



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 9NQ7 / pdb_00009nq7
EMDB ID : EMD-49645
Title : Cryo-EM structure of Csm/AcrIIIA2/enolase 4:3 complex
Authors : Goswami, H.N.; Li, H.
Deposited on : 2025-03-11
Resolution : 2.72 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:

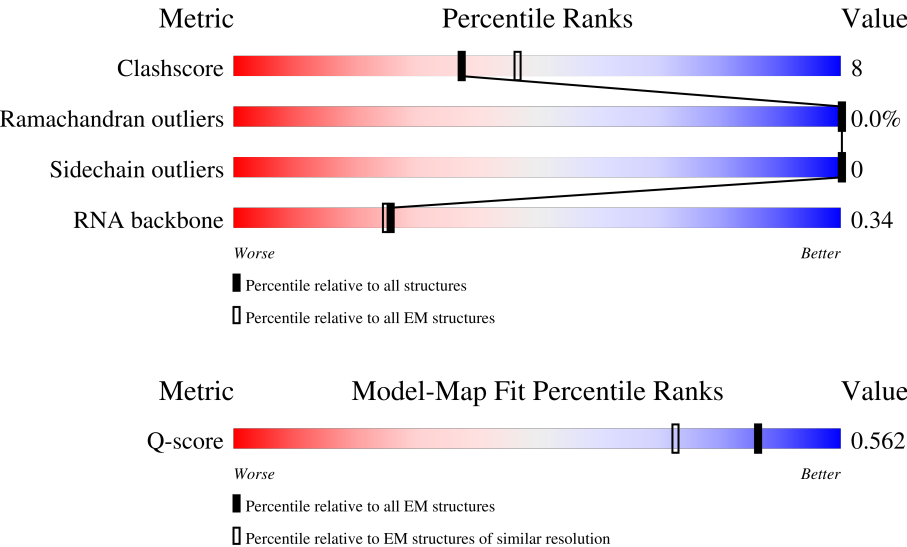
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.72 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	10355 (2.22 - 3.22)

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	R	41	
2	H	357	
3	A	758	

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Mol	Chain	Length	Quality of chain
4	B	299	
5	C	220	
5	E	220	
5	F	220	
5	G	220	
6	D	136	
6	I	136	
6	J	136	
7	K	434	
7	L	434	
7	M	434	
7	N	434	
7	O	434	
7	P	434	
7	Q	434	
7	S	434	
8	T	105	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 49556 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 RNA chain called RNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	41	Total	C	N	O	P	0	0
			863	389	151	283	40		

- Molecule 2 is a protein called CRISPR system Cms protein Csm5.

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

- Molecule 3 is a protein called CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

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

- Molecule 4 is a protein called CRISPR system Cms protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	297	Total	C	N	O	S	0	0
			2321	1485	384	447	5		

- Molecule 5 is a protein called CRISPR system Cms endoribonuclease Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	219	Total	C	N	O	S	0	0
			1707	1079	290	336	2		
5	C	220	Total	C	N	O	S	0	0
			1711	1083	292	333	3		
5	E	219	Total	C	N	O	S	0	0
			1706	1079	289	336	2		
5	G	219	Total	C	N	O	S	0	0
			1709	1081	290	336	2		

- Molecule 6 is a protein called CRISPR system Cms protein Csm2.

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

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP A0A8D6U6W4
D	-4	HIS	-	expression tag	UNP A0A8D6U6W4
D	-3	HIS	-	expression tag	UNP A0A8D6U6W4
D	-2	HIS	-	expression tag	UNP A0A8D6U6W4
D	-1	HIS	-	expression tag	UNP A0A8D6U6W4
D	0	HIS	-	expression tag	UNP A0A8D6U6W4
I	-5	HIS	-	expression tag	UNP A0A8D6U6W4
I	-4	HIS	-	expression tag	UNP A0A8D6U6W4
I	-3	HIS	-	expression tag	UNP A0A8D6U6W4
I	-2	HIS	-	expression tag	UNP A0A8D6U6W4
I	-1	HIS	-	expression tag	UNP A0A8D6U6W4
I	0	HIS	-	expression tag	UNP A0A8D6U6W4
J	-5	HIS	-	expression tag	UNP A0A8D6U6W4
J	-4	HIS	-	expression tag	UNP A0A8D6U6W4
J	-3	HIS	-	expression tag	UNP A0A8D6U6W4
J	-2	HIS	-	expression tag	UNP A0A8D6U6W4
J	-1	HIS	-	expression tag	UNP A0A8D6U6W4
J	0	HIS	-	expression tag	UNP A0A8D6U6W4

- Molecule 7 is a protein called Enolase.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	434	Total	C	N	O	S	0	0
			3305	2082	557	657	9		
7	N	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
S	253	HIS	ARG	conflict	UNP Q03LI0
S	257	GLY	ASP	conflict	UNP Q03LI0
L	253	HIS	ARG	conflict	UNP Q03LI0
L	257	GLY	ASP	conflict	UNP Q03LI0
P	253	HIS	ARG	conflict	UNP Q03LI0
P	257	GLY	ASP	conflict	UNP Q03LI0
K	253	HIS	ARG	conflict	UNP Q03LI0
K	257	GLY	ASP	conflict	UNP Q03LI0
M	253	HIS	ARG	conflict	UNP Q03LI0
M	257	GLY	ASP	conflict	UNP Q03LI0
O	253	HIS	ARG	conflict	UNP Q03LI0
O	257	GLY	ASP	conflict	UNP Q03LI0
N	253	HIS	ARG	conflict	UNP Q03LI0
N	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	T	105	Total	C	N	O	S	0	0
			859	543	153	159	4		

There is a discrepancy between the modelled and reference sequences:

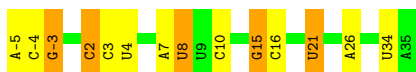
Chain	Residue	Modelled	Actual	Comment	Reference
T	105	VAL	-	expression tag	UNP A0A3G8FB66

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.

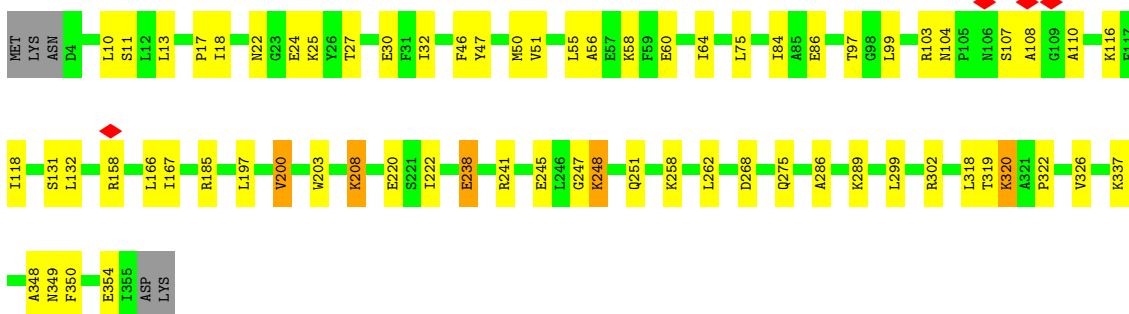
- Molecule 1: RNA (41-MER)

Chain R: 



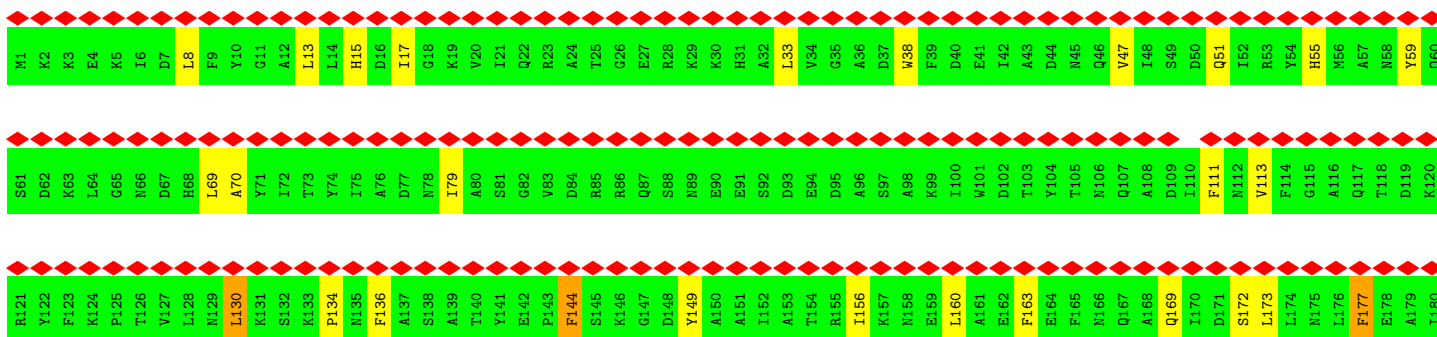
- Molecule 2: CRISPR system Cms protein Csm5

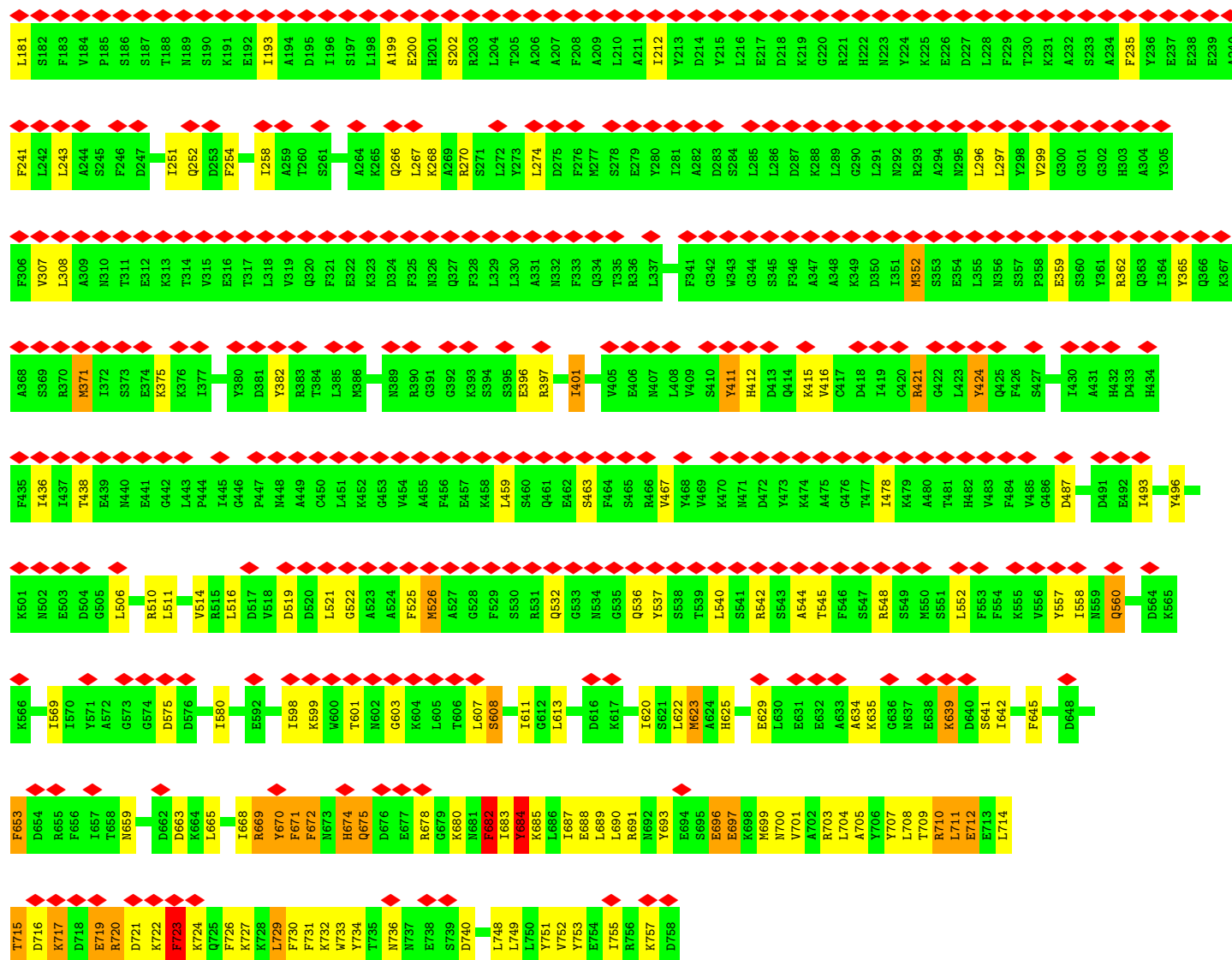
Chain H: 



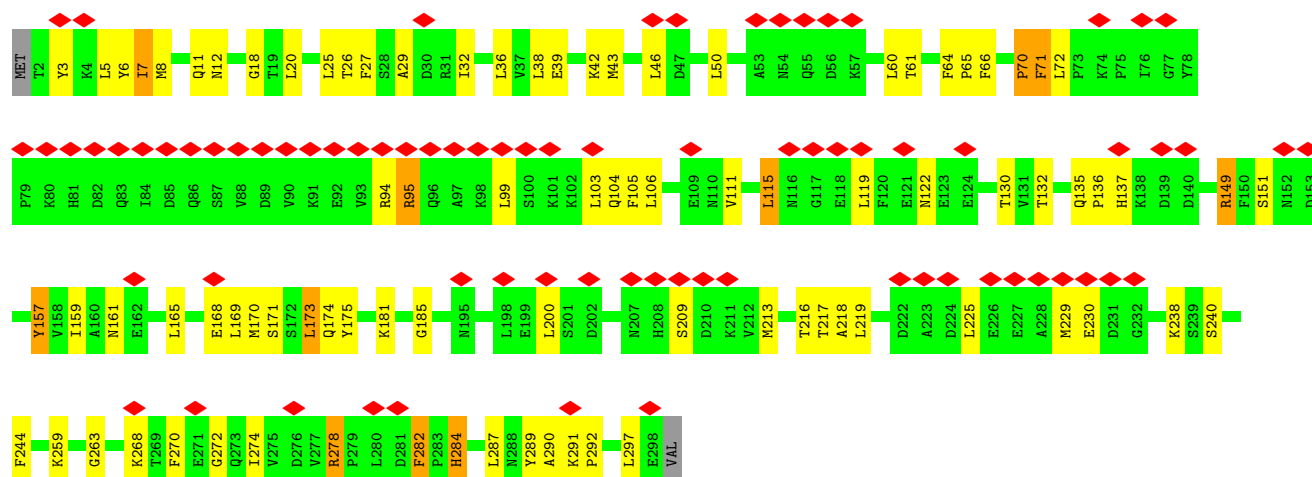
- Molecule 3: CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A)

Chain A: 

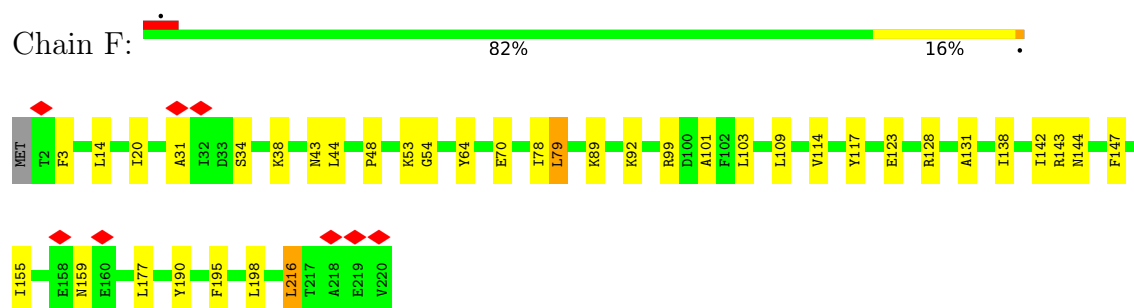




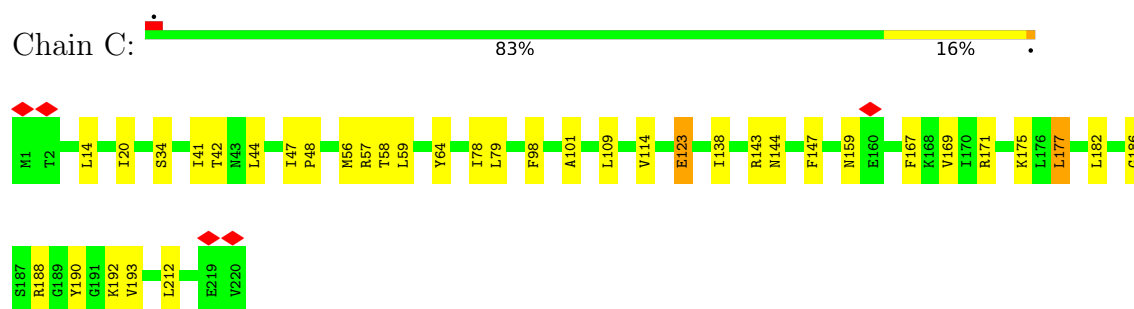
• Molecule 4: CRISPR system Cms protein Csm4



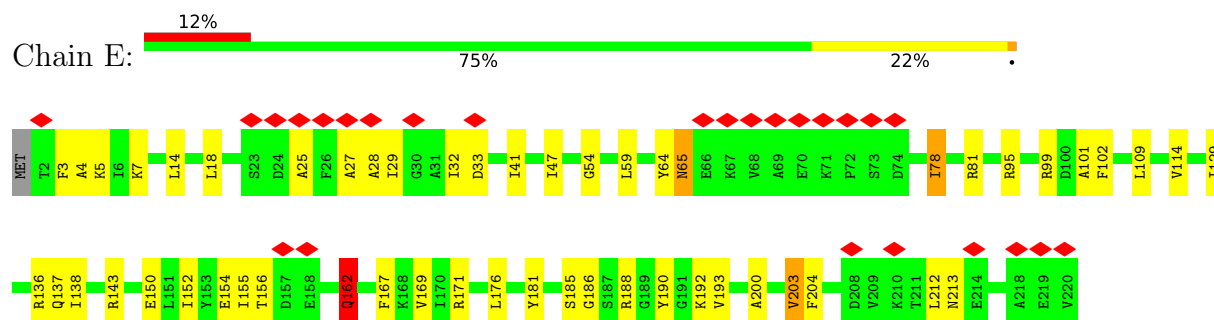
- Molecule 5: CRISPR system Cms endoribonuclease Csm3



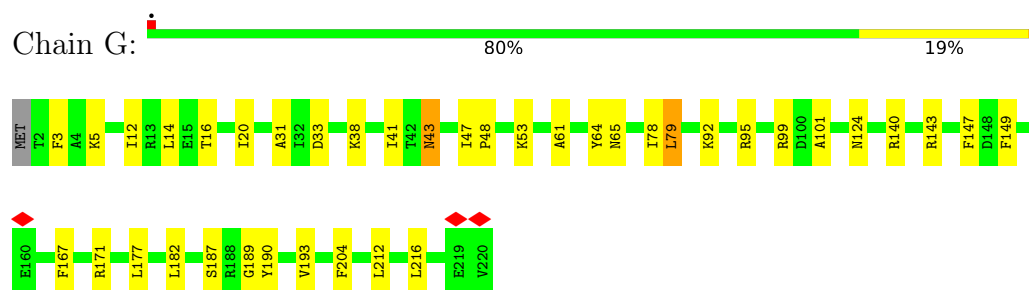
- Molecule 5: CRISPR system Cms endoribonuclease Csm3



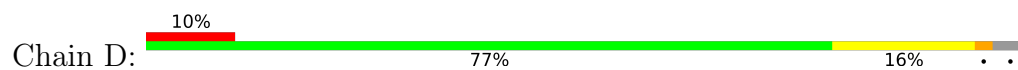
- Molecule 5: CRISPR system Cms endoribonuclease Csm3

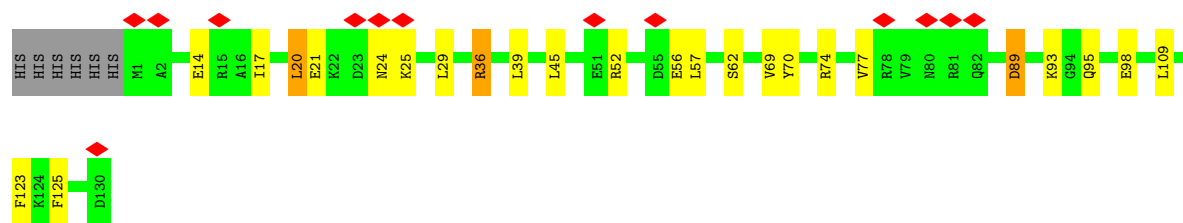


- Molecule 5: CRISPR system Cms endoribonuclease Csm3

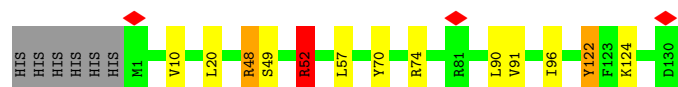
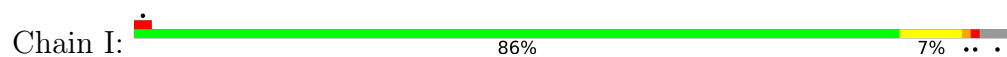


- Molecule 6: CRISPR system Cms protein Csm2

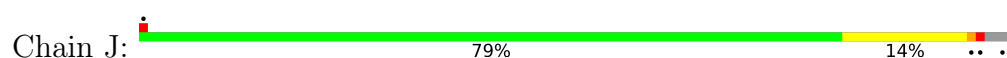




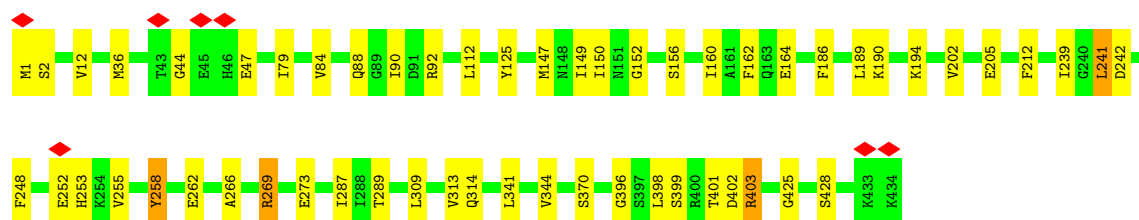
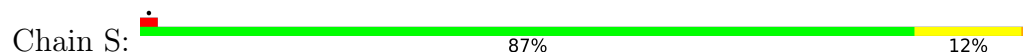
- Molecule 6: CRISPR system Cms protein Csm2



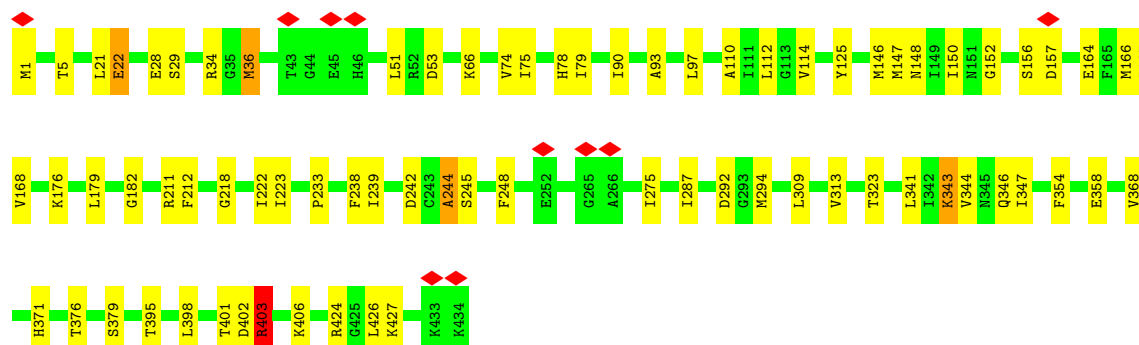
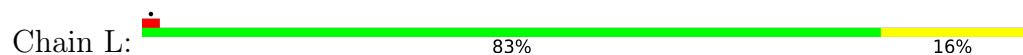
- Molecule 6: CRISPR system Cms protein Csm2



- Molecule 7: Enolase

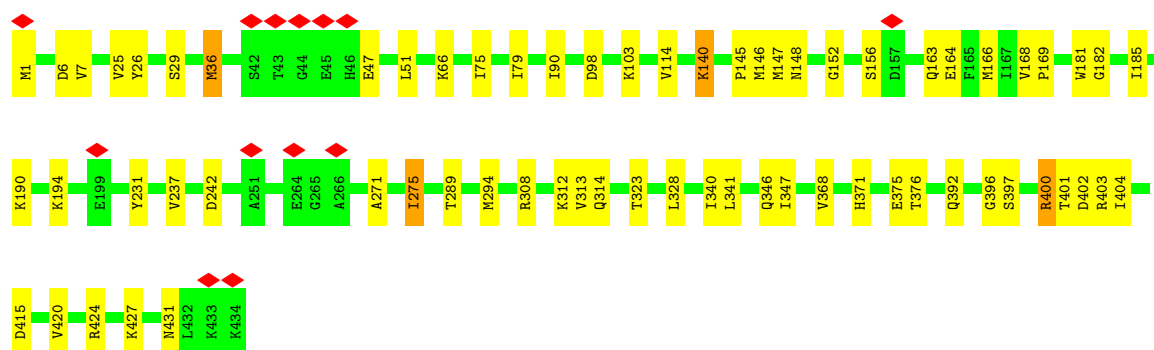


- Molecule 7: Enolase



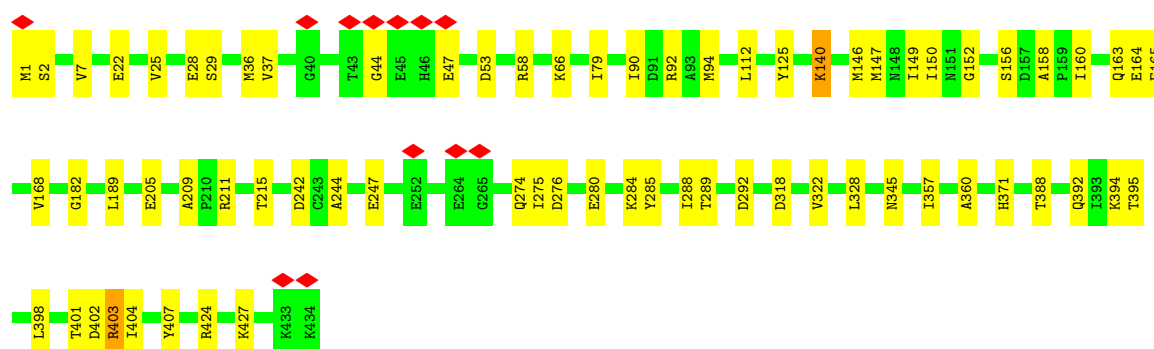
- Molecule 7: Enolase

Chain P:  85% 15%



• Molecule 7: Enolase

Chain K:  84% 16%



• Molecule 7: Enolase

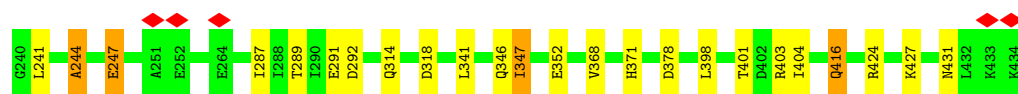
Chain M:  85% 14%



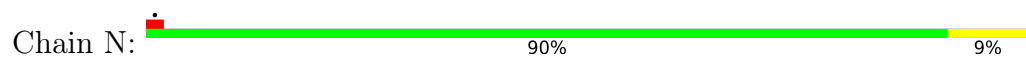
• Molecule 7: Enolase

Chain O:  88% 11%

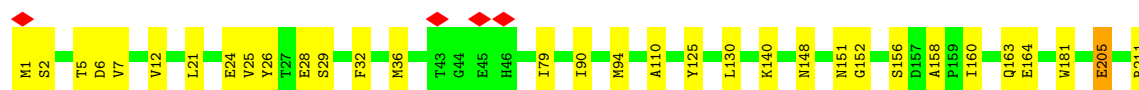
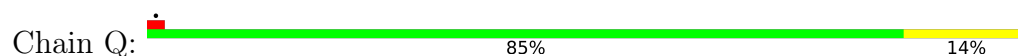




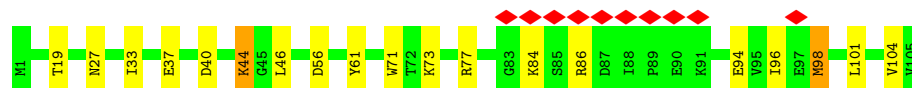
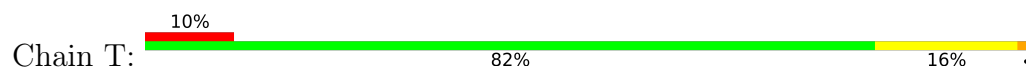
• Molecule 7: Enolase



• Molecule 7: Enolase



• Molecule 8: AcrIIA2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325120	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	1.920	Depositor
Minimum map value	-0.716	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.19	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 ⓘ

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	R	0.36	0/964	0.52	0/1498
2	H	0.87	9/2930 (0.3%)	0.87	12/3940 (0.3%)
3	A	0.96	50/6264 (0.8%)	1.03	37/8436 (0.4%)
4	B	0.87	15/2373 (0.6%)	0.81	8/3215 (0.2%)
5	C	0.55	2/1736 (0.1%)	0.62	1/2338 (0.0%)
5	E	0.77	4/1731 (0.2%)	0.77	1/2335 (0.0%)
5	F	0.54	4/1732 (0.2%)	0.61	1/2335 (0.0%)
5	G	0.62	4/1734 (0.2%)	0.69	4/2337 (0.2%)
6	D	0.70	3/1095 (0.3%)	0.66	0/1465
6	I	0.85	4/1095 (0.4%)	0.70	5/1465 (0.3%)
6	J	1.01	9/1095 (0.8%)	1.13	15/1465 (1.0%)
7	K	0.54	6/3362 (0.2%)	0.59	2/4548 (0.0%)
7	L	0.61	7/3362 (0.2%)	0.67	7/4548 (0.2%)
7	M	0.54	7/3362 (0.2%)	0.68	8/4548 (0.2%)
7	N	0.49	3/3362 (0.1%)	0.60	4/4548 (0.1%)
7	O	0.59	9/3362 (0.3%)	0.63	2/4548 (0.0%)
7	P	0.53	4/3362 (0.1%)	0.61	4/4548 (0.1%)
7	Q	0.46	3/3362 (0.1%)	0.55	3/4548 (0.1%)
7	S	0.46	5/3362 (0.1%)	0.52	1/4548 (0.0%)
8	T	0.85	3/880 (0.3%)	0.80	2/1184 (0.2%)
All	All	0.68	151/50525 (0.3%)	0.73	117/68397 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2
3	A	0	8
4	B	0	1
5	E	0	2
6	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	I	0	1
6	J	0	2
7	L	0	1
7	N	0	1
7	O	0	2
7	P	0	1
8	T	0	1
All	All	0	23

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	167	ILE	CA-C	-28.10	1.31	1.53
6	I	48	ARG	CB-CG	-16.55	1.02	1.52
3	A	715	THR	CB-CG2	-16.54	0.97	1.52
4	B	157	TYR	CZ-OH	-15.29	1.05	1.38
3	A	699	MET	CB-CG	-14.36	1.09	1.52
5	E	203	VAL	CB-CG1	-13.64	1.07	1.52
3	A	130	LEU	C-O	-13.29	1.08	1.24
3	A	719	GLU	CG-CD	-13.26	1.19	1.52
8	T	98	MET	SD-CE	-13.10	1.46	1.79
3	A	719	GLU	CD-OE1	-12.36	1.01	1.25
3	A	487	ASP	CG-OD1	-12.18	1.02	1.25
6	I	48	ARG	CG-CD	11.94	1.88	1.52
3	A	682	PHE	CA-CB	-11.80	1.32	1.53
4	B	95	ARG	CZ-NH1	-11.74	1.16	1.32
6	J	17	ILE	CG1-CD1	-11.47	1.07	1.51
3	A	696	GLU	CD-OE1	-11.32	1.03	1.25
3	A	682	PHE	CG-CD1	11.02	1.61	1.38
6	J	52	ARG	NE-CZ	-10.77	1.21	1.33
5	G	216	LEU	CG-CD1	-10.39	1.18	1.52
7	L	36	MET	SD-CE	-10.35	1.53	1.79
3	A	268	LYS	CD-CE	-10.29	1.21	1.52
7	K	244	ALA	CA-CB	-10.10	1.36	1.53
6	I	52	ARG	CZ-NH1	-10.04	1.18	1.32
2	H	167	ILE	N-CA	10.02	1.53	1.46
8	T	44	LYS	CE-NZ	-9.92	1.19	1.49
2	H	167	ILE	C-N	9.53	1.46	1.33
7	L	5	THR	CB-CG2	-9.37	1.21	1.52
6	J	52	ARG	CD-NE	-9.35	1.33	1.46
3	A	684	TYR	CA-C	-9.21	1.41	1.52
6	J	14	GLU	CD-OE1	-9.04	1.08	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	60	ASP	CG-OD1	-9.03	1.08	1.25
3	A	723	PHE	CD2-CE2	-8.86	1.12	1.38
3	A	684	TYR	C-O	-8.81	1.13	1.24
3	A	421	ARG	CZ-NH1	-8.80	1.20	1.32
7	K	392	GLN	CD-NE2	-8.78	1.14	1.33
7	O	347	ILE	CG1-CD1	-8.37	1.19	1.51
3	A	421	ARG	CG-CD	-8.34	1.27	1.52
6	D	20	LEU	CG-CD1	-8.22	1.25	1.52
3	A	672	PHE	CE1-CZ	-8.13	1.14	1.38
6	J	48	ARG	CZ-NH1	-8.04	1.21	1.32
7	N	334	GLU	CD-OE1	-8.01	1.10	1.25
7	S	252	GLU	CD-OE1	-7.99	1.10	1.25
7	P	294	MET	SD-CE	-7.95	1.59	1.79
7	O	247	GLU	CD-OE1	-7.80	1.10	1.25
3	A	421	ARG	NE-CZ	-7.71	1.24	1.33
3	A	401	ILE	CG1-CD1	-7.66	1.21	1.51
3	A	560	GLN	CD-NE2	-7.64	1.17	1.33
7	L	294	MET	SD-CE	-7.62	1.60	1.79
5	C	123	GLU	CD-OE1	-7.60	1.10	1.25
3	A	712	GLU	CG-CD	-7.52	1.33	1.52
3	A	639	LYS	CE-NZ	-7.48	1.26	1.49
2	H	248	LYS	CD-CE	-7.47	1.30	1.52
7	L	244	ALA	CA-CB	-7.42	1.41	1.53
4	B	282	PHE	CE2-CZ	-7.36	1.16	1.38
3	A	688	GLU	CD-OE1	-7.24	1.11	1.25
4	B	157	TYR	CD1-CE1	-7.10	1.17	1.38
7	Q	398	LEU	CG-CD2	-7.08	1.29	1.52
3	A	371	MET	SD-CE	-7.07	1.61	1.79
2	H	167	ILE	C-O	7.06	1.33	1.24
3	A	144	PHE	CD1-CE1	-6.86	1.18	1.38
6	J	48	ARG	CZ-NH2	-6.84	1.24	1.33
5	C	159	ASN	CG-OD1	-6.75	1.10	1.23
7	M	223	ILE	CG1-CD1	-6.71	1.25	1.51
3	A	674	HIS	CA-CB	-6.69	1.43	1.53
7	M	163	GLN	CD-NE2	-6.65	1.19	1.33
3	A	560	GLN	CD-OE1	-6.63	1.10	1.23
5	F	216	LEU	CG-CD1	-6.60	1.30	1.52
5	G	79	LEU	CG-CD1	-6.58	1.30	1.52
3	A	552	LEU	CG-CD1	-6.56	1.30	1.52
4	B	278	ARG	CG-CD	-6.51	1.32	1.52
7	P	36	MET	SD-CE	-6.49	1.63	1.79
7	O	241	LEU	CG-CD2	-6.45	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	86	GLU	CD-OE2	-6.43	1.13	1.25
7	S	241	LEU	CG-CD2	-6.39	1.31	1.52
4	B	70	PRO	N-CD	6.37	1.56	1.47
4	B	157	TYR	CE1-CZ	-6.36	1.23	1.38
7	O	291	GLU	CD-OE1	-6.34	1.13	1.25
7	K	140	LYS	CD-CE	-6.34	1.33	1.52
7	M	227	GLU	CD-OE1	-6.33	1.13	1.25
7	S	403	ARG	CG-CD	-6.26	1.33	1.52
3	A	682	PHE	CB-CG	6.23	1.65	1.50
3	A	266	GLN	CB-CG	-6.21	1.33	1.52
7	N	252	GLU	CG-CD	-6.21	1.36	1.52
3	A	177	PHE	CD2-CE2	-6.16	1.20	1.38
3	A	675	GLN	CB-CG	-6.12	1.34	1.52
7	L	22	GLU	CD-OE2	-6.09	1.13	1.25
5	F	159	ASN	CG-OD1	-6.06	1.12	1.23
5	E	65	ASN	CG-ND2	-6.06	1.20	1.33
6	J	48	ARG	CG-CD	-6.03	1.34	1.52
3	A	308	LEU	CG-CD1	-6.01	1.32	1.52
7	M	347	ILE	CB-CG1	-6.01	1.41	1.53
3	A	177	PHE	CE1-CZ	-6.01	1.20	1.38
8	T	73	LYS	CD-CE	-6.00	1.34	1.52
2	H	208	LYS	CE-NZ	-6.00	1.31	1.49
3	A	723	PHE	CE1-CZ	-6.00	1.20	1.38
6	D	89	ASP	CG-OD1	-5.97	1.14	1.25
7	P	140	LYS	CD-CE	-5.91	1.34	1.52
4	B	7	ILE	CG1-CD1	-5.91	1.28	1.51
7	S	269	ARG	CZ-NH1	-5.90	1.24	1.32
3	A	599	LYS	CD-CE	-5.89	1.34	1.52
2	H	200	VAL	CB-CG1	-5.88	1.33	1.52
7	M	252	GLU	CB-CG	-5.86	1.34	1.52
3	A	682	PHE	CG-CD2	5.84	1.51	1.38
7	L	403	ARG	CZ-NH1	-5.82	1.24	1.32
5	G	65	ASN	CG-OD1	-5.80	1.12	1.23
7	O	194	LYS	CE-NZ	-5.79	1.31	1.49
4	B	282	PHE	CG-CD2	-5.78	1.26	1.38
3	A	711	LEU	CG-CD2	-5.73	1.33	1.52
7	L	358	GLU	CD-OE1	-5.69	1.14	1.25
3	A	697	GLU	CD-OE1	-5.67	1.14	1.25
5	E	65	ASN	CB-CG	-5.61	1.38	1.52
3	A	623	MET	SD-CE	-5.58	1.65	1.79
7	O	244	ALA	CA-CB	-5.57	1.44	1.53
7	M	252	GLU	CG-CD	-5.55	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	275	ILE	CG1-CD1	-5.54	1.30	1.51
3	A	424	TYR	CZ-OH	-5.48	1.26	1.38
7	P	415	ASP	CG-OD2	-5.47	1.15	1.25
4	B	132	THR	CB-CG2	-5.45	1.34	1.52
3	A	729	LEU	CB-CG	-5.44	1.42	1.53
7	Q	151	ASN	CB-CG	-5.44	1.38	1.52
6	J	122	TYR	CB-CG	-5.42	1.39	1.51
4	B	278	ARG	CB-CG	-5.42	1.36	1.52
3	A	653	PHE	CE1-CZ	-5.40	1.22	1.38
5	G	43	ASN	CG-OD1	-5.40	1.13	1.23
3	A	670	TYR	CZ-OH	5.36	1.49	1.38
4	B	70	PRO	N-CA	-5.35	1.40	1.47
4	B	157	TYR	CE2-CZ	-5.34	1.25	1.38
6	D	14	GLU	CD-OE2	-5.34	1.15	1.25
3	A	671	PHE	C-O	-5.34	1.17	1.24
4	B	230	GLU	CD-OE1	-5.33	1.15	1.25
5	F	43	ASN	CG-OD1	-5.31	1.13	1.23
3	A	411	TYR	CA-CB	-5.27	1.43	1.53
7	N	88	GLN	CD-OE1	-5.27	1.13	1.23
7	O	88	GLN	CD-OE1	-5.25	1.13	1.23
3	A	653	PHE	CD2-CE2	-5.24	1.23	1.38
3	A	526	MET	SD-CE	-5.22	1.66	1.79
3	A	653	PHE	CG-CD2	-5.18	1.27	1.38
7	O	131	TYR	CD2-CE2	-5.18	1.23	1.38
6	I	122	TYR	CE1-CZ	-5.15	1.25	1.38
2	H	354	GLU	CD-OE1	-5.13	1.15	1.25
3	A	608	SER	CA-CB	-5.13	1.43	1.53
7	K	274	GLN	CG-CD	-5.11	1.39	1.52
7	Q	205	GLU	CD-OE2	-5.07	1.15	1.25
4	B	200	LEU	CG-CD2	-5.07	1.35	1.52
7	O	346	GLN	CB-CG	-5.06	1.37	1.52
3	A	200	GLU	CG-CD	-5.06	1.39	1.52
7	S	258	TYR	CE2-CZ	-5.05	1.26	1.38
7	K	392	GLN	CG-CD	-5.05	1.39	1.52
5	F	79	LEU	CG-CD1	-5.03	1.35	1.52
7	M	325	THR	CB-CG2	-5.01	1.36	1.52
5	E	78	ILE	CG1-CD1	-5.00	1.32	1.51

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	699	MET	CA-CB-CG	27.82	169.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	167	ILE	O-C-N	-20.70	106.85	121.55
2	H	167	ILE	CA-C-O	20.30	130.49	119.12
3	A	723	PHE	CZ-CE2-CD2	18.59	153.46	120.00
3	A	696	GLU	OE1-CD-OE2	-17.49	80.92	122.90
3	A	684	TYR	CA-C-O	-17.02	102.38	120.42
3	A	699	MET	N-CA-CB	16.93	136.85	110.44
6	J	48	ARG	NH1-CZ-NH2	-15.68	98.92	119.30
3	A	723	PHE	CG-CD2-CE2	-15.59	94.19	120.70
2	H	326	VAL	CG1-CB-CG2	-15.44	76.83	110.80
3	A	711	LEU	CB-CG-CD2	-14.35	67.66	110.70
3	A	672	PHE	CE1-CZ-CE2	13.82	144.87	120.00
3	A	723	PHE	CE1-CZ-CE2	-13.56	95.58	120.00
3	A	688	GLU	CG-CD-OE1	-12.49	89.67	118.40
6	J	48	ARG	CD-NE-CZ	-12.47	106.94	124.40
6	J	60	ASP	CB-CG-OD2	12.14	146.33	118.40
6	J	48	ARG	CG-CD-NE	11.99	138.37	112.00
3	A	696	GLU	CG-CD-OE2	11.47	144.78	118.40
3	A	699	MET	CB-CA-C	-10.85	87.52	109.55
6	J	52	ARG	NE-CZ-NH2	-10.78	109.50	119.20
6	J	60	ASP	OD1-CG-OD2	-10.36	98.04	122.90
7	M	252	GLU	CG-CD-OE2	-10.19	94.97	118.40
3	A	674	HIS	CA-CB-CG	10.17	123.97	113.80
3	A	421	ARG	NE-CZ-NH1	-9.10	112.41	121.50
4	B	278	ARG	CG-CD-NE	8.82	131.41	112.00
2	H	326	VAL	CA-CB-CG2	-8.39	96.14	110.40
7	P	275	ILE	CA-CB-CG2	-8.38	96.26	110.50
6	I	48	ARG	CB-CG-CD	8.18	130.11	111.30
6	I	52	ARG	NE-CZ-NH1	-8.06	113.44	121.50
2	H	167	ILE	CA-C-N	7.95	127.94	119.76
2	H	167	ILE	C-N-CA	7.95	127.94	119.76
3	A	401	ILE	CB-CG1-CD1	-7.82	97.38	113.80
3	A	688	GLU	OE1-CD-OE2	7.78	141.56	122.90
6	J	52	ARG	CB-CG-CD	-7.55	93.93	111.30
8	T	98	MET	CG-SD-CE	7.50	117.40	100.90
6	J	17	ILE	CB-CG1-CD1	-7.38	98.30	113.80
7	P	415	ASP	CB-CG-OD2	-7.27	101.68	118.40
8	T	73	LYS	CD-CE-NZ	7.10	134.61	111.90
3	A	545	THR	CA-CB-CG2	7.00	122.40	110.50
3	A	672	PHE	CD1-CE1-CZ	-6.99	107.41	120.00
3	A	352	MET	CG-SD-CE	-6.90	85.72	100.90
7	K	403	ARG	CB-CG-CD	6.86	127.07	111.30
3	A	421	ARG	CD-NE-CZ	-6.85	114.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	371	MET	CG-SD-CE	-6.81	85.91	100.90
7	L	403	ARG	CB-CG-CD	6.79	126.92	111.30
3	A	699	MET	CB-CG-SD	-6.79	92.33	112.70
5	E	162	GLN	CG-CD-NE2	-6.57	106.54	116.40
7	M	403	ARG	CB-CG-CD	6.56	126.38	111.30
6	I	52	ARG	NH1-CZ-NH2	-6.54	110.80	119.30
6	J	52	ARG	CD-NE-CZ	6.50	133.51	124.40
6	I	48	ARG	N-CA-CB	-6.50	99.81	110.40
6	J	57	LEU	CB-CG-CD2	-6.47	91.28	110.70
4	B	149	ARG	CG-CD-NE	6.44	126.16	112.00
3	A	684	TYR	CA-C-N	6.40	128.86	120.28
3	A	684	TYR	C-N-CA	6.40	128.86	120.28
7	N	296	GLU	OE1-CD-OE2	-6.37	107.61	122.90
7	M	359	MET	CG-SD-CE	-6.36	86.91	100.90
6	J	52	ARG	NE-CZ-NH1	-6.34	115.16	121.50
2	H	166	LEU	CA-C-N	-6.28	118.33	122.60
2	H	166	LEU	C-N-CA	-6.28	118.33	122.60
7	M	253	HIS	N-CA-CB	6.24	119.99	110.44
7	P	294	MET	CG-SD-CE	-6.18	87.31	100.90
3	A	712	GLU	O-C-N	-6.13	113.85	122.06
3	A	130	LEU	O-C-N	-6.11	115.64	122.12
3	A	675	GLN	CB-CG-CD	6.11	122.98	112.60
3	A	699	MET	CG-SD-CE	-6.07	87.55	100.90
3	A	712	GLU	CA-C-O	6.05	127.90	119.80
7	L	358	GLU	CG-CD-OE1	-6.04	104.52	118.40
6	I	52	ARG	NE-CZ-NH2	6.03	124.63	119.20
7	L	343	LYS	CG-CD-CE	5.93	124.94	111.30
4	B	284	HIS	O-C-N	-5.92	114.74	122.97
3	A	672	PHE	CZ-CE2-CD2	-5.89	109.40	120.00
3	A	70	ALA	N-CA-CB	5.84	119.33	110.28
4	B	71	PHE	O-C-N	-5.84	115.81	123.16
7	O	346	GLN	CG-CD-NE2	-5.76	107.75	116.40
6	J	52	ARG	NH1-CZ-NH2	5.66	126.66	119.30
2	H	320	LYS	CG-CD-CE	5.65	124.29	111.30
6	J	48	ARG	CB-CG-CD	-5.63	98.35	111.30
6	J	48	ARG	NE-CZ-NH2	5.61	124.25	119.20
7	L	403	ARG	CG-CD-NE	5.57	124.24	112.00
7	N	296	GLU	CG-CD-OE2	5.54	131.15	118.40
2	H	302	ARG	CG-CD-NE	-5.53	99.83	112.00
5	F	38	LYS	CG-CD-CE	5.53	124.02	111.30
7	Q	401	THR	OG1-CB-CG2	5.53	120.36	109.30
2	H	238	GLU	CB-CG-CD	5.53	122.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	157	TYR	CE1-CZ-CE2	5.51	131.32	120.30
5	G	61	ALA	CA-C-N	-5.47	113.51	122.54
5	G	61	ALA	C-N-CA	-5.47	113.51	122.54
7	M	346	GLN	N-CA-C	-5.46	106.29	113.17
4	B	115	LEU	CB-CG-CD1	-5.38	94.56	110.70
3	A	684	TYR	O-C-N	5.35	128.25	122.15
7	N	334	GLU	CG-CD-OE2	5.34	130.68	118.40
7	L	36	MET	CG-SD-CE	5.33	112.62	100.90
5	C	177	LEU	CB-CG-CD1	-5.30	94.79	110.70
4	B	173	LEU	CD1-CG-CD2	-5.29	99.16	110.80
4	B	278	ARG	CD-NE-CZ	-5.27	117.02	124.40
7	O	47	GLU	OE1-CD-OE2	-5.27	110.25	122.90
7	M	321	PHE	CB-CA-C	-5.26	102.38	111.23
7	M	352	GLU	CB-CA-C	5.26	120.97	109.99
7	N	319	ASP	CA-CB-CG	5.26	117.86	112.60
7	P	415	ASP	CB-CG-OD1	5.24	130.46	118.40
3	A	719	GLU	CG-CD-OE2	-5.22	106.40	118.40
3	A	696	GLU	CG-CD-OE1	5.15	130.25	118.40
7	L	358	GLU	CG-CD-OE2	5.14	130.23	118.40
7	L	354	PHE	CA-C-O	-5.12	115.45	120.82
6	J	52	ARG	CG-CD-NE	5.12	123.26	112.00
5	G	216	LEU	CD1-CG-CD2	-5.11	99.56	110.80
7	S	252	GLU	CG-CD-OE2	5.11	130.14	118.40
5	G	177	LEU	CB-CG-CD1	-5.10	95.39	110.70
3	A	688	GLU	CB-CG-CD	5.10	121.27	112.60
2	H	326	VAL	CA-CB-CG1	5.05	118.98	110.40
3	A	623	MET	CG-SD-CE	-5.05	89.80	100.90
7	M	347	ILE	CB-CG1-CD1	5.03	124.37	113.80
3	A	682	PHE	CA-CB-CG	-5.03	108.77	113.80
7	Q	205	GLU	CG-CD-OE1	5.03	129.96	118.40
7	K	392	GLN	CG-CD-NE2	-5.03	108.86	116.40
7	Q	399	SER	CA-C-O	-5.01	113.92	119.08

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	669	ARG	Sidechain
3	A	678	ARG	Sidechain
3	A	682	PHE	Sidechain
3	A	684	TYR	Mainchain
3	A	691	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	A	710	ARG	Sidechain
3	A	720	ARG	Sidechain
3	A	723	PHE	Sidechain
4	B	278	ARG	Sidechain
6	D	36	ARG	Sidechain
5	E	162	GLN	Sidechain
5	E	65	ASN	Sidechain
2	H	158	ARG	Sidechain
2	H	30	GLU	Sidechain
6	I	52	ARG	Sidechain
6	J	48	ARG	Sidechain
6	J	52	ARG	Sidechain
7	L	403	ARG	Sidechain
7	N	330	LYS	Mainchain
7	O	416	GLN	Sidechain
7	O	47	GLU	Sidechain
7	P	400	ARG	Sidechain
8	T	86	ARG	Sidechain

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	R	863	0	441	12	0
2	H	2863	0	2898	44	0
3	A	6137	0	5989	168	0
4	B	2321	0	2224	75	0
5	C	1711	0	1697	26	0
5	E	1706	0	1686	45	0
5	F	1707	0	1688	30	0
5	G	1709	0	1695	28	0
6	D	1080	0	1099	22	0
6	I	1080	0	1099	13	0
6	J	1080	0	1099	15	0
7	K	3305	0	3241	46	0
7	L	3305	0	3241	48	0
7	M	3305	0	3241	40	0
7	N	3305	0	3241	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	3305	0	3241	34	0
7	P	3305	0	3241	47	0
7	Q	3305	0	3241	40	0
7	S	3305	0	3241	39	0
8	T	859	0	854	19	0
All	All	49556	0	48397	738	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 (738) 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)
6:I:48:ARG:CD	6:I:48:ARG:CG	1.88	1.51
3:A:715:THR:HB	3:A:720:ARG:HG2	1.23	1.08
3:A:680:LYS:HD3	3:A:755:ILE:HD12	1.38	1.06
3:A:675:GLN:HG2	3:A:723:PHE:CZ	1.94	1.03
6:D:52:ARG:HB3	6:D:56:GLU:OE2	1.68	0.94
6:J:80:ASN:HB3	8:T:46:LEU:HD22	1.49	0.93
7:M:347:ILE:HG13	7:M:352:GLU:HG3	1.53	0.90
3:A:79:ILE:HA	3:A:352:MET:HE1	1.54	0.90
3:A:715:THR:HG22	3:A:716:ASP:H	1.36	0.88
4:B:115:LEU:HD11	4:B:297:LEU:HD12	1.56	0.87
3:A:397:ARG:HD3	3:A:415:LYS:HG3	1.60	0.84
4:B:238:LYS:HE2	4:B:240:SER:CB	2.07	0.83
7:L:78:HIS:HE1	7:L:93:ALA:HB1	1.44	0.83
3:A:674:HIS:HB3	3:A:719:GLU:OE2	1.78	0.83
5:E:25:ALA:HA	5:E:29:ILE:HD13	1.62	0.82
6:D:21:GLU:HG2	6:D:89:ASP:OD2	1.80	0.81
3:A:212:ILE:HD12	3:A:235:PHE:HZ	1.45	0.81
3:A:113:VAL:HA	3:A:532:GLN:HE22	1.46	0.80
7:P:400:ARG:HE	7:Q:400:ARG:HG2	1.46	0.80
6:J:17:ILE:HD11	6:J:122:TYR:HB3	1.62	0.79
3:A:212:ILE:HD12	3:A:235:PHE:CZ	2.18	0.79
6:D:21:GLU:OE1	6:D:93:LYS:HE2	1.83	0.78
4:B:238:LYS:HE2	4:B:240:SER:HB3	1.62	0.78
7:K:1:MET:HB2	7:K:29:SER:HB3	1.65	0.78
3:A:8:LEU:HB2	3:A:69:LEU:HD23	1.66	0.77
3:A:371:MET:HE2	3:A:375:LYS:HE3	1.66	0.77
3:A:753:TYR:OH	5:E:29:ILE:HG23	1.85	0.77
3:A:511:LEU:HD11	3:A:623:MET:HE1	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:715:THR:HG22	3:A:716:ASP:N	1.96	0.77
7:M:347:ILE:CG1	7:M:352:GLU:HG3	2.15	0.76
7:P:275:ILE:HG21	7:P:308:ARG:HH11	1.50	0.76
5:E:4:ALA:HA	5:E:204:PHE:O	1.85	0.76
4:B:219:LEU:H	4:B:290:ALA:HB1	1.51	0.76
3:A:382:TYR:HA	4:B:229:MET:HE3	1.68	0.75
6:D:17:ILE:HA	6:D:20:LEU:HD13	1.68	0.75
7:S:205:GLU:HA	7:S:403:ARG:HE	1.51	0.74
7:Q:90:ILE:HG22	7:Q:94:MET:HE2	1.68	0.74
4:B:238:LYS:HE2	4:B:240:SER:OG	1.88	0.73
7:M:269:ARG:HD2	7:M:273:GLU:HB3	1.68	0.73
7:Q:148:ASN:HD22	7:Q:205:GLU:HG3	1.52	0.73
3:A:715:THR:HB	3:A:720:ARG:CG	2.11	0.73
7:O:401:THR:HA	7:O:404:ILE:HB	1.69	0.72
3:A:371:MET:CE	3:A:375:LYS:HE3	2.21	0.71
5:F:31:ALA:H	6:D:36:ARG:NH1	1.86	0.71
7:K:395:THR:O	7:K:403:ARG:HG3	1.91	0.70
3:A:639:LYS:NZ	4:B:95:ARG:HH12	1.89	0.70
7:L:395:THR:O	7:L:403:ARG:HG3	1.91	0.70
7:P:400:ARG:NE	7:Q:400:ARG:HG2	2.04	0.70
7:L:78:HIS:CE1	7:L:93:ALA:HB1	2.26	0.70
5:F:31:ALA:H	6:D:36:ARG:HH12	1.39	0.70
7:N:296:GLU:OE2	7:N:319:ASP:HB3	1.91	0.69
3:A:749:LEU:HD21	5:E:29:ILE:HG21	1.74	0.69
6:D:69:VAL:HG21	6:I:122:TYR:CE1	2.26	0.69
5:C:182:LEU:HD12	5:C:193:VAL:HG11	1.74	0.69
7:M:343:LYS:HD3	7:M:346:GLN:NE2	2.06	0.69
7:K:284:LYS:HD2	7:K:285:TYR:CZ	2.28	0.69
4:B:66:PHE:HB2	4:B:157:TYR:HD1	1.58	0.68
5:C:192:LYS:HD2	5:G:99:ARG:HD2	1.74	0.68
4:B:42:LYS:HG2	5:E:156:THR:HG21	1.75	0.68
7:P:275:ILE:HG21	7:P:308:ARG:NH1	2.09	0.68
3:A:749:LEU:HD11	3:A:753:TYR:CZ	2.28	0.68
4:B:103:LEU:HD21	4:B:106:LEU:HD21	1.77	0.67
7:M:344:VAL:HG12	7:M:353:THR:HG21	1.78	0.66
3:A:639:LYS:NZ	4:B:95:ARG:NH1	2.43	0.66
5:G:182:LEU:HD12	5:G:193:VAL:HG11	1.76	0.66
7:O:190:LYS:HG2	7:O:194:LYS:NZ	2.10	0.66
7:K:164:GLU:HB2	7:K:242:ASP:HB3	1.78	0.66
3:A:675:GLN:HG2	3:A:723:PHE:CE1	2.30	0.66
3:A:729:LEU:HA	3:A:732:LYS:HZ3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:395:THR:O	7:M:403:ARG:HG3	1.96	0.66
3:A:177:PHE:CE2	3:A:199:ALA:HA	2.31	0.66
7:L:22:GLU:OE2	7:L:34:ARG:HD3	1.95	0.65
5:F:138:ILE:HD11	5:F:190:TYR:HE2	1.61	0.65
7:L:176:LYS:HE2	7:K:58:ARG:HH22	1.62	0.65
8:T:98:MET:SD	8:T:101:LEU:HD13	2.36	0.65
7:S:396:GLY:HA3	7:S:403:ARG:HG2	1.77	0.65
7:M:164:GLU:HB2	7:M:242:ASP:HB3	1.78	0.65
7:L:147:MET:SD	7:L:398:LEU:HD21	2.37	0.65
3:A:683:ILE:HD12	3:A:752:VAL:HG22	1.78	0.65
7:M:401:THR:HA	7:M:404:ILE:HB	1.78	0.65
7:Q:341:LEU:HD11	7:Q:370:SER:HB2	1.79	0.65
3:A:675:GLN:NE2	3:A:723:PHE:CE2	2.65	0.64
5:E:14:LEU:HD23	5:E:193:VAL:HG12	1.78	0.64
7:L:150:ILE:HD12	7:L:222:ILE:HD11	1.78	0.64
2:H:25:LYS:HB2	6:J:74:ARG:HH22	1.62	0.64
7:M:323:THR:HG21	7:M:343:LYS:H	1.63	0.64
7:S:79:ILE:HD12	7:S:90:ILE:HG23	1.79	0.64
3:A:671:PHE:O	3:A:723:PHE:HE1	1.81	0.64
7:N:341:LEU:HD11	7:N:370:SER:HB2	1.80	0.64
2:H:13:LEU:CD1	8:T:98:MET:HE1	2.27	0.63
3:A:672:PHE:HZ	3:A:726:PHE:CE2	2.17	0.63
7:K:163:GLN:NE2	7:K:247:GLU:HG3	2.14	0.63
7:Q:289:THR:HG22	7:Q:314:GLN:HE21	1.64	0.63
7:L:1:MET:HB2	7:L:29:SER:HB3	1.80	0.63
2:H:238:GLU:HA	2:H:241:ARG:HE	1.63	0.63
2:H:18:ILE:HD11	2:H:348:ALA:HB2	1.81	0.62
7:K:90:ILE:HG22	7:K:94:MET:HE2	1.81	0.62
7:O:190:LYS:HG2	7:O:194:LYS:HZ2	1.62	0.62
3:A:521:LEU:HD13	3:A:575:ASP:HB3	1.80	0.62
4:B:185:GLY:HA2	5:E:99:ARG:HA	1.82	0.62
6:D:89:ASP:OD1	6:D:93:LYS:HD2	1.99	0.62
7:S:341:LEU:HD11	7:S:370:SER:HB2	1.80	0.62
7:M:205:GLU:HG2	7:M:403:ARG:HH21	1.65	0.62
7:O:314:GLN:HG3	7:O:431:ASN:HD21	1.65	0.62
7:Q:36:MET:HB2	7:Q:378:ASP:HB2	1.82	0.62
6:D:69:VAL:HG21	6:I:122:TYR:HE1	1.65	0.61
7:N:158:ALA:HA	7:N:211:ARG:HH11	1.66	0.61
4:B:5:LEU:HD21	4:B:70:PRO:HG3	1.82	0.61
3:A:693:TYR:CZ	3:A:697:GLU:HG2	2.35	0.61
7:K:160:ILE:HG23	7:K:215:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:48:ARG:HG3	6:I:52:ARG:NH1	2.16	0.61
7:P:146:MET:HE1	7:P:289:THR:HG21	1.83	0.61
7:K:288:ILE:HG23	7:K:289:THR:HG23	1.83	0.61
7:M:2:SER:HB2	7:M:84:VAL:HG12	1.83	0.60
6:I:48:ARG:HE	6:I:52:ARG:CZ	2.14	0.60
3:A:130:LEU:O	3:A:560:GLN:NE2	2.34	0.60
5:C:64:TYR:HB2	5:C:79:LEU:HD11	1.82	0.60
5:G:38:LYS:HD3	5:G:43:ASN:OD1	2.02	0.60
7:O:371:HIS:HD2	7:O:403:ARG:HH21	1.47	0.60
1:R:2:C:H5'	5:E:54:GLY:HA3	1.83	0.60
6:I:70:TYR:CZ	6:I:74:ARG:HD3	2.36	0.60
3:A:459:LEU:HD22	3:A:478:ILE:HD13	1.84	0.60
2:H:13:LEU:HD11	8:T:98:MET:HE1	1.84	0.59
5:F:131:ALA:HB3	5:G:92:LYS:HD2	1.84	0.59
7:S:164:GLU:HG2	7:S:242:ASP:HB3	1.84	0.59
1:R:2:C:H2'	4:B:136:PRO:HD3	1.83	0.59
3:A:709:THR:HG22	3:A:727:LYS:HD2	1.83	0.59
7:Q:164:GLU:HB2	7:Q:242:ASP:HB3	1.85	0.59
7:M:79:ILE:HD12	7:M:90:ILE:HG23	1.85	0.59
2:H:247:GLY:O	2:H:248:LYS:HG3	2.01	0.59
2:H:103:ARG:HD2	2:H:110:ALA:HA	1.85	0.58
7:O:37:VAL:HG13	7:O:112:LEU:HD23	1.84	0.58
3:A:212:ILE:HD11	3:A:241:PHE:CZ	2.38	0.58
3:A:522:GLY:HA3	4:B:94:ARG:HH12	1.69	0.58
7:K:149:ILE:HG23	7:K:150:ILE:HG12	1.84	0.58
2:H:208:LYS:HD3	8:T:61:TYR:CD2	2.38	0.58
3:A:557:TYR:HA	3:A:560:GLN:OE1	2.04	0.58
7:L:146:MET:HG2	7:L:168:VAL:HG22	1.84	0.58
3:A:177:PHE:CZ	3:A:199:ALA:HA	2.39	0.58
7:Q:401:THR:HA	7:Q:404:ILE:HB	1.85	0.58
5:F:20:ILE:HD13	5:F:48:PRO:HD2	1.86	0.58
7:K:401:THR:HA	7:K:404:ILE:HB	1.83	0.58
7:Q:148:ASN:ND2	7:Q:205:GLU:HG3	2.18	0.58
7:M:347:ILE:HG13	7:M:352:GLU:CG	2.31	0.58
3:A:712:GLU:O	3:A:712:GLU:HG2	2.03	0.58
5:E:25:ALA:HA	5:E:29:ILE:CD1	2.34	0.57
3:A:163:PHE:HZ	3:A:173:LEU:HB2	1.69	0.57
7:M:312:LYS:HG3	7:M:313:VAL:HG23	1.86	0.57
3:A:436:ILE:HG22	3:A:467:VAL:HG12	1.85	0.57
5:F:99:ARG:NE	5:E:192:LYS:HD2	2.18	0.57
7:M:97:LEU:HD22	7:M:106:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:47:VAL:HG12	3:A:51:GLN:HE21	1.68	0.57
5:F:198:LEU:HG	5:F:216:LEU:HD23	1.85	0.57
7:P:181:TRP:CD1	7:P:231:TYR:HH	2.22	0.57
5:C:144:ASN:HB2	5:G:41:ILE:HD12	1.85	0.57
2:H:25:LYS:HB2	6:J:74:ARG:NH2	2.18	0.57
3:A:684:TYR:O	3:A:687:ILE:HB	2.03	0.57
7:S:262:GLU:HB2	7:S:266:ALA:HB2	1.87	0.57
7:L:164:GLU:HB2	7:L:242:ASP:HB3	1.86	0.57
5:G:3:PHE:HZ	5:G:5:LYS:HE3	1.70	0.57
7:P:402:ASP:CG	7:P:403:ARG:HH11	2.13	0.57
5:E:7:LYS:HD2	5:E:150:GLU:OE2	2.03	0.57
7:Q:288:ILE:HG23	7:Q:289:THR:HG23	1.86	0.57
3:A:674:HIS:HB2	3:A:723:PHE:CZ	2.40	0.56
7:P:314:GLN:HG3	7:P:431:ASN:HD21	1.69	0.56
3:A:516:LEU:HD21	3:A:607:LEU:HD13	1.87	0.56
3:A:613:LEU:HG	3:A:645:PHE:CD1	2.39	0.56
3:A:721:ASP:HA	3:A:724:LYS:HE2	1.87	0.56
7:P:140:LYS:HE3	7:O:88:GLN:OE1	2.05	0.56
5:E:14:LEU:HD21	5:E:18:LEU:HD22	1.86	0.56
3:A:506:LEU:HD11	3:A:757:LYS:HE3	1.86	0.56
5:F:78:ILE:HG23	5:F:79:LEU:HD12	1.86	0.56
5:E:185:SER:O	5:E:190:TYR:HD2	1.89	0.56
7:M:146:MET:HG2	7:M:168:VAL:HG22	1.86	0.56
5:F:128:ARG:HH12	5:C:58:THR:HA	1.71	0.56
7:N:371:HIS:HD1	7:N:371:HIS:H	1.54	0.56
3:A:134:PRO:HB2	3:A:136:PHE:CE2	2.39	0.56
7:L:79:ILE:HD12	7:L:90:ILE:HG23	1.87	0.56
3:A:675:GLN:CG	3:A:723:PHE:CZ	2.80	0.56
5:G:78:ILE:HG23	5:G:79:LEU:HD12	1.87	0.56
7:S:190:LYS:HG2	7:S:194:LYS:HE2	1.88	0.56
7:O:347:ILE:HD12	7:O:352:GLU:HB2	1.88	0.56
7:K:152:GLY:HA2	7:K:156:SER:HB3	1.87	0.56
7:Q:181:TRP:CD1	7:Q:231:TYR:HH	2.23	0.56
4:B:72:LEU:HD12	4:B:111:VAL:HG21	1.86	0.55
7:O:150:ILE:HD13	7:O:212:PHE:HE2	1.71	0.55
7:Q:344:VAL:HG12	7:Q:353:THR:HG21	1.89	0.55
2:H:27:THR:HB	6:J:74:ARG:HE	1.71	0.55
3:A:177:PHE:CE1	3:A:181:LEU:HD12	2.41	0.55
4:B:66:PHE:HB2	4:B:157:TYR:CD1	2.39	0.55
7:P:36:MET:SD	7:P:376:THR:HB	2.46	0.55
7:O:36:MET:HB2	7:O:378:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:379:SER:HA	7:L:406:LYS:HE3	1.88	0.55
7:P:328:LEU:HD13	7:P:340:ILE:HD12	1.88	0.55
7:K:147:MET:SD	7:K:398:LEU:HD21	2.46	0.55
7:Q:396:GLY:HA3	7:Q:403:ARG:HD2	1.89	0.55
3:A:721:ASP:OD1	3:A:724:LYS:HE2	2.05	0.55
4:B:8:MET:HE1	4:B:27:PHE:HZ	1.71	0.55
7:S:147:MET:SD	7:S:398:LEU:HD21	2.46	0.55
3:A:720:ARG:HH21	3:A:720:ARG:HB3	1.71	0.55
7:O:74:VAL:HG12	7:O:97:LEU:HD21	1.87	0.55
3:A:715:THR:HG21	3:A:723:PHE:CD2	2.42	0.55
7:S:2:SER:HB2	7:S:84:VAL:HG12	1.89	0.55
7:P:164:GLU:CD	7:P:242:ASP:HB3	2.32	0.55
3:A:411:TYR:CE2	3:A:412:HIS:CD2	2.96	0.55
3:A:680:LYS:HD3	3:A:755:ILE:CD1	2.26	0.54
3:A:690:LEU:HD11	3:A:730:PHE:CZ	2.43	0.54
2:H:97:THR:HG23	2:H:322:PRO:HG3	1.88	0.54
4:B:64:PHE:HB2	4:B:157:TYR:CZ	2.42	0.54
4:B:99:LEU:HB3	4:B:119:LEU:HD11	1.90	0.54
7:S:205:GLU:HA	7:S:403:ARG:HH21	1.73	0.54
7:M:341:LEU:HD12	7:M:368:VAL:HB	1.89	0.54
7:Q:323:THR:HA	7:Q:340:ILE:HD11	1.89	0.54
3:A:729:LEU:HA	3:A:732:LYS:NZ	2.22	0.54
7:Q:160:ILE:HD11	7:Q:212:PHE:HB2	1.88	0.54
5:F:34:SER:HB2	5:F:138:ILE:HB	1.90	0.54
5:E:95:ARG:HH12	5:E:162:GLN:CD	2.16	0.54
7:K:163:GLN:HE21	7:K:247:GLU:HG3	1.72	0.54
8:T:98:MET:SD	8:T:101:LEU:HD22	2.48	0.54
4:B:32:ILE:HG23	4:B:60:LEU:HD21	1.90	0.54
7:P:1:MET:HB3	7:P:29:SER:HB3	1.90	0.54
2:H:203:TRP:HB2	2:H:318:LEU:O	2.07	0.54
5:E:32:ILE:HA	5:E:137:GLN:NE2	2.23	0.54
7:P:400:ARG:HH21	7:Q:400:ARG:HA	1.73	0.54
4:B:39:GLU:HG3	4:B:173:LEU:HD22	1.90	0.54
7:S:205:GLU:HA	7:S:403:ARG:NE	2.22	0.54
3:A:753:TYR:OH	5:E:29:ILE:CG2	2.54	0.54
7:K:205:GLU:HG3	7:K:403:ARG:NH2	2.23	0.54
1:R:21:U:H5"	5:C:123:GLU:HA	1.89	0.54
3:A:705:ALA:O	3:A:709:THR:HG23	2.08	0.54
4:B:104:GLN:HG3	4:B:105:PHE:CD2	2.43	0.54
7:M:181:TRP:CD1	7:M:231:TYR:HH	2.25	0.54
7:O:424:ARG:HB3	7:O:427:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:ASN:HB3	2:H:107:SER:HB2	1.89	0.53
3:A:639:LYS:HZ1	4:B:95:ARG:NH1	2.04	0.53
5:C:78:ILE:HG21	5:C:169:VAL:HG21	1.90	0.53
7:K:205:GLU:HG3	7:K:403:ARG:HH21	1.74	0.53
6:D:95:GLN:HG3	6:D:98:GLU:OE2	2.08	0.53
7:N:357:ILE:HD13	7:N:388:THR:HG21	1.89	0.53
7:L:223:ILE:HG23	7:L:233:PRO:HG2	1.89	0.53
7:L:402:ASP:CG	7:L:403:ARG:HH11	2.15	0.53
7:M:258:TYR:HE2	7:M:269:ARG:NH2	2.06	0.53
7:P:375:GLU:HG3	7:P:376:THR:N	2.24	0.53
7:P:145:PRO:HB2	7:P:147:MET:SD	2.49	0.53
3:A:38:TRP:HH2	3:A:160:LEU:HD12	1.74	0.53
7:Q:6:ASP:HB2	7:Q:26:TYR:HB2	1.91	0.53
2:H:55:LEU:HD22	2:H:58:LYS:HD3	1.91	0.53
3:A:721:ASP:OD1	3:A:724:LYS:CE	2.56	0.53
5:G:47:ILE:HB	5:G:101:ALA:HB3	1.91	0.53
6:I:52:ARG:HG2	6:I:52:ARG:HH11	1.74	0.53
6:J:100:LEU:HD23	6:J:103:ILE:HD12	1.90	0.53
7:Q:163:GLN:HG2	7:Q:164:GLU:HG3	1.91	0.53
5:C:175:LYS:HE2	5:G:204:PHE:HD1	1.74	0.52
3:A:296:LEU:HD21	3:A:299:VAL:HG12	1.90	0.52
5:E:5:LYS:HG2	5:E:154:GLU:HG2	1.91	0.52
7:K:357:ILE:HD13	7:K:388:THR:HG21	1.91	0.52
7:O:148:ASN:HA	7:O:166:MET:HG3	1.91	0.52
3:A:536:GLN:HE21	3:A:537:TYR:HE1	1.57	0.52
7:O:131:TYR:HE2	7:O:416:GLN:NE2	2.07	0.52
4:B:175:TYR:HB3	5:E:152:ILE:HD13	1.92	0.52
4:B:175:TYR:CE2	5:E:203:VAL:HG11	2.45	0.52
7:K:147:MET:HE1	7:K:182:GLY:HA3	1.90	0.52
3:A:267:LEU:HD22	3:A:620:ILE:HD13	1.90	0.52
7:S:253:HIS:HB2	7:S:255:VAL:HG22	1.92	0.52
5:C:56:MET:SD	5:C:98:PHE:HE2	2.32	0.52
7:P:36:MET:HG2	7:P:376:THR:HG21	1.92	0.52
7:O:371:HIS:CD2	7:O:403:ARG:HH21	2.26	0.52
2:H:185:ARG:HG2	5:G:187:SER:HA	1.92	0.52
3:A:659:ASN:O	3:A:663:ASP:HB3	2.10	0.52
7:M:257:GLY:HA2	7:M:268:VAL:HG22	1.91	0.52
3:A:690:LEU:HD11	3:A:730:PHE:HZ	1.74	0.51
5:F:70:GLU:HG3	5:E:129:ILE:HD11	1.92	0.51
7:Q:152:GLY:HA2	7:Q:156:SER:HB3	1.92	0.51
3:A:709:THR:HG22	3:A:727:LYS:CD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:274:ILE:HG22	4:B:287:LEU:HD22	1.93	0.51
7:P:341:LEU:HD12	7:P:368:VAL:HB	1.92	0.51
3:A:113:VAL:HA	3:A:532:GLN:NE2	2.20	0.51
3:A:297:LEU:HD13	3:A:540:LEU:HD11	1.92	0.51
7:S:112:LEU:HD11	7:S:344:VAL:HG22	1.92	0.51
7:K:292:ASP:OD2	7:K:318:ASP:HB3	2.10	0.51
5:F:128:ARG:HH22	5:C:57:ARG:HG2	1.75	0.51
7:M:145:PRO:HB2	7:M:147:MET:SD	2.51	0.51
7:Q:79:ILE:HD12	7:Q:90:ILE:HG23	1.92	0.51
2:H:46:PHE:CZ	2:H:50:MET:HE3	2.46	0.51
5:C:42:THR:HB	5:C:44:LEU:HG	1.93	0.51
7:K:146:MET:HG2	7:K:168:VAL:HG22	1.93	0.51
7:M:288:ILE:HG23	7:M:289:THR:HG23	1.92	0.51
3:A:258:ILE:HG23	3:A:401:ILE:HG23	1.92	0.51
4:B:135:GLN:HG2	4:B:137:HIS:CE1	2.46	0.51
7:N:147:MET:SD	7:N:182:GLY:HA3	2.51	0.51
7:O:2:SER:HB3	7:O:125:TYR:CZ	2.45	0.51
7:O:289:THR:HG23	7:O:314:GLN:HE21	1.76	0.51
1:R:15:G:H5''	5:F:123:GLU:HA	1.92	0.51
4:B:270:PHE:CE2	4:B:292:PRO:HG3	2.46	0.51
5:F:138:ILE:HD11	5:F:190:TYR:CE2	2.45	0.51
7:P:375:GLU:HG3	7:P:376:THR:H	1.75	0.51
7:Q:7:VAL:HG22	7:Q:25:VAL:HG22	1.93	0.51
3:A:401:ILE:HD11	3:A:424:TYR:OH	2.10	0.50
7:S:149:ILE:HG23	7:S:150:ILE:HG12	1.93	0.50
7:N:74:VAL:HG12	7:N:97:LEU:HD21	1.92	0.50
2:H:60:GLU:O	2:H:64:ILE:HG12	2.11	0.50
6:I:48:ARG:HG3	6:I:52:ARG:HH12	1.76	0.50
1:R:-5:A:H5'	4:B:244:PHE:HD2	1.77	0.50
6:J:30:LEU:HD21	6:J:90:LEU:HD22	1.94	0.50
7:Q:1:MET:HB2	7:Q:29:SER:HB3	1.92	0.50
3:A:598:ILE:CD1	3:A:603:GLY:HA2	2.42	0.50
5:C:47:ILE:HB	5:C:101:ALA:HB3	1.92	0.50
1:R:26:A:H1'	2:H:131:SER:HA	1.93	0.50
3:A:537:TYR:HA	3:A:542:ARG:HH11	1.77	0.50
3:A:670:TYR:CZ	3:A:722:LYS:NZ	2.73	0.50
4:B:12:ASN:HD21	5:E:102:PHE:HZ	1.60	0.50
6:D:24:ASN:OD1	6:D:25:LYS:HG3	2.12	0.50
7:L:424:ARG:HB3	7:L:427:LYS:HB2	1.94	0.50
7:K:156:SER:HB2	7:K:209:ALA:HB1	1.94	0.50
7:S:152:GLY:HA2	7:S:156:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:7:VAL:HG22	7:K:25:VAL:HG22	1.93	0.49
4:B:12:ASN:OD1	4:B:149:ARG:HD3	2.12	0.49
3:A:680:LYS:O	3:A:683:ILE:HG12	2.12	0.49
3:A:696:GLU:HG3	3:A:696:GLU:O	2.12	0.49
4:B:36:LEU:HD21	4:B:170:MET:HE2	1.94	0.49
4:B:209:SER:HA	4:B:268:LYS:HG3	1.93	0.49
7:S:402:ASP:HB3	7:N:401:THR:OG1	2.11	0.49
7:P:146:MET:HE2	7:P:166:MET:SD	2.52	0.49
7:M:160:ILE:HD11	7:M:212:PHE:HB2	1.93	0.49
2:H:99:LEU:HD23	2:H:320:LYS:HE3	1.94	0.49
5:G:20:ILE:HD13	5:G:48:PRO:HD2	1.95	0.49
7:P:401:THR:HA	7:P:404:ILE:HB	1.95	0.49
7:K:284:LYS:HD2	7:K:285:TYR:CE2	2.48	0.49
3:A:668:ILE:O	3:A:672:PHE:HB2	2.12	0.49
3:A:715:THR:CB	3:A:720:ARG:HG2	2.17	0.49
5:G:95:ARG:NH2	5:G:158:GLU:HG3	2.27	0.49
3:A:730:PHE:CE2	3:A:748:LEU:HD11	2.48	0.49
3:A:751:TYR:CE2	3:A:755:ILE:HD13	2.48	0.49
4:B:259:LYS:HE2	4:B:290:ALA:HB2	1.94	0.49
6:D:29:LEU:HD22	6:D:77:VAL:HG21	1.94	0.49
7:L:36:MET:SD	7:L:376:THR:HB	2.52	0.49
7:P:312:LYS:HG3	7:P:313:VAL:HG13	1.94	0.49
7:K:79:ILE:HD12	7:K:90:ILE:HG23	1.94	0.49
3:A:696:GLU:HB3	3:A:700:ASN:ND2	2.28	0.49
7:M:147:MET:HE1	7:M:169:PRO:HG3	1.93	0.49
7:M:343:LYS:HD3	7:M:346:GLN:HE22	1.74	0.49
8:T:98:MET:O	8:T:98:MET:HG2	2.11	0.49
5:E:95:ARG:HH22	5:E:162:GLN:NE2	2.10	0.49
3:A:697:GLU:O	3:A:701:VAL:HG23	2.13	0.49
5:E:3:PHE:HA	5:E:155:ILE:O	2.12	0.49
5:E:167:PHE:CD2	5:E:212:LEU:HD13	2.48	0.49
7:N:147:MET:SD	7:N:398:LEU:HD21	2.53	0.49
8:T:33:ILE:HB	8:T:37:GLU:HG3	1.94	0.49
2:H:103:ARG:HD3	2:H:108:ALA:HB3	1.95	0.49
2:H:275:GLN:HB2	2:H:349:ASN:HB3	1.95	0.49
3:A:669:ARG:HA	3:A:751:TYR:CE1	2.48	0.49
4:B:65:PRO:O	4:B:157:TYR:HE1	1.95	0.49
7:S:269:ARG:HB3	7:S:273:GLU:HB2	1.94	0.49
7:L:112:LEU:HD11	7:L:344:VAL:HG12	1.95	0.49
3:A:675:GLN:CG	3:A:723:PHE:CE1	2.96	0.48
4:B:11:GLN:O	4:B:149:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:147:MET:HB2	7:N:167:ILE:HG13	1.95	0.48
7:Q:238:PHE:CE1	7:Q:426:LEU:HD21	2.48	0.48
7:S:12:VAL:HG21	7:S:36:MET:HE3	1.94	0.48
7:S:44:GLY:HA3	7:S:47:GLU:HG2	1.95	0.48
7:L:244:ALA:HA	7:L:292:ASP:HB3	1.95	0.48
7:K:402:ASP:CG	7:K:403:ARG:HH11	2.21	0.48
3:A:693:TYR:CE2	3:A:697:GLU:HG2	2.48	0.48
6:J:48:ARG:HH11	6:J:48:ARG:HD2	1.42	0.48
6:J:52:ARG:HG2	6:J:56:GLU:HB2	1.95	0.48
6:J:68:PHE:CE1	6:J:96:ILE:HG21	2.48	0.48
2:H:251:GLN:NE2	8:T:104:VAL:HG11	2.28	0.48
5:F:14:LEU:HB2	5:F:143:ARG:O	2.14	0.48
6:I:20:LEU:HD11	6:I:90:LEU:HD13	1.95	0.48
4:B:151:SER:HB2	5:E:41:ILE:HD13	1.96	0.48
7:K:140:LYS:HE2	7:N:88:GLN:OE1	2.14	0.48
3:A:685:LYS:HE2	3:A:707:TYR:CE2	2.49	0.48
4:B:289:TYR:CZ	4:B:291:LYS:HB2	2.49	0.48
6:D:62:SER:HB3	6:I:10:VAL:HG21	1.96	0.48
5:F:144:ASN:HB2	5:C:41:ILE:HD12	1.95	0.48
7:P:147:MET:HE1	7:P:169:PRO:HG3	1.95	0.48
5:G:167:PHE:CE2	5:G:212:LEU:HD22	2.49	0.47
7:S:88:GLN:OE1	7:Q:140:LYS:HE2	2.14	0.47
7:P:47:GLU:OE2	7:P:346:GLN:HG3	2.15	0.47
3:A:716:ASP:O	3:A:717:LYS:C	2.57	0.47
3:A:720:ARG:C	3:A:722:LYS:H	2.21	0.47
5:F:53:LYS:HD3	5:E:188:ARG:HG2	1.97	0.47
5:C:56:MET:SD	5:C:98:PHE:CE2	3.07	0.47
3:A:625:HIS:O	3:A:629:GLU:HG2	2.14	0.47
4:B:169:LEU:O	4:B:173:LEU:HD23	2.14	0.47
5:G:64:TYR:HB2	5:G:79:LEU:HD11	1.96	0.47
7:L:341:LEU:HD12	7:L:368:VAL:HB	1.96	0.47
7:L:371:HIS:CD2	7:L:403:ARG:HH21	2.32	0.47
3:A:671:PHE:O	3:A:723:PHE:CE1	2.64	0.47
3:A:675:GLN:NE2	3:A:723:PHE:HE2	2.13	0.47
7:L:218:GLY:O	7:L:222:ILE:HG12	2.15	0.47
8:T:84:LYS:HD2	8:T:84:LYS:O	2.14	0.47
2:H:22:ASN:HB3	2:H:118:ILE:HD12	1.95	0.47
3:A:401:ILE:HG21	3:A:401:ILE:HD13	1.66	0.47
3:A:537:TYR:HA	3:A:542:ARG:NH1	2.29	0.47
3:A:719:GLU:OE2	3:A:723:PHE:CZ	2.67	0.47
4:B:25:LEU:HG	4:B:26:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:103:LEU:HD12	4:B:122:ASN:OD1	2.14	0.47
4:B:171:SER:O	4:B:174:GLN:HG2	2.14	0.47
5:C:59:LEU:HD12	5:C:177:LEU:HD23	1.97	0.47
7:P:314:GLN:HE22	7:P:392:GLN:HE22	1.62	0.47
5:G:3:PHE:CZ	5:G:5:LYS:HE3	2.47	0.47
7:L:53:ASP:HA	7:L:66:LYS:HD2	1.97	0.47
4:B:289:TYR:CE1	4:B:291:LYS:HD3	2.50	0.47
5:F:31:ALA:N	6:D:36:ARG:HH12	2.09	0.47
5:C:14:LEU:HB2	5:C:143:ARG:O	2.15	0.47
5:E:81:ARG:HB2	5:E:95:ARG:NH2	2.30	0.47
7:K:2:SER:HB3	7:K:125:TYR:CZ	2.50	0.47
2:H:238:GLU:HA	2:H:241:ARG:HH21	1.79	0.47
3:A:382:TYR:HE1	4:B:225:LEU:HD12	1.80	0.47
7:L:75:ILE:HG21	7:L:114:VAL:HG21	1.97	0.47
7:K:424:ARG:HB3	7:K:427:LYS:HB2	1.97	0.47
7:O:146:MET:HG2	7:O:168:VAL:HG22	1.97	0.47
3:A:715:THR:CG2	3:A:719:GLU:OE1	2.64	0.46
5:C:20:ILE:HD13	5:C:48:PRO:HD2	1.95	0.46
7:K:37:VAL:HG13	7:K:112:LEU:HD23	1.96	0.46
3:A:608:SER:HB2	3:A:635:LYS:HE3	1.98	0.46
3:A:685:LYS:HE2	3:A:707:TYR:CZ	2.51	0.46
3:A:705:ALA:HB1	6:D:125:PHE:CG	2.49	0.46
3:A:729:LEU:HD12	3:A:732:LYS:HZ3	1.80	0.46
7:S:258:TYR:CE2	7:S:269:ARG:NH1	2.83	0.46
2:H:10:LEU:HD22	2:H:132:LEU:HD21	1.97	0.46
4:B:272:GLY:HA3	4:B:291:LYS:HA	1.97	0.46
5:E:171:ARG:NH1	5:E:212:LEU:HD12	2.31	0.46
3:A:519:ASP:OD2	3:A:639:LYS:HB3	2.15	0.46
6:J:91:VAL:HG13	6:J:96:ILE:HB	1.97	0.46
7:M:90:ILE:HD13	7:M:118:VAL:HG11	1.98	0.46
7:M:205:GLU:HG2	7:M:403:ARG:NH2	2.27	0.46
3:A:15:HIS:HD2	3:A:55:HIS:CD2	2.32	0.46
4:B:175:TYR:CZ	5:E:203:VAL:HG11	2.50	0.46
6:J:45:LEU:HD21	6:J:109:LEU:HD11	1.98	0.46
3:A:705:ALA:HB1	6:D:125:PHE:HB2	1.98	0.46
7:K:158:ALA:HB2	7:K:211:ARG:HA	1.96	0.46
3:A:708:LEU:HD13	3:A:727:LYS:HA	1.97	0.46
7:L:309:LEU:HB3	7:L:313:VAL:HG12	1.98	0.46
7:P:152:GLY:HA2	7:P:156:SER:HB3	1.98	0.46
7:P:323:THR:HG23	7:P:347:ILE:HB	1.97	0.46
1:R:26:A:C6	2:H:289:LYS:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:359:GLU:HA	3:A:362:ARG:HE	1.80	0.46
3:A:717:LYS:O	3:A:720:ARG:HD3	2.16	0.46
5:F:177:LEU:HD23	5:F:195:PHE:CZ	2.51	0.46
1:R:-3:G:C8	4:B:18:GLY:HA2	2.51	0.46
7:N:296:GLU:CD	7:N:319:ASP:HB3	2.41	0.46
5:E:181:TYR:CG	5:E:186:GLY:HA3	2.51	0.46
7:L:147:MET:SD	7:L:182:GLY:HA3	2.56	0.46
7:O:341:LEU:HD12	7:O:368:VAL:HB	1.98	0.46
6:J:65:ARG:HH22	6:J:101:LYS:NZ	2.14	0.45
7:N:424:ARG:HB3	7:N:427:LYS:HB2	1.98	0.45
8:T:19:THR:HB	8:T:56:ASP:HB3	1.97	0.45
7:S:341:LEU:HA	7:S:341:LEU:HD12	1.76	0.45
7:M:396:GLY:HA3	7:M:403:ARG:HG2	1.99	0.45
3:A:33:LEU:HD21	3:A:59:TYR:CZ	2.51	0.45
3:A:169:GLN:OE1	3:A:172:SER:HB2	2.16	0.45
3:A:704:LEU:HD23	3:A:731:PHE:CD1	2.51	0.45
3:A:736:ASN:OD1	3:A:740:ASP:HB2	2.17	0.45
5:F:64:TYR:HB2	5:F:79:LEU:HD11	1.98	0.45
6:I:124:LYS:HB3	6:I:124:LYS:HE3	1.74	0.45
3:A:163:PHE:CZ	3:A:169:GLN:HG3	2.51	0.45
7:L:148:ASN:HA	7:L:166:MET:HG2	1.97	0.45
7:L:343:LYS:HB2	7:L:346:GLN:CD	2.41	0.45
7:K:44:GLY:HA3	7:K:47:GLU:HG3	1.98	0.45
4:B:218:ALA:HA	4:B:290:ALA:HB1	1.99	0.45
7:K:1:MET:HG3	7:K:125:TYR:CE1	2.51	0.45
7:K:92:ARG:HD3	7:K:92:ARG:HA	1.75	0.45
8:T:40:ASP:OD1	8:T:44:LYS:NZ	2.49	0.45
1:R:4:U:H1'	4:B:136:PRO:HB3	1.99	0.45
3:A:544:ALA:O	3:A:548:ARG:HG3	2.17	0.45
7:L:150:ILE:HD13	7:L:212:PHE:HE2	1.81	0.45
7:P:98:ASP:OD2	7:P:103:LYS:HA	2.16	0.45
7:N:37:VAL:HG13	7:N:112:LEU:HD23	1.99	0.45
2:H:24:GLU:HB3	2:H:116:LYS:HE3	1.99	0.45
2:H:208:LYS:HD3	8:T:61:TYR:CE2	2.52	0.45
7:K:53:ASP:HA	7:K:66:LYS:HD2	1.99	0.45
3:A:163:PHE:CZ	3:A:173:LEU:HB2	2.50	0.45
3:A:682:PHE:CD2	3:A:711:LEU:HG	2.51	0.45
5:G:14:LEU:HB2	5:G:143:ARG:O	2.17	0.45
7:S:239:ILE:O	7:S:287:ILE:HA	2.17	0.45
7:P:371:HIS:CD2	7:P:403:ARG:HH21	2.34	0.45
7:K:371:HIS:HD2	7:K:394:LYS:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:VAL:HG11	3:A:424:TYR:CE2	2.52	0.45
3:A:522:GLY:HA3	4:B:94:ARG:NH1	2.32	0.45
5:G:16:THR:HG21	5:G:189:GLY:O	2.16	0.45
7:S:150:ILE:HD11	7:S:189:LEU:HD21	1.98	0.45
7:K:47:GLU:HB3	7:K:322:VAL:HG11	1.99	0.45
7:Q:158:ALA:HB2	7:Q:211:ARG:HA	1.99	0.45
6:D:45:LEU:HD21	6:D:109:LEU:HD11	1.98	0.44
7:S:160:ILE:HD11	7:S:212:PHE:HB2	1.99	0.44
7:P:420:VAL:HG11	7:O:88:GLN:HB3	1.98	0.44
3:A:254:PHE:CD2	3:A:274:LEU:HD21	2.52	0.44
5:F:89:LYS:HA	5:F:92:LYS:HE2	2.00	0.44
5:G:31:ALA:HB1	5:G:33:ASP:OD2	2.16	0.44
7:O:163:GLN:CD	7:O:244:ALA:HB3	2.42	0.44
7:N:21:LEU:HD21	7:N:109:ASN:HB2	1.99	0.44
3:A:729:LEU:HD11	3:A:733:TRP:CZ2	2.53	0.44
6:D:17:ILE:HD12	6:D:123:PHE:HB2	1.98	0.44
5:C:188:ARG:HG2	5:G:53:LYS:HD3	2.00	0.44
7:P:51:LEU:HD21	7:P:66:LYS:HB3	1.98	0.44
3:A:270:ARG:O	3:A:274:LEU:HD23	2.18	0.44
3:A:558:ILE:HG12	3:A:569:ILE:HD13	1.99	0.44
4:B:3:TYR:HB2	4:B:161:ASN:HA	2.00	0.44
5:G:3:PHE:HA	5:G:155:ILE:O	2.18	0.44
7:P:79:ILE:HD12	7:P:90:ILE:HG23	1.99	0.44
7:M:36:MET:HB2	7:M:378:ASP:HB2	1.98	0.44
3:A:13:LEU:HD12	3:A:202:SER:OG	2.17	0.44
4:B:225:LEU:O	4:B:229:MET:HG2	2.17	0.44
6:D:56:GLU:HG2	6:D:57:LEU:HD12	1.99	0.44
8:T:94:GLU:HG3	8:T:96:ILE:HD13	1.98	0.44
7:P:6:ASP:HB3	7:P:26:TYR:HB2	2.00	0.44
7:P:271:ALA:O	7:P:275:ILE:HG12	2.17	0.44
7:P:400:ARG:HG2	7:Q:400:ARG:CZ	2.48	0.44
3:A:680:LYS:CD	3:A:755:ILE:HD12	2.27	0.44
4:B:5:LEU:HD12	4:B:159:ILE:HG12	1.99	0.44
4:B:46:LEU:O	4:B:50:LEU:HD23	2.18	0.44
5:E:136:ARG:HE	5:E:138:ILE:HD11	1.81	0.44
5:C:167:PHE:O	5:C:171:ARG:HG3	2.18	0.44
5:E:3:PHE:CD1	5:E:156:THR:HG22	2.52	0.44
5:G:64:TYR:CB	5:G:79:LEU:HD11	2.48	0.44
5:G:167:PHE:O	5:G:171:ARG:HG3	2.17	0.44
7:P:146:MET:HG2	7:P:168:VAL:HG22	2.00	0.44
7:N:150:ILE:HB	7:N:165:PHE:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:LEU:HD13	8:T:98:MET:HE1	1.97	0.43
3:A:193:ILE:HD12	3:A:537:TYR:HE2	1.83	0.43
7:L:152:GLY:HA2	7:L:156:SER:HB3	2.00	0.43
7:O:239:ILE:O	7:O:287:ILE:HA	2.18	0.43
2:H:11:SER:O	2:H:350:PHE:HA	2.18	0.43
3:A:537:TYR:O	3:A:542:ARG:HD2	2.18	0.43
3:A:674:HIS:CB	3:A:719:GLU:OE2	2.59	0.43
3:A:710:ARG:O	3:A:714:LEU:HG	2.18	0.43
5:E:167:PHE:CZ	5:E:212:LEU:HD22	2.53	0.43
7:L:21:LEU:HD11	7:L:110:ALA:HA	2.00	0.43
7:P:7:VAL:HG22	7:P:25:VAL:HG22	2.00	0.43
7:K:276:ASP:O	7:K:280:GLU:HG2	2.18	0.43
3:A:416:VAL:HG11	3:A:424:TYR:HE2	1.83	0.43
3:A:525:PHE:CD2	3:A:526:MET:HE2	2.53	0.43
5:E:171:ARG:HH11	5:E:212:LEU:HD12	1.83	0.43
7:P:400:ARG:NH2	7:Q:400:ARG:HA	2.33	0.43
7:M:7:VAL:HG22	7:M:25:VAL:HG22	2.00	0.43
7:Q:21:LEU:HD11	7:Q:110:ALA:HA	2.01	0.43
3:A:521:LEU:CD1	3:A:575:ASP:HB3	2.48	0.43
3:A:672:PHE:HZ	3:A:726:PHE:CZ	2.35	0.43
4:B:213:MET:SD	4:B:263:GLY:HA3	2.58	0.43
7:P:147:MET:HE3	7:P:182:GLY:HA3	2.00	0.43
7:K:1:MET:HA	7:K:28:GLU:HB3	1.99	0.43
7:O:220:GLU:O	7:O:224:LYS:HG2	2.19	0.43
7:N:314:GLN:HG3	7:N:431:ASN:HD21	1.83	0.43
3:A:17:ILE:HD11	3:A:156:ILE:HD13	2.00	0.43
5:C:64:TYR:CZ	5:C:169:VAL:HG22	2.54	0.43
7:S:205:GLU:HA	7:S:403:ARG:NH2	2.33	0.43
7:N:75:ILE:HG21	7:N:114:VAL:HG21	2.01	0.43
7:Q:417:LEU:HB2	7:Q:421:ALA:HB2	2.01	0.43
5:F:117:TYR:C	5:F:142:ILE:HG12	2.44	0.43
2:H:197:LEU:HD13	2:H:220:GLU:OE2	2.17	0.43
3:A:111:PHE:CZ	3:A:601:THR:HG22	2.54	0.43
3:A:243:LEU:HD21	3:A:365:TYR:CD1	2.54	0.43
3:A:623:MET:HE2	3:A:623:MET:HB3	1.84	0.43
5:F:44:LEU:HD13	5:F:103:LEU:HD23	2.00	0.43
7:O:6:ASP:HB3	7:O:26:TYR:HB2	2.00	0.43
7:Q:130:LEU:HD21	7:Q:380:THR:HG23	2.01	0.43
2:H:32:ILE:HD11	2:H:75:LEU:HD23	2.01	0.43
2:H:50:MET:HE1	2:H:84:ILE:HG12	2.01	0.43
4:B:216:THR:HB	4:B:292:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:162:PHE:CE2	7:S:241:LEU:HD13	2.54	0.43
7:O:148:ASN:CA	7:O:166:MET:HG3	2.48	0.43
8:T:71:TRP:CH2	8:T:77:ARG:HD3	2.54	0.43
7:S:202:VAL:HG11	7:S:399:SER:OG	2.19	0.43
7:L:323:THR:O	7:L:347:ILE:HD13	2.19	0.43
7:P:163:GLN:HB3	7:P:164:GLU:OE1	2.19	0.43
7:O:131:TYR:CE2	7:O:416:GLN:NE2	2.86	0.43
7:Q:379:SER:HA	7:Q:406:LYS:HE3	2.01	0.43
4:B:217:THR:O	4:B:259:LYS:HD3	2.19	0.42
5:C:138:ILE:HD11	5:C:190:TYR:CE2	2.53	0.42
5:E:109:LEU:O	5:E:114:VAL:HG22	2.19	0.42
7:M:180:ARG:HG3	7:O:59:TYR:CE2	2.54	0.42
6:J:17:ILE:HA	6:J:20:LEU:HG	2.00	0.42
7:S:205:GLU:CA	7:S:403:ARG:HE	2.26	0.42
7:S:309:LEU:HB3	7:S:313:VAL:HG12	2.01	0.42
7:L:150:ILE:HD13	7:L:212:PHE:CE2	2.54	0.42
7:L:157:ASP:HB2	7:L:211:ARG:CZ	2.49	0.42
7:M:323:THR:CG2	7:M:343:LYS:H	2.30	0.42
7:Q:342:ILE:HG13	7:Q:367:ALA:HB1	2.01	0.42
3:A:634:ALA:O	3:A:641:SER:HB2	2.19	0.42
5:E:27:ALA:O	5:E:28:ALA:HB3	2.18	0.42
5:E:59:LEU:HD13	5:E:176:LEU:HB3	2.01	0.42
7:S:1:MET:HG2	7:S:125:TYR:HE1	1.85	0.42
7:L:147:MET:HB2	7:L:167:ILE:HG13	2.01	0.42
3:A:719:GLU:O	3:A:722:LYS:HB3	2.19	0.42
4:B:165:LEU:HD12	4:B:168:GLU:OE2	2.19	0.42
5:C:186:GLY:HA2	5:C:190:TYR:H	1.85	0.42
3:A:493:ILE:HA	3:A:496:TYR:CD2	2.55	0.42
5:F:3:PHE:HA	5:F:155:ILE:O	2.18	0.42
2:H:47:TYR:O	2:H:51:VAL:HG13	2.19	0.42
3:A:696:GLU:HG2	3:A:703:ARG:HH12	1.84	0.42
5:E:47:ILE:HB	5:E:101:ALA:HB3	2.02	0.42
7:P:75:ILE:HG21	7:P:114:VAL:HG21	2.01	0.42
7:P:323:THR:CG2	7:P:346:GLN:HB3	2.49	0.42
7:O:190:LYS:C	7:O:194:LYS:HZ3	2.27	0.42
3:A:514:VAL:HG23	3:A:611:ILE:HG12	2.00	0.42
3:A:720:ARG:HB3	3:A:720:ARG:NH2	2.34	0.42
3:A:720:ARG:O	3:A:724:LYS:HG3	2.20	0.42
5:F:109:LEU:O	5:F:114:VAL:HG22	2.19	0.42
5:C:109:LEU:O	5:C:114:VAL:HG22	2.20	0.42
7:S:1:MET:HG2	7:S:125:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:396:GLY:HA3	7:P:403:ARG:HG2	2.01	0.42
7:Q:402:ASP:OD1	7:Q:403:ARG:HG2	2.19	0.42
3:A:144:PHE:HE1	3:A:149:TYR:CZ	2.38	0.42
3:A:411:TYR:CE2	3:A:412:HIS:HD2	2.37	0.42
3:A:639:LYS:HZ2	4:B:95:ARG:NH1	2.17	0.42
5:E:200:ALA:H	5:E:213:ASN:ND2	2.18	0.42
7:L:1:MET:HE2	7:L:125:TYR:HE1	1.84	0.42
7:P:148:ASN:O	7:P:397:SER:HB2	2.20	0.42
7:K:149:ILE:HG12	7:K:189:LEU:HD23	2.02	0.42
7:Q:5:THR:HG21	7:Q:28:GLU:OE1	2.18	0.42
2:H:51:VAL:HG12	2:H:56:ALA:HB2	2.01	0.42
3:A:682:PHE:CZ	3:A:714:LEU:HD12	2.54	0.42
3:A:712:GLU:O	3:A:712:GLU:CG	2.67	0.42
3:A:729:LEU:HD12	3:A:732:LYS:NZ	2.35	0.42
4:B:282:PHE:CZ	4:B:284:HIS:CE1	3.08	0.42
7:L:1:MET:HA	7:L:28:GLU:HB3	2.01	0.42
7:L:51:LEU:HD12	7:L:51:LEU:HA	1.90	0.42
7:N:258:TYR:HB2	7:N:267:ALA:O	2.19	0.42
7:N:289:THR:HG23	7:N:314:GLN:HE21	1.85	0.42
3:A:254:PHE:CE2	3:A:274:LEU:HD21	2.55	0.42
3:A:525:PHE:HD2	3:A:526:MET:HE2	1.84	0.42
3:A:608:SER:HA	3:A:653:PHE:HZ	1.84	0.42
6:D:36:ARG:HH21	6:D:39:LEU:HB2	1.85	0.42
5:G:12:ILE:HG13	5:G:149:PHE:HB2	2.02	0.42
6:J:124:LYS:HB3	6:J:124:LYS:HE3	1.84	0.42
7:S:289:THR:HG23	7:S:314:GLN:HE21	1.85	0.42
7:L:238:PHE:CE1	7:L:426:LEU:HD21	2.55	0.42
7:L:245:SER:HA	7:L:248:PHE:CE2	2.55	0.42
7:Q:341:LEU:HA	7:Q:341:LEU:HD12	1.78	0.42
3:A:608:SER:HA	3:A:653:PHE:CZ	2.55	0.41
3:A:665:LEU:O	3:A:669:ARG:HG3	2.20	0.41
4:B:32:ILE:HD11	4:B:170:MET:HE1	2.02	0.41
5:C:101:ALA:HB1	5:C:147:PHE:HB3	2.02	0.41
7:L:79:ILE:HD13	7:L:79:ILE:HA	1.88	0.41
7:L:275:ILE:HD12	7:L:275:ILE:HG23	1.70	0.41
7:P:424:ARG:O	7:P:427:LYS:HE2	2.18	0.41
7:K:150:ILE:HB	7:K:165:PHE:HB2	2.02	0.41
7:M:53:ASP:HA	7:M:66:LYS:HE3	2.01	0.41
7:N:36:MET:HB2	7:N:378:ASP:HB2	2.01	0.41
7:N:341:LEU:HA	7:N:341:LEU:HD12	1.79	0.41
3:A:493:ILE:HD13	3:A:580:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:674:HIS:C	3:A:723:PHE:HZ	2.28	0.41
4:B:7:ILE:HG21	4:B:7:ILE:HD13	1.84	0.41
5:C:34:SER:H	5:C:138:ILE:HA	1.86	0.41
7:K:205:GLU:HA	7:K:403:ARG:CZ	2.50	0.41
7:M:306:THR:HG21	7:M:336:ALA:HA	2.02	0.41
2:H:200:VAL:HB	2:H:319:THR:OG1	2.20	0.41
4:B:39:GLU:O	4:B:43:MET:HG3	2.20	0.41
5:F:138:ILE:HG21	5:F:138:ILE:HD13	1.86	0.41
5:E:33:ASP:H	5:E:137:GLN:HE21	1.68	0.41
6:I:49:SER:HA	6:I:57:LEU:HD11	2.03	0.41
7:L:36:MET:HG2	7:L:376:THR:HG21	2.02	0.41
7:N:343:LYS:HD3	7:N:346:GLN:NE2	2.34	0.41
2:H:258:LYS:HA	2:H:262:LEU:HB2	2.01	0.41
4:B:29:ALA:HA	4:B:32:ILE:HG22	2.03	0.41
5:F:131:ALA:CB	5:G:92:LYS:HD2	2.49	0.41
7:S:401:THR:OG1	7:N:402:ASP:HB3	2.19	0.41
7:M:350:LEU:HD23	7:M:350:LEU:HA	1.89	0.41
7:O:149:ILE:HD12	7:O:189:LEU:HD22	2.03	0.41
7:N:160:ILE:HD11	7:N:212:PHE:HB2	2.01	0.41
8:T:94:GLU:HG3	8:T:96:ILE:CD1	2.49	0.41
4:B:61:THR:HA	4:B:216:THR:OG1	2.21	0.41
5:F:64:TYR:CD1	5:F:78:ILE:HD13	2.56	0.41
5:F:101:ALA:HB1	5:F:147:PHE:HB3	2.01	0.41
7:S:92:ARG:HA	7:S:92:ARG:HD3	1.85	0.41
7:O:163:GLN:HE22	7:O:247:GLU:CD	2.29	0.41
7:O:292:ASP:OD2	7:O:318:ASP:HB3	2.20	0.41
8:T:33:ILE:HB	8:T:37:GLU:CG	2.51	0.41
2:H:99:LEU:HD23	2:H:320:LYS:HB3	2.03	0.41
3:A:438:THR:HG22	3:A:463:SER:O	2.20	0.41
5:G:140:ARG:HD3	5:G:190:TYR:CE2	2.56	0.41
7:S:186:PHE:CZ	7:S:399:SER:HB2	2.55	0.41
7:L:74:VAL:HG12	7:L:97:LEU:HD21	2.02	0.41
7:O:95:ILE:HG12	7:O:103:LYS:HE3	2.01	0.41
4:B:65:PRO:O	4:B:71:PHE:HB2	2.20	0.41
5:C:167:PHE:CE2	5:C:212:LEU:HD22	2.55	0.41
5:E:64:TYR:CE2	5:E:169:VAL:HG22	2.55	0.41
7:P:190:LYS:O	7:P:194:LYS:HG3	2.20	0.41
7:Q:312:LYS:HG3	7:Q:313:VAL:HG23	2.02	0.41
3:A:510:ARG:HH21	5:E:25:ALA:HB2	1.86	0.41
3:A:622:LEU:HD21	4:B:130:THR:HG21	2.03	0.41
7:P:185:ILE:HD11	7:P:237:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:147:MET:HG3	7:M:407:TYR:OH	2.21	0.41
7:M:359:MET:HE3	7:M:359:MET:HB2	1.87	0.41
1:R:8:U:H5'	5:F:54:GLY:HA3	2.02	0.41
2:H:17:PRO:HA	2:H:222:ILE:O	2.21	0.41
2:H:103:ARG:HD2	2:H:110:ALA:CA	2.50	0.41
2:H:245:GLU:HG2	2:H:248:LYS:HE3	2.02	0.41
2:H:268:ASP:HA	2:H:337:LYS:HB2	2.01	0.41
3:A:297:LEU:HD11	3:A:307:VAL:HG23	2.01	0.41
3:A:382:TYR:HB2	4:B:229:MET:HG3	2.03	0.41
3:A:642:ILE:HB	3:A:653:PHE:CE1	2.55	0.41
3:A:696:GLU:O	3:A:700:ASN:HB2	2.21	0.41
4:B:6:TYR:CE2	4:B:170:MET:HG3	2.56	0.41
4:B:135:GLN:HE21	4:B:137:HIS:HE1	1.67	0.41
6:D:70:TYR:CZ	6:D:74:ARG:HD3	2.56	0.41
6:I:91:VAL:HG13	6:I:96:ILE:HB	2.03	0.41
7:S:248:PHE:CE2	7:S:258:TYR:HE1	2.39	0.41
7:L:1:MET:HE2	7:L:125:TYR:CE1	2.55	0.41
7:M:306:THR:HG21	7:M:335:HIS:O	2.20	0.41
7:O:371:HIS:H	7:O:371:HIS:HD1	1.69	0.41
1:R:-5:A:H3'	4:B:38:LEU:HD11	2.03	0.41
2:H:286:ALA:HB1	2:H:299:LEU:HD21	2.03	0.41
3:A:411:TYR:CD1	3:A:421:ARG:NH1	2.89	0.41
7:L:239:ILE:O	7:L:287:ILE:HA	2.21	0.41
7:K:112:LEU:HD22	7:K:345:ASN:HA	2.03	0.41
7:M:152:GLY:HA2	7:M:156:SER:OG	2.21	0.41
7:O:147:MET:SD	7:O:398:LEU:HD21	2.61	0.41
3:A:689:LEU:O	3:A:734:TYR:OH	2.39	0.40
5:G:101:ALA:HB1	5:G:147:PHE:HB3	2.03	0.40
7:S:248:PHE:CE2	7:S:258:TYR:CE1	3.09	0.40
7:L:401:THR:OG1	7:K:402:ASP:HB3	2.21	0.40
7:M:346:GLN:HE21	7:M:372:ARG:NH1	2.19	0.40
7:Q:2:SER:HB3	7:Q:125:TYR:CZ	2.57	0.40
2:H:238:GLU:OE1	2:H:241:ARG:NH2	2.54	0.40
3:A:251:ILE:HG13	3:A:252:GLN:N	2.35	0.40
3:A:716:ASP:O	3:A:719:GLU:N	2.48	0.40
5:E:14:LEU:HB2	5:E:143:ARG:O	2.21	0.40
7:K:328:LEU:HD21	7:K:360:ALA:HB2	2.03	0.40
7:Q:24:GLU:HG2	7:Q:32:PHE:CZ	2.56	0.40
8:T:27:ASN:HB3	8:T:33:ILE:HD13	2.03	0.40
1:R:26:A:H5'	5:G:124:ASN:O	2.21	0.40
7:L:157:ASP:HB2	7:L:211:ARG:NE	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:22:GLU:HB3	7:K:36:MET:HG2	2.03	0.40
4:B:20:LEU:HD11	4:B:181:LYS:HE2	2.03	0.40
4:B:135:GLN:NE2	4:B:137:HIS:CE1	2.90	0.40
6:D:45:LEU:CD2	6:D:109:LEU:HD11	2.52	0.40
5:E:78:ILE:H	5:E:78:ILE:HD12	1.87	0.40
7:S:425:GLY:O	7:S:428:SER:HB2	2.22	0.40
7:L:147:MET:HE1	7:L:179:LEU:HA	2.03	0.40
3:A:396:GLU:OE1	3:A:397:ARG:HB2	2.22	0.40
4:B:71:PHE:O	4:B:157:TYR:OH	2.38	0.40
5:E:95:ARG:HH12	5:E:162:GLN:NE2	2.19	0.40
5:G:156:THR:H	5:G:159:ASN:HD22	1.69	0.40
7:K:147:MET:HG2	7:K:407:TYR:OH	2.21	0.40
7:Q:12:VAL:HG21	7:Q:36:MET:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	350/357 (98%)	331 (95%)	19 (5%)	0	100	100
3	A	756/758 (100%)	731 (97%)	24 (3%)	1 (0%)	48	72
4	B	295/299 (99%)	279 (95%)	16 (5%)	0	100	100
5	C	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
5	E	217/220 (99%)	205 (94%)	12 (6%)	0	100	100
5	F	217/220 (99%)	210 (97%)	7 (3%)	0	100	100
5	G	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
6	D	128/136 (94%)	126 (98%)	2 (2%)	0	100	100
6	I	128/136 (94%)	127 (99%)	1 (1%)	0	100	100
6	J	128/136 (94%)	126 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	K	432/434 (100%)	418 (97%)	14 (3%)	0	100	100
7	L	432/434 (100%)	419 (97%)	13 (3%)	0	100	100
7	M	432/434 (100%)	420 (97%)	12 (3%)	0	100	100
7	N	432/434 (100%)	423 (98%)	9 (2%)	0	100	100
7	O	432/434 (100%)	419 (97%)	13 (3%)	0	100	100
7	P	432/434 (100%)	422 (98%)	10 (2%)	0	100	100
7	Q	432/434 (100%)	420 (97%)	12 (3%)	0	100	100
7	S	432/434 (100%)	420 (97%)	12 (3%)	0	100	100
8	T	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
All	All	6213/6279 (99%)	6016 (97%)	196 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	717	LYS

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	
2	H	306/312 (98%)	306 (100%)	0	100	100
3	A	649/649 (100%)	649 (100%)	0	100	100
4	B	247/263 (94%)	247 (100%)	0	100	100
5	C	180/188 (96%)	180 (100%)	0	100	100
5	E	181/188 (96%)	181 (100%)	0	100	100
5	F	181/188 (96%)	181 (100%)	0	100	100
5	G	182/188 (97%)	182 (100%)	0	100	100
6	D	119/125 (95%)	119 (100%)	0	100	100
6	I	119/125 (95%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	119/125 (95%)	119 (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	N	338/338 (100%)	338 (100%)	0	100	100
7	O	338/338 (100%)	338 (100%)	0	100	100
7	P	338/338 (100%)	338 (100%)	0	100	100
7	Q	338/338 (100%)	338 (100%)	0	100	100
7	S	338/338 (100%)	338 (100%)	0	100	100
8	T	94/94 (100%)	94 (100%)	0	100	100
All	All	5081/5149 (99%)	5081 (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 (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	65	GLN
2	H	115	ASN
2	H	124	ASN
2	H	154	ASN
3	A	15	HIS
3	A	107	GLN
3	A	412	HIS
3	A	532	GLN
3	A	692	ASN
3	A	700	ASN
4	B	134	ASN
4	B	137	HIS
5	F	11	GLN
5	F	134	ASN
5	F	144	ASN
6	D	75	ASN
5	C	137	GLN
5	E	134	ASN
5	E	162	GLN
5	E	213	ASN
5	G	161	ASN

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Mol	Chain	Res	Type
6	J	67	GLN
6	J	75	ASN
7	L	65	GLN
7	L	78	HIS
7	L	346	GLN
7	P	65	GLN
7	P	314	GLN
7	P	371	HIS
7	K	65	GLN
7	K	148	ASN
7	K	163	GLN
7	K	371	HIS
7	M	18	ASN
7	M	46	HIS
7	M	65	GLN
7	M	213	ASN
7	M	346	GLN
7	O	65	GLN
7	O	163	GLN
7	O	416	GLN
7	N	65	GLN
7	N	346	GLN
7	Q	65	GLN
7	Q	148	ASN
7	Q	274	GLN
7	Q	346	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	40/41 (97%)	11 (27%)	1 (2%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	-4	C
1	R	-3	G
1	R	2	C
1	R	3	C
1	R	7	A
1	R	8	U

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Mol	Chain	Res	Type
1	R	10	C
1	R	15	G
1	R	16	C
1	R	21	U
1	R	34	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

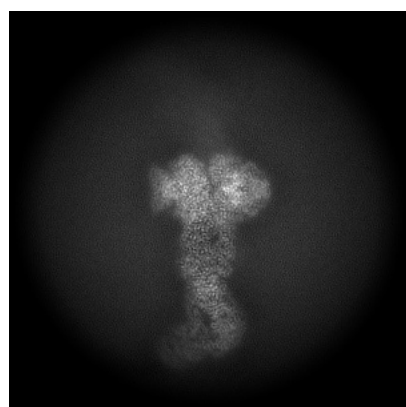
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49645. These allow visual inspection of the internal detail of the map and identification of artifacts.

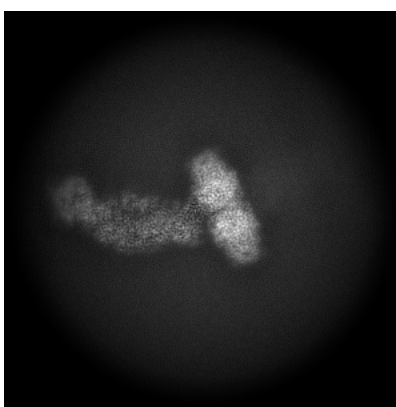
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

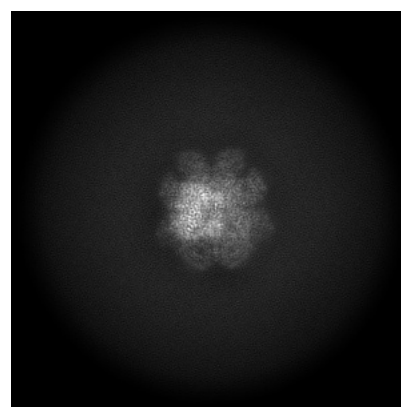
6.1.1 Primary map



X



Y

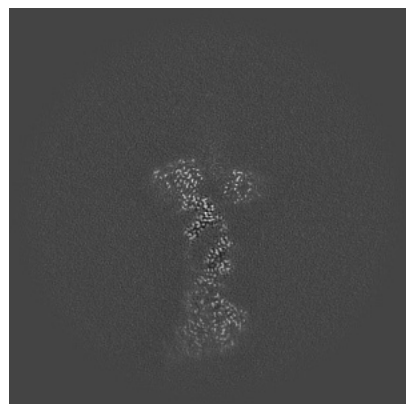


Z

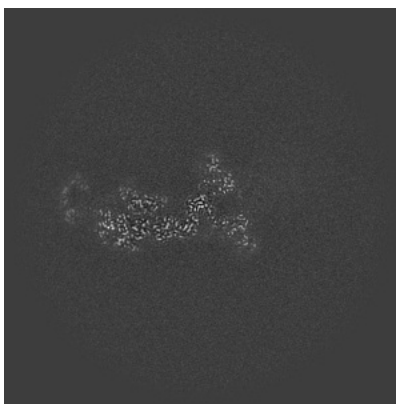
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

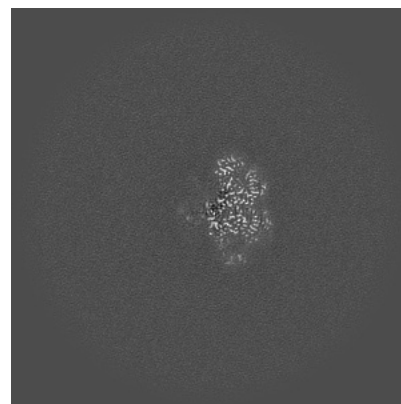
6.2.1 Primary map



X Index: 280



Y Index: 280

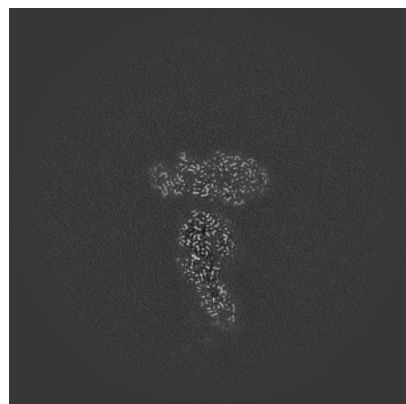


Z Index: 280

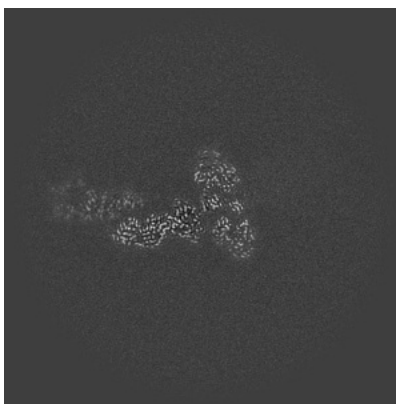
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

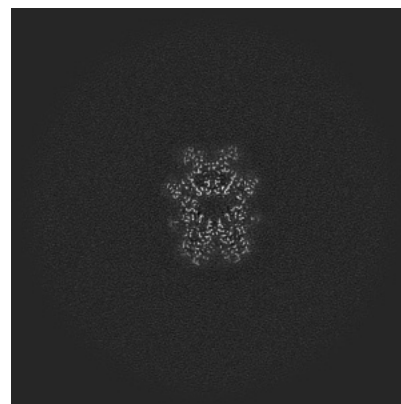
6.3.1 Primary map



X Index: 257



Y Index: 264



Z Index: 310

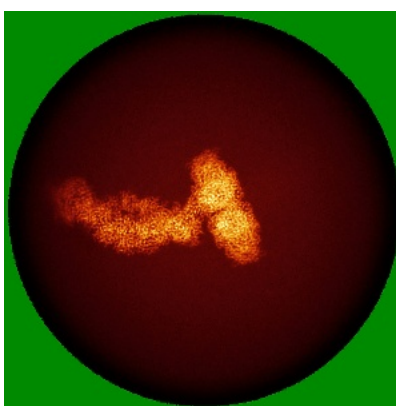
The images above show the largest variance slices of the map in three orthogonal directions.

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

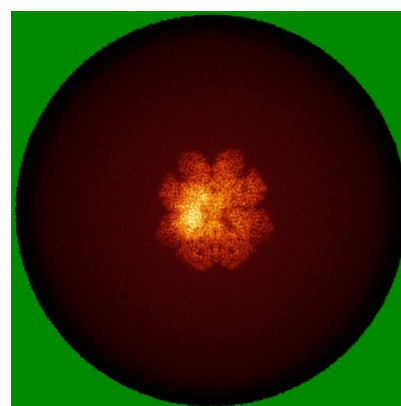
6.4.1 Primary map



X



Y

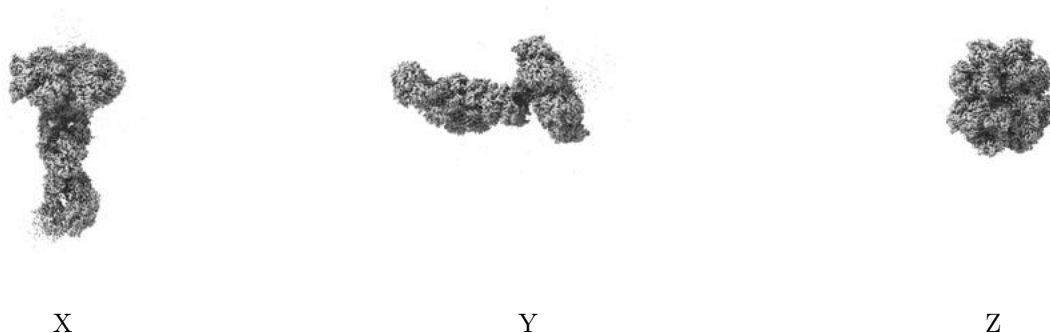


Z

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 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

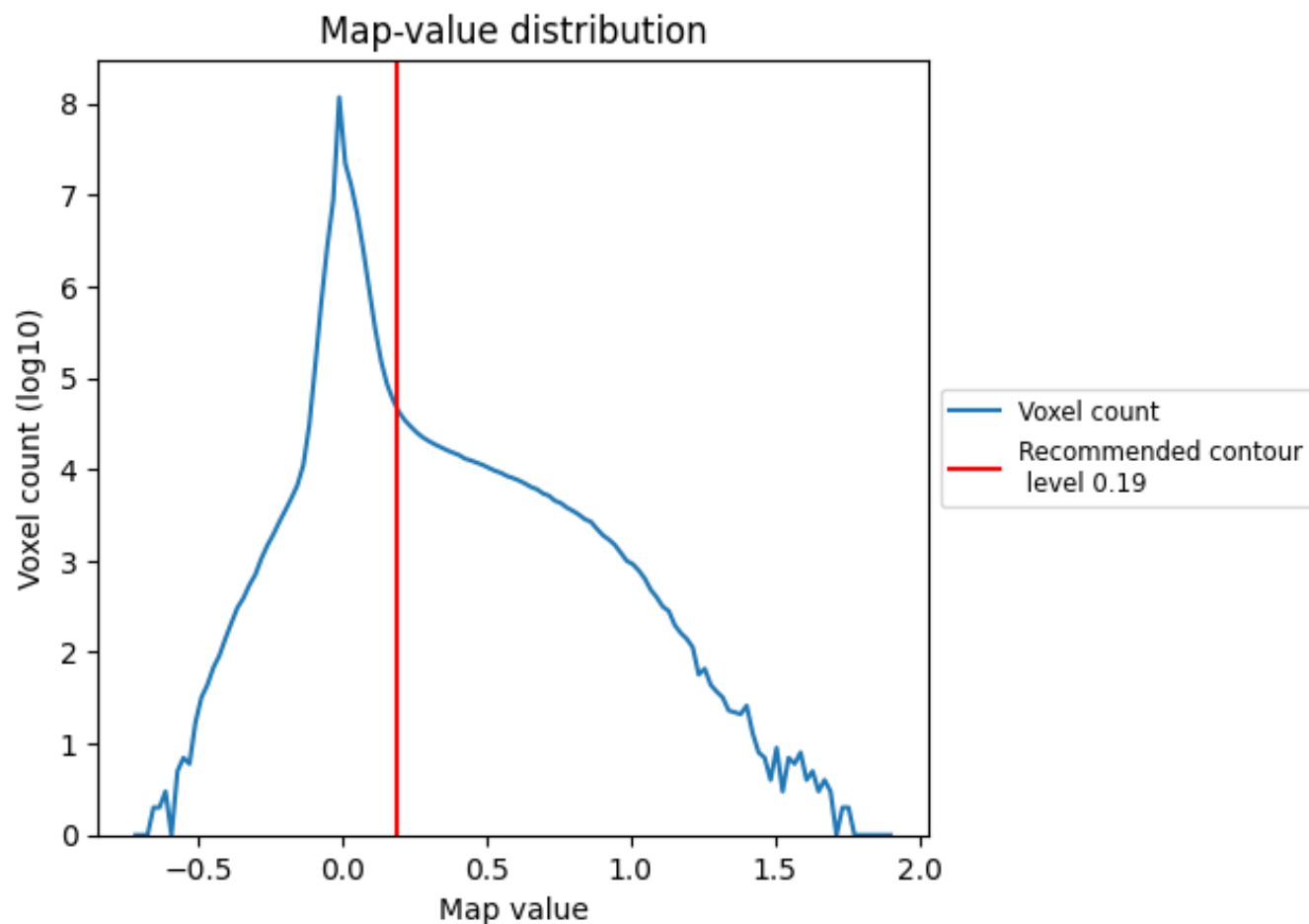
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

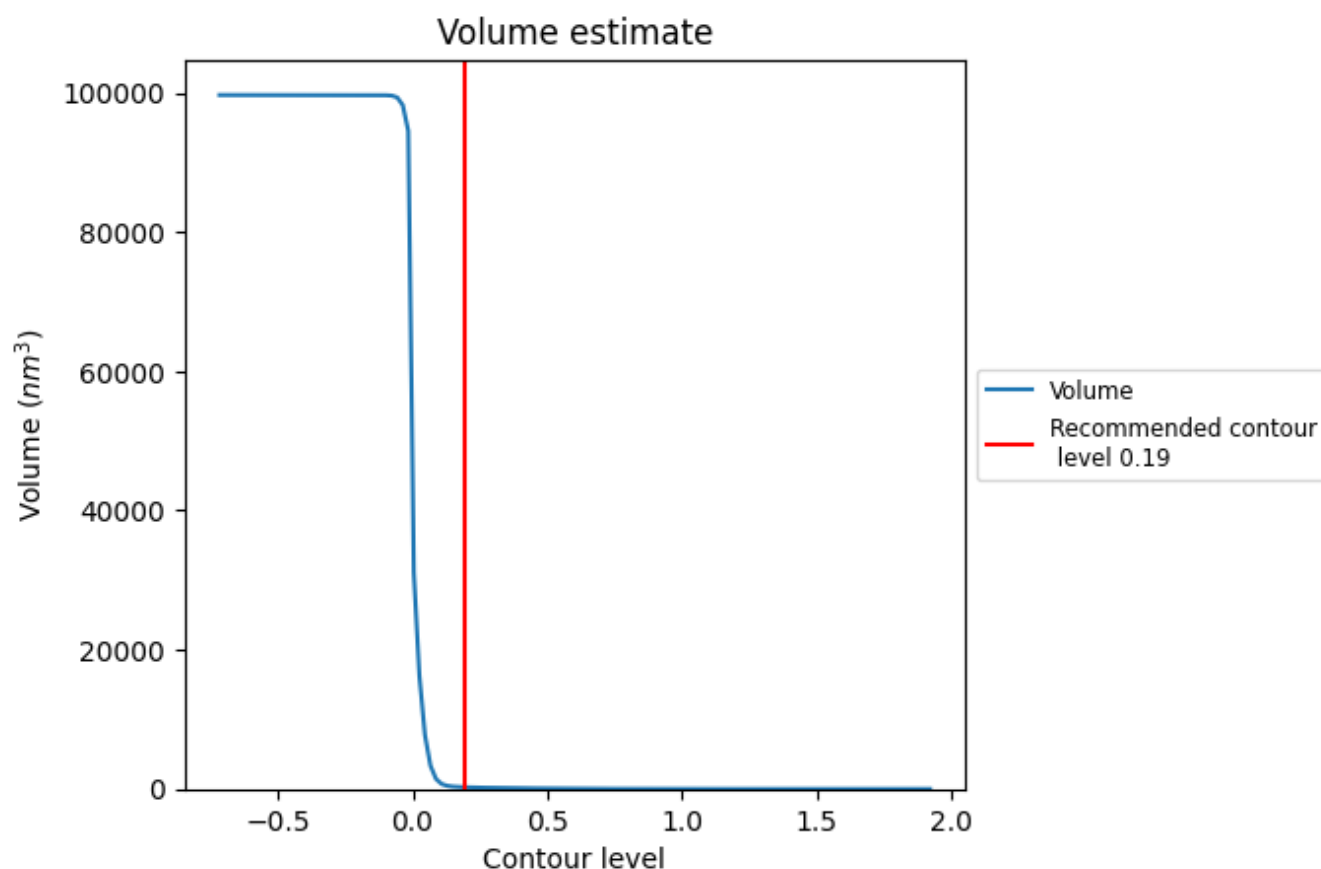
This section contains the results of statistical analysis of the map.

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.

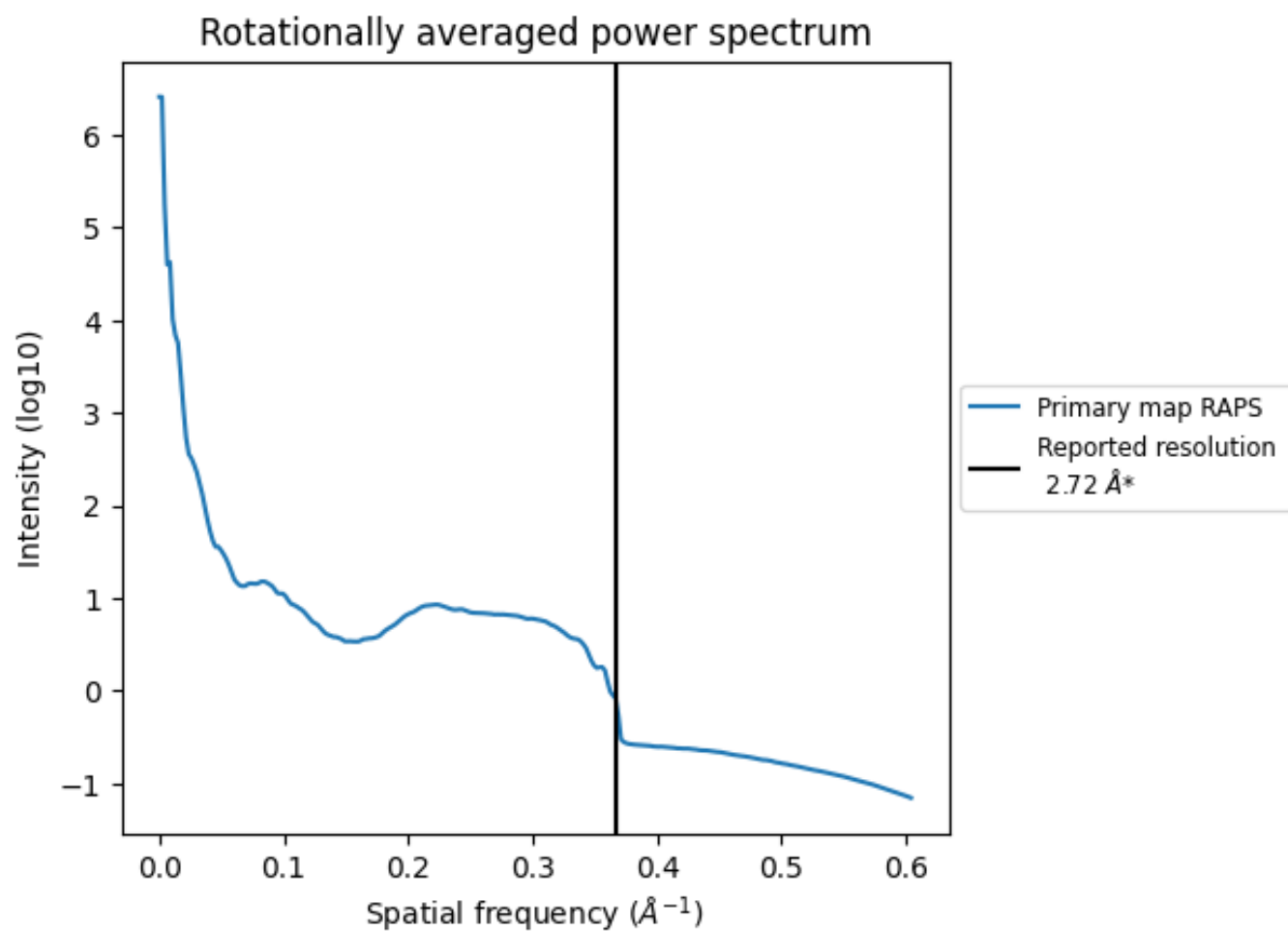
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm³; this corresponds to an approximate mass of 227 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 0.368 Å⁻¹

8 Fourier-Shell correlation

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

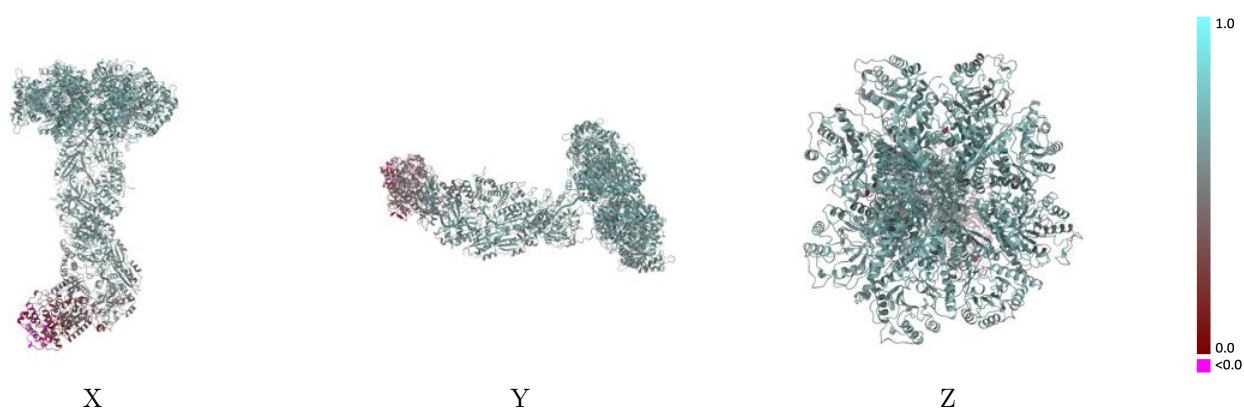
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49645 and PDB model 9NQ7. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

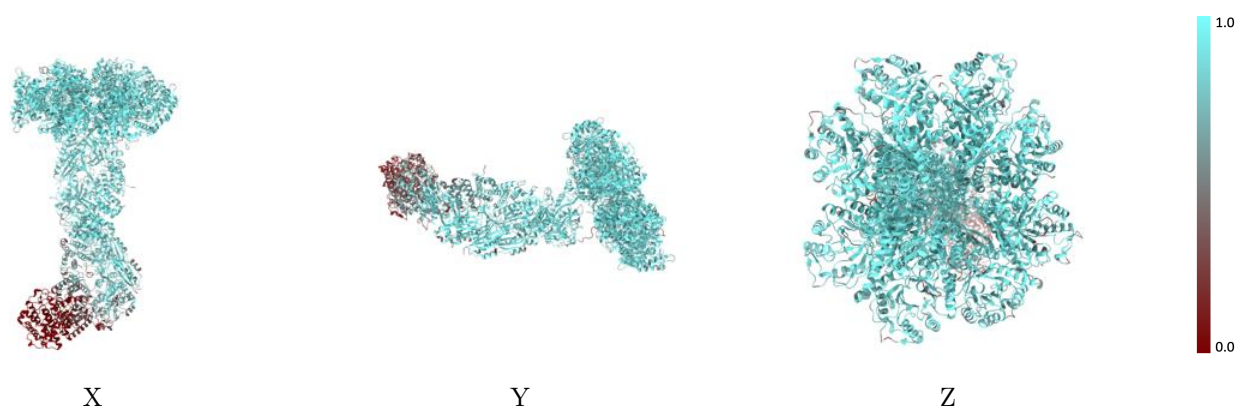
This section was not generated.

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



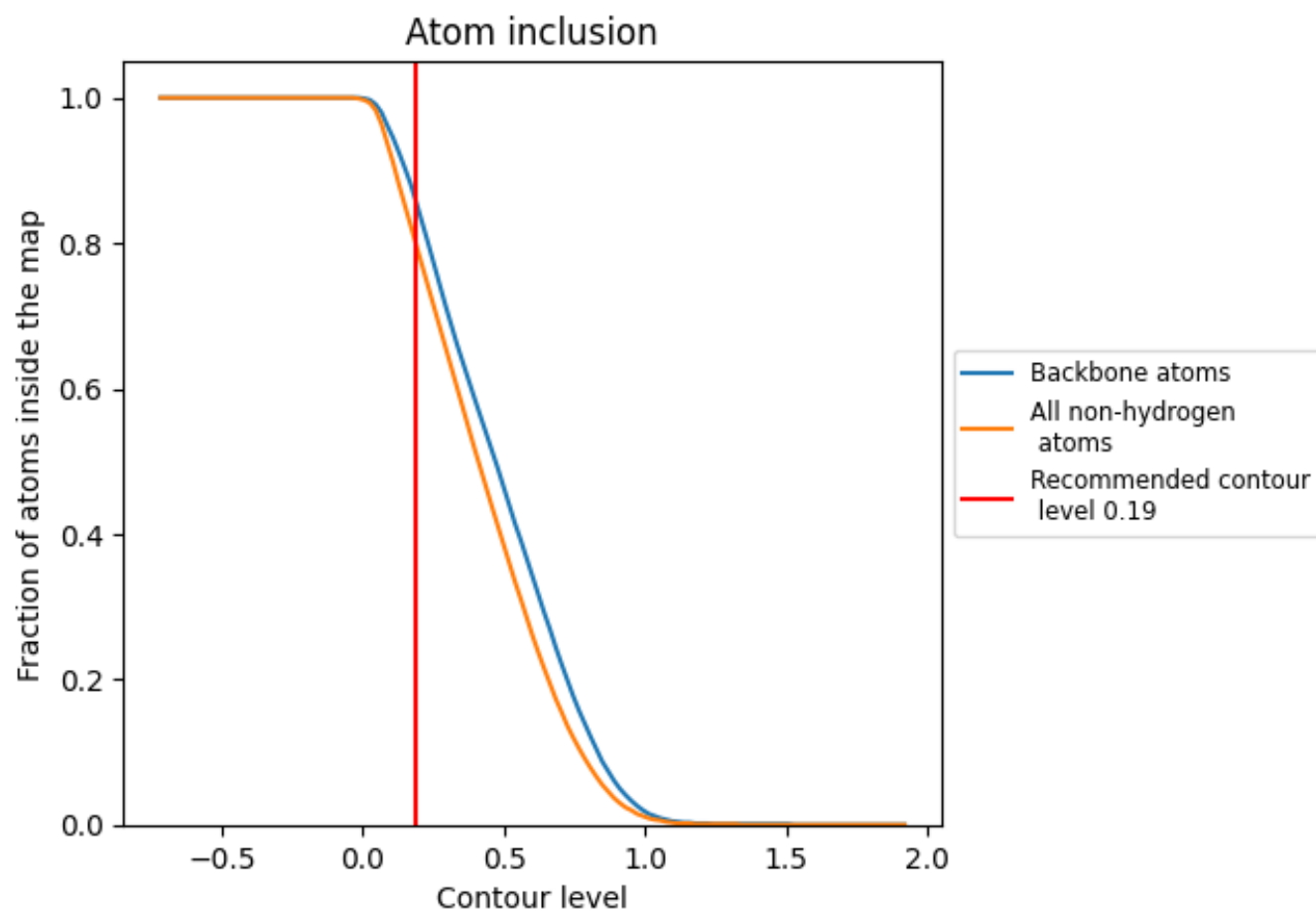
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.5620
A	 0.2710	 0.3300
B	 0.5930	 0.4630
C	 0.8990	 0.6050
D	 0.7780	 0.5510
E	 0.7570	 0.5360
F	 0.8730	 0.5900
G	 0.8960	 0.5960
H	 0.9090	 0.6030
I	 0.8720	 0.5850
J	 0.8780	 0.5820
K	 0.8970	 0.6130
L	 0.9000	 0.6110
M	 0.8940	 0.6150
N	 0.9100	 0.6190
O	 0.8900	 0.6090
P	 0.8890	 0.6060
Q	 0.8930	 0.6140
R	 0.9660	 0.6020
S	 0.9120	 0.6200
T	 0.8350	 0.5650

