Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 11:23 AM JST

PDB ID	:	7WE6
EMDB ID	:	EMD-32440
Title	:	Structure of Csy-AcrIF24-dsDNA
Authors	:	Zhang, L.; Feng, Y.
Deposited on	:	2021-12-22
Resolution	:	3.20 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:

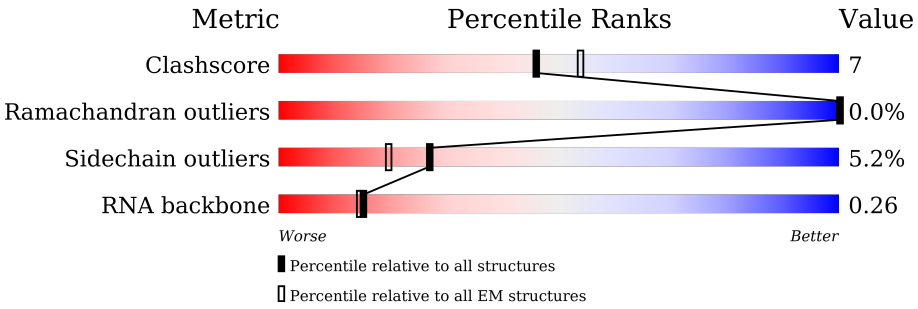
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	327	68% 68% 23% • 7%
1	L	327	66% 71% 21% • 7%
2	C	342	40% 73% 13% 14%
2	D	342	12% 84% 14% •
2	E	342	5% 84% 14% ••
2	F	342	5% 82% 15% ••
2	G	342	• 77% 18% ••

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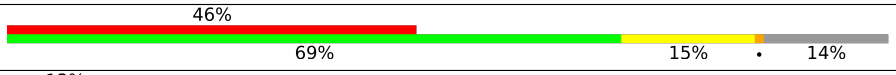
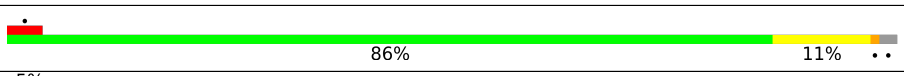
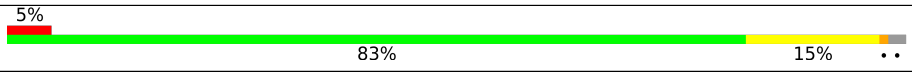
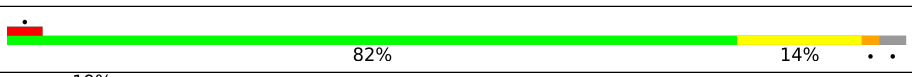
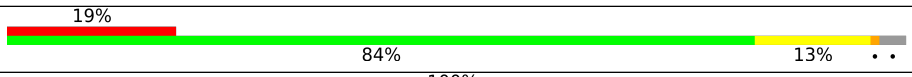
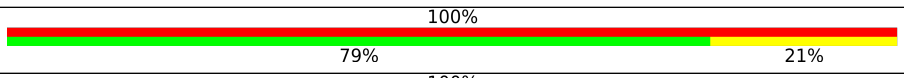
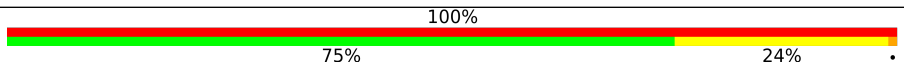
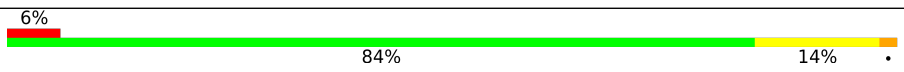
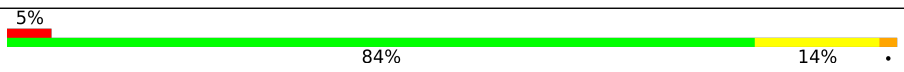
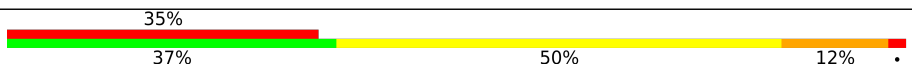
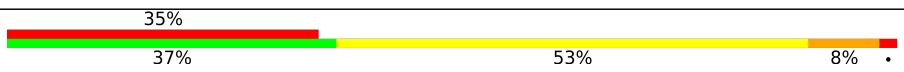
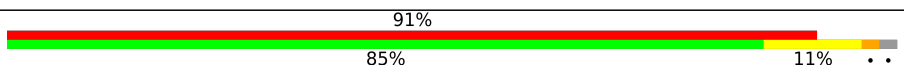
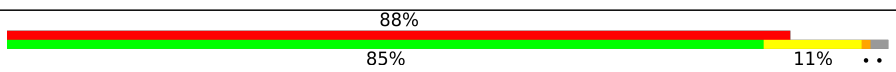
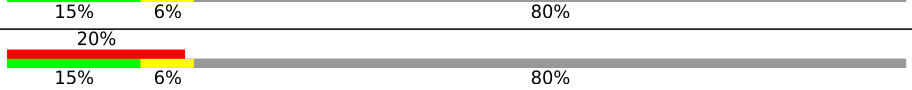
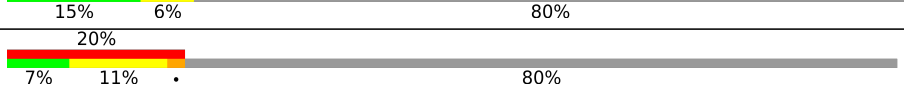
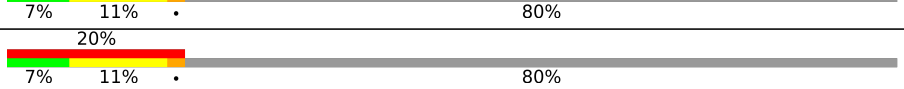
Mol	Chain	Length	Quality of chain
2	H	342	
2	M	342	
2	N	342	
2	O	342	
2	P	342	
2	Q	342	
2	R	342	
3	I	187	
3	S	187	
4	U	228	
4	V	228	
5	J	60	
5	T	60	
6	A	434	
6	X	434	
7	K	54	
7	Y	54	
8	W	54	
8	Z	54	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 48324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR type I-F/YPEST-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	305	Total	C	N	O	S	0	0
			2198	1386	400	409	3		
1	L	305	Total	C	N	O	S	0	0
			2321	1471	431	414	5		

- Molecule 2 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	293	Total	C	N	O	S	0	0
			2144	1350	379	413	2		
2	D	334	Total	C	N	O	S	0	0
			2531	1590	454	485	2		
2	E	337	Total	C	N	O	S	0	0
			2587	1626	469	490	2		
2	F	335	Total	C	N	O	S	0	0
			2577	1619	470	486	2		
2	G	329	Total	C	N	O	S	0	0
			2523	1586	459	476	2		
2	H	332	Total	C	N	O	S	0	0
			2487	1555	452	478	2		
2	M	293	Total	C	N	O	S	0	0
			2227	1406	396	423	2		
2	N	335	Total	C	N	O	S	0	0
			2571	1613	468	488	2		
2	O	334	Total	C	N	O	S	0	0
			2562	1611	467	482	2		
2	P	335	Total	C	N	O	S	0	0
			2581	1622	471	486	2		
2	Q	333	Total	C	N	O	S	0	0
			2552	1605	465	480	2		
2	R	333	Total	C	N	O	S	0	0
			2529	1588	461	479	1		

- Molecule 3 is a protein called Type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	187	Total	C	N	O	S	0	0
			1445	919	264	258	4		
3	S	187	Total	C	N	O	S	1	0
			1445	918	264	258	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	PHE	SER	conflict	UNP A0A0C6F3X3
S	183	PHE	SER	conflict	UNP A0A0C6F3X3

- Molecule 4 is a protein called AcrIF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	227	Total	C	N	O	S	0	0
			1758	1124	308	323	3		
4	V	227	Total	C	N	O	S	0	0
			1758	1124	308	323	3		

- Molecule 5 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
5	T	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		

- Molecule 6 is a protein called Type I-F CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	424	Total	C	N	O	0	0
			2251	1290	491	470		
6	X	424	Total	C	N	O	0	0
			2251	1290	491	470		

- Molecule 7 is a DNA chain called DNA (5'-D(P*GP*GP*AP*TP*GP*GP*CP*TP*TP*CP *C)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Y	11	Total	C	O	P	0	0
			121	55	55	11		
7	K	11	Total	C	O	P	0	0
			121	55	55	11		

- Molecule 8 is a DNA chain called DNA-r.

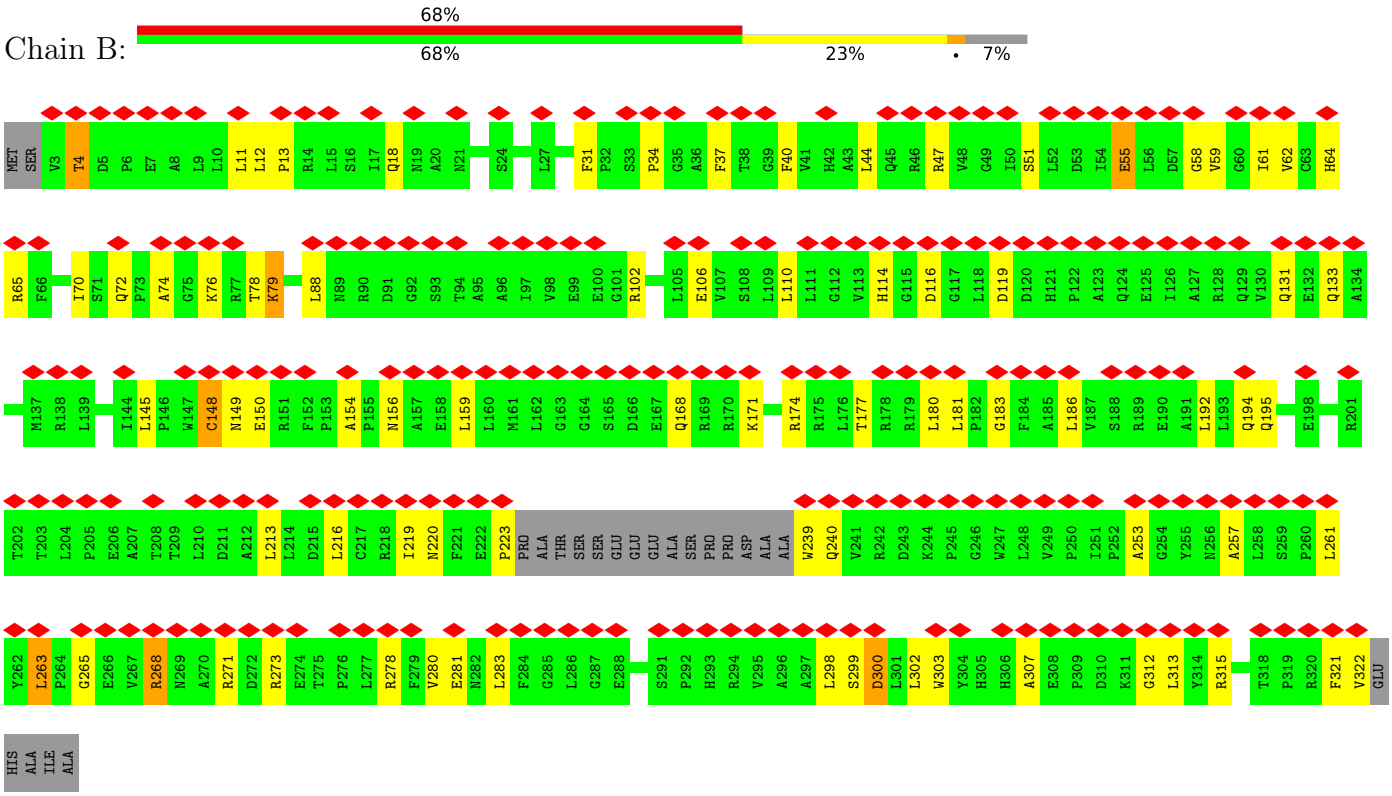
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Z	11	Total	C	O	P	0	0
			121	55	55	11		
8	W	11	Total	C	O	P	0	0
			121	55	55	11		

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.

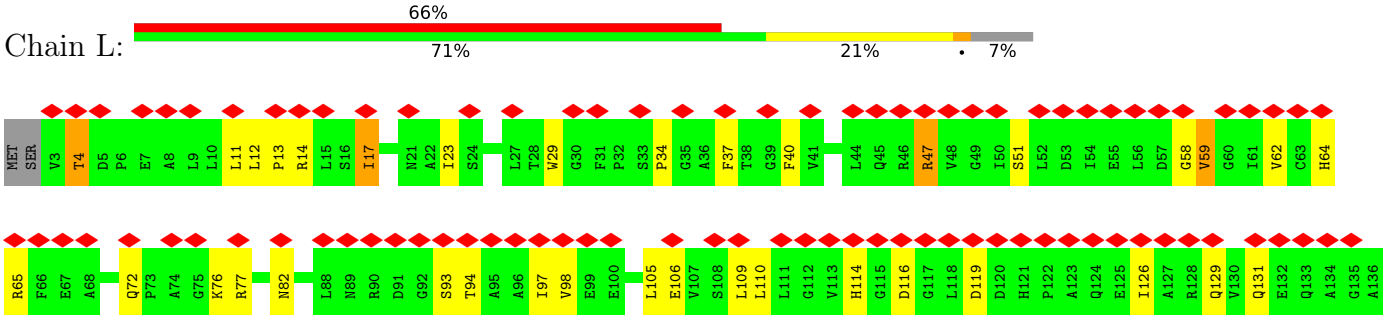
• Molecule 1: CRISPR type I-F/YPEST-associated protein Csy2

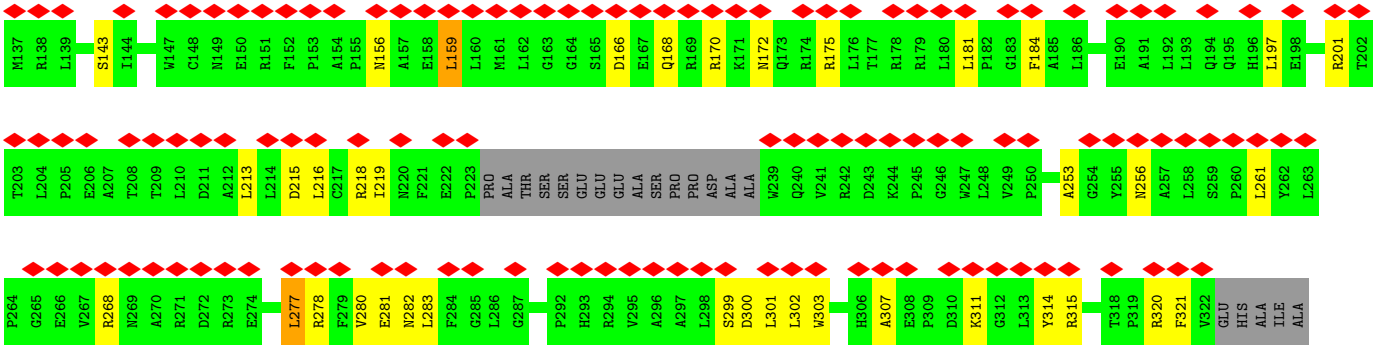
Chain B:



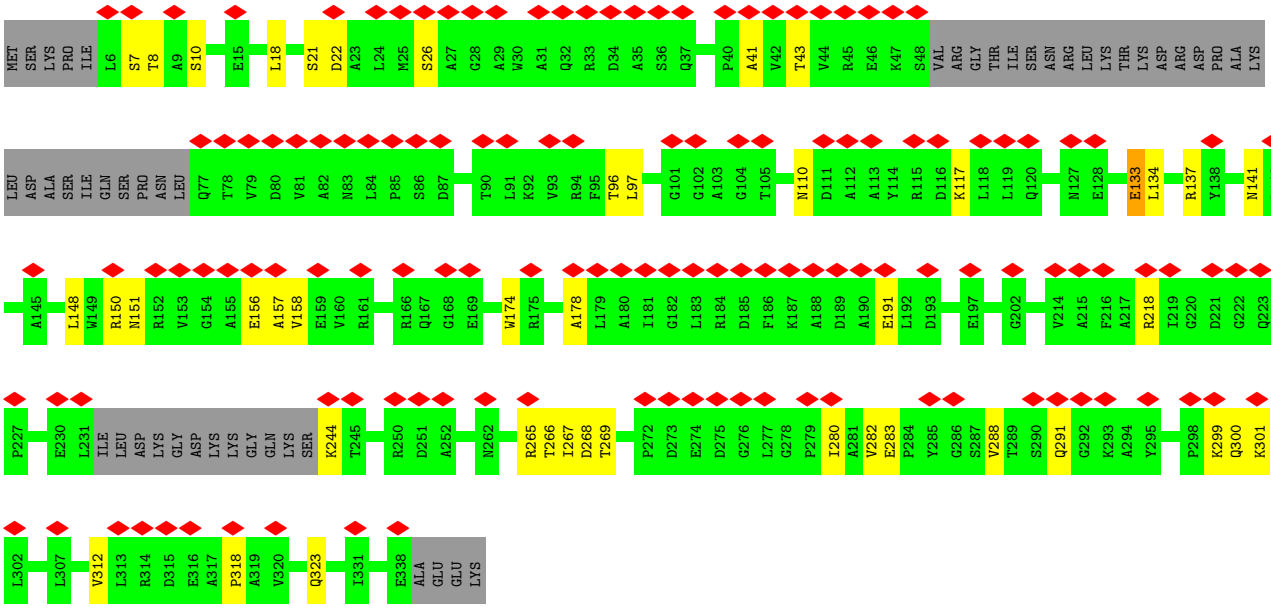
• Molecule 1: CRISPR type I-F/YPEST-associated protein Csy2

Chain L:

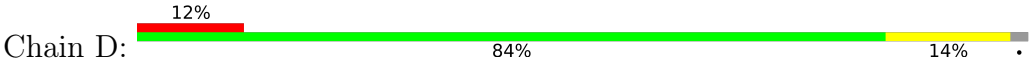


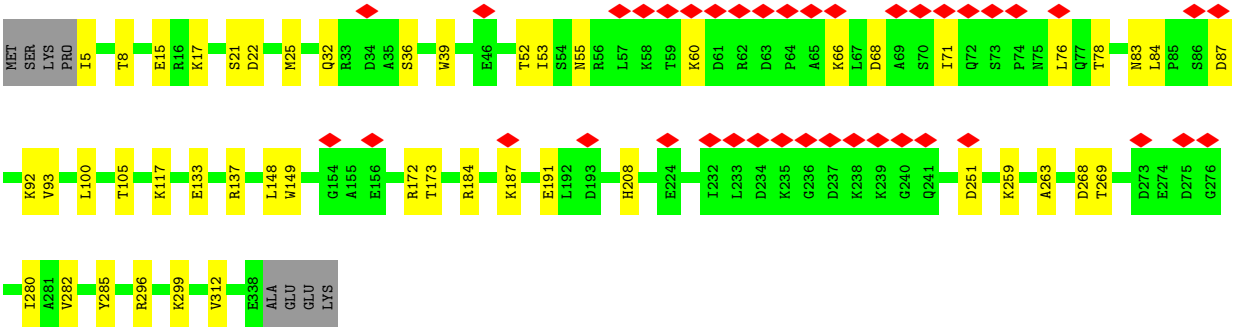


• Molecule 2: CRISPR-associated protein Csy3

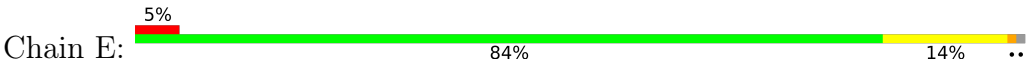


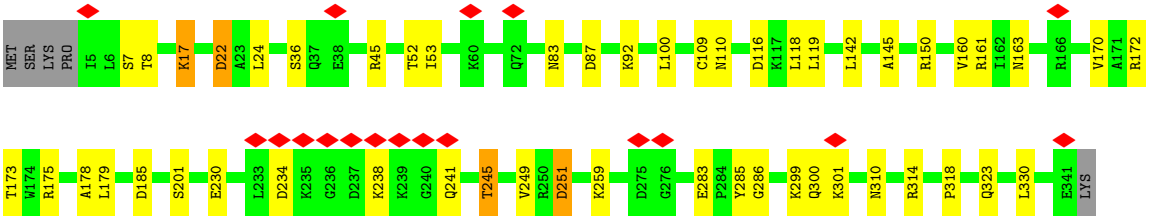
• Molecule 2: CRISPR-associated protein Csy3





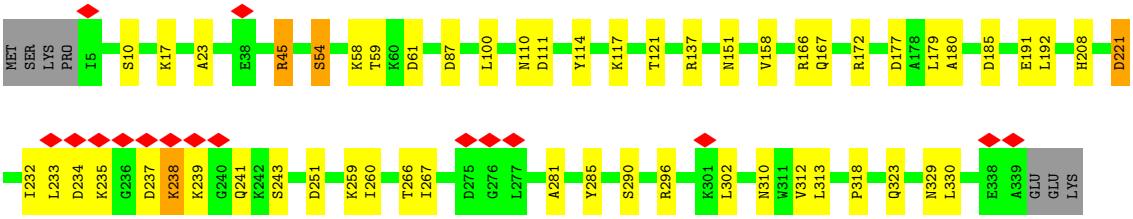
• Molecule 2: CRISPR-associated protein Csy3





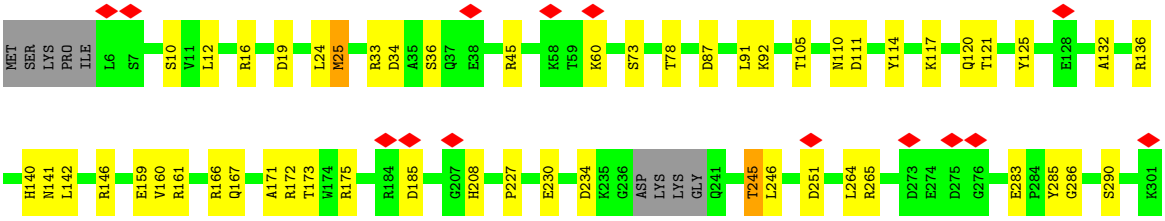
• Molecule 2: CRISPR-associated protein Csy3

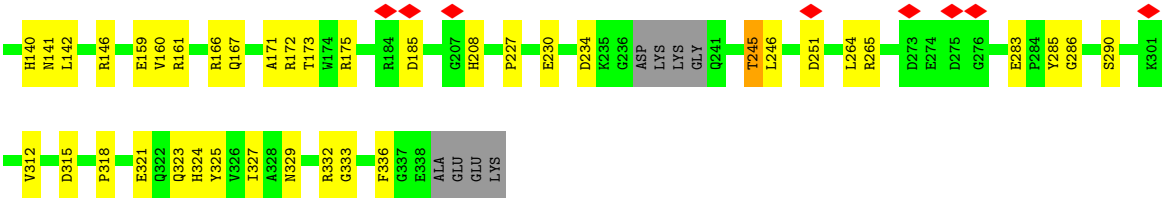
Chain F:



• Molecule 2: CRISPR-associated protein Csy3

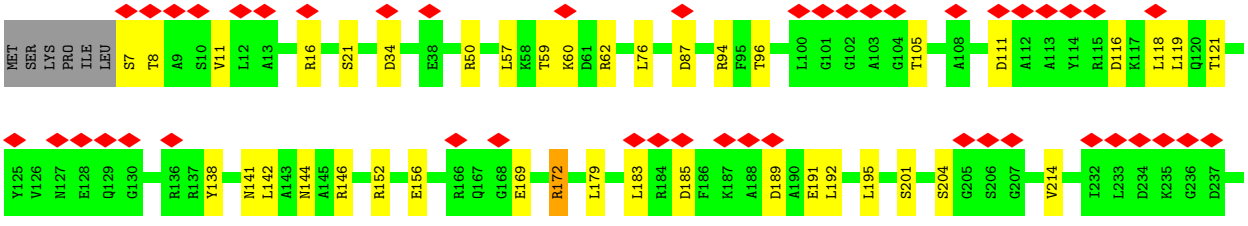
Chain G:

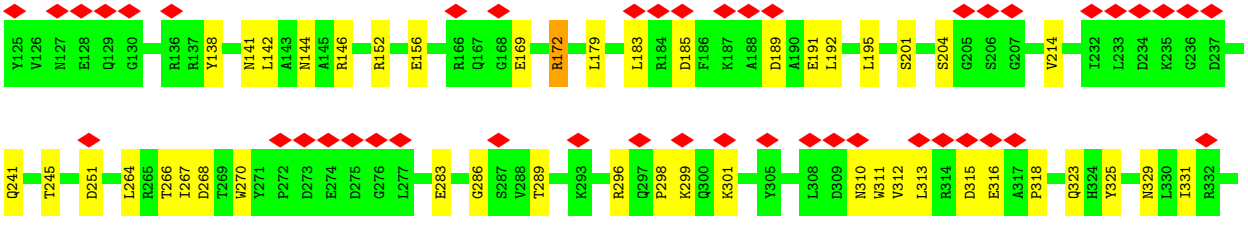


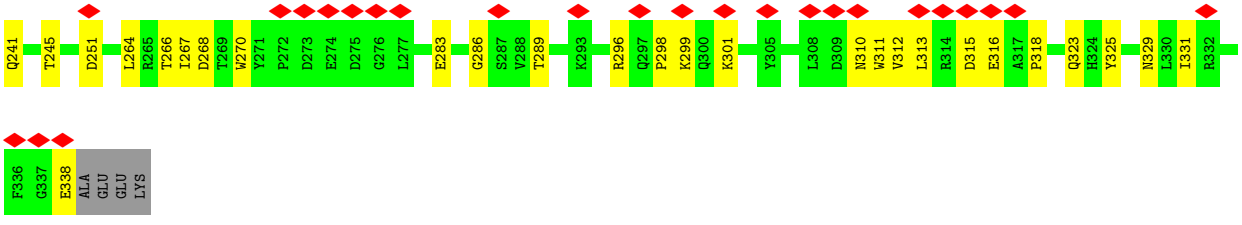


• Molecule 2: CRISPR-associated protein Csy3

Chain H:

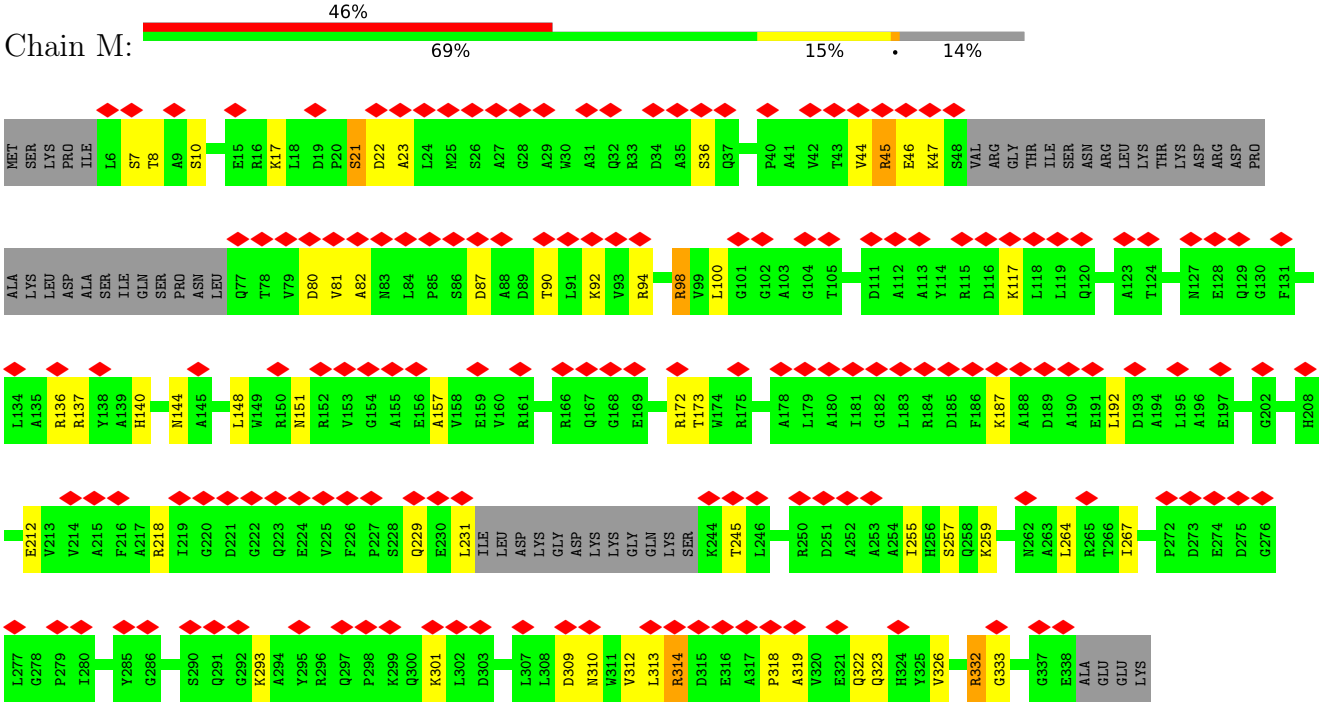






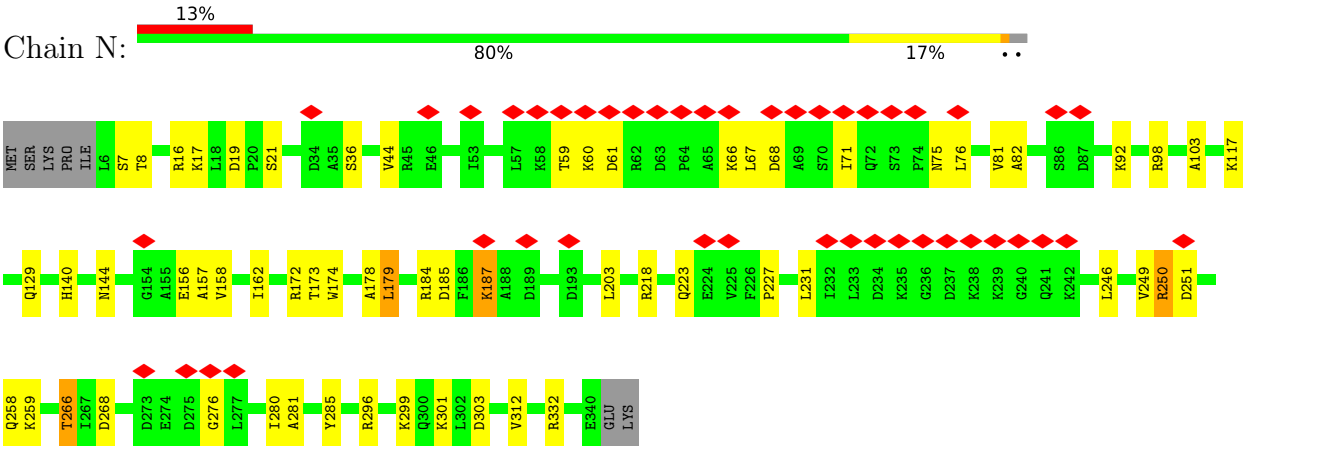
• Molecule 2: CRISPR-associated protein Csy3

Chain M:



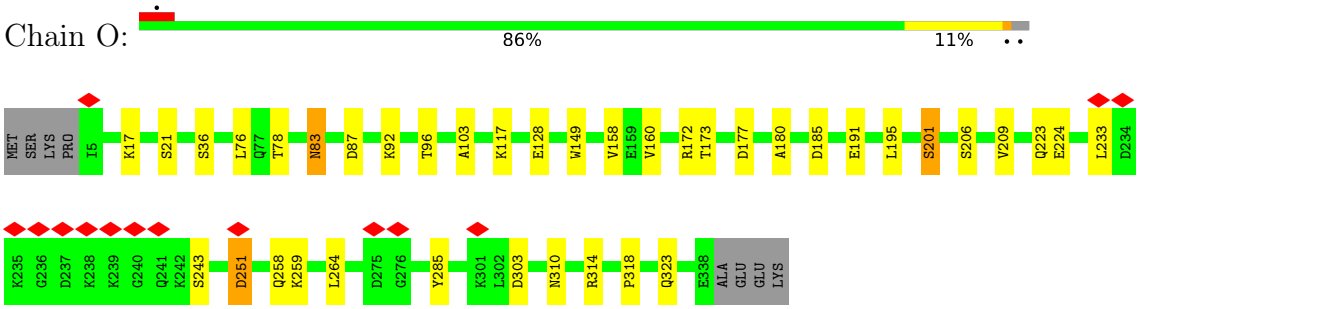
• Molecule 2: CRISPR-associated protein Csy3

Chain N:

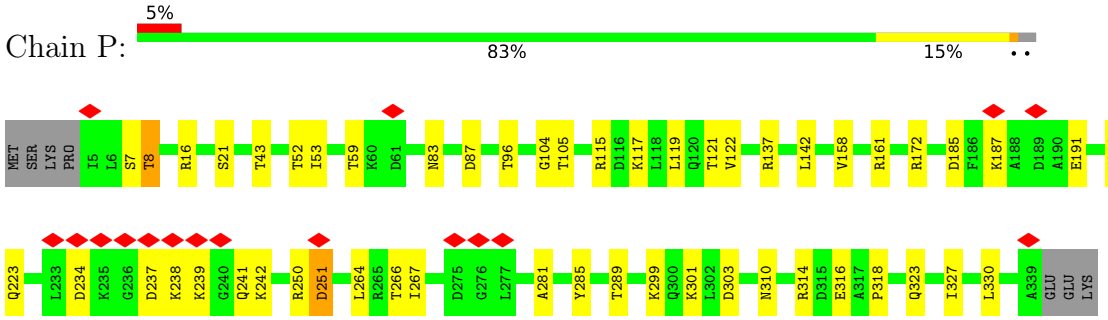


• Molecule 2: CRISPR-associated protein Csy3

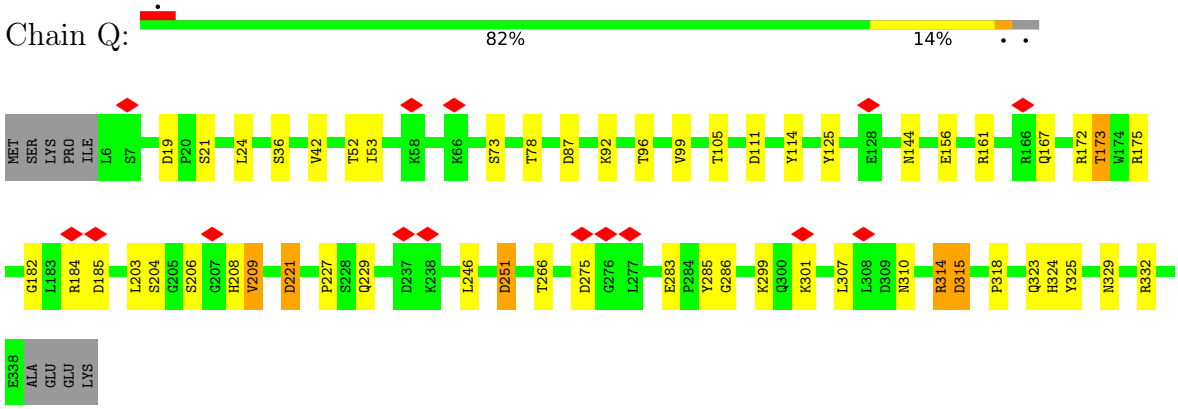
Chain O:



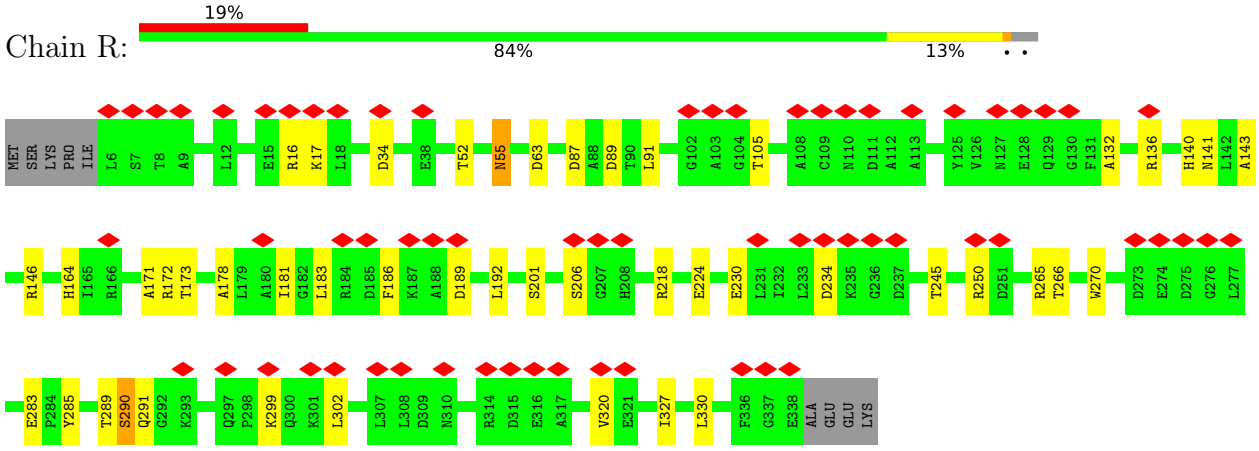
• Molecule 2: CRISPR-associated protein Csy3



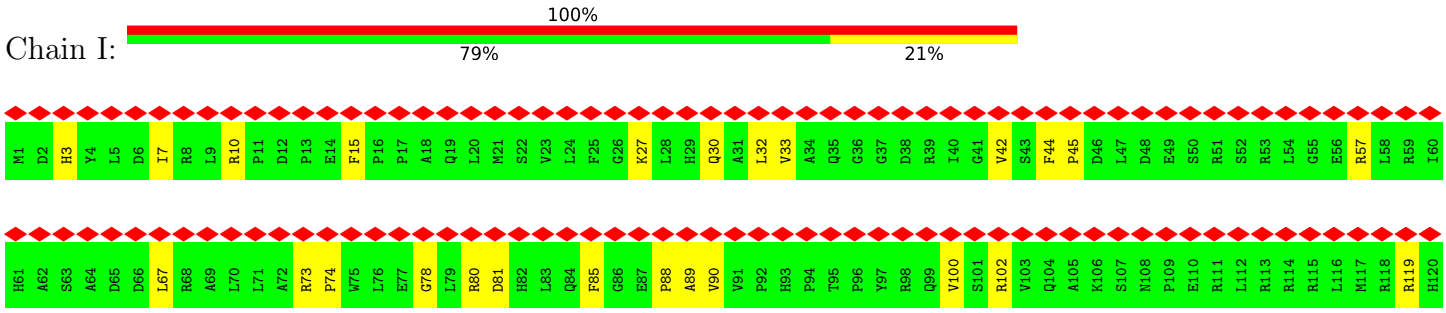
• Molecule 2: CRISPR-associated protein Csy3

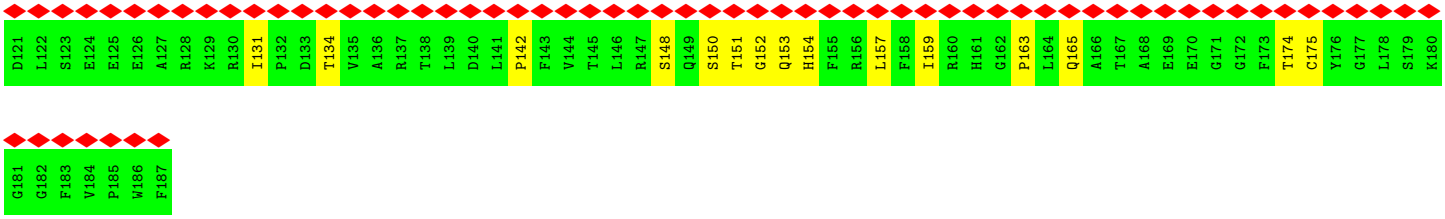


• Molecule 2: CRISPR-associated protein Csy3

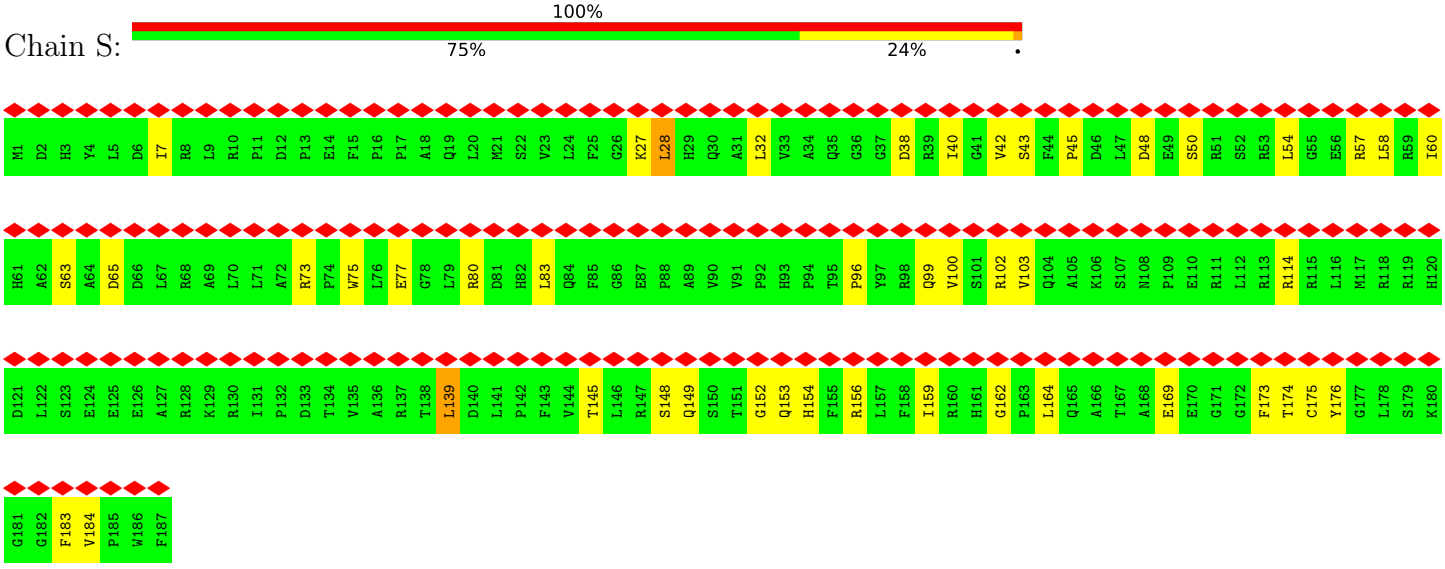


• Molecule 3: Type I-F CRISPR-associated endoribonuclease Cas6/Csy4

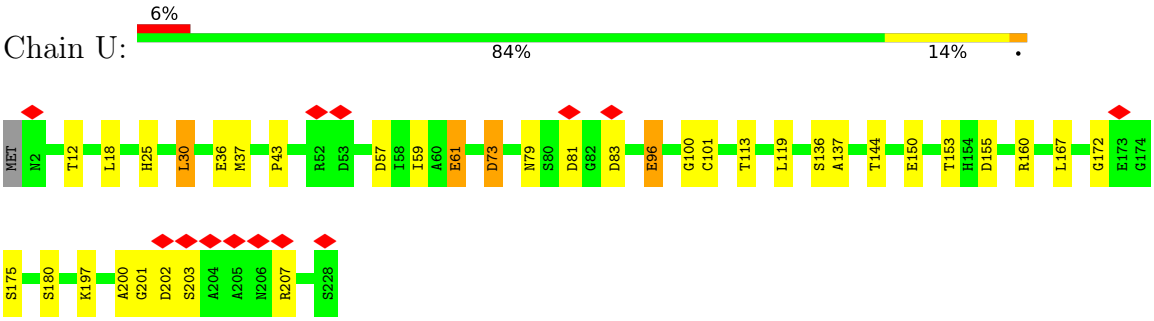




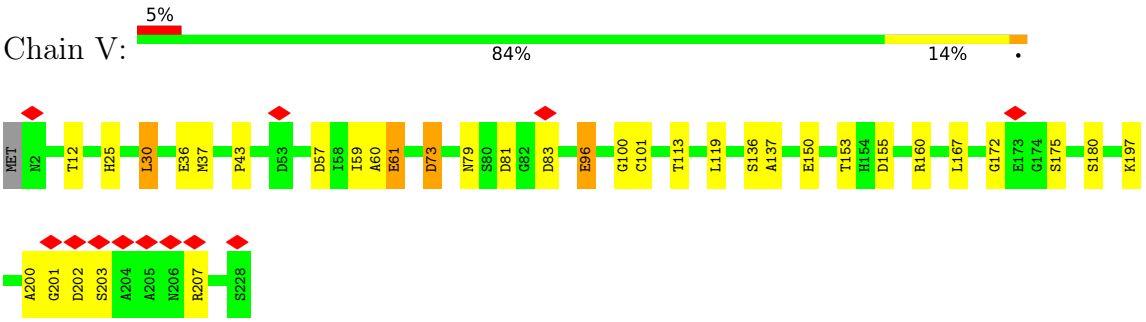
• Molecule 3: Type I-F CRISPR-associated endoribonuclease Cas6/Csy4



• Molecule 4: AcrIF24

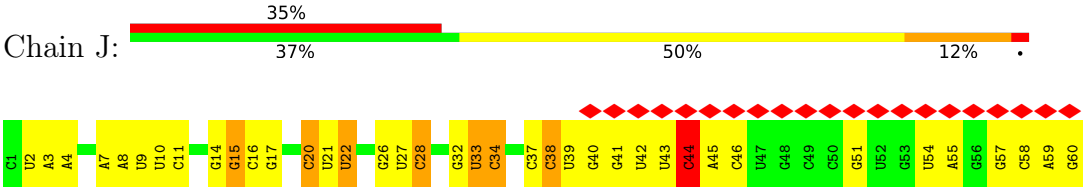


• Molecule 4: AcrIF24



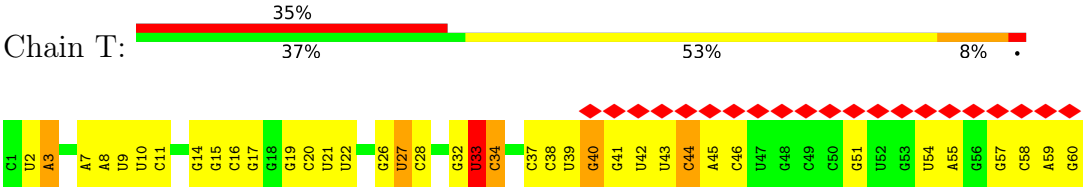
• Molecule 5: RNA (60-MER)

Chain J:



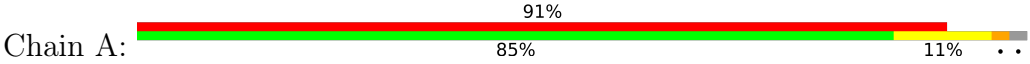
• Molecule 5: RNA (60-MER)

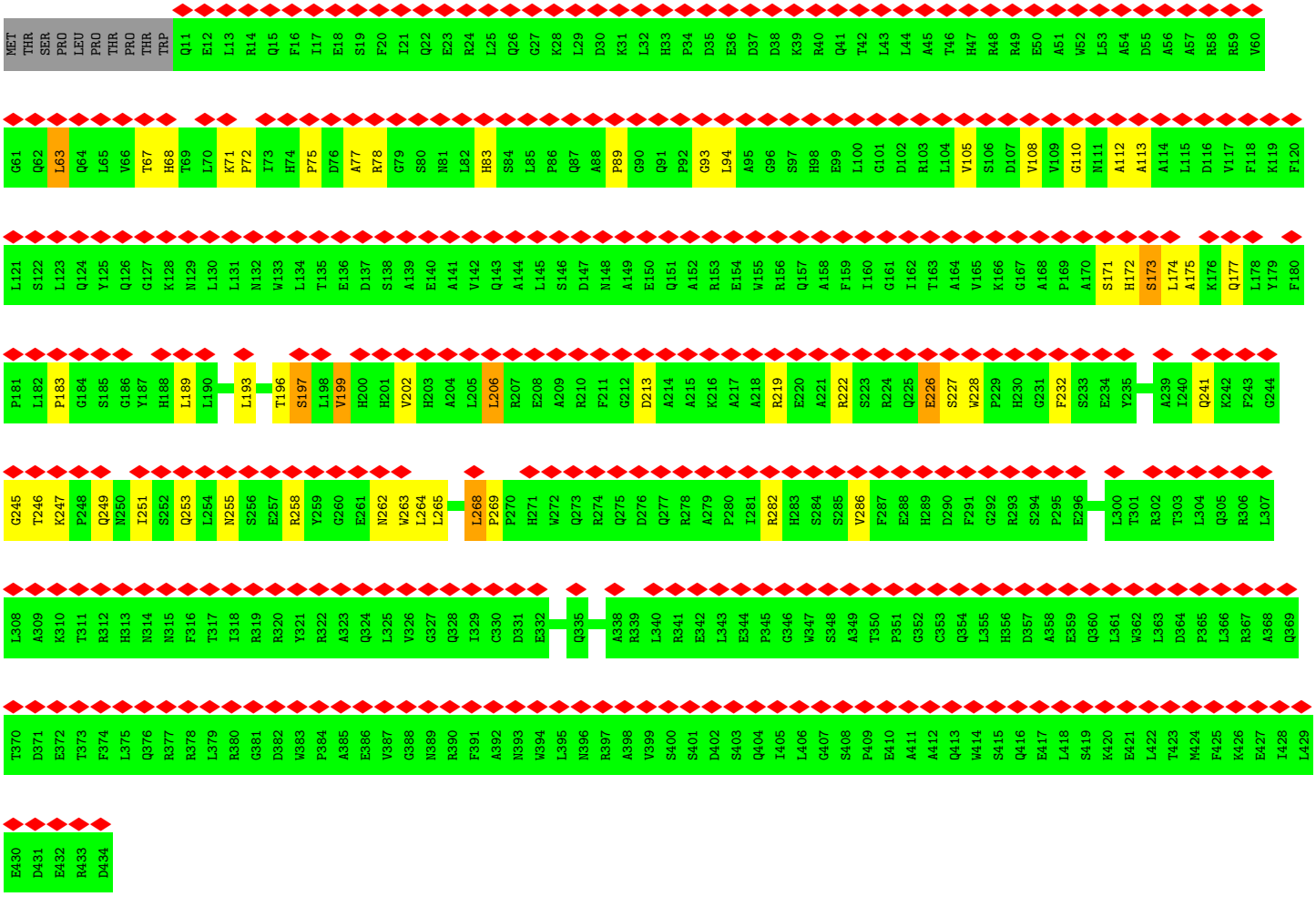
Chain T:



• Molecule 6: Type I-F CRISPR-associated protein Csy1

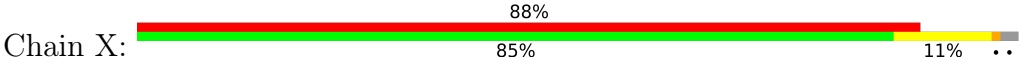
Chain A:

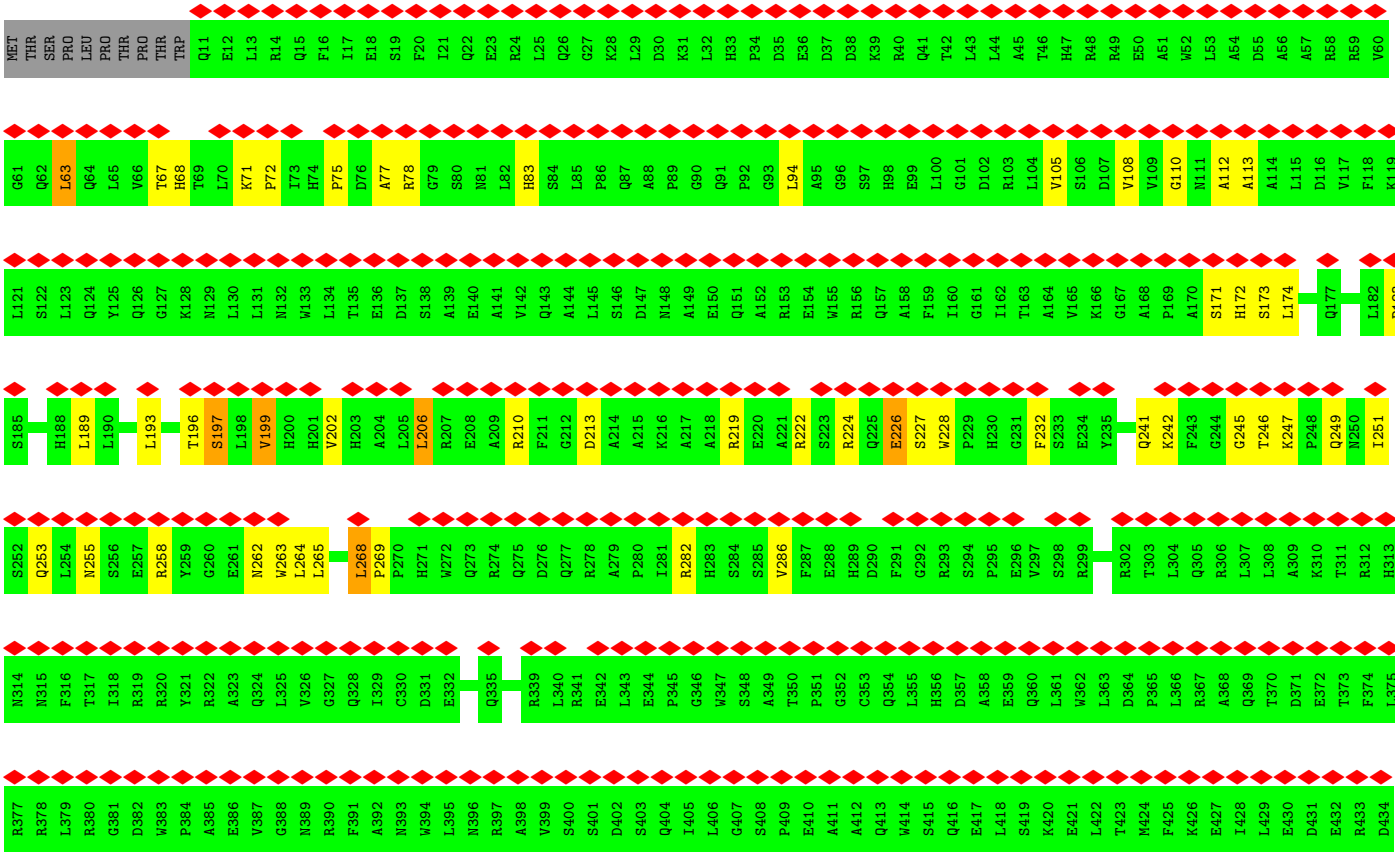




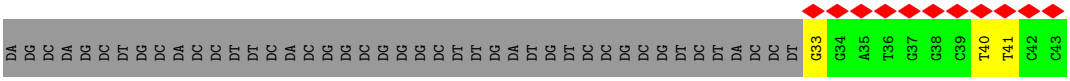
• Molecule 6: Type I-F CRISPR-associated protein Csy1

Chain X:

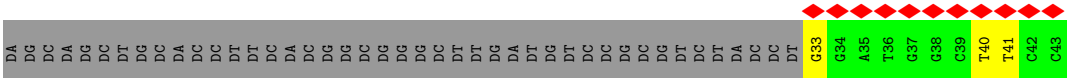




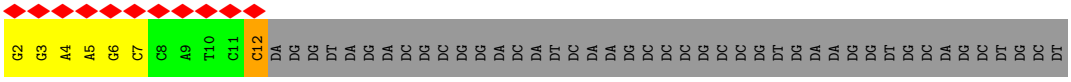
• Molecule 7: DNA (5'-D(P*GP*GP*AP*TP*GP*GP*CP*TP*TP*CP*C)-3')



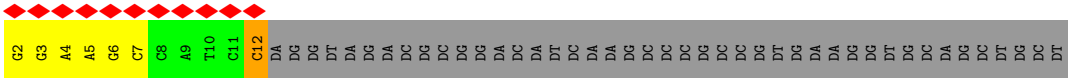
• Molecule 7: DNA (5'-D(P*GP*GP*AP*TP*GP*GP*CP*TP*TP*CP*C)-3')



• Molecule 8: DNA-r



• Molecule 8: DNA-r


G2 G3 A4 A5 G6 C7 C8 A9 T10 C11 C12 DA DG DG DT DA DG DA DC DG DC DG DG DA DC DA DT DC DA DA DG DC DC DC DG DC DC DG DT DG DA DA DG DG DT DG DC DA DG DC DT DG DC DT

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474421	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	B	0.31	0/2248	0.57	2/3077 (0.1%)
1	L	0.31	0/2378	0.58	2/3246 (0.1%)
2	C	0.31	0/2182	0.53	1/2977 (0.0%)
2	D	0.39	0/2578	0.53	0/3507
2	E	0.42	0/2634	0.53	0/3575
2	F	0.42	0/2624	0.55	1/3561 (0.0%)
2	G	0.40	0/2569	0.52	0/3488
2	H	0.33	0/2530	0.52	0/3440
2	M	0.31	0/2269	0.52	0/3087
2	N	0.40	0/2618	0.53	0/3555
2	O	0.42	0/2609	0.53	0/3542
2	P	0.43	0/2628	0.52	0/3565
2	Q	0.40	0/2599	0.51	0/3528
2	R	0.34	0/2576	0.52	0/3502
3	I	0.31	0/1484	0.59	0/2016
3	S	0.30	0/1487	0.66	2/2020 (0.1%)
4	U	0.46	0/1809	0.55	2/2474 (0.1%)
4	V	0.46	0/1809	0.55	2/2474 (0.1%)
5	J	0.68	0/1419	1.14	16/2208 (0.7%)
5	T	0.68	0/1419	1.14	15/2208 (0.7%)
6	A	0.29	0/2292	0.52	1/3000 (0.0%)
6	X	0.29	0/2292	0.52	1/3000 (0.0%)
7	K	0.34	0/131	1.11	0/194
7	Y	0.34	0/131	1.11	0/194
8	W	1.50	0/131	1.17	1/194 (0.5%)
8	Z	1.50	0/131	1.17	1/194 (0.5%)
All	All	0.41	0/49577	0.61	47/67826 (0.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	38	C	N1-C2-O2	9.42	124.55	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	38	C	N1-C2-O2	9.30	124.48	118.90
3	S	28	LEU	CA-CB-CG	7.80	133.24	115.30
5	T	38	C	N3-C2-O2	-7.64	116.55	121.90
5	J	38	C	N3-C2-O2	-7.51	116.65	121.90
5	J	33	U	C2-N1-C1'	7.50	126.70	117.70
5	T	33	U	C2-N1-C1'	7.49	126.69	117.70
5	J	38	C	C2-N1-C1'	7.38	126.92	118.80
5	T	38	C	C2-N1-C1'	7.37	126.91	118.80
2	F	251	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	181	LEU	CA-CB-CG	7.15	131.75	115.30
5	J	33	U	N1-C2-O2	7.03	127.72	122.80
5	T	33	U	N1-C2-O2	7.00	127.70	122.80
5	T	44	C	N1-C2-O2	6.89	123.03	118.90
4	V	61	GLU	CA-CB-CG	6.86	128.49	113.40
5	J	44	C	N1-C2-O2	6.83	123.00	118.90
4	U	61	GLU	CA-CB-CG	6.80	128.35	113.40
5	T	46	C	C6-N1-C2	-6.77	117.59	120.30
1	L	277	LEU	CA-CB-CG	6.76	130.85	115.30
5	J	46	C	C6-N1-C2	-6.70	117.62	120.30
5	J	44	C	C2-N1-C1'	6.50	125.95	118.80
5	T	44	C	C2-N1-C1'	6.47	125.91	118.80
1	L	181	LEU	CA-CB-CG	6.18	129.52	115.30
4	V	96	GLU	CA-CB-CG	6.15	126.92	113.40
4	U	96	GLU	CA-CB-CG	6.13	126.89	113.40
6	A	226	GLU	CA-CB-CG	6.09	126.80	113.40
6	X	226	GLU	CA-CB-CG	6.08	126.78	113.40
5	T	33	U	N3-C2-O2	-6.08	117.95	122.20
5	J	33	U	N3-C2-O2	-6.05	117.97	122.20
5	T	46	C	C5-C6-N1	5.88	123.94	121.00
5	J	46	C	C5-C6-N1	5.83	123.92	121.00
5	J	37	C	N1-C2-O2	5.77	122.36	118.90
5	T	37	C	N1-C2-O2	5.68	122.31	118.90
5	J	33	U	C6-N1-C1'	-5.59	113.37	121.20
5	T	33	U	C6-N1-C1'	-5.59	113.38	121.20
2	C	18	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	263	LEU	CA-CB-CG	5.50	127.95	115.30
8	Z	12	DC	O4'-C4'-C3'	-5.36	102.36	104.50
5	J	37	C	N3-C2-O2	-5.36	118.15	121.90
5	T	37	C	N3-C2-O2	-5.33	118.17	121.90
5	T	38	C	C6-N1-C1'	-5.29	114.45	120.80
5	J	38	C	C6-N1-C1'	-5.28	114.46	120.80
5	T	44	C	N3-C2-O2	-5.23	118.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	12	DC	O4'-C4'-C3'	-5.21	102.42	104.50
3	S	139	LEU	CA-CB-CG	5.21	127.28	115.30
5	J	44	C	N3-C2-O2	-5.14	118.30	121.90
5	J	20	C	N1-C2-O2	5.00	121.90	118.90

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	2198	0	2017	53	0
1	L	2321	0	2248	48	0
2	C	2144	0	2026	24	0
2	D	2531	0	2464	23	0
2	E	2587	0	2563	27	0
2	F	2577	0	2562	29	0
2	G	2523	0	2492	36	0
2	H	2487	0	2405	42	0
2	M	2227	0	2167	33	0
2	N	2571	0	2537	35	0
2	O	2562	0	2540	22	0
2	P	2581	0	2573	27	0
2	Q	2552	0	2531	31	0
2	R	2529	0	2471	28	0
3	I	1445	0	1387	24	0
3	S	1445	0	1383	28	0
4	U	1758	0	1720	18	0
4	V	1758	0	1720	17	0
5	J	1271	0	647	14	0
5	T	1271	0	647	13	0
6	A	2251	0	1413	42	0
6	X	2251	0	1413	39	0
7	K	121	0	67	4	0
7	Y	121	0	67	5	0
8	W	121	0	67	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Z	121	0	67	12	0
All	All	48324	0	44194	611	0

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

All (611) 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:A:245:GLY:HA3	7:Y:33:DG:OP2	1.45	1.17
6:X:245:GLY:HA3	7:K:33:DG:OP2	1.45	1.15
6:A:112:ALA:C	8:Z:12:DC:H4'	1.72	1.10
6:X:112:ALA:C	8:W:12:DC:H4'	1.72	1.09
6:X:112:ALA:O	8:W:12:DC:H4'	1.69	0.92
6:A:112:ALA:O	8:Z:12:DC:H4'	1.69	0.90
6:A:245:GLY:CA	7:Y:33:DG:OP2	2.21	0.89
6:X:245:GLY:CA	7:K:33:DG:OP2	2.21	0.88
6:A:112:ALA:C	8:Z:12:DC:C4'	2.50	0.80
6:X:112:ALA:C	8:W:12:DC:C4'	2.50	0.79
5:J:51:G:H21	5:J:55:A:H62	1.30	0.79
6:X:246:THR:N	7:K:33:DG:OP2	2.15	0.79
6:A:246:THR:N	7:Y:33:DG:OP2	2.15	0.78
5:T:51:G:H21	5:T:55:A:H62	1.29	0.76
5:T:51:G:N2	5:T:55:A:H62	1.88	0.72
5:J:51:G:N2	5:J:55:A:H62	1.88	0.70
8:W:2:DG:H2"	8:W:3:DG:H5'	1.74	0.69
8:Z:2:DG:H2"	8:Z:3:DG:H5'	1.74	0.68
2:M:148:LEU:HB3	2:M:151:ASN:HB3	1.76	0.68
2:H:144:ASN:HB2	2:H:152:ARG:HH12	1.59	0.67
6:X:112:ALA:CA	8:W:12:DC:H4'	2.25	0.67
6:A:112:ALA:CA	8:Z:12:DC:H4'	2.25	0.67
1:L:307:ALA:HB3	6:X:183:PRO:HD3	1.76	0.67
4:U:201:GLY:H	4:U:207:ARG:HD2	1.61	0.66
4:V:201:GLY:H	4:V:207:ARG:HD2	1.61	0.66
2:M:45:ARG:HH12	2:M:47:LYS:HB2	1.62	0.65
2:E:249:VAL:HG12	2:F:45:ARG:HH12	1.62	0.65
1:L:12:LEU:HD13	1:L:156:ASN:HD21	1.62	0.64
6:A:255:ASN:HA	6:A:258:ARG:HG2	1.80	0.63
2:M:98:ARG:HD3	2:N:223:GLN:HG2	1.81	0.63
1:L:159:LEU:HD11	1:L:172:ASN:HB2	1.80	0.62
1:B:11:LEU:HD21	1:B:180:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:78:GLY:H	3:I:80:ARG:HH21	1.47	0.62
2:R:146:ARG:NH2	2:R:183:LEU:O	2.32	0.62
1:L:300:ASP:HB3	1:L:321:PHE:HA	1.82	0.62
1:B:313:LEU:HD21	6:A:89:PRO:HB3	1.81	0.62
6:X:67:THR:HG22	6:X:83:HIS:HA	1.82	0.62
6:X:108:VAL:HG13	6:X:253:GLN:HE22	1.65	0.62
6:X:255:ASN:HA	6:X:258:ARG:HG2	1.80	0.61
5:T:51:G:H21	5:T:55:A:N6	1.98	0.61
6:A:108:VAL:HG13	6:A:253:GLN:HE22	1.65	0.61
1:L:213:LEU:HD12	1:L:216:LEU:HD21	1.82	0.61
2:P:87:ASP:OD1	2:P:87:ASP:N	2.34	0.61
2:N:162:ILE:HB	2:N:174:TRP:HB2	1.83	0.60
6:A:67:THR:HG22	6:A:83:HIS:HA	1.82	0.60
3:I:119:ARG:NH1	5:J:51:G:O6	2.34	0.60
1:B:148:CYS:SG	1:B:149:ASN:N	2.75	0.59
1:L:58:GLY:HA3	1:L:302:LEU:HB3	1.83	0.59
5:J:4:A:N6	6:A:175:ALA:O	2.34	0.59
5:J:51:G:H21	5:J:55:A:N6	1.98	0.59
2:N:185:ASP:N	2:N:185:ASP:OD1	2.35	0.59
2:N:259:LYS:NZ	5:T:34:C:OP1	2.35	0.59
2:D:149:TRP:HE1	2:D:263:ALA:HB2	1.67	0.59
1:L:4:THR:HG1	1:L:114:HIS:HE2	1.50	0.59
1:L:278:ARG:NH2	1:L:314:TYR:OH	2.34	0.59
1:L:82:ASN:ND2	2:R:230:GLU:OE1	2.35	0.59
2:E:310:ASN:OD1	2:E:314:ARG:NH2	2.35	0.58
2:G:117:LYS:HD2	2:G:120:GLN:HE21	1.68	0.58
2:M:310:ASN:OD1	2:M:314:ARG:NH2	2.36	0.58
2:N:140:HIS:O	2:N:144:ASN:ND2	2.36	0.58
1:B:219:ILE:HB	6:A:232:PHE:HD1	1.69	0.58
3:I:163:PRO:O	3:I:165:GLN:NE2	2.36	0.58
1:L:215:ASP:OD1	1:L:215:ASP:N	2.35	0.58
2:H:311:TRP:HE3	2:H:318:PRO:HD2	1.69	0.58
2:Q:310:ASN:OD1	2:Q:314:ARG:NH2	2.36	0.58
1:L:72:GLN:NE2	1:L:76:LYS:O	2.37	0.58
2:G:234:ASP:OD1	2:G:234:ASP:N	2.36	0.58
2:H:146:ARG:NH1	2:H:266:THR:HG1	2.02	0.58
1:L:213:LEU:O	1:L:218:ARG:NH1	2.36	0.58
2:N:172:ARG:NH1	2:N:173:THR:O	2.37	0.58
2:Q:87:ASP:OD1	2:Q:87:ASP:N	2.37	0.58
2:F:185:ASP:OD1	2:F:185:ASP:N	2.36	0.58
1:B:40:PHE:HD1	5:J:2:U:H3	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:132:ALA:O	2:R:136:ARG:HB2	2.03	0.57
1:B:4:THR:OG1	1:B:114:HIS:NE2	2.38	0.57
2:H:172:ARG:NH2	2:H:191:GLU:OE1	2.37	0.57
2:R:141:ASN:OD1	2:R:146:ARG:NH1	2.37	0.57
2:G:166:ARG:HG2	2:G:171:ALA:HB2	1.85	0.57
2:M:21:SER:OG	2:M:22:ASP:N	2.38	0.57
2:O:310:ASN:OD1	2:O:314:ARG:NH2	2.37	0.57
2:Q:172:ARG:NH1	2:Q:173:THR:O	2.38	0.57
2:C:265:ARG:NH1	2:C:282:VAL:O	2.37	0.57
2:P:185:ASP:OD1	2:P:185:ASP:N	2.36	0.57
1:B:78:THR:OG1	1:B:79:LYS:N	2.38	0.57
2:C:21:SER:OG	2:C:22:ASP:N	2.37	0.57
2:R:146:ARG:NH1	2:R:266:THR:HG1	2.03	0.57
2:E:87:ASP:OD1	2:E:87:ASP:N	2.37	0.57
1:B:34:PRO:HA	1:B:37:PHE:HD2	1.70	0.57
2:N:299:LYS:O	2:N:301:LYS:NZ	2.38	0.57
2:G:185:ASP:OD1	2:G:185:ASP:N	2.35	0.57
4:V:203:SER:HA	4:V:207:ARG:HB3	1.87	0.57
2:D:21:SER:OG	2:D:22:ASP:N	2.38	0.56
2:G:87:ASP:OD1	2:G:87:ASP:N	2.34	0.56
2:P:318:PRO:O	2:P:323:GLN:NE2	2.38	0.56
6:A:171:SER:OG	6:A:172:HIS:N	2.38	0.56
2:M:23:ALA:HB3	2:M:255:ILE:HB	1.87	0.56
2:O:185:ASP:OD1	2:O:185:ASP:N	2.39	0.56
2:R:87:ASP:OD1	2:R:87:ASP:N	2.37	0.56
6:A:113:ALA:N	8:Z:12:DC:H5'	2.21	0.56
2:H:318:PRO:O	2:H:323:GLN:NE2	2.38	0.56
2:H:121:THR:HG1	2:H:311:TRP:HE1	1.52	0.56
4:U:203:SER:HA	4:U:207:ARG:HB3	1.87	0.56
4:V:100:GLY:HA2	4:V:119:LEU:HA	1.88	0.56
1:B:131:GLN:NE2	1:B:156:ASN:OD1	2.39	0.55
1:B:239:TRP:HA	6:A:222:ARG:HD2	1.88	0.55
6:X:171:SER:OG	6:X:172:HIS:N	2.38	0.55
2:E:22:ASP:OD1	2:E:22:ASP:N	2.38	0.55
2:R:172:ARG:HH11	2:R:173:THR:H	1.54	0.55
3:I:148:SER:HB3	3:I:152:GLY:HA2	1.89	0.55
2:H:325:TYR:O	2:H:329:ASN:ND2	2.40	0.55
2:M:117:LYS:NZ	2:M:312:VAL:O	2.39	0.55
2:O:318:PRO:O	2:O:323:GLN:NE2	2.40	0.55
2:D:133:GLU:OE2	2:D:137:ARG:NH1	2.40	0.55
2:H:146:ARG:NH1	2:H:266:THR:OG1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:318:PRO:O	2:Q:323:GLN:NE2	2.39	0.55
4:U:100:GLY:HA2	4:U:119:LEU:HA	1.88	0.55
6:X:113:ALA:N	8:W:12:DC:H5'	2.21	0.55
1:B:194:GLN:HE22	6:A:93:GLY:HA3	1.72	0.55
2:C:265:ARG:NH2	5:J:38:C:OP2	2.38	0.55
2:E:161:ARG:HG2	2:E:175:ARG:HD2	1.88	0.55
1:B:58:GLY:HA3	1:B:302:LEU:HB3	1.87	0.55
2:G:318:PRO:O	2:G:323:GLN:NE2	2.40	0.55
3:I:73:ARG:HD2	3:I:74:PRO:HD2	1.88	0.55
2:R:146:ARG:NH1	2:R:266:THR:OG1	2.40	0.55
2:G:34:ASP:OD1	2:G:161:ARG:NH2	2.40	0.54
2:M:136:ARG:O	2:M:140:HIS:ND1	2.40	0.54
3:S:73:ARG:HB3	3:S:75:TRP:HD1	1.72	0.54
2:H:268:ASP:OD1	2:H:296:ARG:NH2	2.40	0.54
2:M:318:PRO:O	2:M:323:GLN:NE2	2.40	0.54
1:B:116:ASP:HB2	1:B:119:ASP:HB2	1.89	0.54
2:E:36:SER:O	2:E:92:LYS:NZ	2.40	0.54
2:H:298:PRO:O	2:H:301:LYS:NZ	2.40	0.54
2:M:229:GLN:HE21	5:T:40:G:H5"	1.71	0.54
2:R:265:ARG:NH1	2:R:283:GLU:OE2	2.41	0.54
2:E:185:ASP:N	2:E:185:ASP:OD1	2.40	0.54
2:G:332:ARG:NH1	2:G:333:GLY:O	2.41	0.54
2:P:266:THR:HA	2:P:281:ALA:HA	1.89	0.54
5:J:58:C:H2'	5:J:59:A:H8	1.73	0.54
7:Y:40:DT:H2"	7:Y:41:DT:H2'	1.89	0.54
7:K:40:DT:H2"	7:K:41:DT:H2'	1.89	0.54
2:F:87:ASP:OD1	2:F:87:ASP:N	2.40	0.54
2:C:268:ASP:HB3	2:C:280:ILE:HB	1.89	0.54
2:E:52:THR:OG1	2:E:53:ILE:N	2.42	0.53
2:D:259:LYS:NZ	5:J:34:C:OP1	2.39	0.53
2:N:303:ASP:OD1	2:N:303:ASP:N	2.40	0.53
2:O:17:LYS:HE3	2:O:103:ALA:HA	1.89	0.53
2:R:201:SER:O	2:R:206:SER:OG	2.26	0.53
2:H:121:THR:OG1	2:H:311:TRP:NE1	2.42	0.53
2:N:16:ARG:NE	2:N:19:ASP:OD2	2.41	0.53
2:Q:167:GLN:OE1	2:R:218:ARG:NH1	2.41	0.53
1:B:64:HIS:HB2	1:B:106:GLU:HB3	1.91	0.53
3:I:7:ILE:HG22	3:I:85:PHE:HA	1.91	0.53
2:N:7:SER:OG	2:N:8:THR:N	2.42	0.53
6:X:105:VAL:O	6:X:197:SER:OG	2.27	0.53
2:D:117:LYS:NZ	2:D:312:VAL:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:36:SER:O	2:Q:92:LYS:NZ	2.41	0.53
1:L:172:ASN:HA	1:L:175:ARG:HG2	1.90	0.53
2:N:227:PRO:HG2	2:N:246:LEU:HD12	1.90	0.53
6:A:199:VAL:HA	6:A:202:VAL:HG22	1.91	0.53
6:X:268:LEU:HD12	6:X:269:PRO:HD2	1.91	0.53
2:G:117:LYS:NZ	2:G:312:VAL:O	2.41	0.53
6:A:268:LEU:HD12	6:A:269:PRO:HD2	1.91	0.53
2:C:157:ALA:H	2:C:218:ARG:HB2	1.73	0.53
1:L:116:ASP:HB3	1:L:119:ASP:HB2	1.90	0.53
2:G:167:GLN:NE2	2:H:156:GLU:OE2	2.41	0.53
1:L:77:ARG:HH21	6:X:210:ARG:HD3	1.74	0.53
2:N:44:VAL:HA	2:N:82:ALA:HB2	1.90	0.53
2:Q:161:ARG:HH21	2:Q:175:ARG:HH12	1.56	0.53
5:T:58:C:H2'	5:T:59:A:H8	1.73	0.53
8:Z:5:DA:H2"	8:Z:6:DG:OP2	2.08	0.53
1:B:74:ALA:HB3	2:H:241:GLN:HE21	1.73	0.53
2:N:36:SER:O	2:N:92:LYS:NZ	2.42	0.53
2:O:87:ASP:OD1	2:O:87:ASP:N	2.38	0.53
2:G:141:ASN:OD1	2:G:146:ARG:NH1	2.42	0.52
2:P:234:ASP:O	2:P:238:LYS:NZ	2.43	0.52
2:H:21:SER:HG	2:H:96:THR:H	1.56	0.52
2:H:50:ARG:N	5:J:15:G:OP2	2.42	0.52
2:H:94:ARG:HB2	2:H:214:VAL:HG22	1.92	0.52
2:C:10:SER:OG	2:C:110:ASN:ND2	2.43	0.52
2:C:21:SER:HB3	2:C:96:THR:H	1.73	0.52
2:D:172:ARG:NH1	2:D:173:THR:O	2.42	0.52
2:G:16:ARG:NE	2:G:19:ASP:OD1	2.42	0.52
4:U:172:GLY:O	4:U:175:SER:OG	2.26	0.52
8:W:5:DA:H2"	8:W:6:DG:OP2	2.08	0.52
1:B:257:ALA:HA	1:B:280:VAL:HA	1.91	0.52
2:F:10:SER:OG	2:F:110:ASN:ND2	2.43	0.52
2:G:227:PRO:HG2	2:G:246:LEU:HD22	1.92	0.52
2:N:268:ASP:HB3	2:N:280:ILE:HG13	1.90	0.52
3:S:27:LYS:HG3	3:S:75:TRP:HE3	1.74	0.52
2:R:136:ARG:O	2:R:140:HIS:ND1	2.42	0.52
6:A:72:PRO:HG3	6:A:251:ILE:HD12	1.92	0.52
6:A:105:VAL:O	6:A:197:SER:OG	2.27	0.52
2:Q:227:PRO:HG2	2:Q:246:LEU:HD22	1.90	0.52
2:H:141:ASN:OD1	2:H:146:ARG:NH1	2.42	0.52
3:I:174:THR:OG1	3:I:175:CYS:N	2.43	0.52
2:M:87:ASP:OD1	2:M:87:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:ALA:HB3	2:M:218:ARG:HD3	1.91	0.52
3:S:102:ARG:NH1	5:T:58:C:OP2	2.42	0.52
6:X:199:VAL:HA	6:X:202:VAL:HG22	1.91	0.52
1:B:273:ARG:NH1	2:H:111:ASP:OD1	2.43	0.51
2:E:299:LYS:O	2:E:301:LYS:NZ	2.41	0.51
1:L:11:LEU:O	1:L:156:ASN:ND2	2.43	0.51
2:C:148:LEU:HB3	2:C:151:ASN:HB3	1.91	0.51
4:U:73:ASP:OD1	4:U:73:ASP:N	2.44	0.51
1:B:281:GLU:HG3	6:A:68:HIS:HE2	1.75	0.51
4:V:73:ASP:OD1	4:V:73:ASP:N	2.44	0.51
4:V:172:GLY:O	4:V:175:SER:OG	2.26	0.51
2:F:17:LYS:HG3	2:F:100:LEU:HB2	1.93	0.51
2:R:290:SER:OG	2:R:291:GLN:NE2	2.42	0.51
1:B:257:ALA:H	1:B:312:GLY:HA3	1.75	0.51
2:G:325:TYR:O	2:G:329:ASN:ND2	2.44	0.51
2:C:299:LYS:O	2:C:301:LYS:NZ	2.44	0.51
2:E:7:SER:OG	2:E:8:THR:N	2.44	0.51
2:H:7:SER:OG	2:H:8:THR:N	2.43	0.51
1:L:126:ILE:HA	1:L:129:GLN:HE21	1.76	0.51
2:M:332:ARG:NH1	2:M:333:GLY:O	2.44	0.51
4:V:83:ASP:OD1	4:V:83:ASP:N	2.39	0.51
2:G:117:LYS:O	2:G:121:THR:OG1	2.25	0.51
3:I:3:HIS:HE1	3:I:90:VAL:HG12	1.76	0.51
1:B:131:GLN:NE2	1:B:154:ALA:O	2.44	0.50
2:D:25:MET:HG2	2:D:93:VAL:HG12	1.92	0.50
1:L:281:GLU:HG3	6:X:68:HIS:HE2	1.76	0.50
2:R:146:ARG:HG3	2:R:183:LEU:HD11	1.92	0.50
1:B:65:ARG:HG2	1:B:106:GLU:HB2	1.93	0.50
2:N:117:LYS:NZ	2:N:312:VAL:O	2.43	0.50
4:U:81:ASP:OD1	4:U:81:ASP:N	2.44	0.50
1:B:307:ALA:HB3	6:A:183:PRO:HD3	1.93	0.50
3:I:27:LYS:HD3	3:I:30:GLN:HE21	1.77	0.50
3:S:148:SER:HB3	3:S:152:GLY:HA2	1.92	0.50
2:D:36:SER:O	2:D:92:LYS:NZ	2.44	0.50
6:A:113:ALA:CA	8:Z:12:DC:H5'	2.41	0.50
1:L:12:LEU:HB2	1:L:109:LEU:HB2	1.92	0.50
2:P:21:SER:HG	2:P:96:THR:H	1.59	0.50
2:Q:19:ASP:OD1	2:Q:19:ASP:N	2.37	0.50
4:V:25:HIS:HA	4:V:43:PRO:HA	1.93	0.50
6:X:72:PRO:HG3	6:X:251:ILE:HD12	1.92	0.50
2:C:318:PRO:O	2:C:323:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:283:GLU:HB2	2:E:286:GLY:HA2	1.92	0.50
2:Q:144:ASN:ND2	2:Q:182:GLY:O	2.44	0.50
2:R:327:ILE:HA	2:R:330:LEU:HD12	1.93	0.50
2:C:137:ARG:NH1	2:C:267:ILE:O	2.45	0.50
3:I:10:ARG:NH1	3:I:81:ASP:O	2.45	0.50
2:O:36:SER:O	2:O:92:LYS:NZ	2.45	0.50
4:U:150:GLU:OE2	4:U:160:ARG:NE	2.42	0.50
6:X:113:ALA:CA	8:W:12:DC:H5'	2.41	0.50
2:N:68:ASP:HA	2:N:71:ILE:HD12	1.94	0.49
2:R:140:HIS:CE1	2:R:186:PHE:HB2	2.47	0.49
4:U:200:ALA:HB3	4:U:207:ARG:HB2	1.93	0.49
4:V:200:ALA:HB3	4:V:207:ARG:HB2	1.93	0.49
2:H:146:ARG:HH11	2:H:266:THR:HG1	1.60	0.49
3:I:142:PRO:O	3:I:159:ILE:N	2.42	0.49
2:P:299:LYS:O	2:P:301:LYS:NZ	2.43	0.49
2:Q:283:GLU:HG2	2:Q:286:GLY:HA2	1.93	0.49
2:C:117:LYS:NZ	2:C:312:VAL:O	2.42	0.49
2:F:221:ASP:N	2:F:221:ASP:OD1	2.46	0.49
2:R:89:ASP:OD1	2:R:89:ASP:N	2.45	0.49
4:V:150:GLU:OE2	4:V:160:ARG:NE	2.42	0.49
2:D:17:LYS:HG3	2:D:100:LEU:HB2	1.93	0.49
2:P:172:ARG:NH2	2:P:191:GLU:OE1	2.45	0.49
4:V:202:ASP:OD1	4:V:202:ASP:N	2.45	0.49
6:X:262:ASN:OD1	6:X:262:ASN:N	2.45	0.49
2:E:172:ARG:NH1	2:E:173:THR:O	2.46	0.49
2:F:234:ASP:O	2:F:238:LYS:NZ	2.43	0.49
2:F:259:LYS:NZ	5:J:22:U:OP1	2.36	0.49
4:V:81:ASP:OD1	4:V:81:ASP:N	2.44	0.49
2:C:265:ARG:HH12	2:C:283:GLU:HG3	1.78	0.49
2:N:59:THR:HG23	2:N:60:LYS:HD2	1.94	0.49
2:P:137:ARG:NH1	2:P:267:ILE:O	2.46	0.49
2:D:137:ARG:NH2	2:D:269:THR:OG1	2.45	0.49
1:L:4:THR:OG1	1:L:114:HIS:NE2	2.38	0.49
3:I:73:ARG:HH11	3:I:74:PRO:HD2	1.77	0.49
4:U:202:ASP:N	4:U:202:ASP:OD1	2.45	0.49
1:B:59:VAL:H	1:B:303:TRP:H	1.61	0.49
1:B:300:ASP:HB3	1:B:321:PHE:HA	1.94	0.49
2:F:318:PRO:O	2:F:323:GLN:NE2	2.45	0.49
2:H:116:ASP:HA	2:H:119:LEU:HB2	1.93	0.49
1:L:168:GLN:O	1:L:172:ASN:ND2	2.46	0.49
6:A:262:ASN:OD1	6:A:262:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD13	1:B:216:LEU:HD11	1.94	0.48
2:G:265:ARG:NH1	2:G:283:GLU:OE2	2.36	0.48
2:Q:185:ASP:N	2:Q:185:ASP:OD1	2.43	0.48
2:N:61:ASP:OD1	2:N:61:ASP:N	2.46	0.48
2:R:164:HIS:O	2:R:171:ALA:N	2.42	0.48
2:G:251:ASP:OD1	2:G:251:ASP:N	2.47	0.48
1:L:17:ILE:HD12	1:L:105:LEU:HB2	1.96	0.48
1:L:65:ARG:HD2	2:R:250:ARG:HH22	1.78	0.48
4:U:25:HIS:HA	4:U:43:PRO:HA	1.93	0.48
2:M:309:ASP:HA	2:M:313:LEU:HD13	1.95	0.48
2:O:258:GLN:NE2	5:T:27:U:OP2	2.33	0.48
2:P:303:ASP:N	2:P:303:ASP:OD1	2.45	0.48
2:Q:221:ASP:OD1	2:Q:221:ASP:N	2.46	0.48
6:X:112:ALA:CA	8:W:12:DC:C4'	2.90	0.48
1:B:47:ARG:HH11	1:B:133:GLN:HG2	1.78	0.48
2:H:310:ASN:O	2:H:316:GLU:N	2.47	0.48
1:B:64:HIS:N	1:B:106:GLU:O	2.45	0.48
2:C:150:ARG:HE	3:I:15:PHE:HE2	1.62	0.48
2:Q:229:GLN:HB3	2:Q:246:LEU:HD23	1.96	0.48
3:S:145:THR:HA	3:S:156:ARG:HA	1.96	0.48
6:A:282:ARG:O	6:A:286:VAL:N	2.45	0.48
2:O:251:ASP:N	2:O:251:ASP:OD1	2.44	0.48
2:P:237:ASP:OD1	2:P:237:ASP:N	2.42	0.48
1:L:166:ASP:OD1	1:L:170:ARG:NH1	2.47	0.48
2:N:187:LYS:HB3	2:N:187:LYS:HE3	1.57	0.48
2:Q:52:THR:OG1	2:Q:53:ILE:N	2.47	0.48
6:X:247:LYS:HB3	6:X:249:GLN:HE22	1.78	0.48
2:H:201:SER:O	2:H:204:SER:OG	2.32	0.47
2:M:90:THR:HG22	2:M:218:ARG:HG2	1.95	0.47
2:P:119:LEU:HA	2:P:122:VAL:HG22	1.95	0.47
2:R:189:ASP:HB3	2:R:192:LEU:HB3	1.95	0.47
6:A:247:LYS:HB3	6:A:249:GLN:HE22	1.78	0.47
2:F:312:VAL:HG12	2:F:313:LEU:HD23	1.96	0.47
2:M:45:ARG:NH2	2:M:46:GLU:O	2.47	0.47
2:Q:266:THR:O	2:Q:266:THR:OG1	2.29	0.47
4:U:136:SER:OG	4:U:137:ALA:N	2.48	0.47
2:C:26:SER:HA	2:C:41:ALA:HA	1.95	0.47
2:F:233:LEU:O	2:F:235:LYS:NZ	2.38	0.47
1:L:64:HIS:N	1:L:106:GLU:O	2.47	0.47
6:X:282:ARG:O	6:X:286:VAL:N	2.45	0.47
2:G:12:LEU:HB3	2:G:336:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:16:ARG:NH1	5:T:7:A:OP1	2.48	0.47
1:B:263:LEU:HD23	1:B:265:GLY:H	1.79	0.47
2:F:137:ARG:NH1	2:F:267:ILE:O	2.46	0.47
2:Q:125:TYR:OH	2:Q:324:HIS:ND1	2.39	0.47
2:Q:315:ASP:N	2:Q:315:ASP:OD1	2.47	0.47
1:B:168:GLN:HA	1:B:171:LYS:HG2	1.97	0.47
2:P:251:ASP:OD1	2:P:251:ASP:N	2.47	0.47
2:Q:21:SER:HG	2:Q:96:THR:H	1.60	0.47
2:Q:204:SER:HG	2:Q:206:SER:HG	1.60	0.47
2:F:61:ASP:OD1	2:F:61:ASP:N	2.45	0.47
2:G:172:ARG:NH1	2:G:173:THR:O	2.48	0.47
3:S:43:SER:HB3	3:S:184:VAL:HG21	1.96	0.47
6:A:112:ALA:CA	8:Z:12:DC:C4’	2.90	0.47
1:B:72:GLN:NE2	1:B:76:LYS:O	2.44	0.47
3:S:38:ASP:O	3:S:173:PHE:N	2.48	0.47
6:X:63:LEU:HD22	6:X:110:GLY:HA3	1.97	0.47
1:B:268:ARG:NH2	2:H:338:GLU:OE2	2.48	0.46
1:B:315:ARG:HH22	6:A:94:LEU:HD11	1.80	0.46
2:H:16:ARG:NE	5:J:7:A:OP1	2.48	0.46
3:I:30:GLN:HA	3:I:33:VAL:HG12	1.97	0.46
3:I:150:SER:OG	3:I:151:THR:N	2.48	0.46
2:R:178:ALA:HA	2:R:181:ILE:HD12	1.97	0.46
1:B:261:LEU:HA	1:B:278:ARG:HD3	1.96	0.46
2:M:7:SER:OG	2:M:8:THR:N	2.47	0.46
3:S:153:GLN:NE2	3:S:154:HIS:O	2.49	0.46
4:V:60:ALA:HB1	6:X:224:ARG:HH22	1.79	0.46
3:I:32:LEU:HD22	3:I:175:CYS:HA	1.97	0.46
6:X:206:LEU:HD13	6:X:263:TRP:HE3	1.81	0.46
1:B:116:ASP:N	1:B:116:ASP:OD1	2.48	0.46
2:D:268:ASP:HB3	2:D:280:ILE:HB	1.97	0.46
2:G:159:GLU:OE2	2:G:175:ARG:NH1	2.49	0.46
2:H:59:THR:HA	2:H:62:ARG:HG3	1.97	0.46
2:P:142:LEU:HD13	2:P:264:LEU:HD21	1.97	0.46
1:B:223:PRO:HD3	1:B:240:GLN:HE22	1.80	0.46
1:B:299:SER:O	1:B:299:SER:OG	2.32	0.46
2:N:75:ASN:OD1	2:N:75:ASN:N	2.49	0.46
2:O:83:ASN:HB3	2:O:224:GLU:HA	1.98	0.46
4:V:30:LEU:HD23	4:V:37:MET:HB2	1.97	0.46
6:A:63:LEU:HD22	6:A:110:GLY:HA3	1.97	0.46
2:C:141:ASN:ND2	2:C:266:THR:O	2.47	0.46
2:G:10:SER:HB3	2:G:110:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:GLN:NE2	1:L:156:ASN:OD1	2.48	0.46
3:S:96:PRO:HB2	3:S:164:LEU:HD12	1.97	0.46
1:L:213:LEU:HG	1:L:218:ARG:HH11	1.81	0.46
2:G:36:SER:O	2:G:92:LYS:NZ	2.49	0.46
2:F:172:ARG:NH2	2:F:191:GLU:OE1	2.46	0.46
2:N:17:LYS:HE2	2:N:103:ALA:HA	1.97	0.46
2:O:177:ASP:OD2	2:O:180:ALA:N	2.49	0.46
3:S:73:ARG:HH11	3:S:75:TRP:HB3	1.80	0.46
4:U:30:LEU:HD23	4:U:37:MET:HB2	1.97	0.46
2:D:52:THR:OG1	2:D:53:ILE:N	2.49	0.45
2:D:55:ASN:OD1	2:D:55:ASN:N	2.48	0.45
2:F:166:ARG:HG3	2:F:167:GLN:H	1.81	0.45
1:L:219:ILE:HB	6:X:232:PHE:HD1	1.82	0.45
2:Q:251:ASP:OD1	2:Q:251:ASP:N	2.49	0.45
3:S:63:SER:OG	3:S:65:ASP:OD2	2.32	0.45
1:B:18:GLN:HB3	1:B:145:LEU:HD21	1.98	0.45
2:N:299:LYS:HA	2:N:299:LYS:HD3	1.82	0.45
3:S:48:ASP:OD2	3:S:50:SER:OG	2.32	0.45
2:M:46:GLU:HA	2:M:80:ASP:HA	1.97	0.45
2:P:83:ASN:N	2:P:83:ASN:OD1	2.50	0.45
4:V:136:SER:OG	4:V:137:ALA:N	2.48	0.45
2:C:137:ARG:NH2	2:C:269:THR:OG1	2.40	0.45
2:P:52:THR:OG1	2:P:53:ILE:N	2.49	0.45
1:B:62:VAL:HG22	1:B:183:GLY:HA3	1.97	0.45
2:M:319:ALA:HB3	2:M:322:GLN:HG2	1.97	0.45
2:Q:299:LYS:O	2:Q:301:LYS:NZ	2.50	0.45
2:E:238:LYS:H	2:E:241:GLN:HE22	1.63	0.45
2:G:132:ALA:O	2:G:136:ARG:HB2	2.16	0.45
2:R:224:GLU:OE1	2:R:224:GLU:N	2.47	0.45
3:S:7:ILE:HD11	3:S:83:LEU:HD13	1.99	0.45
2:D:5:ILE:HD12	2:D:5:ILE:HA	1.84	0.45
2:D:15:GLU:OE2	2:E:150:ARG:NE	2.50	0.45
2:E:318:PRO:O	2:E:323:GLN:NE2	2.47	0.45
2:H:251:ASP:N	2:H:251:ASP:OD1	2.48	0.45
2:M:137:ARG:HD3	2:M:267:ILE:HB	1.98	0.45
2:Q:325:TYR:O	2:Q:329:ASN:ND2	2.44	0.45
2:E:299:LYS:NZ	2:E:300:GLN:OE1	2.41	0.45
2:H:11:VAL:HG22	6:A:173:SER:HB2	1.99	0.45
1:L:315:ARG:HH22	6:X:94:LEU:HD11	1.81	0.45
2:M:94:ARG:NH2	2:M:212:GLU:OE2	2.50	0.45
2:P:239:LYS:NZ	2:P:242:LYS:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:79:ASN:OD1	4:U:79:ASN:N	2.41	0.45
6:A:206:LEU:HD13	6:A:263:TRP:HE3	1.81	0.45
2:F:266:THR:HA	2:F:281:ALA:HA	1.99	0.44
1:L:40:PHE:HD1	5:T:2:U:H3	1.65	0.44
1:L:59:VAL:HG23	1:L:303:TRP:HB2	2.00	0.44
3:I:102:ARG:HD2	3:I:157:LEU:HD23	1.98	0.44
2:N:249:VAL:HG12	2:N:250:ARG:HG2	1.99	0.44
1:B:11:LEU:HD13	1:B:110:LEU:HD13	1.99	0.44
1:B:51:SER:O	1:B:51:SER:OG	2.35	0.44
2:D:68:ASP:HA	2:D:71:ILE:HD12	1.99	0.44
3:I:154:HIS:O	5:J:44:C:O2'	2.36	0.44
1:L:299:SER:O	1:L:320:ARG:NH1	2.50	0.44
2:N:156:GLU:HB3	2:N:218:ARG:HB3	1.99	0.44
2:O:303:ASP:OD1	2:O:303:ASP:N	2.46	0.44
3:S:73:ARG:HB3	3:S:75:TRP:CD1	2.52	0.44
3:I:3:HIS:ND1	3:I:89:ALA:O	2.51	0.44
3:I:153:GLN:NE2	3:I:154:HIS:O	2.50	0.44
2:P:117:LYS:O	2:P:121:THR:OG1	2.31	0.44
4:U:57:ASP:OD1	4:U:57:ASP:N	2.50	0.44
8:Z:6:DG:H2"	8:Z:7:DC:O5'	2.17	0.44
2:G:60:LYS:HB2	2:G:60:LYS:HE2	1.80	0.44
1:B:44:LEU:HA	1:B:133:GLN:HE22	1.82	0.44
2:C:158:VAL:HG23	2:C:178:ALA:HB3	1.98	0.44
2:D:187:LYS:HA	2:D:187:LYS:HD3	1.84	0.44
2:O:149:TRP:CE2	2:O:259:LYS:HE2	2.53	0.44
2:O:172:ARG:NH2	2:O:191:GLU:OE1	2.44	0.44
6:X:241:GLN:HB2	6:X:264:LEU:HD11	2.00	0.44
8:W:6:DG:H2"	8:W:7:DC:O5'	2.17	0.44
2:C:174:TRP:NE1	2:C:191:GLU:O	2.49	0.44
2:F:111:ASP:OD2	2:F:114:TYR:N	2.51	0.44
3:I:45:PRO:HG2	3:I:57:ARG:HH11	1.83	0.44
2:R:299:LYS:HE3	2:R:299:LYS:HB3	1.91	0.44
3:S:54:LEU:HD21	3:S:159:ILE:HD13	2.00	0.44
4:V:57:ASP:N	4:V:57:ASP:OD1	2.50	0.44
1:B:70:ILE:HG22	1:B:79:LYS:HG2	2.00	0.43
1:L:253:ALA:N	1:L:283:LEU:O	2.50	0.43
2:M:17:LYS:HD2	2:M:100:LEU:HB2	2.00	0.43
2:N:258:GLN:NE2	5:T:33:U:OP1	2.49	0.43
2:Q:73:SER:O	2:Q:73:SER:OG	2.31	0.43
2:Q:184:ARG:NH2	2:Q:275:ASP:O	2.48	0.43
6:A:241:GLN:HB2	6:A:264:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ARG:HA	1:B:177:THR:HG22	2.00	0.43
1:B:239:TRP:N	1:B:240:GLN:OE1	2.51	0.43
2:C:244:LYS:HD2	2:C:244:LYS:HA	1.86	0.43
2:G:327:ILE:HD13	2:G:327:ILE:HA	1.85	0.43
1:L:283:LEU:HD13	6:X:94:LEU:HD13	2.00	0.43
2:N:157:ALA:HA	2:N:179:LEU:HD21	1.99	0.43
2:H:76:LEU:HD12	4:U:18:LEU:HD13	2.00	0.43
2:E:116:ASP:HA	2:E:119:LEU:HB2	2.01	0.43
2:F:54:SER:O	2:F:54:SER:OG	2.36	0.43
1:L:47:ARG:HD2	1:L:47:ARG:HA	1.72	0.43
1:L:282:ASN:OD1	5:T:3:A:N6	2.50	0.43
2:N:231:LEU:HD11	2:O:76:LEU:HB3	2.00	0.43
6:X:71:LYS:HG2	6:X:75:PRO:HA	2.00	0.43
2:D:83:ASN:OD1	2:D:83:ASN:N	2.52	0.43
6:X:78:ARG:H	6:X:172:HIS:CD2	2.36	0.43
2:F:117:LYS:O	2:F:121:THR:OG1	2.33	0.43
2:E:230:GLU:HB2	2:E:245:THR:HB	2.00	0.43
2:G:33:ARG:O	2:G:36:SER:OG	2.27	0.43
1:L:256:ASN:HB2	1:L:283:LEU:HD11	2.01	0.43
4:U:30:LEU:HD11	4:U:59:ILE:HD11	2.00	0.43
6:A:71:LYS:HG2	6:A:75:PRO:HA	2.00	0.43
1:B:61:ILE:HD11	1:B:186:LEU:HB3	2.01	0.43
2:N:36:SER:O	2:N:36:SER:OG	2.35	0.43
8:W:4:DA:OP1	8:W:4:DA:H3'	2.19	0.43
2:F:239:LYS:O	2:F:241:GLN:NE2	2.52	0.43
3:S:169:GLU:H	3:S:183:PHE:HD2	1.67	0.43
8:Z:4:DA:OP1	8:Z:4:DA:H3'	2.19	0.43
1:B:55:GLU:HG3	1:B:114:HIS:HB2	2.01	0.43
1:L:34:PRO:HA	1:L:37:PHE:HD2	1.84	0.43
2:P:7:SER:OG	2:P:8:THR:N	2.52	0.43
2:R:302:LEU:HD23	2:R:302:LEU:HA	1.91	0.43
3:S:32:LEU:HD23	3:S:175[B]:CYS:HA	2.01	0.43
3:S:77:GLU:HA	3:S:80:ARG:HE	1.84	0.43
2:G:125:TYR:OH	2:G:324:HIS:ND1	2.46	0.42
2:G:283:GLU:HB2	2:G:286:GLY:HA2	2.01	0.42
2:H:146:ARG:HE	2:H:183:LEU:HD12	1.84	0.42
1:L:23:ILE:HA	1:L:29:TRP:HA	2.00	0.42
2:D:184:ARG:HE	2:D:184:ARG:HB3	1.68	0.42
2:R:143:ALA:HB1	2:R:181:ILE:HD13	2.02	0.42
3:S:32:LEU:HD11	3:S:40:ILE:HD13	2.00	0.42
6:A:77:ALA:HB2	6:A:174:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LYS:HE2	1:B:79:LYS:HB2	1.95	0.42
2:E:251:ASP:OD1	2:E:251:ASP:N	2.50	0.42
2:F:296:ARG:NH1	2:F:302:LEU:O	2.49	0.42
2:M:44:VAL:HG22	2:M:82:ALA:HB2	2.00	0.42
2:N:158:VAL:HB	2:N:178:ALA:HB3	2.02	0.42
2:O:233:LEU:HD13	2:O:233:LEU:HA	1.92	0.42
3:S:103:VAL:HG22	3:S:139:LEU:HD11	2.01	0.42
6:X:68:HIS:HB3	6:X:193:LEU:HB3	2.02	0.42
6:X:77:ALA:HB2	6:X:174:LEU:HB2	2.01	0.42
2:G:230:GLU:HB2	2:G:245:THR:HG23	2.02	0.42
1:L:62:VAL:O	1:L:184:PHE:N	2.50	0.42
2:M:36:SER:O	2:M:92:LYS:NZ	2.41	0.42
6:A:68:HIS:HB3	6:A:193:LEU:HB3	2.02	0.42
6:X:189:LEU:HD23	6:X:189:LEU:HA	1.87	0.42
1:B:88:LEU:HG	2:H:289:THR:HG22	2.02	0.42
2:P:239:LYS:O	2:P:241:GLN:NE2	2.39	0.42
2:P:310:ASN:HB3	2:P:316:GLU:HB2	2.02	0.42
4:V:79:ASN:OD1	4:V:79:ASN:N	2.41	0.42
2:O:96:THR:OG1	2:P:223:GLN:NE2	2.51	0.42
2:P:330:LEU:HD23	2:P:330:LEU:HA	1.85	0.42
3:S:32:LEU:HD23	3:S:175[A]:CYS:HA	2.02	0.42
2:D:268:ASP:OD1	2:D:296:ARG:NH2	2.50	0.42
2:F:266:THR:HG22	2:F:281:ALA:HB2	2.02	0.42
3:I:81:ASP:N	3:I:81:ASP:OD1	2.47	0.42
1:L:12:LEU:HD13	1:L:12:LEU:HA	1.92	0.42
1:L:197:LEU:O	1:L:201:ARG:N	2.45	0.42
2:F:179:LEU:HD23	2:F:179:LEU:HA	1.87	0.42
2:G:25:MET:HB3	2:G:91:LEU:HD11	2.01	0.42
2:O:264:LEU:HD23	2:O:264:LEU:HA	1.84	0.42
6:A:78:ARG:H	6:A:172:HIS:CD2	2.37	0.42
2:F:58:LYS:NZ	4:U:144:THR:O	2.41	0.42
2:H:138:TYR:HE1	2:H:267:ILE:HD13	1.84	0.42
2:M:255:ILE:HG23	2:M:259:LYS:HZ3	1.84	0.42
2:P:327:ILE:HD13	2:P:327:ILE:HA	1.87	0.42
3:S:28:LEU:HD11	3:S:58:LEU:HD21	2.01	0.42
2:C:156:GLU:N	2:C:218:ARG:O	2.45	0.42
1:L:261:LEU:HD13	1:L:261:LEU:HA	1.94	0.42
1:L:311:LYS:HE2	1:L:311:LYS:HB2	1.93	0.42
3:S:148:SER:OG	3:S:149:GLN:N	2.53	0.42
2:E:330:LEU:HD23	2:E:330:LEU:HA	1.88	0.41
2:M:36:SER:HB3	2:M:92:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:98:ARG:HD2	2:O:223:GLN:HG3	2.01	0.41
3:S:174:THR:HG23	3:S:176:TYR:H	1.85	0.41
2:H:301:LYS:HA	2:H:301:LYS:HD3	1.81	0.41
2:Q:99:VAL:HB	2:Q:209:VAL:HG23	2.01	0.41
2:Q:301:LYS:HA	2:Q:301:LYS:HD3	1.93	0.41
3:S:45:PRO:HG2	3:S:57:ARG:HE	1.84	0.41
4:V:30:LEU:HD11	4:V:59:ILE:HD11	2.00	0.41
6:X:222:ARG:HD3	6:X:222:ARG:HA	1.96	0.41
2:D:172:ARG:NH2	2:D:191:GLU:OE1	2.49	0.41
2:H:179:LEU:HD23	2:H:179:LEU:HA	1.89	0.41
2:R:172:ARG:NH1	2:R:173:THR:O	2.53	0.41
6:A:241:GLN:OE1	6:A:262:ASN:ND2	2.49	0.41
1:B:12:LEU:HA	1:B:13:PRO:HD3	1.91	0.41
2:E:109:CYS:SG	2:E:110:ASN:N	2.92	0.41
2:E:145:ALA:H	2:E:178:ALA:HB1	1.86	0.41
2:M:323:GLN:HA	2:M:326:VAL:HG22	2.03	0.41
2:Q:204:SER:OG	2:Q:206:SER:OG	2.30	0.41
8:W:4:DA:H2"	8:W:5:DA:OP2	2.21	0.41
1:B:271:ARG:N	6:A:177:GLN:OE1	2.53	0.41
2:F:23:ALA:HB2	2:F:260:ILE:HD11	2.02	0.41
2:H:312:VAL:HG13	2:H:313:LEU:HG	2.03	0.41
2:N:203:LEU:HD23	2:N:203:LEU:HA	1.92	0.41
2:O:117:LYS:HA	2:O:117:LYS:HD2	1.87	0.41
2:Q:307:LEU:HD23	2:Q:307:LEU:HA	1.91	0.41
6:X:112:ALA:C	8:W:12:DC:C5'	2.89	0.41
2:E:163:ASN:HB3	2:E:170:VAL:HG13	2.02	0.41
2:H:299:LYS:HB3	2:H:299:LYS:HE3	1.78	0.41
3:I:42:VAL:HG23	3:I:100:VAL:HG21	2.02	0.41
2:M:187:LYS:HE2	2:M:187:LYS:HB2	1.93	0.41
2:C:133:GLU:HG3	2:C:134:LEU:HD22	2.02	0.41
2:F:302:LEU:HD23	2:F:302:LEU:HA	1.85	0.41
2:G:73:SER:O	2:G:73:SER:OG	2.31	0.41
1:L:110:LEU:HD12	1:L:110:LEU:HA	1.90	0.41
2:M:22:ASP:OD1	2:M:257:SER:N	2.54	0.41
2:M:172:ARG:NH1	2:M:173:THR:O	2.54	0.41
2:N:184:ARG:NH1	2:N:276:GLY:O	2.39	0.41
2:N:268:ASP:OD1	2:N:296:ARG:NH2	2.51	0.41
2:O:195:LEU:HD23	2:O:195:LEU:HA	1.86	0.41
2:P:185:ASP:OD2	2:P:187:LYS:NZ	2.53	0.41
1:B:192:LEU:O	1:B:195:GLN:NE2	2.42	0.41
2:F:177:ASP:OD2	2:F:180:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:330:LEU:HD23	2:F:330:LEU:HA	1.86	0.41
2:G:159:GLU:OE2	2:G:161:ARG:NH1	2.54	0.41
2:H:195:LEU:HD23	2:H:195:LEU:HA	1.92	0.41
2:M:47:LYS:HD2	2:M:47:LYS:HA	1.75	0.41
2:O:243:SER:O	2:O:243:SER:OG	2.37	0.41
2:P:104:GLY:HA3	2:P:122:VAL:HG21	2.03	0.41
3:S:99:GLN:HG3	3:S:162:GLY:HA3	2.03	0.41
2:D:32:GLN:HB2	2:D:39:TRP:HZ2	1.85	0.41
2:E:45:ARG:HH22	2:E:83:ASN:HD21	1.69	0.41
2:G:111:ASP:OD1	2:G:114:TYR:N	2.51	0.41
2:H:264:LEU:HA	2:H:264:LEU:HD23	1.82	0.41
3:I:67:LEU:HD22	3:I:88:PRO:HG3	2.03	0.41
2:M:231:LEU:HD21	2:N:76:LEU:HD12	2.03	0.41
2:Q:111:ASP:OD2	2:Q:114:TYR:N	2.53	0.41
6:A:189:LEU:HD23	6:A:189:LEU:HA	1.87	0.41
6:X:242:LYS:HA	6:X:242:LYS:HD2	1.90	0.41
1:B:220:ASN:N	1:B:240:GLN:O	2.44	0.40
1:B:253:ALA:N	1:B:283:LEU:O	2.54	0.40
2:E:17:LYS:HG3	2:E:100:LEU:HB2	2.01	0.40
2:H:118:LEU:HA	2:H:121:THR:HG22	2.02	0.40
1:L:301:LEU:HD23	1:L:301:LEU:HA	1.93	0.40
2:R:55:ASN:OD1	2:R:55:ASN:N	2.53	0.40
4:U:83:ASP:OD1	4:U:83:ASP:N	2.39	0.40
6:A:112:ALA:C	8:Z:12:DC:C5'	2.89	0.40
2:C:7:SER:OG	2:C:8:THR:N	2.53	0.40
2:E:259:LYS:NZ	5:J:28:C:OP1	2.36	0.40
2:G:321:GLU:HA	2:G:324:HIS:CD2	2.56	0.40
2:H:142:LEU:HD23	2:H:142:LEU:HA	1.92	0.40
2:O:201:SER:O	2:O:206:SER:OG	2.39	0.40
3:S:42:VAL:HA	3:S:60:ILE:HA	2.03	0.40
2:F:232:ILE:HA	2:F:235:LYS:HE2	2.02	0.40
2:G:142:LEU:HD23	2:G:142:LEU:HA	1.89	0.40
2:G:264:LEU:HA	2:G:264:LEU:HD12	1.87	0.40
2:H:331:ILE:HD12	2:H:331:ILE:HA	1.89	0.40
1:L:93:SER:OG	1:L:94:THR:N	2.55	0.40
3:S:100:VAL:HG23	3:S:159:ILE:HG23	2.02	0.40
2:C:288:VAL:HG22	2:C:291:GLN:H	1.86	0.40
2:M:293:LYS:HE2	2:M:293:LYS:HB2	1.96	0.40
2:Q:203:LEU:HD23	2:Q:203:LEU:HA	1.95	0.40
2:D:84:LEU:HD12	2:D:84:LEU:HA	1.80	0.40
2:E:142:LEU:HA	2:E:142:LEU:HD23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:283:GLU:HB2	2:H:286:GLY:HA2	2.04	0.40
1:L:97:ILE:HD13	1:L:97:ILE:HA	1.95	0.40
2:N:266:THR:HA	2:N:281:ALA:HA	2.03	0.40
2:P:16:ARG:NH1	5:T:19:G:OP2	2.54	0.40
6:A:245:GLY:C	7:Y:33:DG:OP2	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	301/327 (92%)	268 (89%)	33 (11%)	0	100	100
1	L	301/327 (92%)	275 (91%)	25 (8%)	1 (0%)	41	74
2	C	287/342 (84%)	268 (93%)	19 (7%)	0	100	100
2	D	332/342 (97%)	312 (94%)	20 (6%)	0	100	100
2	E	335/342 (98%)	312 (93%)	23 (7%)	0	100	100
2	F	333/342 (97%)	312 (94%)	21 (6%)	0	100	100
2	G	325/342 (95%)	306 (94%)	19 (6%)	0	100	100
2	H	330/342 (96%)	302 (92%)	28 (8%)	0	100	100
2	M	287/342 (84%)	273 (95%)	14 (5%)	0	100	100
2	N	333/342 (97%)	316 (95%)	17 (5%)	0	100	100
2	O	332/342 (97%)	307 (92%)	25 (8%)	0	100	100
2	P	333/342 (97%)	313 (94%)	20 (6%)	0	100	100
2	Q	331/342 (97%)	306 (92%)	25 (8%)	0	100	100
2	R	331/342 (97%)	314 (95%)	17 (5%)	0	100	100
3	I	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
3	S	186/187 (100%)	179 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	225/228 (99%)	207 (92%)	18 (8%)	0	100	100
4	V	225/228 (99%)	207 (92%)	18 (8%)	0	100	100
6	A	422/434 (97%)	392 (93%)	30 (7%)	0	100	100
6	X	422/434 (97%)	392 (93%)	30 (7%)	0	100	100
All	All	6156/6456 (95%)	5735 (93%)	420 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	13	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/270 (75%)	191 (94%)	12 (6%)	19	54
1	L	232/270 (86%)	220 (95%)	12 (5%)	23	59
2	C	202/274 (74%)	198 (98%)	4 (2%)	55	80
2	D	253/274 (92%)	240 (95%)	13 (5%)	24	60
2	E	262/274 (96%)	251 (96%)	11 (4%)	30	65
2	F	262/274 (96%)	247 (94%)	15 (6%)	20	56
2	G	255/274 (93%)	243 (95%)	12 (5%)	26	62
2	H	244/274 (89%)	231 (95%)	13 (5%)	22	58
2	M	221/274 (81%)	209 (95%)	12 (5%)	22	58
2	N	260/274 (95%)	248 (95%)	12 (5%)	27	63
2	O	259/274 (94%)	248 (96%)	11 (4%)	30	65
2	P	263/274 (96%)	250 (95%)	13 (5%)	25	61
2	Q	258/274 (94%)	244 (95%)	14 (5%)	22	58
2	R	251/274 (92%)	237 (94%)	14 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	145/160 (91%)	142 (98%)	3 (2%)	53 79
3	S	145/160 (91%)	144 (99%)	1 (1%)	84 94
4	U	181/182 (100%)	168 (93%)	13 (7%)	14 47
4	V	181/182 (100%)	168 (93%)	13 (7%)	14 47
6	A	117/365 (32%)	104 (89%)	13 (11%)	6 25
6	X	117/365 (32%)	104 (89%)	13 (11%)	6 25
All	All	4311/5242 (82%)	4087 (95%)	224 (5%)	27 59

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	THR
1	B	31	PHE
1	B	55	GLU
1	B	79	LYS
1	B	102	ARG
1	B	148	CYS
1	B	150	GLU
1	B	159	LEU
1	B	268	ARG
1	B	298	LEU
1	B	300	ASP
1	B	322	VAL
2	C	43	THR
2	C	97	LEU
2	C	133	GLU
2	C	300	GLN
2	D	8	THR
2	D	60	LYS
2	D	66	LYS
2	D	76	LEU
2	D	78	THR
2	D	87	ASP
2	D	105	THR
2	D	148	LEU
2	D	208	HIS
2	D	251	ASP
2	D	282	VAL
2	D	285	TYR
2	D	299	LYS

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Mol	Chain	Res	Type
2	E	17	LYS
2	E	22	ASP
2	E	24	LEU
2	E	118	LEU
2	E	160	VAL
2	E	179	LEU
2	E	201	SER
2	E	234	ASP
2	E	245	THR
2	E	251	ASP
2	E	285	TYR
2	F	45	ARG
2	F	54	SER
2	F	59	THR
2	F	151	ASN
2	F	158	VAL
2	F	192	LEU
2	F	208	HIS
2	F	221	ASP
2	F	237	ASP
2	F	238	LYS
2	F	243	SER
2	F	285	TYR
2	F	290	SER
2	F	310	ASN
2	F	329	ASN
2	G	24	LEU
2	G	25	MET
2	G	45	ARG
2	G	78	THR
2	G	105	THR
2	G	140	HIS
2	G	160	VAL
2	G	208	HIS
2	G	245	THR
2	G	285	TYR
2	G	290	SER
2	G	315	ASP
2	H	34	ASP
2	H	57	LEU
2	H	60	LYS
2	H	87	ASP

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Mol	Chain	Res	Type
2	H	105	THR
2	H	169	GLU
2	H	172	ARG
2	H	185	ASP
2	H	189	ASP
2	H	192	LEU
2	H	245	THR
2	H	270	TRP
2	H	315	ASP
3	I	44	PHE
3	I	131	ILE
3	I	134	THR
1	L	4	THR
1	L	14	ARG
1	L	17	ILE
1	L	47	ARG
1	L	51	SER
1	L	59	VAL
1	L	98	VAL
1	L	143	SER
1	L	159	LEU
1	L	268	ARG
1	L	277	LEU
1	L	280	VAL
2	M	10	SER
2	M	21	SER
2	M	45	ARG
2	M	81	VAL
2	M	98	ARG
2	M	144	ASN
2	M	192	LEU
2	M	245	THR
2	M	264	LEU
2	M	301	LYS
2	M	314	ARG
2	M	332	ARG
2	N	21	SER
2	N	66	LYS
2	N	67	LEU
2	N	81	VAL
2	N	129	GLN
2	N	179	LEU

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Mol	Chain	Res	Type
2	N	187	LYS
2	N	250	ARG
2	N	251	ASP
2	N	266	THR
2	N	285	TYR
2	N	332	ARG
2	O	21	SER
2	O	78	THR
2	O	83	ASN
2	O	128	GLU
2	O	158	VAL
2	O	160	VAL
2	O	173	THR
2	O	201	SER
2	O	209	VAL
2	O	251	ASP
2	O	285	TYR
2	P	8	THR
2	P	43	THR
2	P	59	THR
2	P	105	THR
2	P	115	ARG
2	P	158	VAL
2	P	161	ARG
2	P	208	HIS
2	P	250	ARG
2	P	251	ASP
2	P	285	TYR
2	P	289	THR
2	P	314	ARG
2	Q	24	LEU
2	Q	42	VAL
2	Q	78	THR
2	Q	105	THR
2	Q	156	GLU
2	Q	173	THR
2	Q	208	HIS
2	Q	209	VAL
2	Q	221	ASP
2	Q	251	ASP
2	Q	285	TYR
2	Q	314	ARG

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Mol	Chain	Res	Type
2	Q	315	ASP
2	Q	332	ARG
2	R	17	LYS
2	R	34	ASP
2	R	52	THR
2	R	55	ASN
2	R	63	ASP
2	R	91	LEU
2	R	105	THR
2	R	234	ASP
2	R	245	THR
2	R	270	TRP
2	R	285	TYR
2	R	289	THR
2	R	290	SER
2	R	320	VAL
3	S	114	ARG
4	U	12	THR
4	U	30	LEU
4	U	36	GLU
4	U	61	GLU
4	U	73	ASP
4	U	96	GLU
4	U	101	CYS
4	U	113	THR
4	U	153	THR
4	U	155	ASP
4	U	167	LEU
4	U	180	SER
4	U	197	LYS
4	V	12	THR
4	V	30	LEU
4	V	36	GLU
4	V	61	GLU
4	V	73	ASP
4	V	96	GLU
4	V	101	CYS
4	V	113	THR
4	V	153	THR
4	V	155	ASP
4	V	167	LEU
4	V	180	SER

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Mol	Chain	Res	Type
4	V	197	LYS
6	A	63	LEU
6	A	173	SER
6	A	196	THR
6	A	197	SER
6	A	199	VAL
6	A	206	LEU
6	A	213	ASP
6	A	219	ARG
6	A	226	GLU
6	A	227	SER
6	A	228	TRP
6	A	265	LEU
6	A	268	LEU
6	X	63	LEU
6	X	173	SER
6	X	196	THR
6	X	197	SER
6	X	199	VAL
6	X	206	LEU
6	X	213	ASP
6	X	219	ARG
6	X	226	GLU
6	X	227	SER
6	X	228	TRP
6	X	265	LEU
6	X	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	B	69	GLN
1	B	86	ASN
2	C	110	ASN
2	C	127	ASN
2	C	129	GLN
2	D	110	ASN
2	E	37	GLN
2	E	297	GLN
2	F	110	ASN
2	G	120	GLN

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Mol	Chain	Res	Type
2	G	323	GLN
2	H	241	GLN
2	H	329	ASN
3	I	30	GLN
3	I	84	GLN
3	I	99	GLN
3	I	120	HIS
3	I	165	GLN
1	L	69	GLN
1	L	104	HIS
1	L	129	GLN
1	L	131	GLN
1	L	156	ASN
1	L	172	ASN
1	L	256	ASN
2	M	144	ASN
2	M	229	GLN
2	N	151	ASN
2	N	297	GLN
2	P	120	GLN
2	Q	223	GLN
2	Q	300	GLN
2	R	75	ASN
2	R	291	GLN
2	R	310	ASN
2	R	329	ASN
4	V	194	ASN
6	A	237	ASN
6	A	249	GLN
6	A	250	ASN
6	X	237	ASN
6	X	249	GLN
6	X	250	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	J	59/60 (98%)	28 (47%)	1 (1%)
5	T	59/60 (98%)	28 (47%)	1 (1%)
All	All	118/120 (98%)	56 (47%)	2 (1%)

All (56) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	J	3	A
5	J	8	A
5	J	9	U
5	J	10	U
5	J	11	C
5	J	14	G
5	J	15	G
5	J	16	C
5	J	17	G
5	J	20	C
5	J	21	U
5	J	22	U
5	J	26	G
5	J	27	U
5	J	28	C
5	J	32	G
5	J	33	U
5	J	34	C
5	J	39	U
5	J	40	G
5	J	41	G
5	J	42	U
5	J	43	U
5	J	44	C
5	J	45	A
5	J	54	U
5	J	57	G
5	J	60	G
5	T	3	A
5	T	8	A
5	T	9	U
5	T	10	U
5	T	11	C
5	T	14	G
5	T	15	G
5	T	16	C
5	T	17	G
5	T	20	C
5	T	21	U
5	T	22	U
5	T	26	G
5	T	27	U
5	T	28	C

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Mol	Chain	Res	Type
5	T	32	G
5	T	33	U
5	T	34	C
5	T	39	U
5	T	40	G
5	T	41	G
5	T	42	U
5	T	43	U
5	T	44	C
5	T	45	A
5	T	54	U
5	T	57	G
5	T	60	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	J	16	C
5	T	16	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

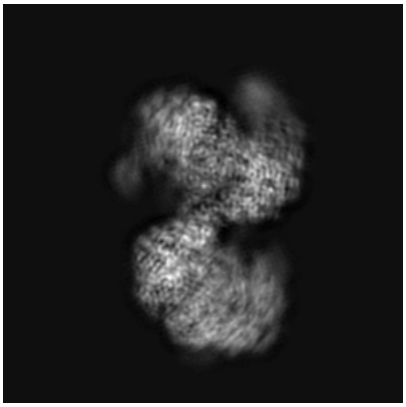
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32440. These allow visual inspection of the internal detail of the map and identification of artifacts.

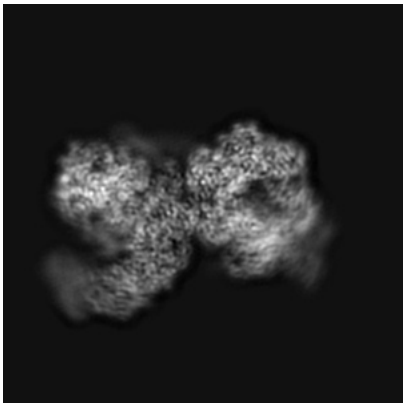
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

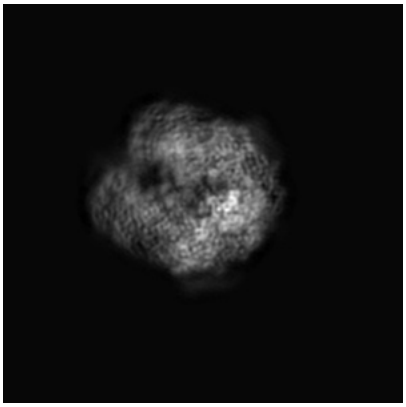
6.1.1 Primary map



X



Y

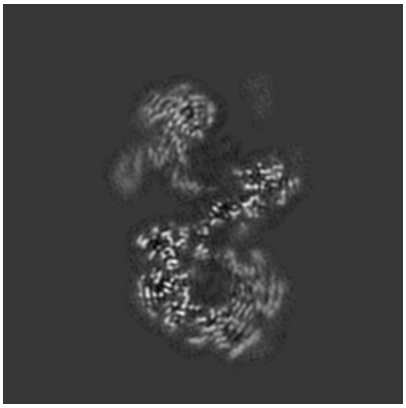


Z

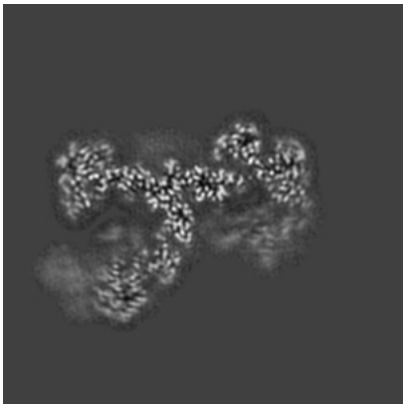
The images above show the map projected in three orthogonal directions.

6.2 Central slices

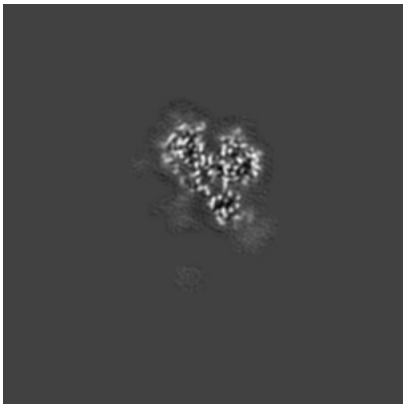
6.2.1 Primary map



X Index: 140



Y Index: 140

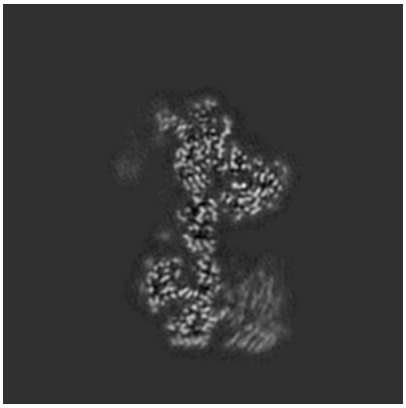


Z Index: 140

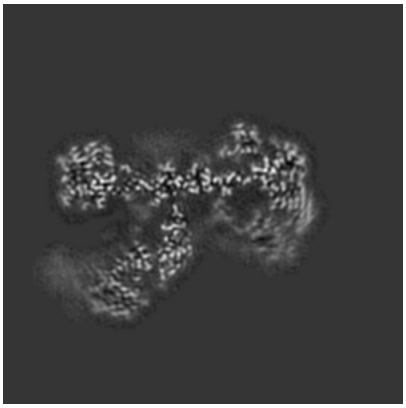
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

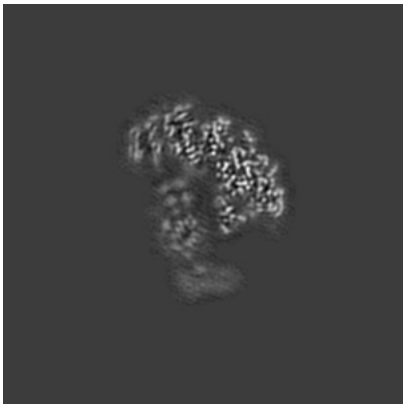
6.3.1 Primary map



X Index: 158



Y Index: 135



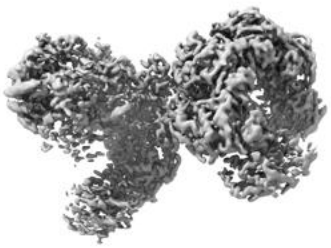
Z Index: 164

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

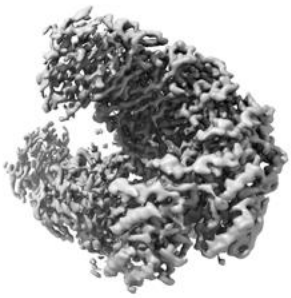
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

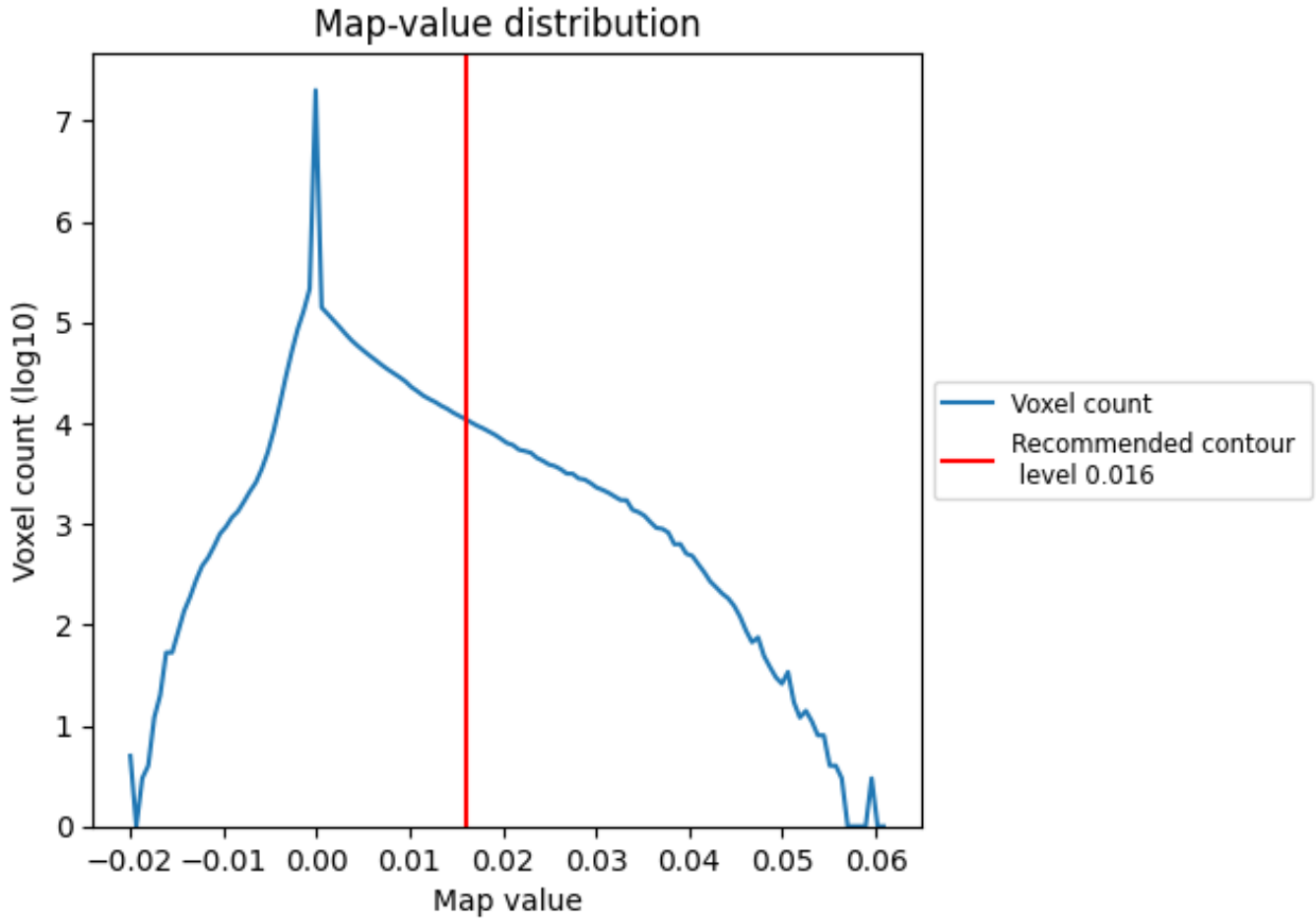
6.5 Mask visualisation (i)

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

7 Map analysis

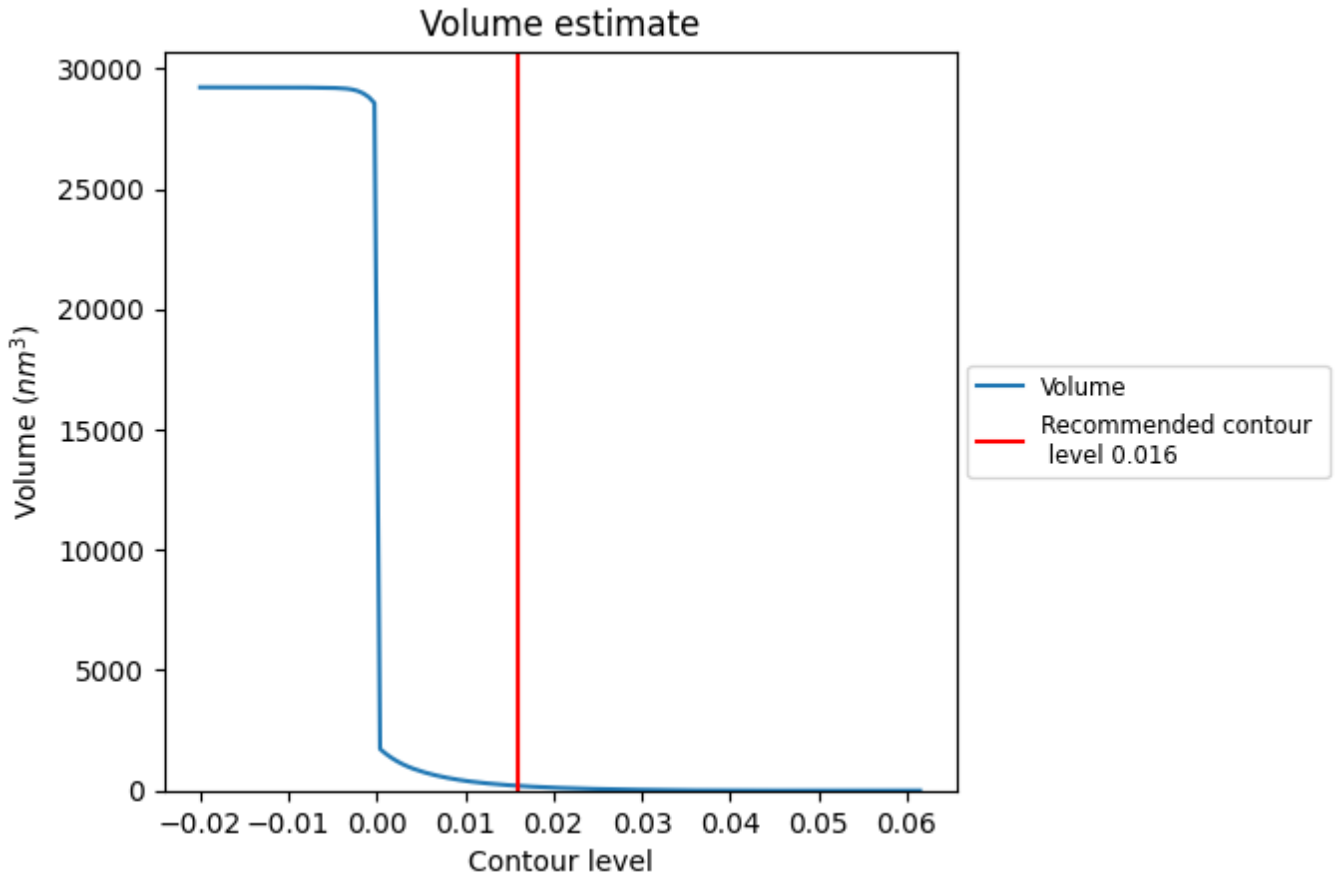
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

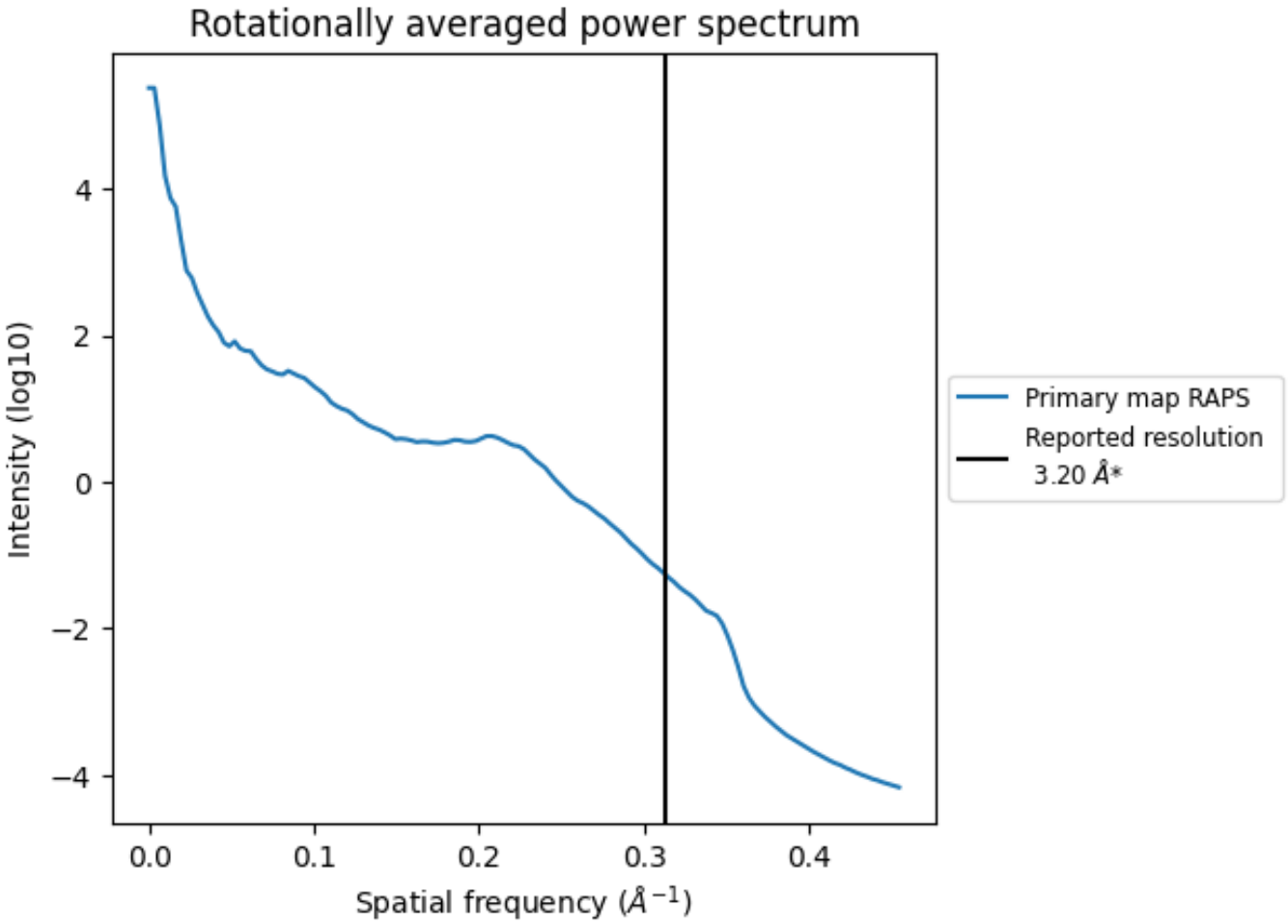
7.2 Volume estimate



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

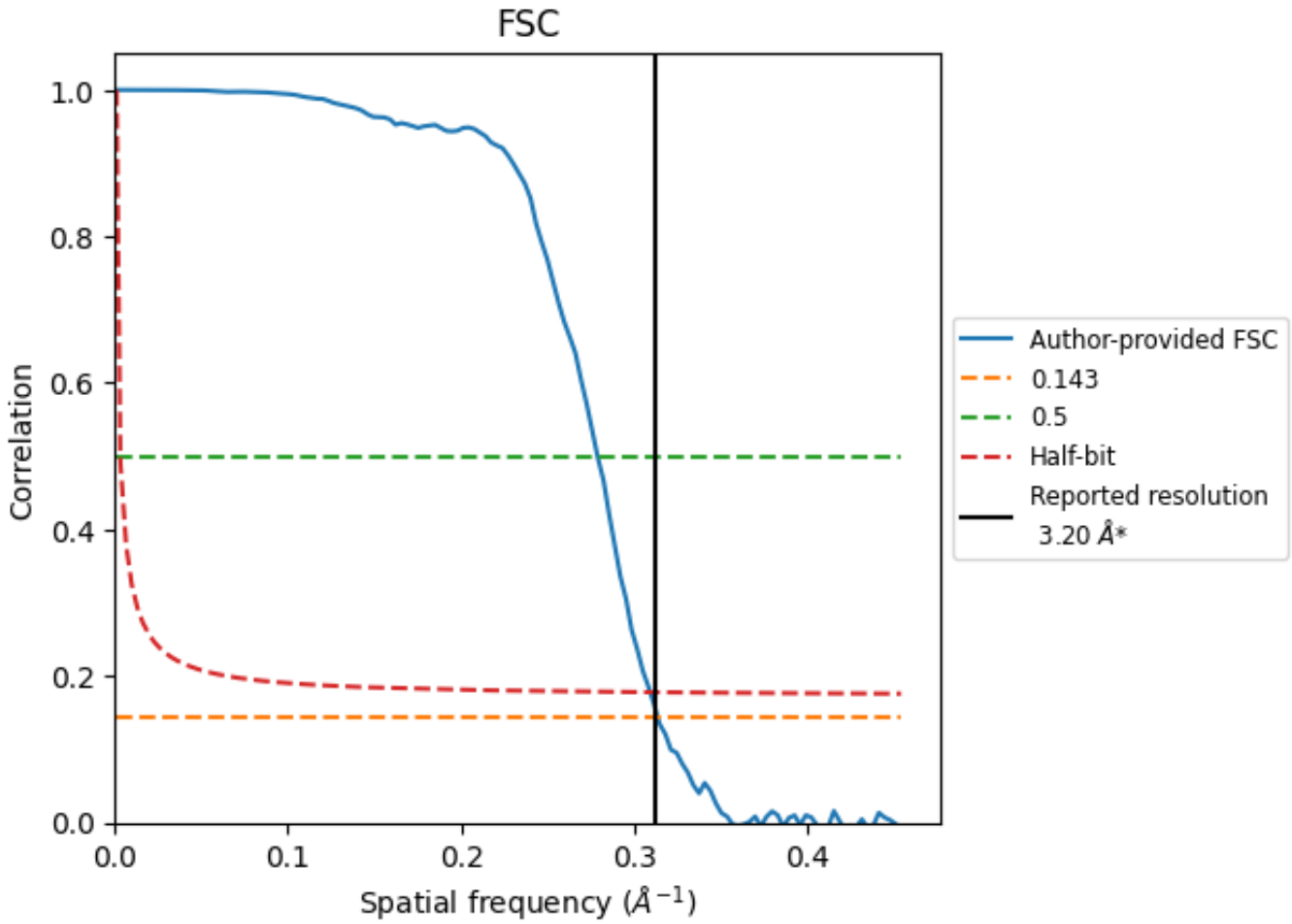


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

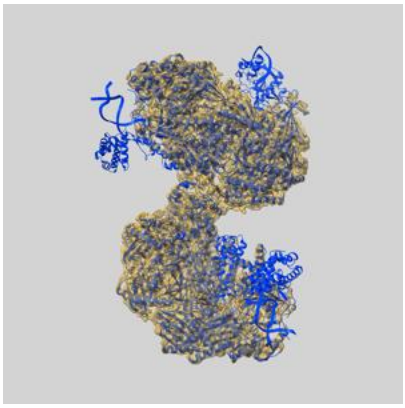
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.58	3.23
Unmasked-calculated*	-	-	-

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

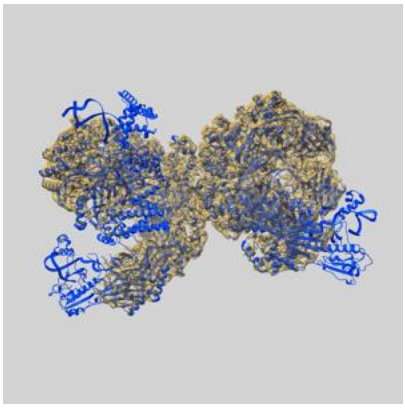
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32440 and PDB model 7WE6. Per-residue inclusion information can be found in section 3 on page 7.

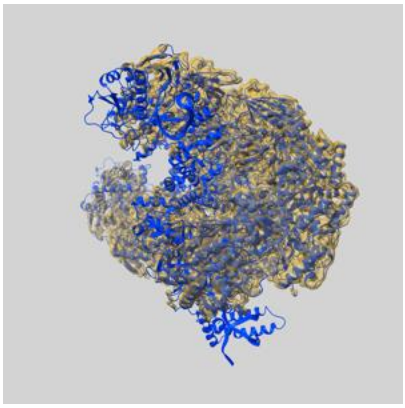
9.1 Map-model overlay



X



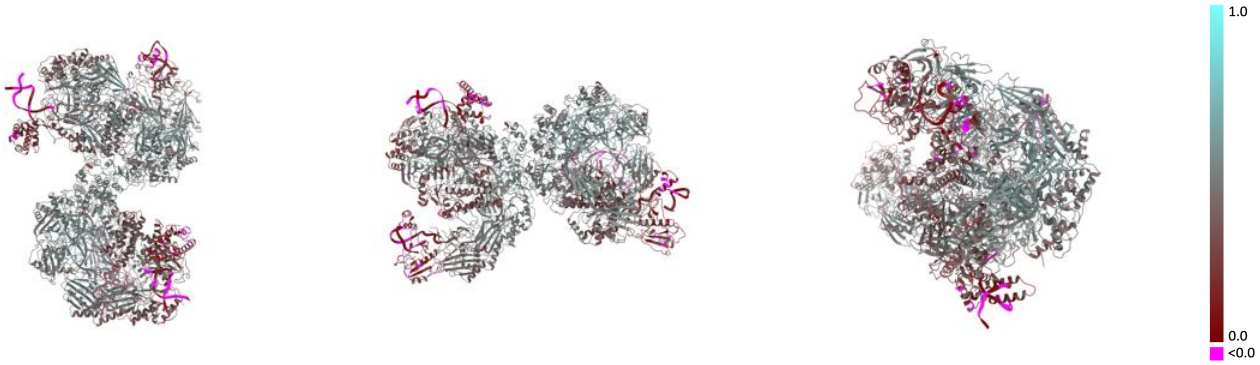
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

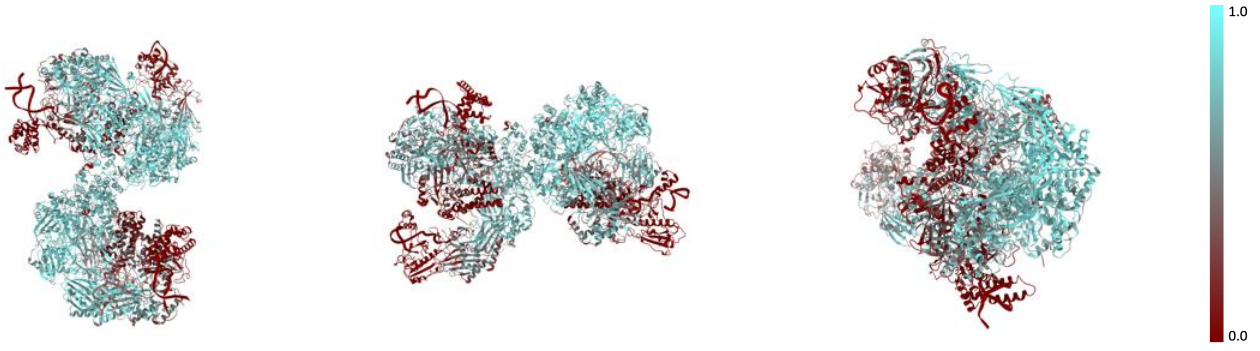
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

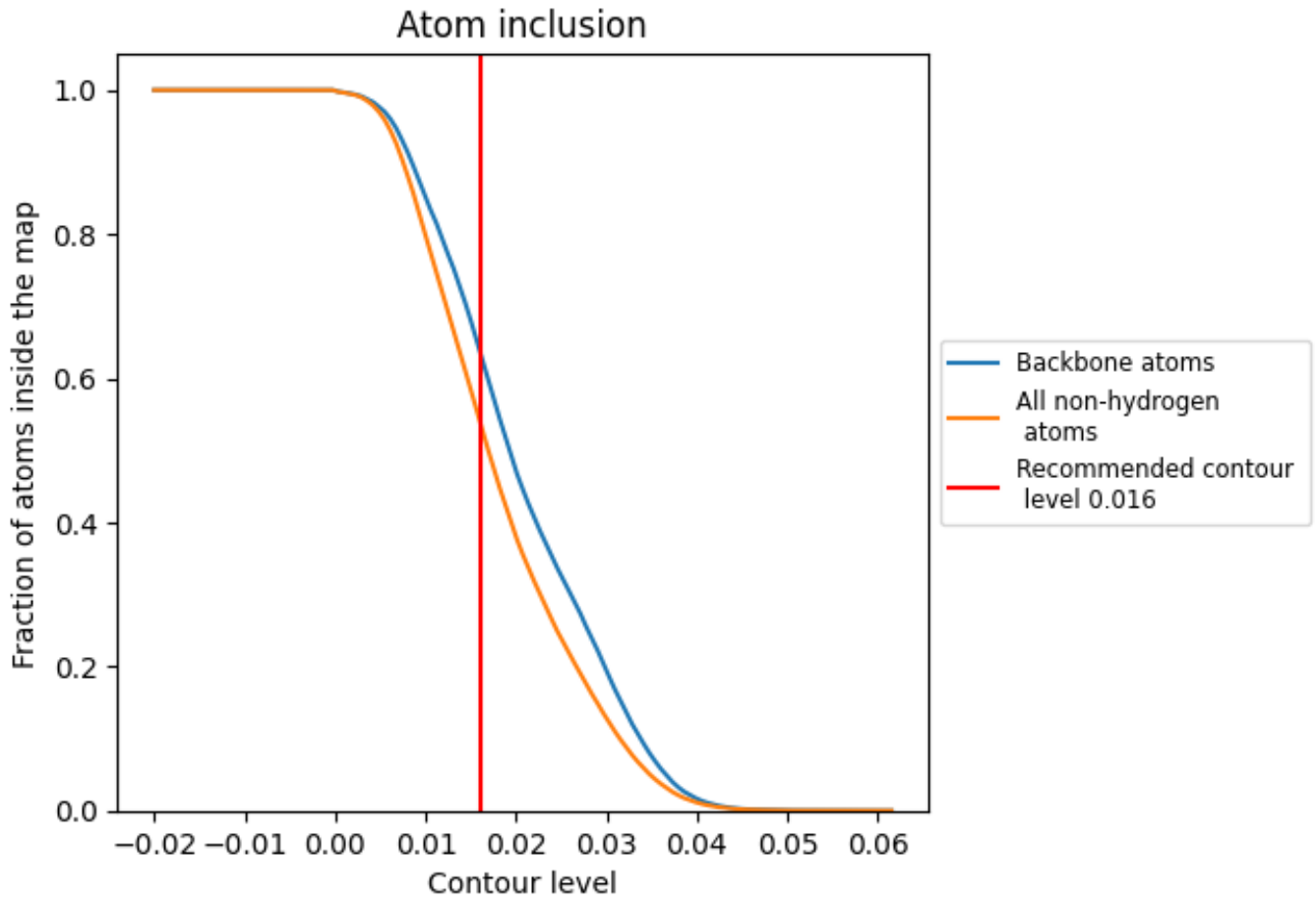
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 54% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5403	0.4360
A	0.1046	0.3140
B	0.2648	0.4070
C	0.4457	0.4360
D	0.6940	0.4900
E	0.7702	0.5140
F	0.7842	0.5170
G	0.7646	0.5030
H	0.6026	0.4480
I	0.0000	0.1880
J	0.5515	0.3860
K	0.0000	0.0120
L	0.2925	0.3940
M	0.3920	0.4250
N	0.6776	0.4860
O	0.7753	0.5200
P	0.7814	0.5170
Q	0.7618	0.5010
R	0.6046	0.4290
S	0.0014	0.1760
T	0.5547	0.3770
U	0.7691	0.5230
V	0.7633	0.5230
W	0.0000	0.0340
X	0.1342	0.3320
Y	0.0000	0.0470
Z	0.0000	0.0280