL:HG21	1.93	0.50
9:A:806:LYS:HB2	9:A:809:SER:HB3	1.94	0.50
4:G:36:ALA:HB1	4:G:221:GLN:HG3	1.94	0.50
4:G:254:SER:HA	4:G:261:ALA:HA	1.93	0.50
4:L:231:ASN:O	4:L:235:THR:OG1	2.29	0.50
6:P:1:G:H1	7:Q:50:DT:H3	1.58	0.50
9:A:135:ARG:HB2	9:A:217:TRP:HD1	1.77	0.50
1:B:122:HIS:O	1:B:126:SER:HB3	2.11	0.50
2:C:12:VAL:HG11	2:C:126:ILE:HB	1.94	0.50
4:I:132:ASN:ND2	4:I:224:MET:SD	2.85	0.50
4:K:61:ASN:OD1	4:K:63:GLN:NE2	2.42	0.50
9:a:6:LYS:HB2	9:a:59:VAL:HG12	1.94	0.50
9:A:385:LEU:HD11	9:A:508:VAL:HG21	1.93	0.50
3:E:73:TRP:HB2	3:E:83:ALA:HB3	1.94	0.50
4:G:277:ALA:HB2	4:G:283:LEU:HD11	1.93	0.50
4:L:23:MET:HE3	4:L:77:LEU:HD21	1.94	0.50
4:I:257:ARG:HB3	4:M:94:LEU:HA	1.93	0.49
4:J:247:ILE:HD13	4:J:262:TYR:HD2	1.77	0.49
4:L:234:ARG:NH2	6:P:30:A:OP2	2.44	0.49
5:H:91:ARG:HA	5:H:162:LEU:HB3	1.92	0.49
8:R:27:DC:H2''	8:R:28:DC:H3'	1.94	0.49
3:d:109:LEU:HD21	3:e:105:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:235:THR:HA	4:L:248:ALA:HA	1.95	0.49
3:d:239:VAL:O	3:d:243:ALA:HB3	2.13	0.49
3:D:50:LEU:HD23	3:D:54:THR:HB	1.94	0.49
3:E:74:THR:HA	3:E:81:MET:HA	1.94	0.49
3:E:209:ALA:HB2	3:E:251:ILE:HG13	1.95	0.49
4:G:131:ARG:NH2	6:P:16:A:OP1	2.45	0.49
9:A:764:THR:OG1	9:A:765:HIS:N	2.45	0.49
5:H:27:LEU:HD22	5:H:32:ILE:HG21	1.95	0.49
4:K:97:GLY:O	4:K:101:ASN:ND2	2.45	0.49
9:A:239:TYR:HA	9:A:314:LEU:HD21	1.93	0.49
9:A:481:ASP:N	9:A:481:ASP:OD1	2.42	0.49
4:K:106:ALA:O	4:K:288:GLN:NE2	2.46	0.49
4:L:118:ARG:NH2	4:L:238:THR:OG1	2.46	0.49
4:L:247:ILE:HD13	4:L:262:TYR:HD2	1.78	0.49
4:M:266:ASN:OD1	4:M:266:ASN:N	2.45	0.49
3:D:122:LEU:HD13	3:D:122:LEU:HA	1.60	0.49
3:E:217:LEU:HD21	3:E:242:VAL:HG21	1.94	0.49
4:G:297:ARG:NH1	4:G:298:GLY:O	2.44	0.49
5:H:22:LYS:HG2	4:L:134:VAL:HG12	1.94	0.49
4:I:11:ALA:HB3	4:I:94:LEU:HB3	1.94	0.49
4:J:23:MET:HB3	4:J:77:LEU:HD11	1.94	0.49
4:J:118:ARG:NH1	4:J:236:ILE:O	2.46	0.49
9:A:87:LYS:HG3	9:A:88:LYS:HD2	1.95	0.49
3:D:224:ASN:HD22	3:E:95:TYR:HE2	1.61	0.48
4:G:141:THR:HB	4:G:152:PHE:HB2	1.94	0.48
9:A:122:ARG:HB3	9:A:127:GLU:HG2	1.95	0.48
9:A:615:HIS:HA	9:A:766:ASN:HD21	1.77	0.48
3:D:13:MET:HG2	3:D:46:VAL:HB	1.95	0.48
9:A:899:LYS:HB3	9:A:899:LYS:HE3	1.67	0.48
4:G:212:SER:OG	7:Q:34:DA:N6	2.46	0.48
2:C:186:TYR:HB3	2:C:208:ALA:HB1	1.95	0.48
4:G:125:ALA:O	4:G:133:ARG:NH1	2.44	0.48
3:d:8:SER:HB3	3:d:286:ILE:HD12	1.94	0.48
3:d:104:TRP:HZ3	3:d:292:LEU:HD21	1.78	0.48
9:A:93:ASP:OD1	9:A:93:ASP:N	2.46	0.48
2:C:13:ASP:OD1	2:C:13:ASP:N	2.46	0.48
3:D:264:SER:H	3:D:267:GLU:HG3	1.78	0.48
4:G:129:LEU:HB3	4:G:132:ASN:HB2	1.96	0.48
4:G:145:VAL:HG22	4:G:185:LEU:HG	1.96	0.48
9:A:291:ASP:OD1	9:A:291:ASP:N	2.44	0.48
4:L:239:TRP:HB3	4:L:286:GLU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:11:U:H5	7:Q:40:DA:H61	1.60	0.48
3:e:250:ILE:HG12	3:e:275:TYR:HE2	1.79	0.48
4:G:231:ASN:O	4:G:235:THR:OG1	2.31	0.48
9:a:40:GLN:HE22	3:d:3:LYS:HG2	1.79	0.48
3:e:267:GLU:HA	3:e:270:ARG:HB3	1.95	0.48
9:A:663:GLN:HG2	9:A:892:ILE:CD1	2.34	0.48
3:e:118:ALA:O	3:e:122:LEU:HG	2.13	0.48
3:e:212:ILE:HG13	3:e:282:LEU:HD12	1.95	0.48
3:d:244:ASP:N	3:d:244:ASP:OD1	2.37	0.47
3:d:263:MET:SD	3:d:263:MET:N	2.87	0.47
4:G:64:THR:O	4:G:212:SER:N	2.42	0.47
4:M:120:VAL:HG11	4:M:169:ILE:HB	1.97	0.47
9:A:338:ILE:HG12	9:A:415:VAL:HG22	1.96	0.47
4:I:257:ARG:HH21	4:M:93:GLU:HG2	1.80	0.47
4:M:145:VAL:HG11	4:M:169:ILE:HG23	1.96	0.47
9:A:83:LYS:HD2	9:A:83:LYS:HA	1.42	0.47
2:C:18:LYS:HA	2:C:24:VAL:HG22	1.97	0.47
4:K:14:ARG:NH1	6:P:-1:G:OP2	2.48	0.47
4:K:21:ALA:HB3	4:K:224:MET:HB2	1.96	0.47
3:d:239:VAL:O	3:d:243:ALA:CB	2.62	0.47
3:d:244:ASP:HA	3:d:247:LYS:HG2	1.96	0.47
3:e:18:ARG:HH21	3:e:53:GLY:HA3	1.79	0.47
9:A:674:ILE:HB	9:A:895:LYS:HD3	1.97	0.47
4:I:97:GLY:O	4:I:101:ASN:ND2	2.48	0.47
4:J:235:THR:HA	4:J:248:ALA:HA	1.96	0.47
9:A:843:ASP:O	9:A:850:PHE:HB2	2.14	0.47
4:M:129:LEU:HD13	4:M:191:MET:HE3	1.96	0.47
3:e:244:ASP:OD1	3:e:247:LYS:NZ	2.39	0.47
3:D:235:ARG:HH11	3:E:95:TYR:H	1.63	0.47
3:D:244:ASP:HA	3:D:247:LYS:HG2	1.97	0.47
4:K:266:ASN:OD1	4:K:266:ASN:N	2.44	0.47
8:R:43:DC:H5''	9:A:399:MET:HG2	1.97	0.47
9:A:367:CYS:HB3	9:A:538:ILE:HA	1.97	0.47
7:U:3:DC:H2''	7:U:4:DA:C8	2.49	0.47
4:I:23:MET:HG2	4:I:79:VAL:HG22	1.96	0.47
4:L:99:TYR:HE1	4:L:274:MET:HE3	1.79	0.47
3:d:220:LEU:HD21	3:d:286:ILE:HG23	1.97	0.47
3:D:174:LYS:HD2	3:D:174:LYS:HA	1.65	0.47
3:D:189:LYS:HD2	3:D:189:LYS:HA	1.47	0.47
4:G:23:MET:HG2	4:G:79:VAL:HG22	1.95	0.47
4:I:89:VAL:HB	4:I:296:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:257:ARG:HH12	6:P:20:U:H5''	1.80	0.47
4:L:130:TRP:CZ2	4:L:232:ALA:HB2	2.49	0.47
4:L:172:MET:HE2	4:L:172:MET:HB3	1.74	0.47
9:A:725:VAL:O	9:A:730:ARG:NH1	2.48	0.47
4:G:239:TRP:HB3	4:G:286:GLU:HB3	1.95	0.46
4:I:277:ALA:HB2	4:I:283:LEU:HD22	1.96	0.46
4:K:73:ASN:OD1	4:K:73:ASN:N	2.47	0.46
4:L:204:GLU:HB2	4:L:214:GLN:HB2	1.97	0.46
3:E:107:LEU:HD11	3:E:117:ALA:HB2	1.97	0.46
5:H:91:ARG:NH1	5:H:92:LYS:O	2.49	0.46
4:I:85:PHE:HB2	4:I:183:VAL:HG12	1.97	0.46
4:K:169:ILE:HA	4:K:172:MET:HE3	1.98	0.46
9:a:10:LYS:HG3	10:V:12:DT:H3'	1.95	0.46
1:B:46:MET:HE1	1:B:62:LEU:HG	1.97	0.46
1:B:50:LYS:HG2	7:Q:52:DA:H2	1.80	0.46
2:C:161:VAL:HG11	2:C:182:MET:HE2	1.96	0.46
4:G:96:GLY:HA2	4:J:258:ASN:HA	1.97	0.46
9:A:94:ASP:OD1	9:A:94:ASP:N	2.46	0.46
9:A:297:ALA:HB2	9:A:309:LEU:HD13	1.98	0.46
2:C:31:THR:OG1	6:P:-5:U:OP1	2.32	0.46
4:K:130:TRP:CH2	4:K:232:ALA:HB2	2.51	0.46
4:L:176:VAL:HG21	4:L:183:VAL:HB	1.97	0.46
3:e:176:LEU:HD12	3:e:248:THR:HB	1.97	0.46
9:A:650:ILE:HG21	9:A:661:VAL:HG11	1.96	0.46
4:J:120:VAL:HG12	4:J:166:VAL:HG13	1.98	0.46
4:L:154:ASP:OD1	4:L:154:ASP:N	2.46	0.46
9:a:17:VAL:O	9:a:21:VAL:HG12	2.16	0.46
9:A:8:PHE:HB2	9:A:57:LYS:HB3	1.96	0.46
9:A:45:LEU:O	9:A:49:LEU:HB2	2.16	0.46
9:A:114:GLY:H	9:A:140:SER:HB3	1.81	0.46
1:B:172:GLN:NE2	2:C:57:PHE:O	2.49	0.46
4:J:65:VAL:HG13	4:J:213:LYS:HB3	1.98	0.46
4:K:131:ARG:NE	6:P:3:C:OP1	2.43	0.46
4:K:254:SER:HA	4:K:261:ALA:HA	1.97	0.46
4:L:78:LEU:HA	4:L:189:HIS:O	2.16	0.46
9:A:357:MET:HE3	9:A:357:MET:HB3	1.82	0.46
2:C:185:GLY:HA3	2:C:238:LYS:HA	1.98	0.46
5:H:92:LYS:HG3	5:H:146:MET:HE2	1.97	0.46
8:R:45:DT:OP1	9:A:425:GLY:N	2.45	0.46
9:A:413:MET:SD	9:A:414:GLY:N	2.89	0.46
9:A:446:GLU:N	9:A:446:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:GLN:HA	4:K:251:PRO:HG2	1.97	0.46
4:K:117:TYR:OH	4:K:163:ASP:OD1	2.33	0.46
4:L:103:LEU:HD12	4:L:103:LEU:HA	1.78	0.46
4:M:254:SER:HA	4:M:261:ALA:HA	1.98	0.46
3:d:166:LEU:HD11	3:d:234:ARG:HB3	1.98	0.46
9:A:370:MET:N	9:A:579:TRP:O	2.45	0.46
9:A:625:ASN:HB3	9:A:770:LEU:HD13	1.98	0.46
5:H:103:ARG:HH12	6:P:39:A:H5''	1.81	0.46
4:M:85:PHE:HB2	4:M:183:VAL:HG12	1.96	0.46
4:M:297:ARG:NH1	4:M:298:GLY:O	2.48	0.46
4:G:218:LEU:HD23	4:G:218:LEU:HA	1.69	0.45
4:M:115:LEU:HD21	4:M:293:ALA:HB2	1.97	0.45
4:M:143:ILE:HG12	4:M:187:VAL:HG13	1.97	0.45
3:D:178:LYS:HD2	3:D:178:LYS:HA	1.40	0.45
4:M:21:ALA:HB3	4:M:224:MET:HB2	1.98	0.45
6:P:16:A:H2'	6:P:17:U:C6	2.52	0.45
2:C:161:VAL:HG11	2:C:182:MET:CE	2.46	0.45
4:K:78:LEU:HD13	4:K:190:TYR:CE1	2.51	0.45
4:K:277:ALA:HB2	4:K:283:LEU:HD22	1.97	0.45
3:e:258:ALA:HA	3:e:263:MET:HE1	1.99	0.45
2:C:182:MET:HG2	2:C:215:ILE:HG12	1.99	0.45
4:J:77:LEU:HD13	4:J:199:VAL:HG11	1.99	0.45
4:L:69:ASN:HA	4:L:198:GLU:HA	1.99	0.45
3:d:77:GLY:HA2	3:d:84:ALA:HB3	1.97	0.45
9:A:4:ARG:HE	9:A:6:LYS:HZ1	1.64	0.45
1:B:115:LEU:HD21	2:C:188:LYS:HZ2	1.81	0.45
4:G:16:ILE:HG21	4:G:233:ILE:HG21	1.98	0.45
4:J:13:SER:N	4:J:93:GLU:OE1	2.50	0.45
4:K:231:ASN:O	4:K:235:THR:OG1	2.34	0.45
4:M:124:ALA:HA	4:M:141:THR:HG21	1.98	0.45
9:A:18:SER:O	9:A:22:SER:HB3	2.17	0.45
4:G:21:ALA:HA	4:G:81:TYR:HB3	1.99	0.45
1:B:22:ARG:HA	1:B:22:ARG:HD3	1.87	0.45
2:C:178:LYS:HD2	2:C:178:LYS:HA	1.61	0.45
4:G:93:GLU:O	4:J:257:ARG:NE	2.41	0.45
5:H:128:CYS:O	6:P:37:G:N2	2.50	0.45
4:I:91:LYS:HB3	4:I:91:LYS:HE3	1.27	0.45
4:K:176:VAL:HG21	4:K:183:VAL:HB	1.98	0.45
3:e:220:LEU:HD21	3:e:286:ILE:HD12	1.99	0.45
9:A:17:VAL:HG12	9:A:52:VAL:HG11	1.98	0.45
9:A:122:ARG:HE	9:A:122:ARG:HB2	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:332:PRO:HG3	9:A:504:HIS:HB3	1.99	0.45
9:A:368:ILE:HG23	9:A:578:TRP:HA	1.97	0.45
9:A:481:ASP:HA	9:A:484:VAL:HG22	1.98	0.45
1:B:23:TYR:HE1	1:B:153:THR:HG21	1.82	0.45
4:G:65:VAL:HG12	4:G:213:LYS:HB3	1.99	0.45
4:K:77:LEU:HD13	4:K:199:VAL:HG11	1.99	0.45
4:M:63:GLN:NE2	6:P:29:A:N1	2.65	0.45
3:d:31:LEU:HD13	3:d:37:VAL:HG22	1.99	0.45
9:A:622:GLN:H	9:A:622:GLN:HG2	1.28	0.45
9:A:656:LYS:HA	9:A:659:VAL:HG22	1.97	0.45
3:D:13:MET:HE1	3:D:276:PHE:HD2	1.82	0.45
3:D:98:THR:OG1	3:E:232:SER:O	2.31	0.45
3:E:290:LYS:O	3:E:294:MET:HB2	2.17	0.45
4:I:89:VAL:HB	4:I:296:ILE:HG22	1.98	0.45
4:J:120:VAL:HG11	4:J:169:ILE:HB	1.99	0.45
4:L:86:VAL:HG11	4:M:134:VAL:HG13	1.98	0.45
9:A:127:GLU:N	9:A:127:GLU:OE2	2.50	0.45
9:A:649:LEU:HD11	9:A:726:VAL:HG11	1.98	0.45
5:H:104:ARG:HH12	6:P:42:C:H5	1.65	0.44
4:M:125:ALA:HB1	4:M:157:VAL:HG22	1.99	0.44
9:A:363:ASP:OD1	9:A:363:ASP:N	2.42	0.44
9:A:370:MET:HE2	9:A:604:ARG:HD3	1.98	0.44
3:D:61:MET:HE1	3:D:71:VAL:HG11	1.99	0.44
4:J:127:ARG:NH2	4:J:157:VAL:O	2.50	0.44
4:K:99:TYR:OH	4:K:275:ASP:OD1	2.35	0.44
4:M:66:ASN:HB2	4:M:214:GLN:HA	1.99	0.44
3:d:92:GLN:HE22	3:e:84:ALA:HB3	1.83	0.44
3:d:227:PRO:HG3	3:d:237:GLY:HA2	2.00	0.44
9:A:820:ASP:H	9:A:833:HIS:CD2	2.35	0.44
9:A:562:VAL:O	9:A:566:ASN:HB2	2.18	0.44
2:C:192:ILE:HG21	2:C:198:MET:HE3	1.98	0.44
4:I:120:VAL:HG12	4:I:166:VAL:HG13	2.00	0.44
4:I:230:GLY:HA2	4:I:233:ILE:HG12	2.00	0.44
1:B:102:PRO:HG2	6:P:-5:U:H1'	1.99	0.44
3:E:14:TYR:O	3:E:49:GLY:N	2.47	0.44
4:G:11:ALA:HA	4:G:300:VAL:HA	1.98	0.44
4:L:23:MET:HG2	4:L:79:VAL:HG22	2.00	0.44
4:M:53:ASN:OD1	4:M:53:ASN:N	2.48	0.44
6:P:22:C:O2'	6:P:23:C:O5'	2.34	0.44
9:A:109:LEU:HD13	9:A:243:LEU:HA	1.99	0.44
9:A:625:ASN:HA	9:A:628:ALA:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:775:LYS:NZ	9:A:785:ASP:OD1	2.44	0.44
3:E:244:ASP:HA	3:E:247:LYS:HD3	2.00	0.44
4:I:235:THR:HA	4:I:248:ALA:HA	1.98	0.44
7:Q:53:DC:H5	8:R:22:DG:H22	1.65	0.44
3:e:113:LYS:HB2	3:e:113:LYS:HE3	1.61	0.44
7:U:4:DA:H2'	7:U:5:DA:C8	2.52	0.44
3:D:109:LEU:HD11	3:E:105:VAL:CG1	2.44	0.44
4:G:21:ALA:HB3	4:G:224:MET:HB2	2.00	0.44
4:G:120:VAL:HG11	4:G:169:ILE:HB	2.00	0.44
4:I:169:ILE:HA	4:I:172:MET:HE3	2.00	0.44
3:e:197:ASN:O	3:e:201:PHE:HB2	2.18	0.44
3:D:114:LYS:HG2	3:D:162:PHE:HZ	1.82	0.44
9:A:90:TYR:CD1	9:A:92:PRO:HD3	2.53	0.44
9:A:116:ALA:HB2	9:A:234:PHE:HZ	1.82	0.44
1:B:103:GLN:HG2	1:B:116:VAL:HG22	2.00	0.43
2:C:105:GLU:N	2:C:105:GLU:OE1	2.51	0.43
4:K:48:GLN:NE2	4:K:60:GLY:O	2.45	0.43
4:K:115:LEU:HG	4:K:289:MET:HG2	1.98	0.43
4:M:127:ARG:HD3	4:M:235:THR:HB	1.99	0.43
9:A:124:LEU:HD22	9:A:299:LEU:HG	1.99	0.43
9:A:260:LEU:HD22	9:A:264:GLN:HE21	1.82	0.43
9:A:280:ASP:HA	9:A:316:VAL:HG22	1.99	0.43
3:D:248:THR:HG22	3:D:252:LEU:HD13	1.99	0.43
3:d:35:GLY:HA3	9:A:85:THR:HG23	2.00	0.43
9:A:16:LYS:NZ	9:A:52:VAL:O	2.43	0.43
5:H:158:ASN:HB3	5:H:164:ILE:HD11	2.00	0.43
4:J:263:ARG:NH1	4:J:268:THR:OG1	2.51	0.43
4:L:39:VAL:HG13	4:L:222:ALA:HB2	2.01	0.43
9:A:117:ASN:N	9:A:117:ASN:OD1	2.51	0.43
3:E:174:LYS:HE2	3:E:174:LYS:HB3	1.91	0.43
3:e:21:VAL:HB	3:e:56:ILE:HG13	1.99	0.43
2:C:24:VAL:HG11	2:C:66:THR:HG21	2.01	0.43
4:I:43:THR:HB	4:M:205:PHE:HB3	1.99	0.43
4:M:133:ARG:HH22	4:M:157:VAL:HG21	1.83	0.43
4:M:235:THR:HA	4:M:248:ALA:HA	2.00	0.43
6:P:43:G:N2	6:P:47:A:H62	2.11	0.43
4:M:78:LEU:HD13	4:M:190:TYR:CE1	2.53	0.43
3:e:99:LYS:H	3:e:99:LYS:HG2	1.48	0.43
3:e:168:HIS:HA	3:e:171:THR:HG22	2.01	0.43
9:A:18:SER:HA	9:A:21:VAL:HG12	2.00	0.43
9:A:282:ASN:HA	9:A:459:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:GLU:HA	9:A:793:GLY:HA3	2.00	0.43
5:H:4:ILE:HD12	5:H:81:PRO:HG3	2.00	0.43
4:J:11:ALA:HA	4:J:300:VAL:HA	2.00	0.43
9:A:181:TRP:NE1	9:A:856:LEU:O	2.46	0.43
9:A:470:LEU:HD11	9:A:482:HIS:HB3	2.00	0.43
3:E:16:LEU:HD11	3:E:48:ILE:HD11	2.00	0.43
3:E:18:ARG:HD3	10:V:1:DA:C6	2.53	0.43
4:G:124:ALA:HA	4:G:141:THR:HG21	2.00	0.43
5:H:101:LEU:HD23	5:H:120:TYR:HE2	1.83	0.43
4:M:152:PHE:HB3	4:M:155:LEU:HD11	2.00	0.43
3:d:100:TYR:CZ	3:d:290:LYS:HE3	2.53	0.43
3:d:178:LYS:HD2	3:d:178:LYS:HA	1.40	0.43
9:A:231:ASP:OD1	9:A:231:ASP:N	2.51	0.43
9:A:322:LYS:HE3	9:A:322:LYS:HB3	1.43	0.43
2:C:18:LYS:HB2	2:C:92:PRO:HD2	2.00	0.43
9:A:654:THR:OG1	9:A:655:ILE:N	2.52	0.43
7:Q:35:DA:H2'	7:Q:36:DG:C8	2.53	0.42
3:d:204:LEU:HD21	3:d:269:LYS:HD3	2.01	0.42
9:A:9:SER:HB2	9:A:13:ILE:HG23	2.00	0.42
9:A:400:VAL:O	9:A:403:THR:OG1	2.28	0.42
3:D:206:ASN:HA	3:D:247:LYS:NZ	2.34	0.42
3:D:206:ASN:HA	3:D:247:LYS:HZ1	1.83	0.42
3:E:21:VAL:HG22	3:E:30:HIS:HB3	2.01	0.42
3:E:258:ALA:HA	3:E:263:MET:HE1	2.00	0.42
4:I:158:ASN:OD1	4:I:158:ASN:N	2.52	0.42
9:A:178:ALA:HB1	9:A:269:LEU:HD11	1.99	0.42
4:I:205:PHE:HA	6:P:19:U:C5	2.54	0.42
4:L:188:GLU:OE2	4:L:188:GLU:N	2.52	0.42
3:e:122:LEU:HD22	3:e:169:GLU:OE1	2.19	0.42
3:e:278:LYS:HB2	3:e:278:LYS:HE3	1.73	0.42
9:A:95:SER:OG	9:A:96:ILE:N	2.53	0.42
9:A:470:LEU:HD13	9:A:476:LEU:HD21	2.00	0.42
9:A:888:THR:HA	9:A:920:TYR:O	2.19	0.42
4:J:211:LEU:HD23	4:J:214:GLN:HB2	2.01	0.42
3:e:246:ILE:HB	3:e:250:ILE:HD12	2.01	0.42
3:D:129:LEU:HD13	3:D:129:LEU:HA	1.91	0.42
4:G:115:LEU:HG	4:G:289:MET:HG2	2.01	0.42
4:I:234:ARG:HB2	4:I:249:VAL:HB	2.00	0.42
9:A:691:MET:HE2	9:A:691:MET:HB2	1.72	0.42
9:A:886:VAL:O	9:A:919:CYS:HA	2.18	0.42
2:C:173:ASP:OD2	2:C:214:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:234:ARG:HG3	4:J:249:VAL:H	1.85	0.42
4:J:241:GLU:OE1	4:J:266:ASN:ND2	2.52	0.42
4:K:234:ARG:HH12	6:P:-1:G:H5"	1.83	0.42
9:a:25:LEU:HB2	9:a:33:TRP:HB3	2.02	0.42
2:C:70:LYS:HG2	4:K:205:PHE:HD2	1.84	0.42
3:d:51:ALA:O	3:d:54:THR:OG1	2.32	0.42
3:d:162:PHE:HA	3:d:165:LEU:HD12	2.01	0.42
3:e:209:ALA:HB2	3:e:251:ILE:HG13	2.02	0.42
3:e:227:PRO:HB3	3:e:237:GLY:HA3	2.00	0.42
9:A:553:TYR:O	9:A:557:SER:OG	2.30	0.42
3:D:145:VAL:HA	3:D:148:ILE:HG22	2.01	0.42
4:J:3:LYS:HA	4:J:3:LYS:HD2	1.87	0.42
4:M:281:LYS:HE2	4:M:281:LYS:HB2	1.83	0.42
3:d:269:LYS:O	3:d:273:VAL:HG23	2.20	0.42
9:A:646:SER:HB2	9:A:736:TRP:HE1	1.85	0.42
5:H:82:LYS:HE2	5:H:82:LYS:HB3	1.83	0.42
4:J:283:LEU:HB3	4:J:287:ASP:HB3	2.02	0.42
9:A:355:VAL:HG21	9:A:383:LYS:HG2	2.00	0.42
9:A:462:ASN:HB3	9:A:463:ALA:H	1.67	0.42
3:D:58:ASN:N	3:E:54:THR:O	2.53	0.42
3:E:187:GLU:OE2	5:H:43:ARG:NH1	2.52	0.42
4:J:169:ILE:HA	4:J:172:MET:HE3	2.02	0.42
4:L:28:TRP:HH2	4:L:140:GLU:HB2	1.85	0.42
3:d:98:THR:OG1	3:e:232:SER:O	2.30	0.42
3:e:19:CYS:SG	3:e:30:HIS:HB2	2.60	0.42
2:C:142:ALA:HA	2:C:147:GLU:HB3	2.01	0.41
4:G:119:TYR:HE1	4:G:234:ARG:HA	1.85	0.41
4:G:258:ASN:HA	4:I:96:GLY:HA2	2.02	0.41
4:I:73:ASN:OD1	4:I:73:ASN:N	2.52	0.41
4:K:120:VAL:HG11	4:K:169:ILE:HB	2.02	0.41
3:e:163:GLU:OE1	3:e:163:GLU:N	2.52	0.41
9:A:706:TYR:C	9:A:708:LYS:N	2.75	0.41
9:A:789:TYR:HD2	9:A:832:GLU:HG2	1.85	0.41
9:A:918:ILE:HD12	9:A:918:ILE:HA	1.80	0.41
1:B:104:ILE:HB	6:P:-6:U:H5"	2.03	0.41
4:I:80:LYS:HG2	4:I:188:GLU:HG2	2.01	0.41
4:J:239:TRP:HB3	4:J:286:GLU:HG2	2.01	0.41
4:K:226:ASP:OD1	4:K:226:ASP:N	2.51	0.41
4:M:260:VAL:HG13	4:M:262:TYR:HE1	1.85	0.41
4:J:58:ASP:OD1	4:J:58:ASP:N	2.50	0.41
4:J:79:VAL:HB	4:J:189:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:25:DT:H2"	7:Q:26:DA:C8	2.55	0.41
3:d:143:LYS:O	3:d:147:SER:HB3	2.20	0.41
9:A:469:LYS:HE2	9:A:469:LYS:HB3	1.93	0.41
3:D:101:MET:HE2	3:D:222:ILE:HA	2.02	0.41
3:E:139:ASP:HB3	3:E:142:ASN:HB2	2.02	0.41
4:I:23:MET:HB3	4:I:77:LEU:HD11	2.03	0.41
4:I:127:ARG:NH2	4:I:157:VAL:O	2.53	0.41
4:L:270:LEU:HD12	4:L:291:VAL:HG22	2.02	0.41
4:L:286:GLU:OE2	4:L:286:GLU:N	2.53	0.41
3:D:156:VAL:HG23	3:D:165:LEU:HD11	2.01	0.41
3:E:5:ILE:HB	3:E:13:MET:HB3	2.02	0.41
3:E:270:ARG:HA	3:E:273:VAL:HG22	2.03	0.41
4:K:163:ASP:OD1	4:K:163:ASP:N	2.52	0.41
9:a:4:ARG:HB2	9:a:34:GLU:HG3	2.03	0.41
9:A:137:GLU:HB3	9:A:186:HIS:CE1	2.56	0.41
3:E:1:MET:HB3	3:E:2:GLN:H	1.66	0.41
4:I:254:SER:HA	4:I:261:ALA:HA	2.02	0.41
4:J:84:LYS:HB2	4:J:84:LYS:HE3	1.71	0.41
3:d:153:ASP:HA	3:d:156:VAL:HG12	2.03	0.41
9:A:506:ASP:HA	9:A:535:ASN:HB3	2.02	0.41
3:E:186:ILE:HD12	3:E:188:PHE:HB2	2.02	0.41
4:L:191:MET:HE3	4:L:191:MET:HB2	1.90	0.41
9:a:36:HIS:O	3:d:44:ASN:ND2	2.54	0.41
3:d:270:ARG:NH1	9:A:64:ASP:OD2	2.54	0.41
3:e:1:MET:N	3:e:17:SER:HB2	2.35	0.41
9:A:12:PRO:O	9:A:16:LYS:HG2	2.20	0.41
9:A:132:ASP:O	9:A:219:ASN:ND2	2.53	0.41
9:A:300:ASP:OD1	9:A:304:ASN:N	2.53	0.41
3:D:61:MET:HE3	3:E:73:TRP:CE2	2.55	0.41
3:E:267:GLU:H	3:E:267:GLU:HG2	1.60	0.41
5:H:17:ASN:OD1	5:H:17:ASN:N	2.54	0.41
4:L:27:ASN:HB2	4:L:30:ASP:HB3	2.02	0.41
9:a:14:ALA:HA	9:a:17:VAL:HG12	2.03	0.41
3:d:50:LEU:HD23	3:d:54:THR:HB	2.02	0.41
2:C:75:ASP:HA	4:K:302:GLY:H	1.85	0.41
4:G:77:LEU:HD13	4:G:199:VAL:HG11	2.03	0.41
4:G:110:THR:HG22	4:G:288:GLN:HB3	2.03	0.41
5:H:76:ILE:HD12	5:H:76:ILE:HA	1.94	0.41
4:J:45:ALA:HA	4:J:61:ASN:O	2.20	0.41
4:K:99:TYR:O	4:K:103:LEU:HB2	2.21	0.41
4:M:70:LEU:O	4:M:196:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:42:C:H2'	6:P:43:G:O4'	2.21	0.41
3:d:110:ASP:HB2	3:d:113:LYS:HB2	2.01	0.41
3:e:31:LEU:O	3:e:32:HIS:C	2.59	0.41
3:e:124:MET:HE3	3:e:124:MET:HB3	1.77	0.41
9:A:83:LYS:HB3	9:A:84:TYR:H	1.20	0.41
9:A:143:ILE:HA	9:A:163:VAL:HG11	2.03	0.41
9:A:679:TYR:HB3	9:A:722:ALA:HB2	2.03	0.41
2:C:159:TYR:CE1	2:C:219:MET:HG2	2.56	0.41
3:D:20:LYS:HG3	3:D:22:LEU:HD23	2.03	0.41
5:H:100:LYS:HE2	6:P:40:G:H22	1.84	0.41
4:J:81:TYR:OH	4:J:189:HIS:NE2	2.51	0.41
9:A:400:VAL:HG13	9:A:424:THR:HG21	2.03	0.41
3:D:29:CYS:HB2	3:D:37:VAL:HG12	2.03	0.40
4:I:24:PHE:HB2	4:I:78:LEU:HD23	2.03	0.40
4:M:75:ASN:OD1	4:M:75:ASN:N	2.55	0.40
6:P:4:A:H2'	6:P:5:A:C4	2.56	0.40
6:P:33:G:OP2	6:P:33:G:N2	2.46	0.40
9:A:169:VAL:HG21	9:A:184:ASN:HD21	1.86	0.40
3:E:3:LYS:HB3	3:E:15:ILE:HB	2.02	0.40
5:H:41:PHE:H	5:H:90:TYR:HE2	1.67	0.40
9:a:13:ILE:HD12	9:a:16:LYS:HE2	2.02	0.40
9:A:160:ILE:HA	9:A:161:PRO:HD3	1.92	0.40
9:A:659:VAL:HG21	9:A:927:TYR:HB3	2.02	0.40
2:C:31:THR:HG21	2:C:127:ALA:HB2	2.03	0.40
2:C:182:MET:HE3	2:C:215:ILE:HG21	2.04	0.40
4:J:186:LYS:HE3	4:J:186:LYS:HB3	1.84	0.40
4:L:145:VAL:HG11	4:L:169:ILE:HG23	2.03	0.40
3:d:70:ILE:HG12	3:d:214:ARG:HB2	2.03	0.40
3:e:13:MET:HA	3:e:47:PHE:HB2	2.04	0.40
3:D:73:TRP:CD2	3:E:61:MET:HG2	2.57	0.40
3:d:108:TRP:HE3	3:d:109:LEU:HD22	1.87	0.40
9:A:463:ALA:HB3	9:A:467:ASN:HB2	2.03	0.40
1:B:45:ASP:HB2	1:B:121:ALA:HB1	2.03	0.40
3:D:18:ARG:NH2	3:D:52:GLU:OE2	2.53	0.40
4:J:5:LYS:HB3	4:J:5:LYS:HE3	1.91	0.40
4:K:234:ARG:NH2	6:P:0:A:OP2	2.53	0.40
4:K:290:PHE:O	4:K:294:ASN:ND2	2.44	0.40
3:e:75:LYS:HA	3:e:75:LYS:HD2	1.86	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	175/178 (98%)	165 (94%)	10 (6%)	0	100	100
2	C	245/248 (99%)	225 (92%)	20 (8%)	0	100	100
3	D	295/295 (100%)	279 (95%)	14 (5%)	2 (1%)	18	46
3	E	293/295 (99%)	286 (98%)	7 (2%)	0	100	100
3	d	295/295 (100%)	278 (94%)	16 (5%)	1 (0%)	36	64
3	e	293/295 (99%)	279 (95%)	14 (5%)	0	100	100
4	G	300/306 (98%)	290 (97%)	10 (3%)	0	100	100
4	I	300/306 (98%)	284 (95%)	16 (5%)	0	100	100
4	J	300/306 (98%)	286 (95%)	11 (4%)	3 (1%)	12	37
4	K	300/306 (98%)	286 (95%)	14 (5%)	0	100	100
4	L	300/306 (98%)	285 (95%)	15 (5%)	0	100	100
4	M	300/306 (98%)	286 (95%)	13 (4%)	1 (0%)	36	64
5	H	163/168 (97%)	148 (91%)	14 (9%)	1 (1%)	21	50
9	A	927/930 (100%)	850 (92%)	69 (7%)	8 (1%)	14	40
9	a	73/930 (8%)	71 (97%)	1 (1%)	1 (1%)	9	29
All	All	4559/5470 (83%)	4298 (94%)	244 (5%)	17 (0%)	31	58

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	62	ILE
9	A	159	ILE
9	A	851	VAL
3	D	5	ILE
4	J	50	VAL
4	J	145	VAL
3	D	294	MET
3	d	5	ILE

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Mol	Chain	Res	Type
9	A	11	GLN
9	A	75	MET
9	A	887	THR
9	A	95	SER
4	J	98	GLU
9	a	63	GLN
9	A	845	ALA
5	H	32	ILE
9	A	81	VAL

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	155/157 (99%)	146 (94%)	9 (6%)	18	47
2	C	208/211 (99%)	195 (94%)	13 (6%)	16	43
3	D	247/254 (97%)	224 (91%)	23 (9%)	8	26
3	E	247/254 (97%)	239 (97%)	8 (3%)	34	66
3	d	250/254 (98%)	232 (93%)	18 (7%)	13	37
3	e	247/254 (97%)	227 (92%)	20 (8%)	11	31
4	G	246/251 (98%)	238 (97%)	8 (3%)	33	65
4	I	241/251 (96%)	227 (94%)	14 (6%)	18	47
4	J	247/251 (98%)	232 (94%)	15 (6%)	17	44
4	K	247/251 (98%)	235 (95%)	12 (5%)	22	52
4	L	244/251 (97%)	225 (92%)	19 (8%)	11	33
4	M	246/251 (98%)	239 (97%)	7 (3%)	38	70
5	H	148/151 (98%)	143 (97%)	5 (3%)	32	65
9	A	792/817 (97%)	743 (94%)	49 (6%)	16	44
9	a	63/817 (8%)	62 (98%)	1 (2%)	55	81
All	All	3828/4675 (82%)	3607 (94%)	221 (6%)	20	47

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	ILE
1	B	4	GLU
1	B	5	MET
1	B	8	ASP
1	B	10	ILE
1	B	87	LEU
1	B	89	LYS
1	B	93	THR
1	B	165	GLN
2	C	21	ASP
2	C	39	MET
2	C	40	SER
2	C	141	VAL
2	C	144	ASP
2	C	147	GLU
2	C	170	ILE
2	C	178	LYS
2	C	179	LEU
2	C	180	GLN
2	C	182	MET
2	C	215	ILE
2	C	218	LYS
3	D	106	ARG
3	D	114	LYS
3	D	122	LEU
3	D	123	LYS
3	D	125	ARG
3	D	126	VAL
3	D	129	LEU
3	D	165	LEU
3	D	166	LEU
3	D	169	GLU
3	D	174	LYS
3	D	176	LEU
3	D	178	LYS
3	D	179	GLU
3	D	183	GLU
3	D	186	ILE
3	D	189	LYS
3	D	194	SER
3	D	222	ILE
3	D	224	ASN

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Mol	Chain	Res	Type
3	D	225	SER
3	D	264	SER
3	D	267	GLU
3	E	99	LYS
3	E	101	MET
3	E	107	LEU
3	E	109	LEU
3	E	124	MET
3	E	125	ARG
3	E	126	VAL
3	E	130	SER
4	G	48	GLN
4	G	49	SER
4	G	50	VAL
4	G	53	ASN
4	G	56	ASP
4	G	58	ASP
4	G	129	LEU
4	G	151	THR
5	H	9	VAL
5	H	12	ASP
5	H	14	VAL
5	H	17	ASN
5	H	44	MET
4	I	9	VAL
4	I	59	LYS
4	I	84	LYS
4	I	89	VAL
4	I	91	LYS
4	I	204	GLU
4	I	206	VAL
4	I	217	ASP
4	I	218	LEU
4	I	226	ASP
4	I	228	LYS
4	I	278	VAL
4	I	283	LEU
4	I	284	THR
4	J	29	SER
4	J	31	ARG
4	J	32	ASP
4	J	35	THR

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Mol	Chain	Res	Type
4	J	84	LYS
4	J	86	VAL
4	J	88	ASP
4	J	89	VAL
4	J	144	THR
4	J	145	VAL
4	J	146	ASN
4	J	151	THR
4	J	226	ASP
4	J	227	GLN
4	J	228	LYS
4	K	30	ASP
4	K	31	ARG
4	K	32	ASP
4	K	34	THR
4	K	50	VAL
4	K	53	ASN
4	K	55	ASN
4	K	58	ASP
4	K	207	GLU
4	K	210	LYS
4	K	212	SER
4	K	218	LEU
4	L	89	VAL
4	L	91	LYS
4	L	93	GLU
4	L	94	LEU
4	L	98	GLU
4	L	102	THR
4	L	103	LEU
4	L	104	GLN
4	L	108	GLU
4	L	109	ASN
4	L	114	THR
4	L	164	VAL
4	L	165	ASP
4	L	168	GLU
4	L	172	MET
4	L	209	SER
4	L	226	ASP
4	L	266	ASN
4	L	288	GLN

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Mol	Chain	Res	Type
4	M	34	THR
4	M	94	LEU
4	M	188	GLU
4	M	195	GLU
4	M	197	SER
4	M	198	GLU
4	M	199	VAL
9	a	13	ILE
3	d	52	GLU
3	d	102	GLN
3	d	113	LYS
3	d	115	LEU
3	d	119	LYS
3	d	120	GLU
3	d	121	ILE
3	d	122	LEU
3	d	123	LYS
3	d	124	MET
3	d	125	ARG
3	d	129	LEU
3	d	178	LYS
3	d	179	GLU
3	d	182	LEU
3	d	186	ILE
3	d	187	GLU
3	d	189	LYS
3	e	6	LEU
3	e	13	MET
3	e	31	LEU
3	e	36	ASN
3	e	37	VAL
3	e	98	THR
3	e	99	LYS
3	e	105	VAL
3	e	106	ARG
3	e	113	LYS
3	e	115	LEU
3	e	116	SER
3	e	120	GLU
3	e	121	ILE
3	e	123	LYS
3	e	124	MET

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Mol	Chain	Res	Type
3	e	125	ARG
3	e	126	VAL
3	e	130	SER
3	e	166	LEU
9	A	72	ASN
9	A	83	LYS
9	A	172	ASP
9	A	175	VAL
9	A	247	ARG
9	A	248	LYS
9	A	251	LEU
9	A	254	LYS
9	A	321	LEU
9	A	322	LYS
9	A	411	LEU
9	A	419	SER
9	A	422	MET
9	A	541	SER
9	A	621	ASP
9	A	622	GLN
9	A	623	ASP
9	A	626	MET
9	A	684	VAL
9	A	686	ASP
9	A	688	LYS
9	A	690	GLN
9	A	695	LEU
9	A	705	GLU
9	A	710	VAL
9	A	714	THR
9	A	716	THR
9	A	837	LEU
9	A	839	LYS
9	A	841	THR
9	A	848	ASN
9	A	849	VAL
9	A	871	LYS
9	A	873	GLU
9	A	874	ASP
9	A	876	VAL
9	A	878	THR
9	A	885	ASN

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Mol	Chain	Res	Type
9	A	888	THR
9	A	889	THR
9	A	893	GLN
9	A	897	TRP
9	A	901	GLN
9	A	903	GLU
9	A	907	ILE
9	A	908	THR
9	A	914	LEU
9	A	916	LYS
9	A	918	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	HIS
2	C	9	ASN
2	C	74	GLN
2	C	78	ASN
3	D	58	ASN
3	D	102	GLN
3	D	103	ASN
3	D	197	ASN
3	D	224	ASN
3	E	44	ASN
3	E	150	ASN
4	G	20	ASN
4	G	104	GLN
4	G	203	GLN
4	I	20	ASN
4	I	33	ASN
4	I	69	ASN
4	J	20	ASN
4	J	33	ASN
4	J	69	ASN
4	J	146	ASN
4	J	148	GLN
4	J	227	GLN
4	K	27	ASN
4	K	53	ASN
4	K	231	ASN
4	L	158	ASN

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Mol	Chain	Res	Type
4	L	266	ASN
4	M	101	ASN
4	M	146	ASN
4	M	148	GLN
9	a	40	GLN
9	a	51	ASN
3	d	9	GLN
3	d	32	HIS
3	d	92	GLN
3	d	102	GLN
3	d	257	HIS
3	d	265	ASN
3	e	30	HIS
9	A	44	ASN
9	A	46	GLN
9	A	168	ASN
9	A	219	ASN
9	A	264	GLN
9	A	298	ASN
9	A	409	GLN
9	A	535	ASN
9	A	592	GLN
9	A	622	GLN
9	A	818	GLN
9	A	833	HIS
9	A	872	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	P	59/60 (98%)	37 (62%)	3 (5%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	P	-6	U
6	P	-5	U
6	P	-2	A
6	P	0	A
6	P	1	G
6	P	2	U

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Mol	Chain	Res	Type
6	P	3	C
6	P	4	A
6	P	5	A
6	P	6	C
6	P	7	C
6	P	8	C
6	P	9	U
6	P	10	U
6	P	11	U
6	P	12	G
6	P	13	C
6	P	14	U
6	P	16	A
6	P	18	C
6	P	19	U
6	P	20	U
6	P	22	C
6	P	23	C
6	P	24	U
6	P	25	A
6	P	26	U
6	P	27	U
6	P	28	U
6	P	29	A
6	P	30	A
6	P	31	A
6	P	36	A
6	P	38	C
6	P	41	C
6	P	42	C
6	P	46	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	P	11	U
6	P	22	C
6	P	41	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

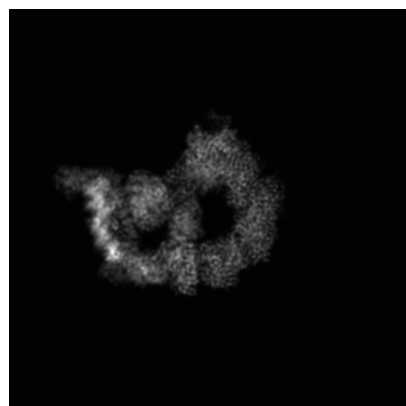
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36825. These allow visual inspection of the internal detail of the map and identification of artifacts.

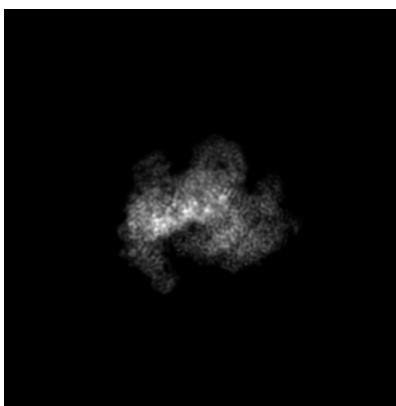
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

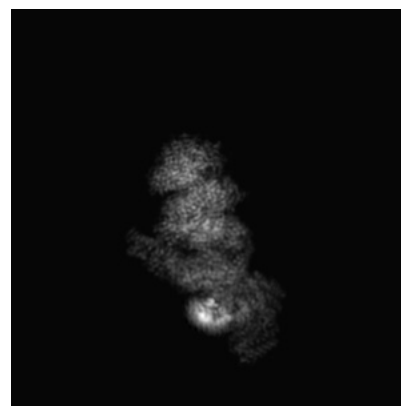
6.1.1 Primary map



X

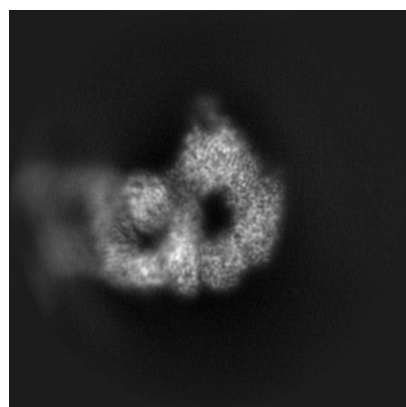


Y

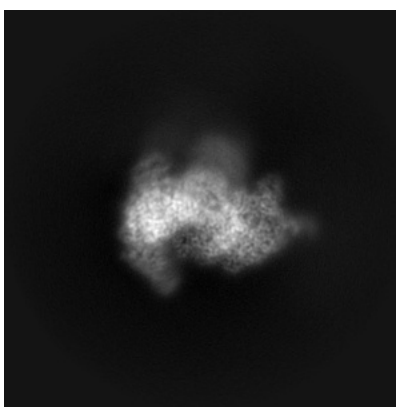


Z

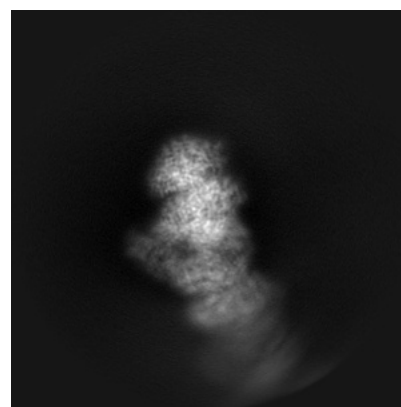
6.1.2 Raw map



X



Y

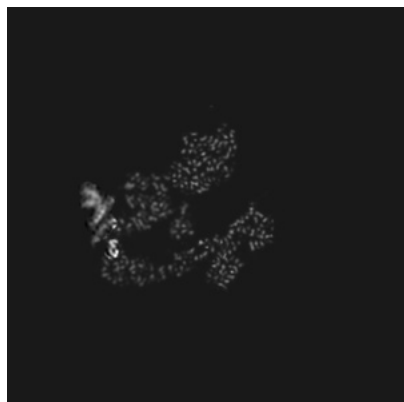


Z

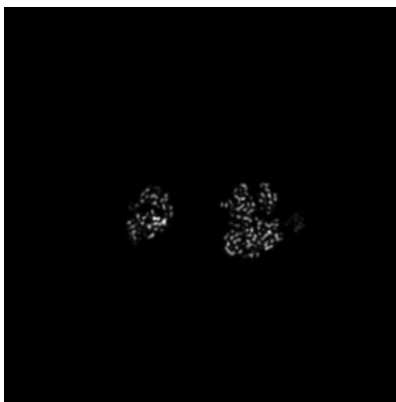
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

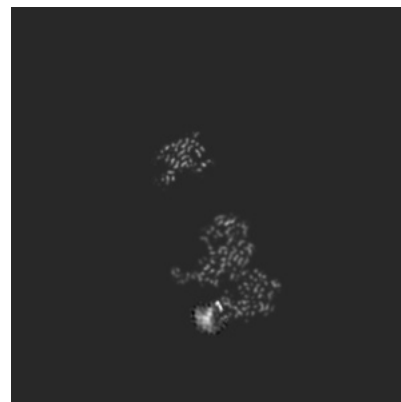
6.2.1 Primary map



X Index: 160

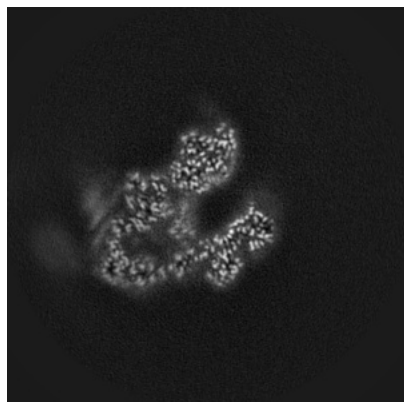


Y Index: 160

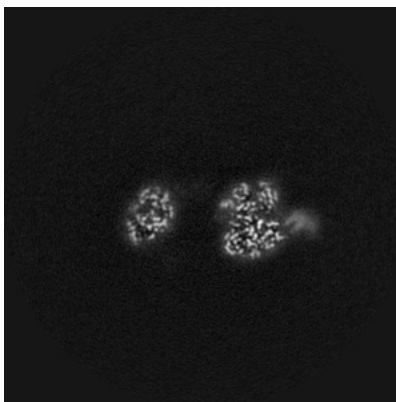


Z Index: 160

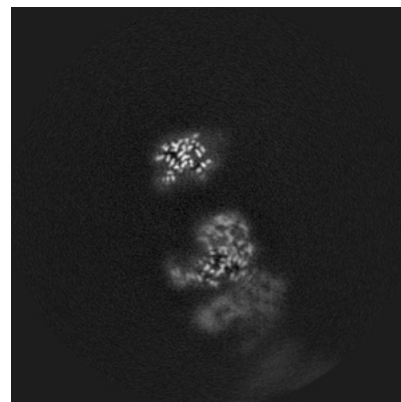
6.2.2 Raw map



X Index: 160



Y Index: 160

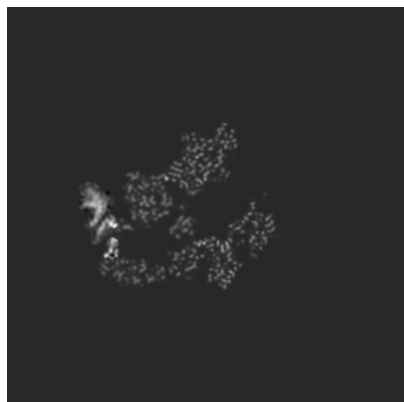


Z Index: 160

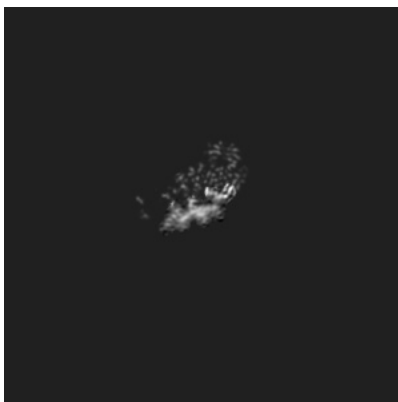
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 158

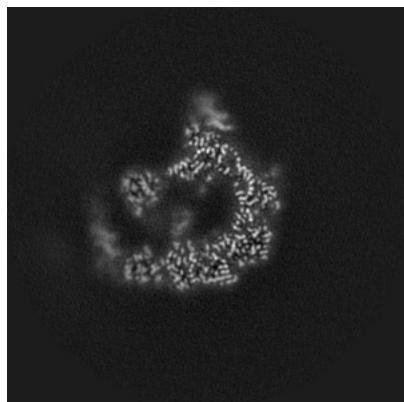


Y Index: 72

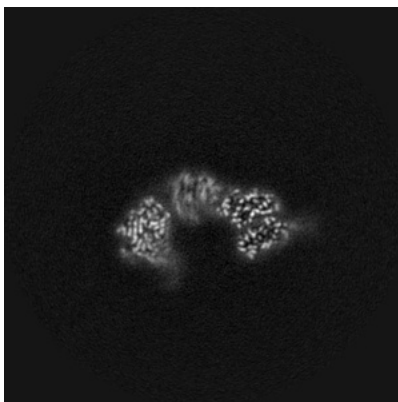


Z Index: 121

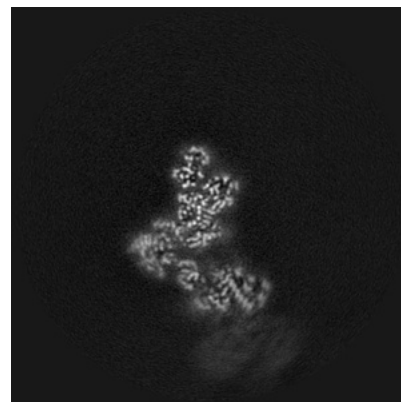
6.3.2 Raw map



X Index: 147



Y Index: 147

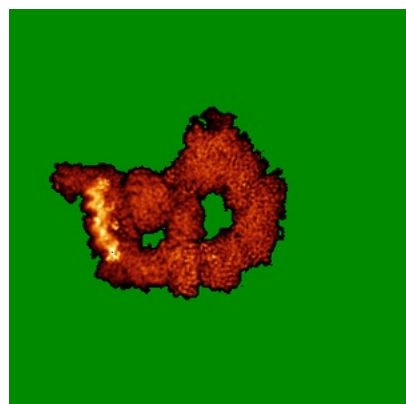


Z Index: 120

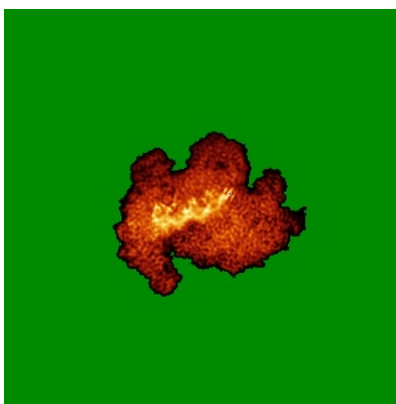
The images above show the largest variance slices of the map in three orthogonal directions.

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

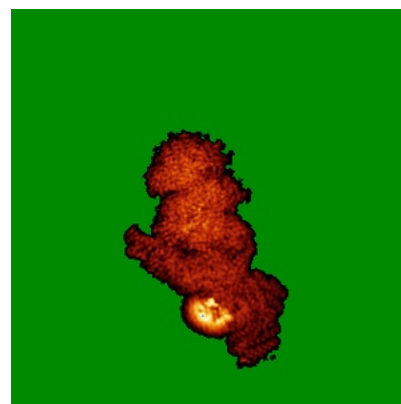
6.4.1 Primary map



X



Y



Z

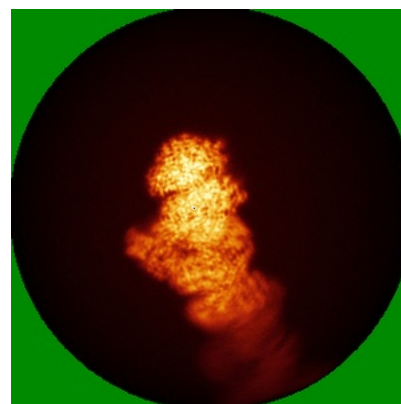
6.4.2 Raw map



X



Y

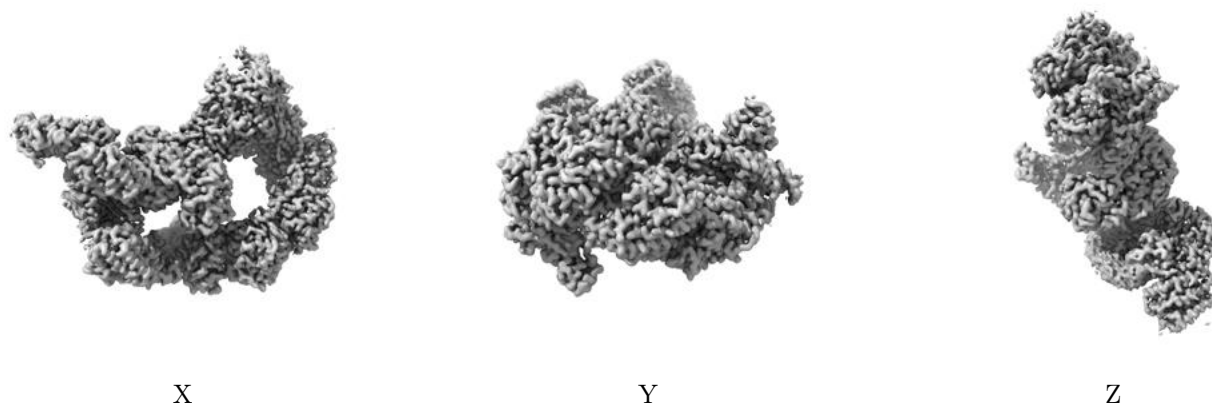


Z

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.

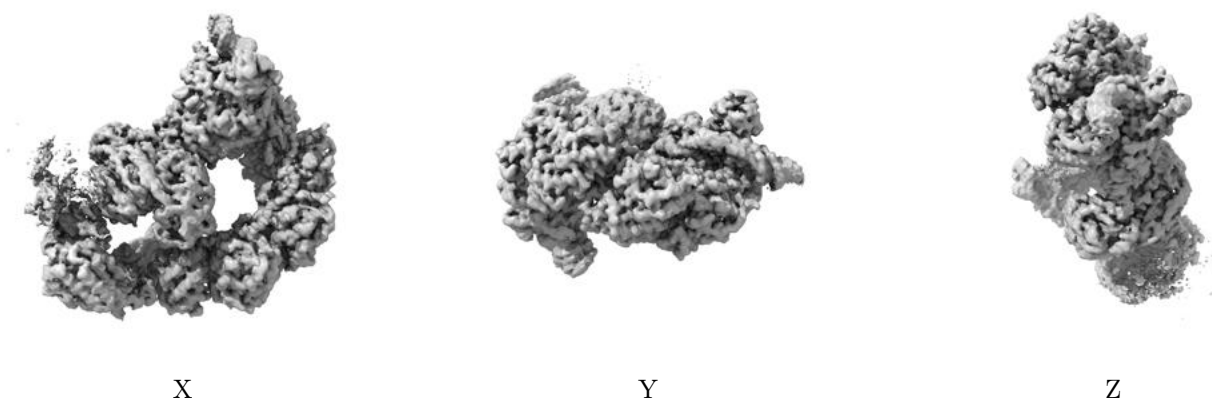
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

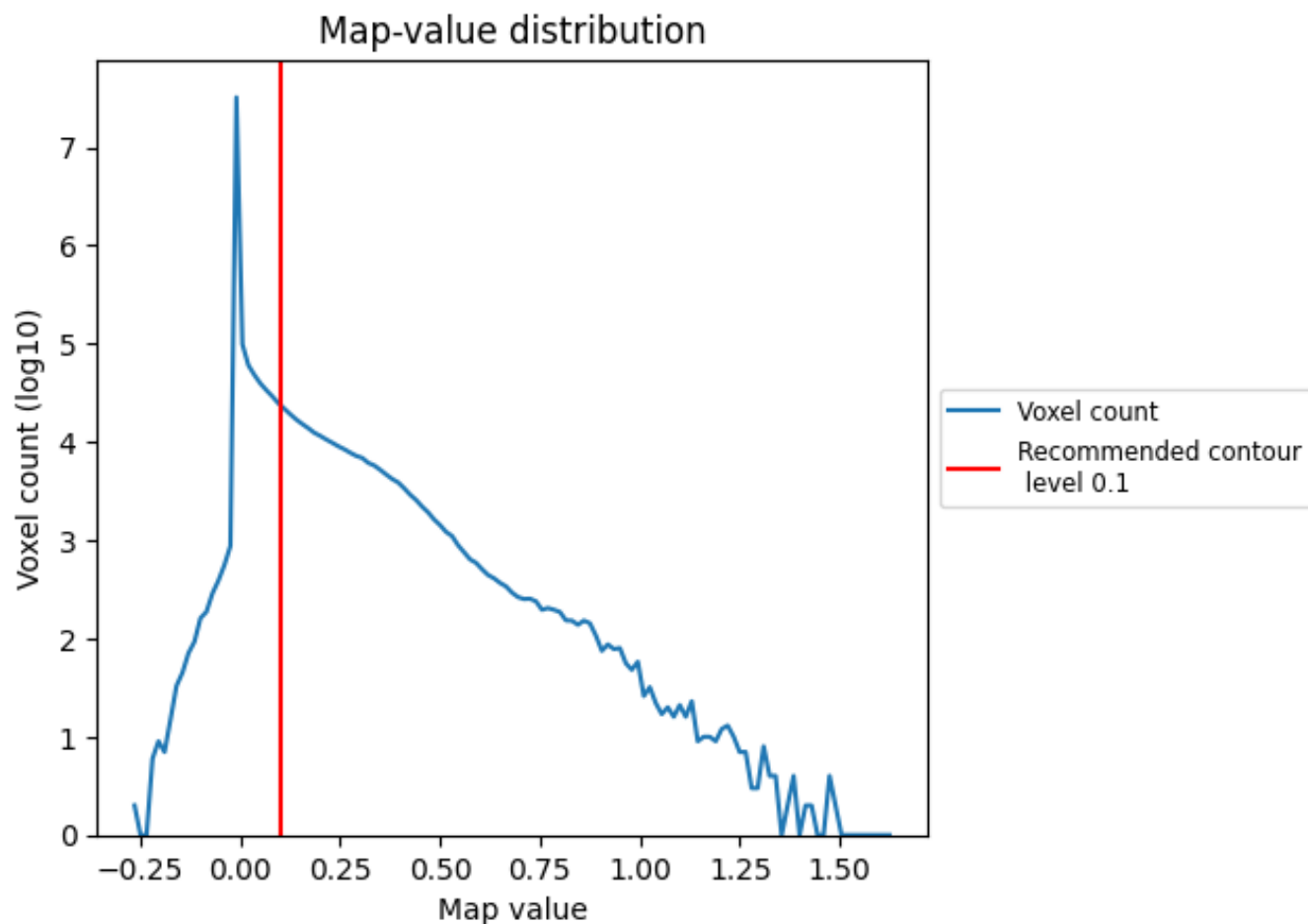
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

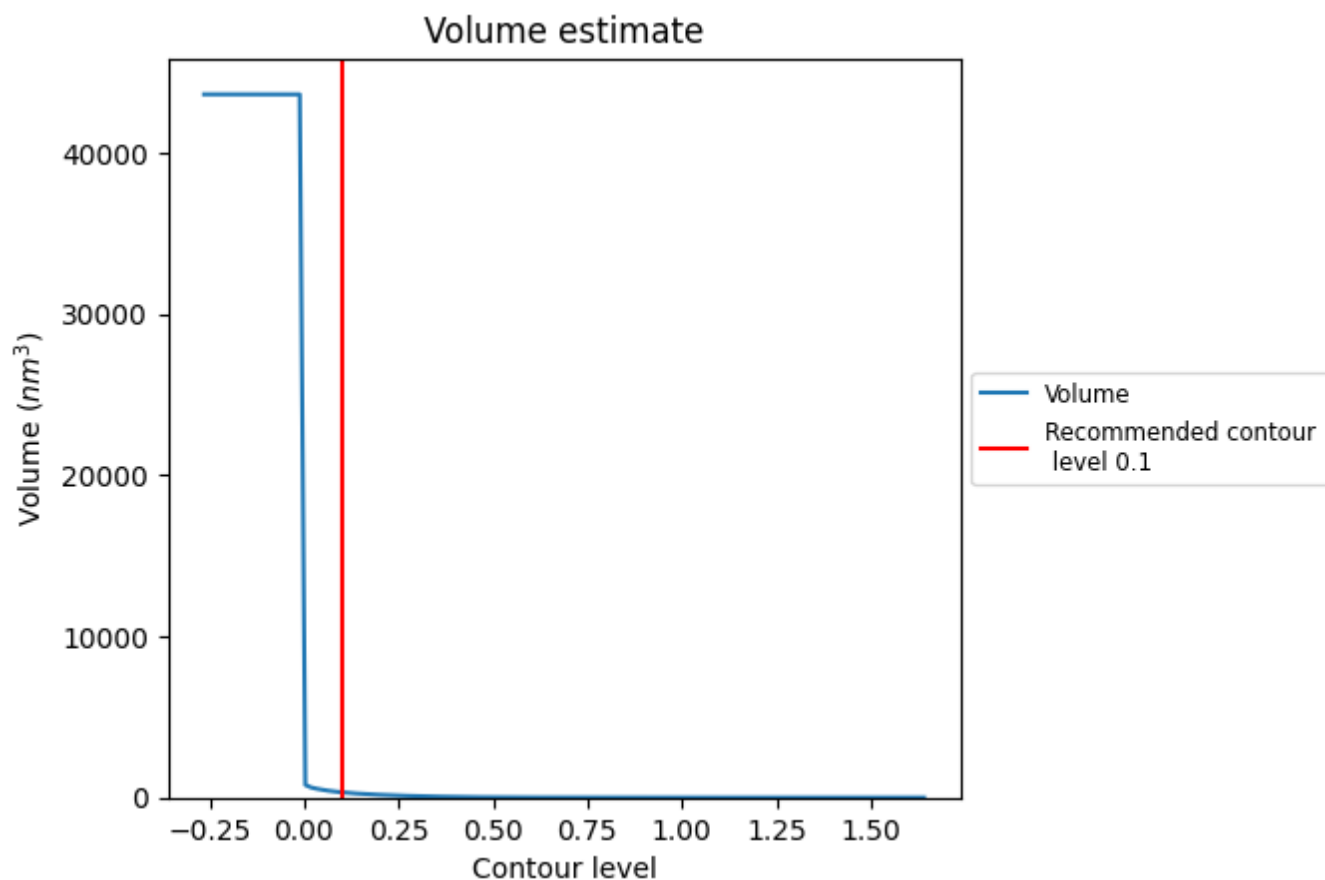
This section contains the results of statistical analysis of the map.

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.

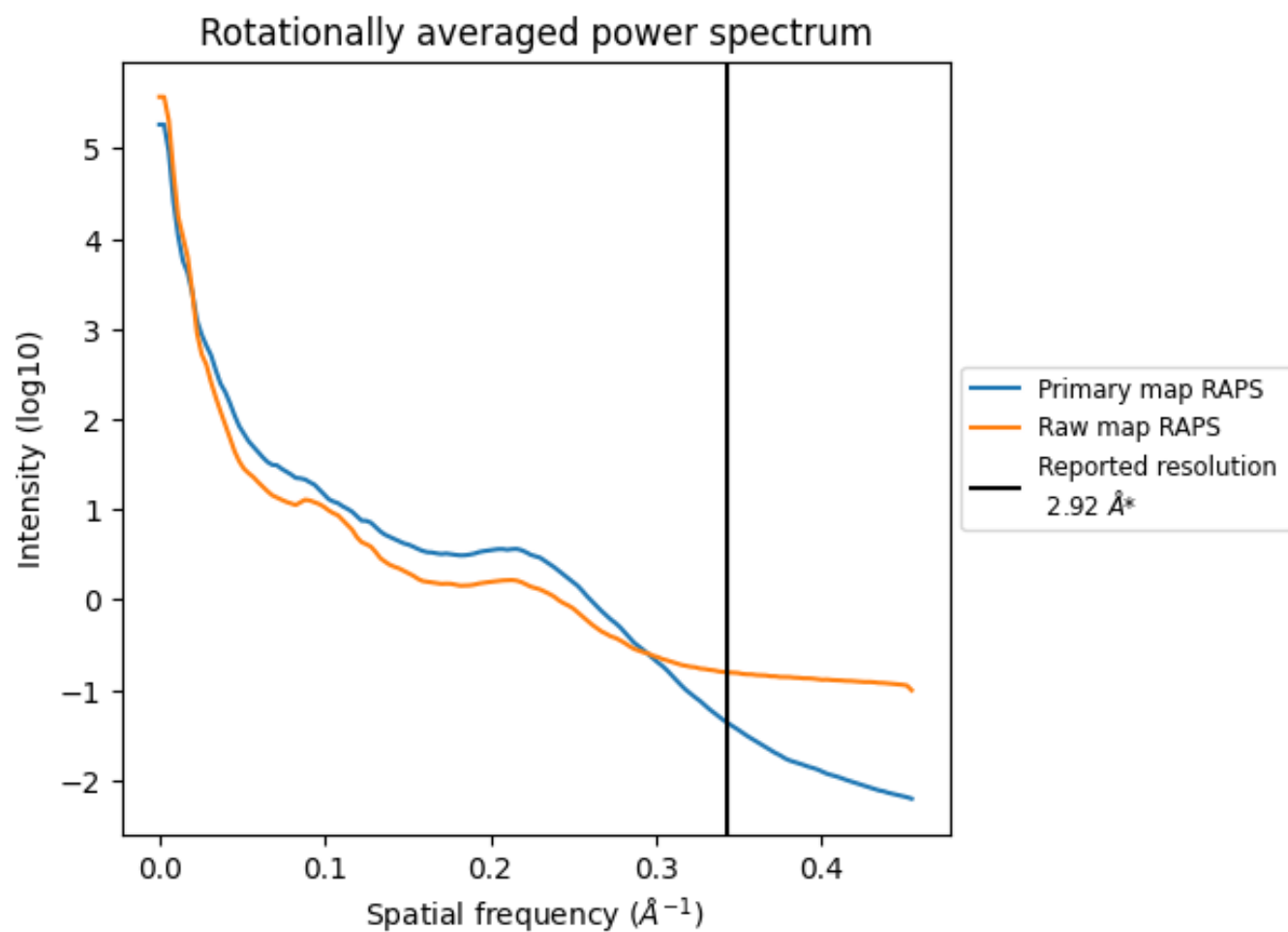
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; this corresponds to an approximate mass of 295 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 ⓘ

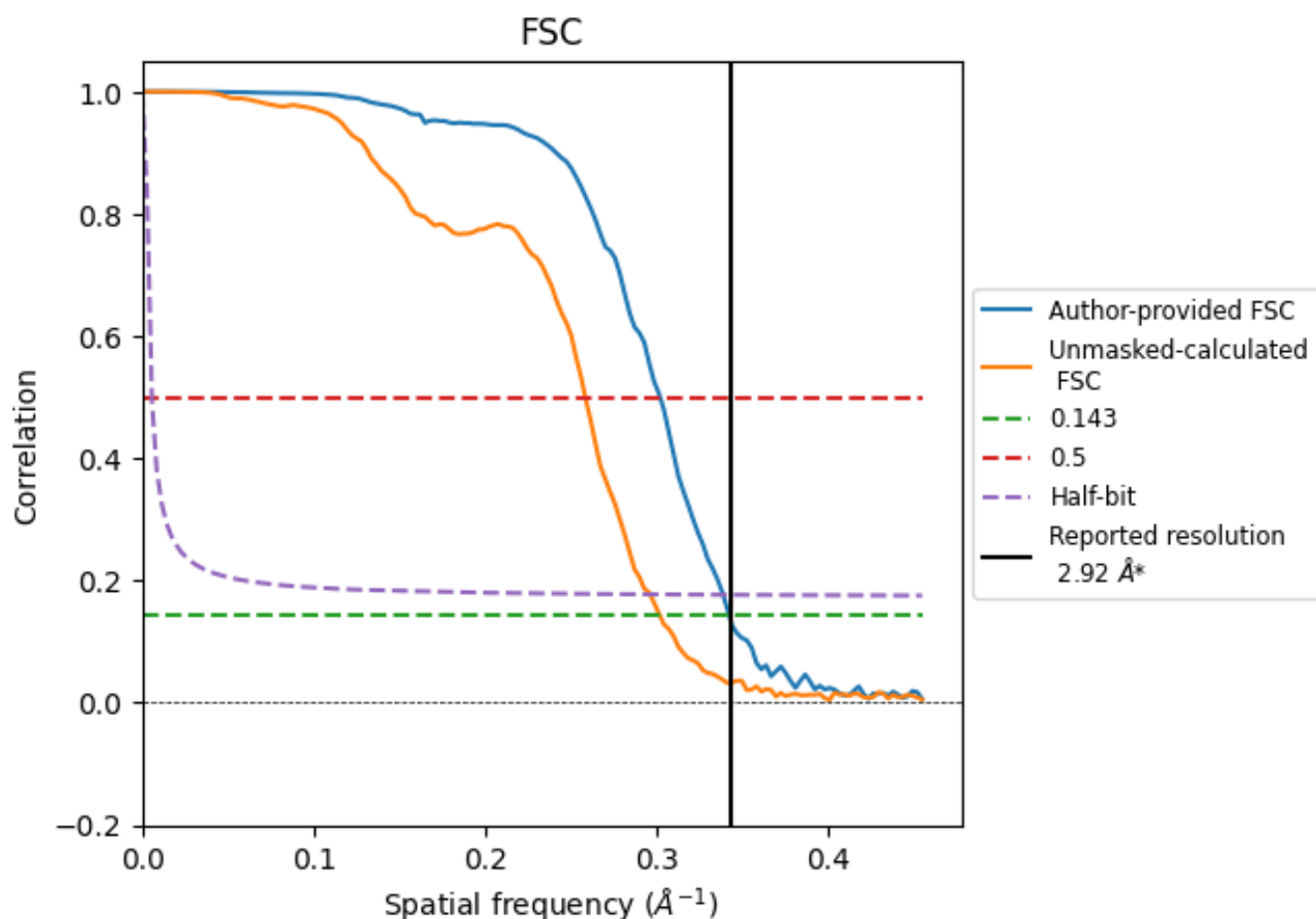


*Reported resolution corresponds to spatial frequency of 0.342 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

8.2 Resolution estimates [i](#)

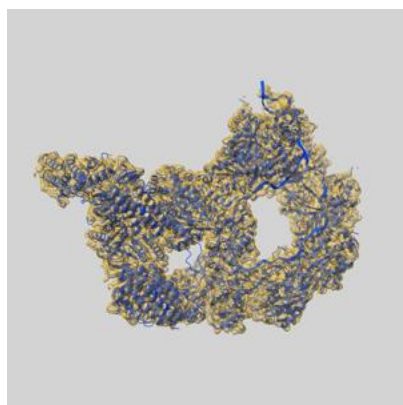
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.31	2.95
Unmasked-calculated*	3.32	3.87	3.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.92 by more than 10 %

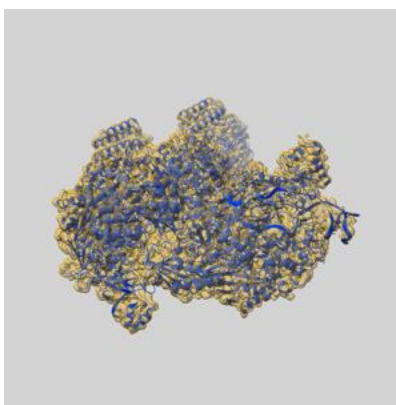
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36825 and PDB model 8K22. Per-residue inclusion information can be found in section [3](#) on page [7](#).

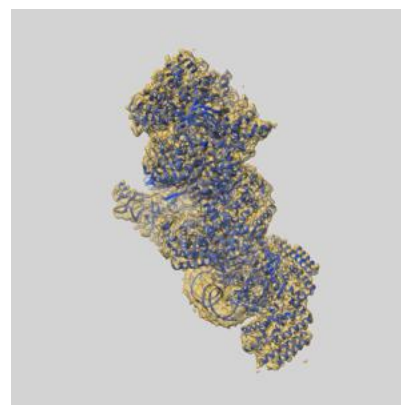
9.1 Map-model overlay [i](#)



X



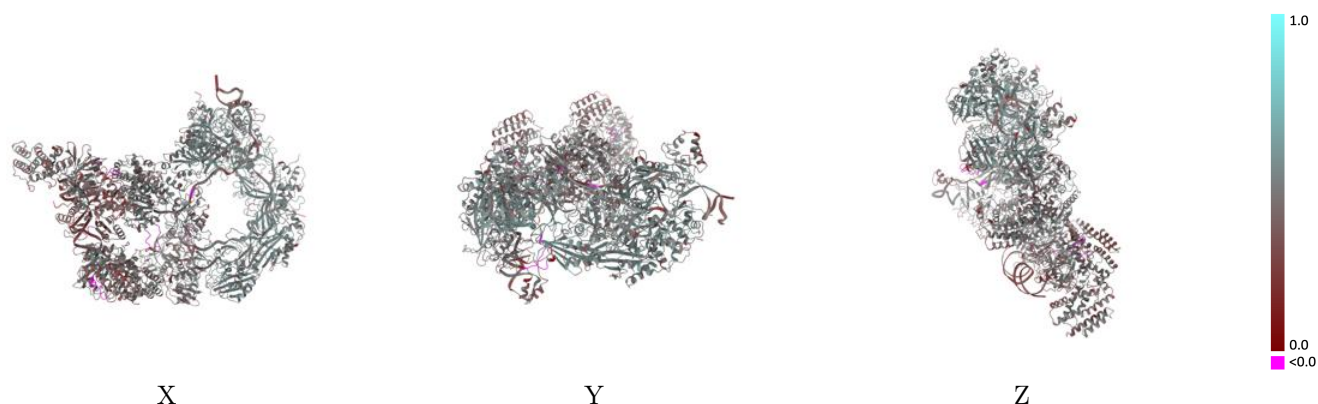
Y



Z

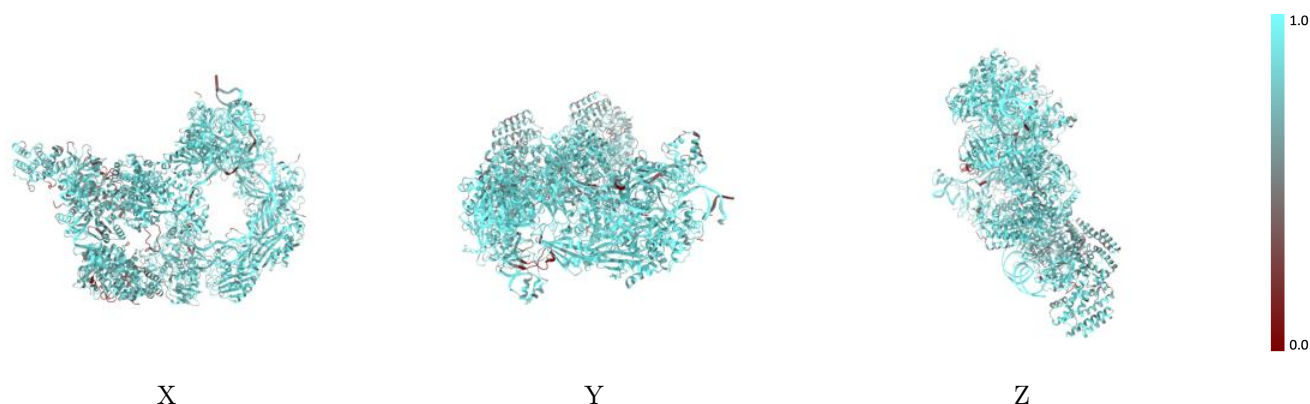
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



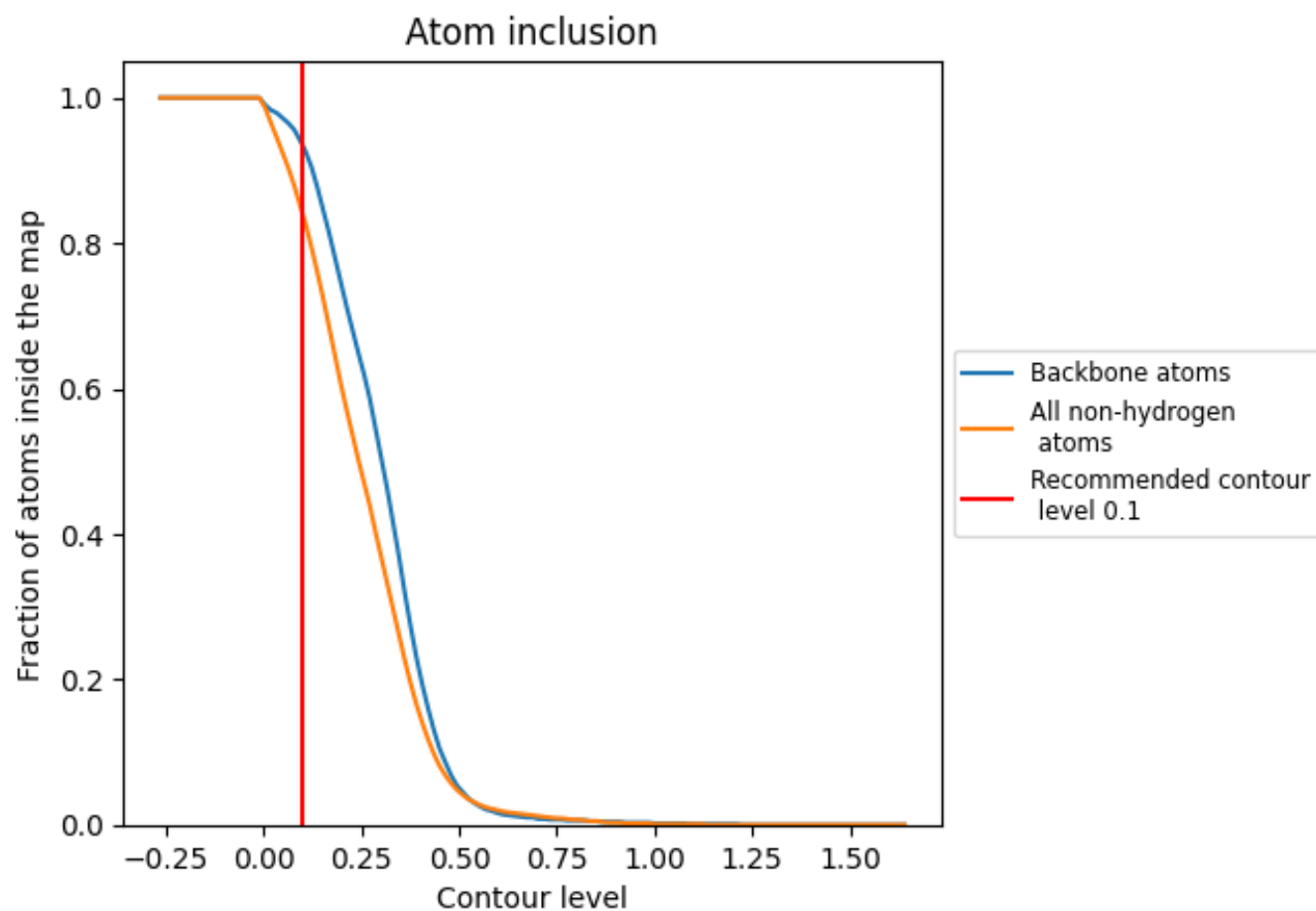
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 84% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.4480
A	 0.8440	 0.4300
B	 0.8570	 0.4840
C	 0.8920	 0.5040
D	 0.7750	 0.4130
E	 0.7700	 0.4250
G	 0.8830	 0.5120
H	 0.8270	 0.4030
I	 0.8780	 0.5110
J	 0.8950	 0.5090
K	 0.8910	 0.5010
L	 0.7970	 0.4240
M	 0.8810	 0.4980
P	 0.9210	 0.4620
Q	 0.8750	 0.4510
R	 0.6770	 0.3810
U	 0.9950	 0.2830
V	 0.9980	 0.2740
a	 0.7080	 0.3310
d	 0.7480	 0.3900
e	 0.7660	 0.4130

