Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 02:59 pm BST

PDB ID	:	7R2K
EMDB ID	:	EMD-14245
Title	:	elongated Cascade complex from type I-A CRISPR-Cas system
Authors	:	Hu, C.; Ni, D.; Nam, K.H.; Terns, M.; Stahlberg, H.; Ke, A.
Deposited on	:	2022-02-04
Resolution	:	3.30 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:

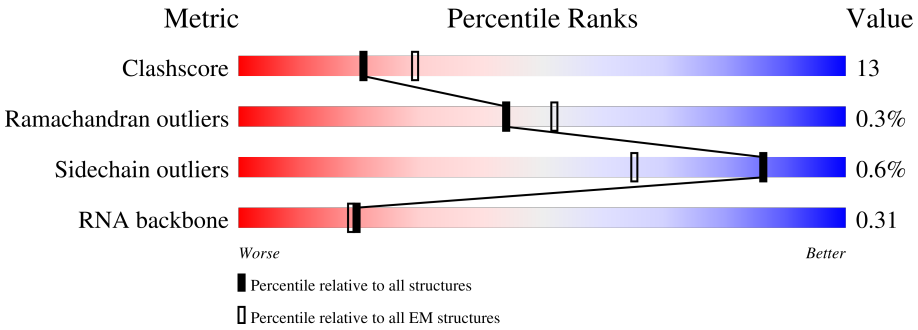
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	A	651	63% 24% 12%
2	C	108	60% 38%
2	E	108	46% 70% 28%
2	F	108	67% 31%
2	G	108	75% 24%
2	H	108	64% 35%
2	I	108	69% 31%

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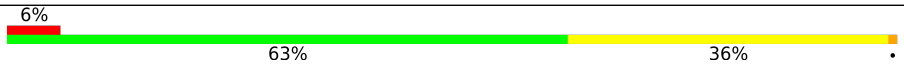
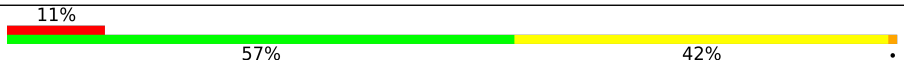
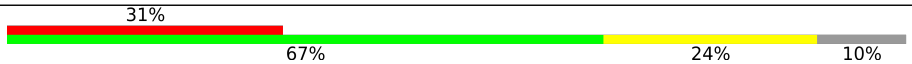
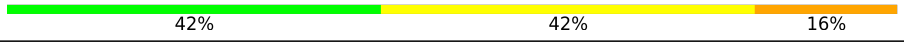
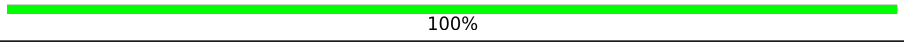
Mol	Chain	Length	Quality of chain
2	J	108	
3	D	9	
4	K	336	
4	L	336	
4	M	336	
4	N	336	
4	O	336	
4	P	336	
4	R	336	
4	T	336	
4	V	336	
4	W	336	
5	Q	238	
6	S	256	
7	U	57	
8	X	4	
9	Y	341	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 43931 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-associated helicase Cas3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	572	Total	C	N	O	S	0	0
			4304	2749	745	802	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	LYS	ARG	conflict	UNP A0A5C0XNV5
A	393	VAL	THR	conflict	UNP A0A5C0XNV5
A	451	PRO	-	insertion	UNP A0A5C0XNV5
A	517	LYS	LEU	conflict	UNP A0A5C0XNV5

- Molecule 2 is a protein called Cas11a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	107	Total	C	N	O	S	0	0
			856	550	144	160	2		
2	E	107	Total	C	N	O	S	0	0
			856	550	144	160	2		
2	F	107	Total	C	N	O	S	0	0
			856	550	144	160	2		
2	G	108	Total	C	N	O	S	0	0
			860	552	145	161	2		
2	H	107	Total	C	N	O	S	0	0
			856	550	144	160	2		
2	I	107	Total	C	N	O	S	0	0
			856	550	144	160	2		
2	J	107	Total	C	N	O	S	0	0
			856	550	144	160	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	9	Total	C	N	O	P	0	0
			189	89	40	51	9		

- Molecule 4 is a protein called Cas7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	335	Total	C	N	O	S	0	0
			2597	1655	450	487	5		
4	L	336	Total	C	N	O	S	0	0
			2603	1659	451	488	5		
4	M	336	Total	C	N	O	S	0	0
			2596	1656	448	487	5		
4	N	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	O	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	P	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	R	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	T	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	V	336	Total	C	N	O	S	0	0
			2597	1656	448	488	5		
4	W	304	Total	C	N	O	S	0	0
			2350	1505	403	438	4		

- Molecule 5 is a protein called CRISPR-associated endonuclease Cas3-HD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	237	Total	C	N	O	S	0	0
			1822	1166	314	329	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	237	ALA	-	expression tag	UNP Q8U336
Q	238	ALA	-	expression tag	UNP Q8U336

- Molecule 6 is a protein called Type I-A CRISPR-associated protein Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	240	Total	C	N	O	S	0	0
			1936	1266	315	349	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	THR	deletion	UNP A0A5C0XNV9

- Molecule 7 is a RNA chain called crRNA (57-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	57	Total	C	N	O	P	0	0
			1215	543	216	400	56		

- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	4	Total	C	N	O	P	0	0
			77	37	11	25	4		

- Molecule 9 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	333	Total	C	N	O	S	0	0
			2662	1730	439	484	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	24	VAL	GLU	conflict	UNP Q8U338
Y	64	SER	GLU	conflict	UNP Q8U338
Y	110	LEU	VAL	conflict	UNP Q8U338
Y	?	-	SER	deletion	UNP Q8U338
Y	?	-	LEU	deletion	UNP Q8U338
Y	?	-	GLY	deletion	UNP Q8U338

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

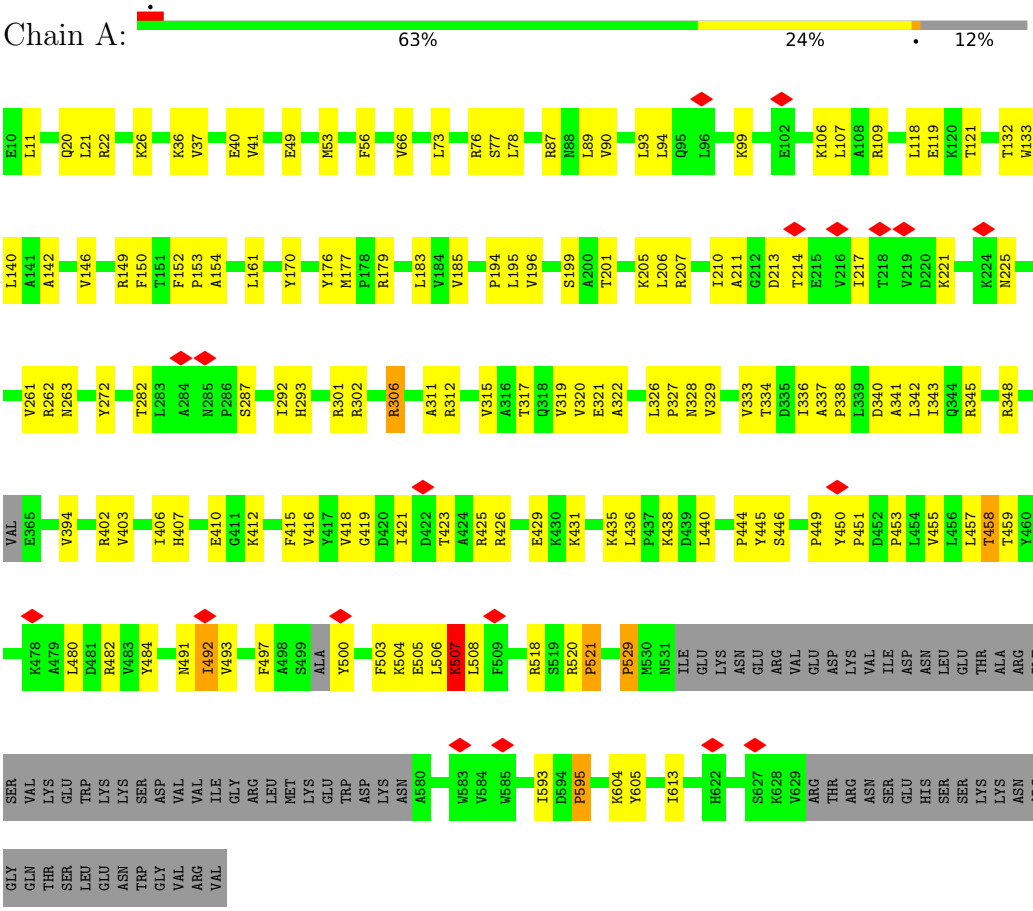
Mol	Chain	Residues	Atoms		AltConf
10	Q	2	Total	Ni	0
			2	2	

3 Residue-property plots (i)

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

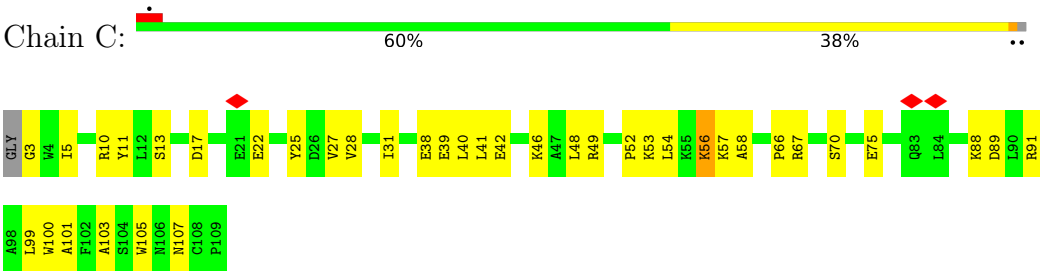
• Molecule 1: CRISPR-associated helicase Cas3

Chain A:



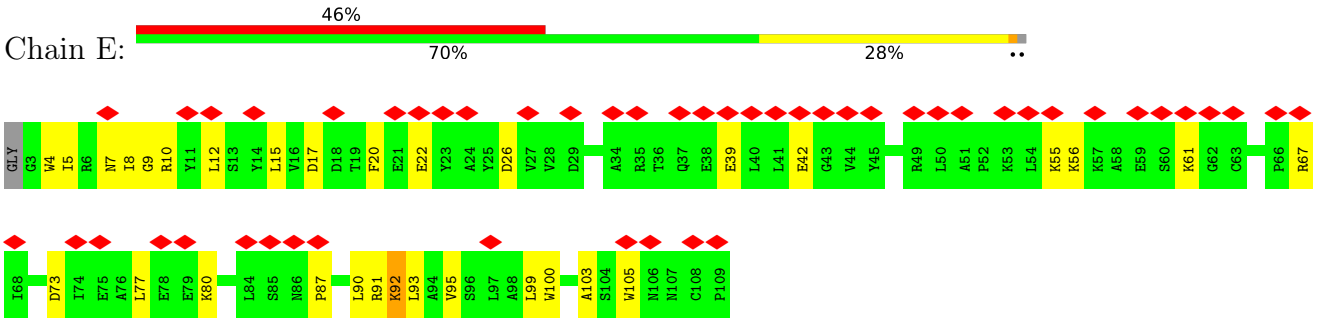
• Molecule 2: Cas11a

Chain C:



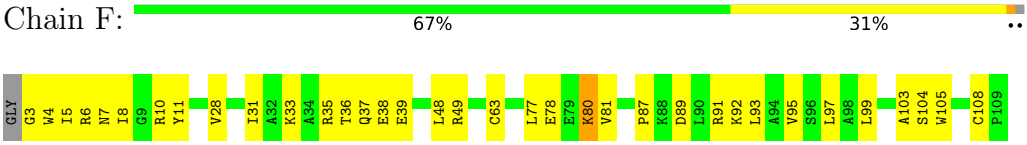
• Molecule 2: Cas11a

Chain E:



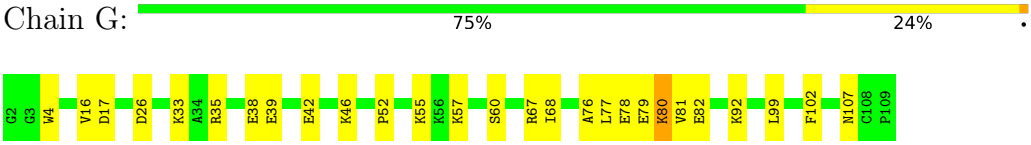
• Molecule 2: Cas11a

Chain F:



• Molecule 2: Cas11a

Chain G:

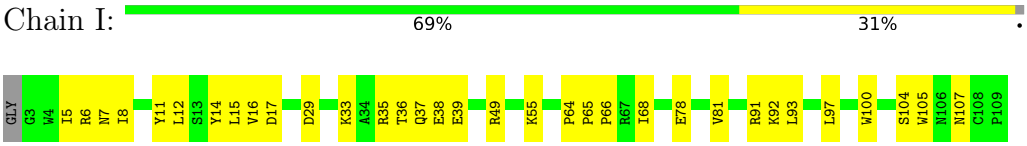


• Molecule 2: Cas11a

Chain H:

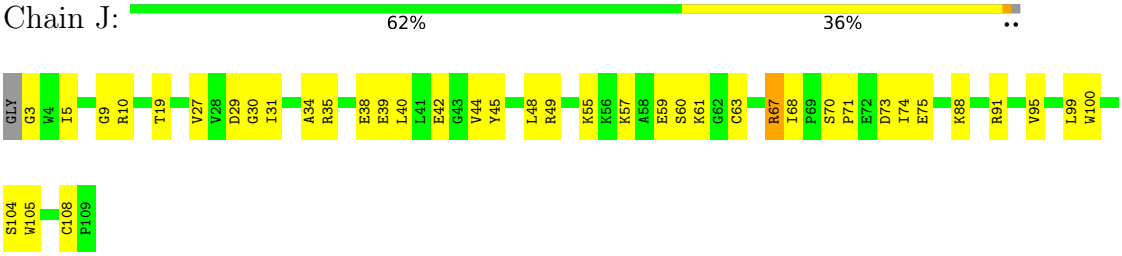
• Molecule 2: Cas11a

Chain I:



• Molecule 2: Cas11a

Chain J:

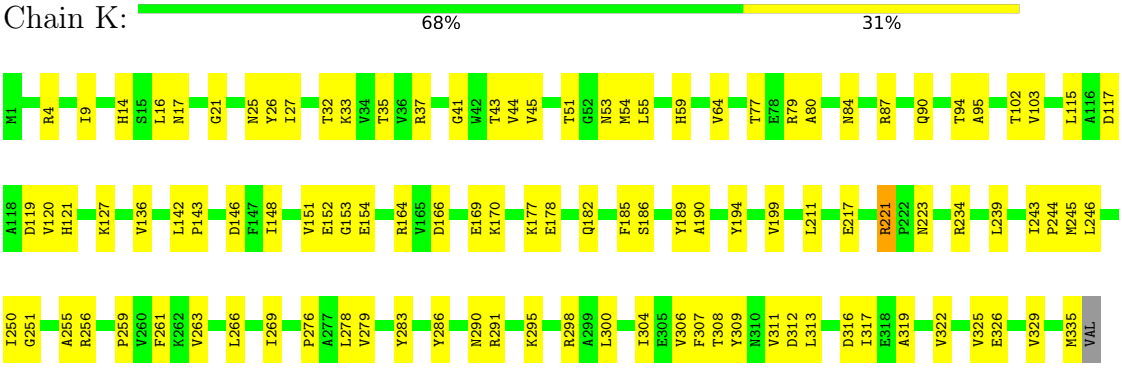


• Molecule 3: DNA (5'-D(P*TP*AP*CP*AP*AP*GP*GP*GP*A)-3')

Chain D:

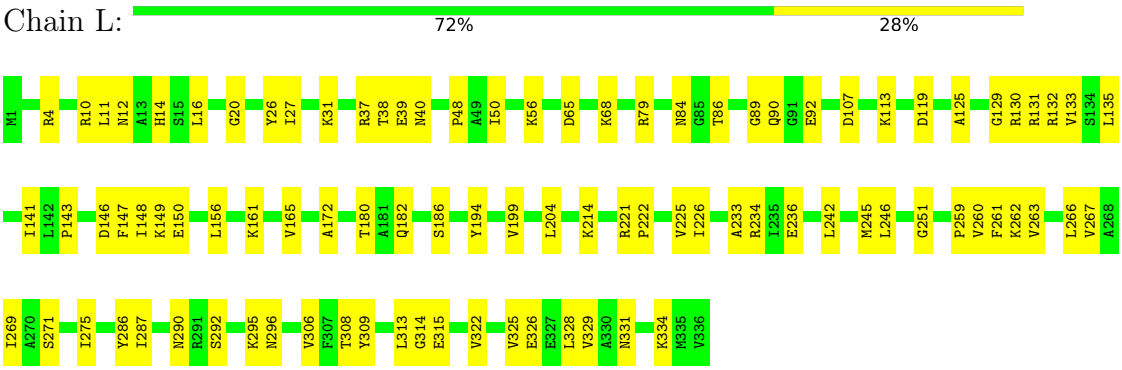
• Molecule 4: Cas7a

Chain K:



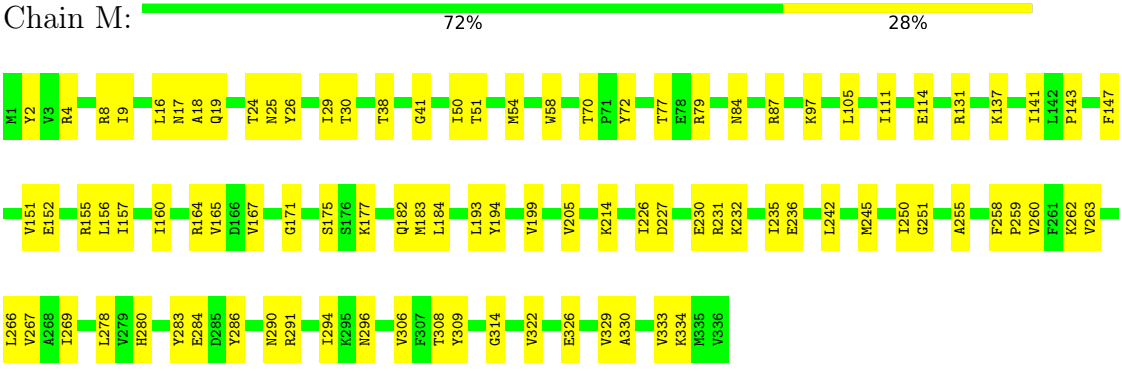
• Molecule 4: Cas7a

Chain L:



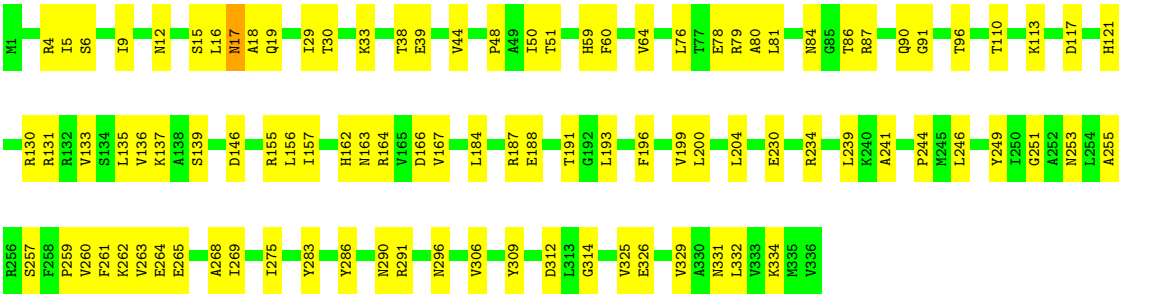
• Molecule 4: Cas7a

Chain M:



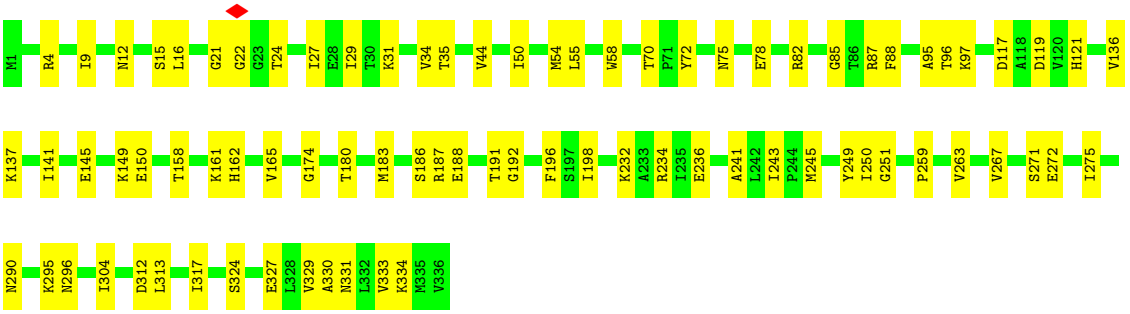
• Molecule 4: Cas7a

Chain N:



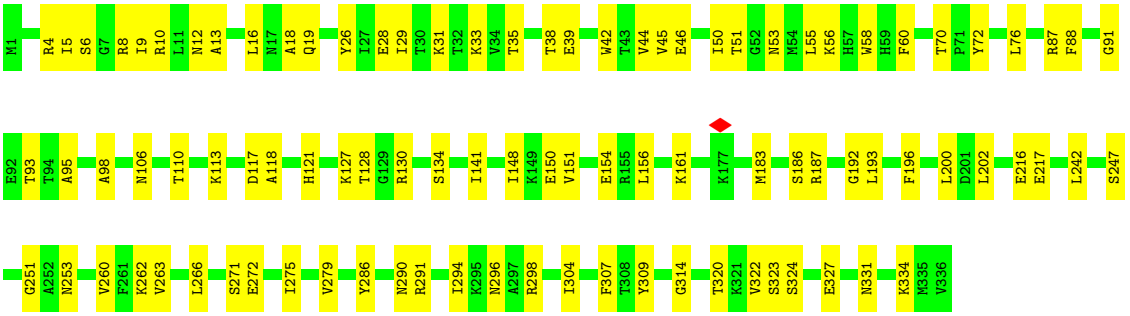
- Molecule 4: Cas7a

Chain O:



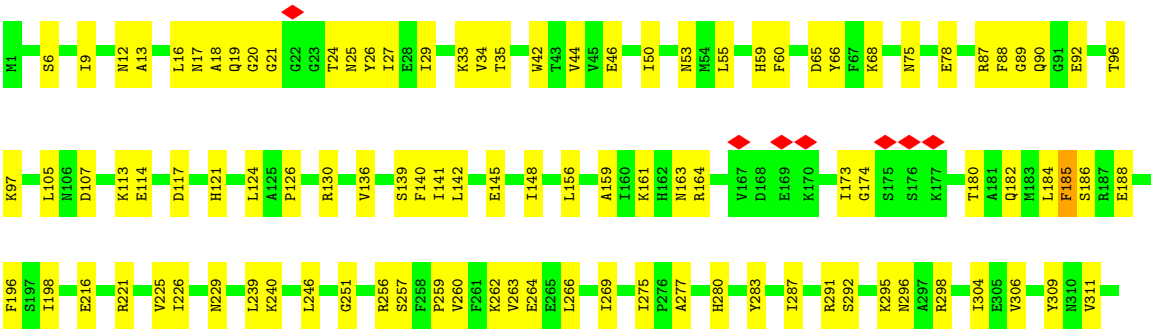
- Molecule 4: Cas7a

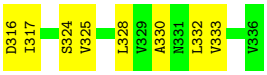
Chain P:



- Molecule 4: Cas7a

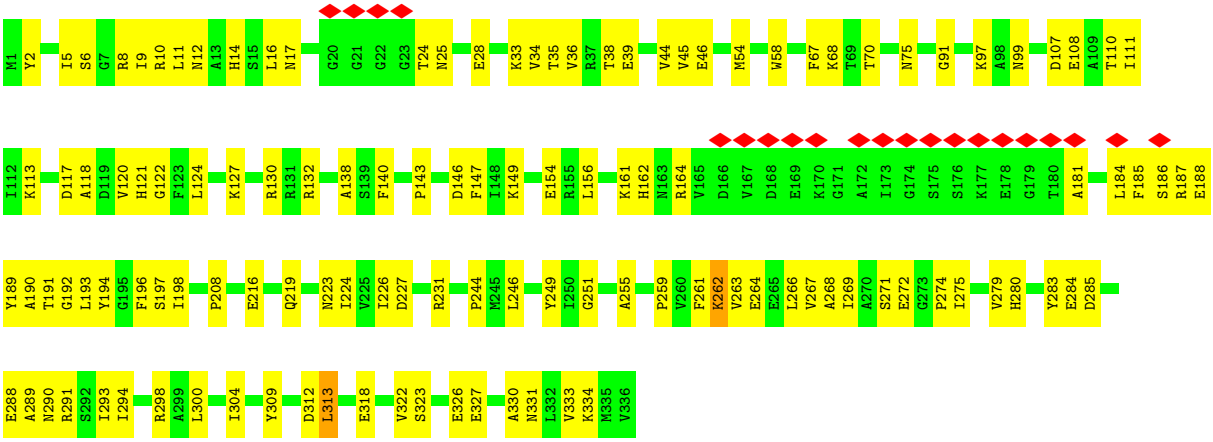
Chain R:





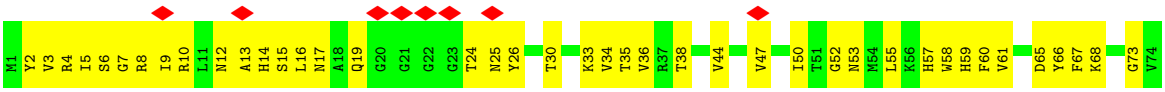
• Molecule 4: Cas7a

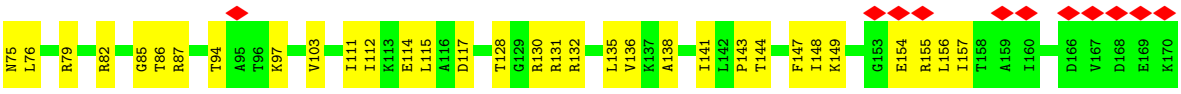
Chain T:

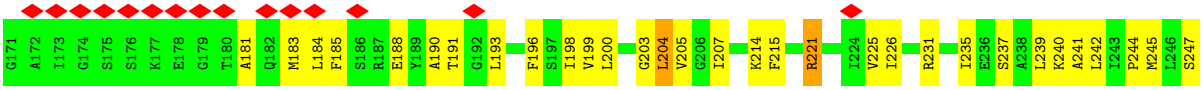


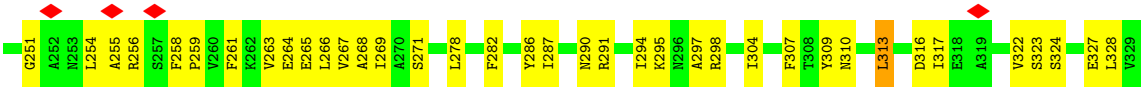
• Molecule 4: Cas7a

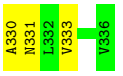
Chain V:





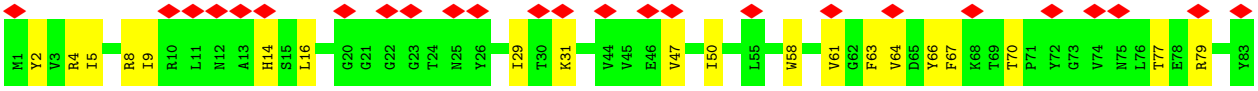


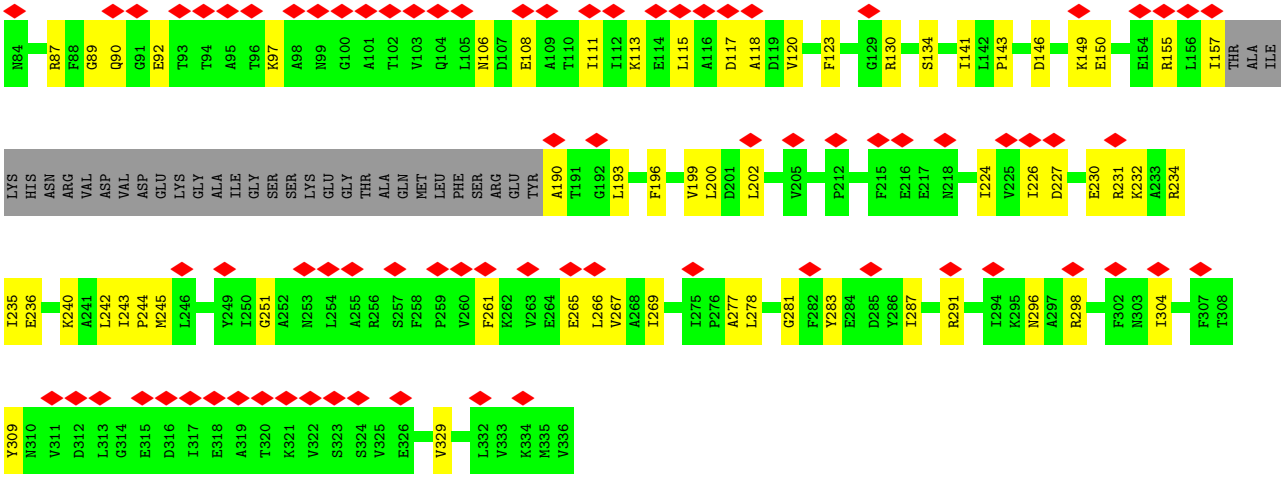




• Molecule 4: Cas7a

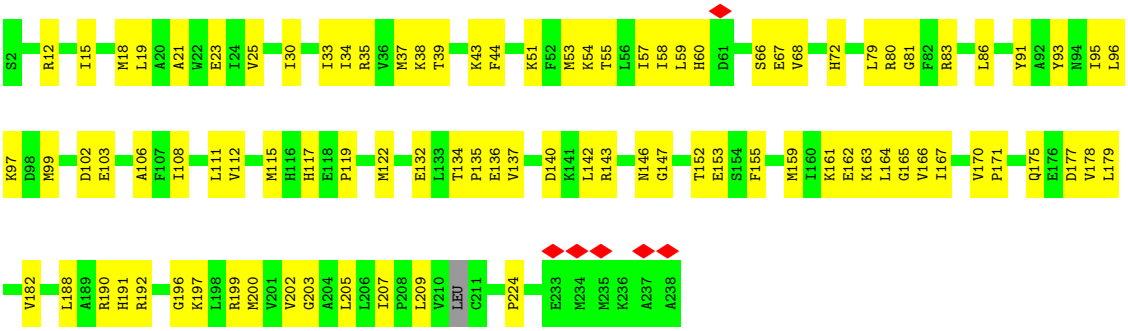
Chain W:





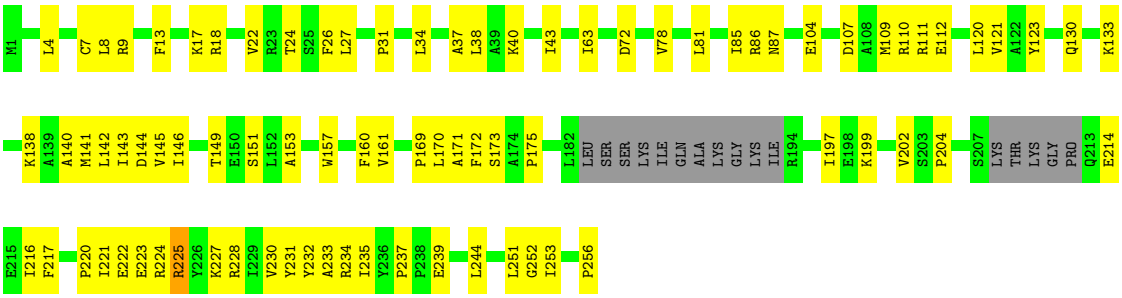
• Molecule 5: CRISPR-associated endonuclease Cas3-HD

Chain Q:



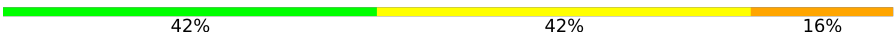
• Molecule 6: Type I-A CRISPR-associated protein Cas5

Chain S:



• Molecule 7: crRNA (57-MER)

Chain U:



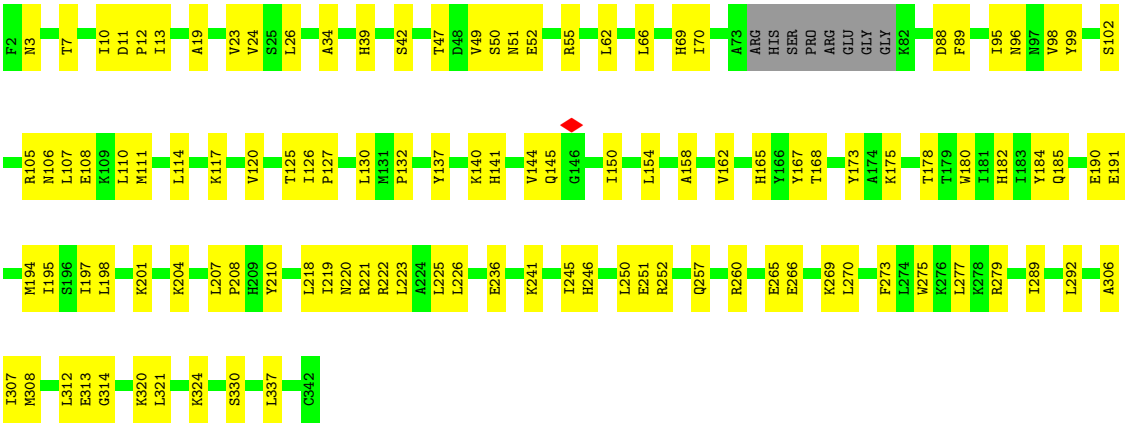
• Molecule 8: DNA (5'-D(P*TP*CP*CP*C)-3')

Chain X:

There are no outlier residues recorded for this chain.

• Molecule 9: Cas8

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49699	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.572	Depositor
Minimum map value	-0.852	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	426.4, 426.4, 426.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3325, 1.3325, 1.3325	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/4376	0.54	3/5945 (0.1%)
2	C	0.27	0/876	0.58	0/1188
2	E	0.25	0/876	0.50	0/1188
2	F	0.25	0/876	0.51	0/1188
2	G	0.28	0/880	0.57	0/1193
2	H	0.26	0/876	0.53	0/1188
2	I	0.25	0/876	0.52	0/1188
2	J	0.27	0/876	0.56	0/1188
3	D	0.42	0/213	0.74	0/327
4	K	0.25	0/2645	0.52	0/3583
4	L	0.25	0/2651	0.51	0/3592
4	M	0.26	0/2644	0.52	0/3584
4	N	0.25	0/2645	0.51	0/3585
4	O	0.25	0/2645	0.51	0/3585
4	P	0.25	0/2645	0.52	0/3585
4	R	0.25	0/2645	0.52	0/3585
4	T	0.26	0/2645	0.55	1/3585 (0.0%)
4	V	0.26	0/2645	0.58	2/3585 (0.1%)
4	W	0.25	0/2394	0.52	0/3248
5	Q	0.26	0/1853	0.58	1/2500 (0.0%)
6	S	0.26	0/1977	0.53	0/2673
7	U	0.18	0/1358	0.76	0/2117
8	X	0.31	0/84	0.68	0/126
9	Y	0.26	0/2723	0.52	0/3684
All	All	0.25	0/44924	0.54	7/61210 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	PRO	N-CA-CB	6.58	111.19	103.30
1	A	595	PRO	N-CA-CB	6.07	110.59	103.30
4	T	313	LEU	CA-CB-CG	5.89	128.85	115.30
4	V	313	LEU	CA-CB-CG	5.83	128.71	115.30
5	Q	224	PRO	N-CA-CB	5.78	110.24	103.30
1	A	521	PRO	N-CA-CB	5.59	110.00	103.30
4	V	204	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4304	0	4175	106	0
2	C	856	0	860	35	0
2	E	856	0	860	25	0
2	F	856	0	860	26	0
2	G	860	0	863	19	0
2	H	856	0	860	29	0
2	I	856	0	860	24	0
2	J	856	0	860	39	0
3	D	189	0	101	5	0
4	K	2597	0	2628	76	0
4	L	2603	0	2635	64	0
4	M	2596	0	2621	69	0
4	N	2597	0	2624	76	0
4	O	2597	0	2624	62	0
4	P	2597	0	2624	70	0
4	R	2597	0	2624	83	0
4	T	2597	0	2624	88	0
4	V	2597	0	2624	101	0
4	W	2350	0	2380	65	0
5	Q	1822	0	1834	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	1936	0	2018	70	0
7	U	1215	0	611	32	0
8	X	77	0	46	0	0
9	Y	2662	0	2668	97	0
10	Q	2	0	0	0	0
All	All	43931	0	43484	1179	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 13.

All (1179) 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)
4:M:164:ARG:O	4:M:182:GLN:HA	1.56	1.01
4:V:269:ILE:HB	4:V:304:ILE:HD11	1.50	0.94
5:Q:115:MET:HG3	5:Q:119:PRO:HB3	1.51	0.91
2:J:34:ALA:O	2:J:91:ARG:NH2	2.08	0.86
4:V:4:ARG:HB3	4:V:278:LEU:HD22	1.57	0.84
4:T:262:LYS:NZ	4:T:264:GLU:OE2	2.11	0.83
4:V:17:ASN:ND2	4:V:30:THR:OG1	2.12	0.82
1:A:426:ARG:HB3	5:Q:190:ARG:HH11	1.43	0.82
6:S:228:ARG:NH2	9:Y:265:GLU:OE1	2.12	0.82
2:C:10:ARG:HH21	2:C:100:TRP:HB3	1.45	0.81
2:J:34:ALA:HB1	2:J:39:GLU:HG3	1.63	0.80
4:V:58:TRP:HA	4:V:61:VAL:HG12	1.63	0.80
1:A:66:VAL:HG11	1:A:161:LEU:HG	1.64	0.79
1:A:292:ILE:HD12	1:A:319:VAL:HB	1.65	0.79
5:Q:79:LEU:HD12	5:Q:81:GLY:H	1.46	0.79
9:Y:95:ILE:HD12	9:Y:250:LEU:HB3	1.64	0.79
4:T:10:ARG:HB2	4:T:262:LYS:HE3	1.65	0.79
1:A:435:LYS:HE2	9:Y:210:TYR:HA	1.63	0.78
4:V:97:LYS:NZ	4:V:114:GLU:O	2.17	0.78
1:A:449:PRO:HB2	1:A:453:PRO:HD3	1.68	0.76
1:A:20:GLN:HE22	1:A:225:ASN:HD22	1.36	0.74
4:K:300:LEU:HD21	6:S:138:LYS:HG2	1.69	0.74
3:D:48:DG:H1'	9:Y:257:GLN:HE21	1.52	0.73
4:V:294:ILE:HD11	4:V:313:LEU:HD21	1.70	0.73
6:S:78:VAL:HG12	6:S:121:VAL:HG12	1.69	0.73
4:R:78:GLU:HG2	4:R:96:THR:HB	1.71	0.73
2:C:88:LYS:NZ	2:J:38:GLU:OE2	2.20	0.73
1:A:604:LYS:HG3	1:A:605:TYR:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:4:ARG:HG3	4:N:199:VAL:HG23	1.70	0.72
4:V:66:TYR:HB3	4:V:240:LYS:HE3	1.72	0.72
4:N:331:ASN:HA	4:N:334:LYS:HD3	1.72	0.72
7:U:3:U:N3	9:Y:140:LYS:O	2.16	0.72
4:K:79:ARG:HB3	4:K:84:ASN:HB3	1.72	0.71
4:V:324:SER:OG	4:W:296:ASN:ND2	2.23	0.71
4:L:172:ALA:HB2	4:N:130:ARG:HE	1.54	0.71
5:Q:39:THR:HG22	5:Q:197:LYS:HE3	1.72	0.71
6:S:4:LEU:HD11	6:S:140:ALA:HB2	1.71	0.70
4:N:79:ARG:HD3	4:N:86:THR:HB	1.73	0.70
4:W:77:THR:HG22	4:W:79:ARG:H	1.57	0.70
4:T:271:SER:HB2	4:T:304:ILE:HG22	1.74	0.70
4:K:151:VAL:O	4:K:153:GLY:N	2.24	0.70
5:Q:96:LEU:HD22	5:Q:106:ALA:HB2	1.74	0.69
4:T:164:ARG:HB3	7:U:55:G:H1’	1.74	0.69
4:W:77:THR:OG1	4:W:97:LYS:NZ	2.25	0.69
9:Y:62:LEU:HD11	9:Y:107:LEU:HD13	1.73	0.69
4:R:156:LEU:HA	4:T:33:LYS:HD2	1.74	0.69
2:H:17:ASP:OD2	2:H:107:ASN:ND2	2.26	0.68
4:O:12:ASN:ND2	4:O:191:THR:OG1	2.24	0.68
5:Q:37:MET:HE3	5:Q:44:PHE:H	1.58	0.68
4:N:16:LEU:HD22	4:N:251:GLY:HA3	1.75	0.68
2:C:54:LEU:HB3	2:C:66:PRO:HG3	1.75	0.68
4:P:87:ARG:HH12	4:P:121:HIS:HB2	1.58	0.68
4:L:221:ARG:HE	4:L:222:PRO:HD2	1.59	0.67
4:N:12:ASN:HA	4:N:191:THR:HG22	1.76	0.67
4:R:19:GLN:HB2	7:U:45:G:H21	1.57	0.67
6:S:225:ARG:NH2	9:Y:266:GLU:OE2	2.27	0.67
4:T:216:GLU:HB2	4:T:219:GLN:HE21	1.59	0.67
5:Q:58:ILE:HG13	5:Q:163:LYS:HD3	1.77	0.66
5:Q:102:ASP:OD1	5:Q:103:GLU:N	2.28	0.66
4:R:13:ALA:HB1	4:T:140:PHE:HD2	1.59	0.66
4:T:331:ASN:HA	4:T:334:LYS:HZ1	1.61	0.66
4:T:331:ASN:HA	4:T:334:LYS:NZ	2.10	0.66
2:H:53:LYS:NZ	4:O:24:THR:OG1	2.26	0.66
4:K:143:PRO:HA	4:K:194:TYR:HA	1.78	0.66
4:N:239:LEU:HD21	4:N:332:LEU:HB3	1.78	0.66
4:K:95:ALA:HB3	4:K:103:VAL:HB	1.79	0.65
1:A:118:LEU:HG	1:A:119:GLU:H	1.60	0.65
4:R:262:LYS:NZ	4:R:264:GLU:OE1	2.29	0.65
2:I:55:LYS:NZ	2:I:66:PRO:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:269:ILE:HG22	4:R:306:VAL:HG12	1.77	0.65
6:S:27:LEU:HG	6:S:86:ARG:HH21	1.61	0.65
2:J:42:GLU:HA	2:J:45:TYR:HD2	1.62	0.65
4:K:16:LEU:HD22	4:K:251:GLY:HA3	1.77	0.65
3:D:43:DA:H2"	4:L:90:GLN:HB3	1.79	0.65
2:F:91:ARG:NH2	9:Y:313:GLU:OE2	2.29	0.65
4:M:131:ARG:HD2	7:U:17:U:H1'	1.79	0.65
4:T:9:ILE:HG22	4:T:263:VAL:HA	1.79	0.65
6:S:22:VAL:HB	6:S:110:ARG:NH1	2.12	0.64
9:Y:140:LYS:HG3	9:Y:141:HIS:H	1.62	0.64
4:R:50:ILE:HB	4:R:141:ILE:HB	1.79	0.64
4:V:50:ILE:HB	4:V:141:ILE:HB	1.79	0.64
4:W:269:ILE:HD11	4:W:304:ILE:HG23	1.78	0.64
4:M:79:ARG:HB3	4:M:84:ASN:HB3	1.79	0.64
4:O:21:GLY:HA3	4:O:27:ILE:HG22	1.80	0.64
4:P:55:LEU:HD11	4:P:141:ILE:HD11	1.79	0.64
9:Y:110:LEU:HD21	9:Y:154:LEU:HB3	1.79	0.64
4:T:288:GLU:HA	4:T:291:ARG:HG2	1.80	0.64
2:J:55:LYS:HD3	2:J:68:ILE:HD11	1.79	0.63
4:N:135:LEU:HD11	4:N:204:LEU:HB2	1.80	0.63
2:F:37:GLN:HE22	2:F:81:VAL:HG13	1.64	0.63
4:P:216:GLU:HG2	4:P:217:GLU:H	1.63	0.63
4:P:271:SER:OG	4:P:272:GLU:N	2.29	0.63
9:Y:23:VAL:HG21	9:Y:197:ILE:HG21	1.81	0.63
4:P:324:SER:OG	4:R:296:ASN:ND2	2.31	0.63
9:Y:99:TYR:HA	9:Y:102:SER:HB3	1.81	0.63
7:U:9:U:O4	9:Y:260:ARG:NH2	2.32	0.63
4:P:51:THR:HG22	4:P:53:ASN:H	1.63	0.62
1:A:262:ARG:H	1:A:317:THR:HA	1.64	0.62
2:J:19:THR:O	2:J:61:LYS:NZ	2.28	0.62
5:Q:54:LYS:HD3	5:Q:163:LYS:HB2	1.81	0.62
2:F:7:ASN:OD1	2:F:8:ILE:N	2.31	0.62
2:C:52:PRO:HG2	2:C:53:LYS:NZ	2.14	0.62
4:W:8:ARG:NH1	4:W:281:GLY:O	2.32	0.62
5:Q:58:ILE:HG22	5:Q:59:LEU:HD22	1.81	0.62
4:V:287:ILE:O	4:V:291:ARG:HG2	2.00	0.62
9:Y:140:LYS:HB3	9:Y:145:GLN:NE2	2.13	0.62
4:T:5:ILE:HD11	4:T:266:LEU:HD13	1.82	0.62
1:A:257:LYS:NZ	1:A:328:ASN:O	2.32	0.62
4:N:163:ASN:HB3	4:N:184:LEU:HG	1.80	0.62
6:S:18:ARG:HH12	9:Y:150:ILE:HD13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:29:ILE:HG13	4:N:188:GLU:HB2	1.81	0.62
4:V:4:ARG:O	4:V:268:ALA:HA	1.99	0.62
4:R:246:LEU:HD12	4:R:263:VAL:HG22	1.81	0.61
4:V:10:ARG:HE	4:V:193:LEU:HD11	1.64	0.61
1:A:142:ALA:HB3	1:A:153:PRO:HG2	1.80	0.61
1:A:292:ILE:HD11	1:A:317:THR:H	1.66	0.61
4:L:214:LYS:NZ	4:L:222:PRO:O	2.34	0.61
4:R:59:HIS:HE1	4:R:136:VAL:HG21	1.66	0.61
4:P:58:TRP:NE1	4:P:251:GLY:O	2.33	0.61
4:R:298:ARG:HE	4:R:304:ILE:HB	1.65	0.61
2:H:53:LYS:NZ	4:O:21:GLY:O	2.29	0.61
1:A:418:VAL:HG21	9:Y:207:LEU:HD23	1.81	0.61
4:K:14:HIS:HB3	4:K:259:PRO:HB3	1.82	0.61
4:P:35:THR:HG22	4:P:44:VAL:HG12	1.83	0.61
4:N:286:TYR:O	4:N:290:ASN:ND2	2.34	0.61
2:C:27:VAL:HG12	2:C:46:LYS:HE3	1.82	0.61
2:G:17:ASP:OD2	2:G:107:ASN:ND2	2.34	0.61
5:Q:86:LEU:HG	5:Q:182:VAL:HG21	1.83	0.61
1:A:22:ARG:HH21	1:A:41:VAL:HB	1.65	0.60
4:V:65:ASP:OD1	4:V:68:LYS:NZ	2.34	0.60
1:A:604:LYS:HG3	1:A:605:TYR:N	2.15	0.60
4:M:165:VAL:O	4:N:86:THR:OG1	2.19	0.60
4:R:65:ASP:OD1	4:R:68:LYS:NZ	2.28	0.60
4:K:21:GLY:HA2	4:K:27:ILE:HG23	1.82	0.60
4:P:31:LYS:HB3	4:P:46:GLU:OE2	2.02	0.60
2:C:13:SER:HB3	2:C:101:ALA:HA	1.83	0.60
4:P:156:LEU:HA	4:R:33:LYS:HD2	1.82	0.60
5:Q:12:ARG:HE	5:Q:12:ARG:HA	1.65	0.60
4:L:133:VAL:HG22	7:U:11:G:H4'	1.83	0.60
4:R:161:LYS:HD2	7:U:51:G:C2	2.37	0.60
4:V:264:GLU:O	4:V:310:ASN:ND2	2.34	0.60
4:M:9:ILE:HG22	4:M:263:VAL:HA	1.83	0.60
4:O:78:GLU:HG2	4:O:96:THR:HB	1.84	0.60
9:Y:7:THR:HG21	9:Y:19:ALA:HB2	1.84	0.60
9:Y:273:PHE:HD2	9:Y:307:ILE:HG23	1.66	0.60
4:P:70:THR:HG22	4:P:72:TYR:H	1.65	0.60
4:P:327:GLU:HB2	4:R:296:ASN:HD22	1.67	0.59
4:T:14:HIS:HB3	4:T:259:PRO:HB3	1.84	0.59
4:P:127:LYS:HG3	4:P:128:THR:HG23	1.83	0.59
4:V:9:ILE:HG22	4:V:263:VAL:HA	1.84	0.59
4:W:266:LEU:HG	4:W:309:TYR:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:78:GLU:O	2:G:81:VAL:HG12	2.03	0.59
4:V:154:GLU:O	4:V:156:LEU:HD12	2.03	0.59
4:O:29:ILE:O	4:O:31:LYS:NZ	2.35	0.59
4:W:89:GLY:HA3	4:W:92:GLU:HG3	1.85	0.59
5:Q:153:GLU:HB2	5:Q:170:VAL:HG11	1.83	0.59
1:A:76:ARG:HG3	1:A:319:VAL:HG13	1.85	0.59
2:G:67:ARG:NH1	2:G:68:ILE:O	2.36	0.59
4:R:9:ILE:HG22	4:R:263:VAL:HA	1.85	0.59
4:T:107:ASP:H	4:T:130:ARG:HH12	1.50	0.59
4:V:67:PHE:HB2	4:V:237:SER:HB2	1.85	0.59
4:L:143:PRO:HG2	4:L:148:ILE:HD11	1.83	0.59
4:M:70:THR:HG22	4:M:72:TYR:H	1.67	0.59
4:N:19:GLN:NE2	4:N:30:THR:HA	2.18	0.59
4:N:164:ARG:HH12	4:N:166:ASP:HB2	1.67	0.59
4:T:25:ASN:HB2	4:T:185:PHE:H	1.67	0.59
1:A:504:LYS:HG3	1:A:505:GLU:HG3	1.84	0.59
2:H:89:ASP:OD1	2:H:92:LYS:NZ	2.35	0.59
4:T:162:HIS:CD2	4:V:53:ASN:HD22	2.21	0.59
1:A:21:LEU:HG	1:A:49:GLU:HG3	1.85	0.58
4:R:266:LEU:HG	4:R:309:TYR:HB3	1.85	0.58
6:S:199:LYS:HD3	6:S:216:ILE:HD13	1.85	0.58
4:L:119:ASP:OD1	4:L:132:ARG:NH2	2.36	0.58
4:V:33:LYS:HE3	4:V:44:VAL:HG11	1.84	0.58
4:V:214:LYS:HB2	4:V:221:ARG:NH1	2.18	0.58
4:W:298:ARG:HG2	4:W:304:ILE:HB	1.84	0.58
2:G:35:ARG:N	2:G:39:GLU:OE2	2.34	0.58
5:Q:93:TYR:O	5:Q:97:LYS:HG2	2.03	0.58
4:V:5:ILE:HD13	4:V:268:ALA:HB2	1.84	0.58
4:M:326:GLU:HA	4:M:329:VAL:HG22	1.85	0.58
4:N:79:ARG:NH1	4:N:87:ARG:O	2.35	0.58
4:P:9:ILE:HG22	4:P:263:VAL:HA	1.84	0.58
4:P:50:ILE:HB	4:P:141:ILE:HB	1.85	0.58
4:K:32:THR:HG23	6:S:87:ASN:HD22	1.69	0.58
4:K:326:GLU:OE2	4:L:296:ASN:HB2	2.03	0.58
2:J:55:LYS:HA	2:J:55:LYS:HE3	1.86	0.58
4:M:8:ARG:HH22	4:M:284:GLU:HA	1.68	0.58
4:M:286:TYR:O	4:M:290:ASN:ND2	2.37	0.58
4:R:163:ASN:ND2	7:U:51:G:O4'	2.35	0.58
6:S:228:ARG:NH2	9:Y:308:MET:SD	2.76	0.58
9:Y:55:ARG:HH12	9:Y:117:LYS:HD3	1.69	0.58
2:I:68:ILE:HB	2:J:104:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:162:HIS:HB2	7:U:33:G:OP2	2.04	0.58
4:T:132:ARG:HH22	4:T:208:PRO:HA	1.69	0.58
2:I:11:TYR:HA	2:I:14:TYR:HD2	1.69	0.58
4:K:279:VAL:HG11	4:K:286:TYR:HB2	1.85	0.58
4:M:25:ASN:ND2	4:M:184:LEU:O	2.36	0.58
5:Q:152:THR:HA	5:Q:155:PHE:CZ	2.38	0.58
4:P:16:LEU:HD22	4:P:251:GLY:HA3	1.85	0.58
4:T:117:ASP:OD1	4:T:118:ALA:N	2.37	0.58
2:J:35:ARG:HD2	2:J:91:ARG:HD2	1.85	0.57
6:S:85:ILE:HG22	6:S:231:TYR:HB3	1.86	0.57
4:T:122:GLY:HA2	4:T:132:ARG:HG2	1.86	0.57
1:A:263:ASN:ND2	1:A:336:ILE:O	2.34	0.57
4:V:266:LEU:HG	4:V:309:TYR:HB3	1.86	0.57
2:I:37:GLN:HB2	2:I:81:VAL:HG22	1.86	0.57
4:T:99:ASN:HB3	4:V:215:PHE:HD2	1.69	0.57
4:M:262:LYS:HB2	4:N:283:TYR:CE2	2.40	0.57
1:A:140:LEU:HA	1:A:154:ALA:HB2	1.87	0.57
4:K:256:ARG:NH1	7:U:12:U:OP2	2.35	0.57
4:M:330:ALA:O	4:M:334:LYS:HG2	2.03	0.57
1:A:185:VAL:HG23	1:A:195:LEU:HD23	1.86	0.57
2:C:38:GLU:HG3	2:E:92:LYS:HB3	1.85	0.57
4:T:312:ASP:OD1	4:T:313:LEU:N	2.35	0.57
1:A:446:SER:O	1:A:482:ARG:NH1	2.36	0.57
2:C:57:LYS:HA	2:C:57:LYS:HE3	1.85	0.57
4:M:266:LEU:HG	4:M:309:TYR:HB3	1.87	0.57
4:K:266:LEU:HG	4:K:309:TYR:HB3	1.85	0.57
4:L:180:THR:HG22	4:L:182:GLN:H	1.69	0.57
1:A:22:ARG:NH2	1:A:40:GLU:O	2.38	0.57
4:O:70:THR:HG22	4:O:72:TYR:H	1.70	0.57
1:A:121:THR:HA	1:A:146:VAL:HG11	1.86	0.57
2:I:100:TRP:HD1	2:I:105:TRP:HE1	1.53	0.57
4:P:60:PHE:HE1	4:P:117:ASP:HB2	1.70	0.57
1:A:137:LEU:HD21	1:A:438:LYS:HG2	1.87	0.56
2:H:10:ARG:HH21	2:H:107:ASN:HA	1.70	0.56
4:O:271:SER:HB2	4:O:304:ILE:HD13	1.87	0.56
4:P:200:LEU:HB3	4:P:202:LEU:HD23	1.86	0.56
6:S:13:PHE:HA	6:S:151:SER:HB2	1.85	0.56
4:T:14:HIS:HB2	4:T:16:LEU:HG	1.87	0.56
4:K:14:HIS:O	4:K:189:TYR:HA	2.06	0.56
1:A:292:ILE:HD13	1:A:320:VAL:HB	1.87	0.56
5:Q:97:LYS:NZ	5:Q:103:GLU:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:16:LEU:HD11	4:V:259:PRO:HG3	1.87	0.56
4:W:8:ARG:HB3	4:W:193:LEU:HD11	1.87	0.56
9:Y:184:TYR:HB3	9:Y:245:ILE:HD11	1.86	0.56
1:A:402:ARG:HE	1:A:406:ILE:HD12	1.69	0.56
2:H:36:THR:HG23	2:H:39:GLU:H	1.71	0.56
5:Q:80:ARG:HD2	5:Q:80:ARG:O	2.06	0.56
5:Q:161:LYS:HA	5:Q:165:GLY:HA2	1.86	0.56
4:V:256:ARG:HH22	4:W:87:ARG:HH12	1.54	0.56
9:Y:111:MET:O	9:Y:114:LEU:N	2.35	0.56
9:Y:178:THR:OG1	9:Y:251:GLU:OE2	2.21	0.56
2:H:4:TRP:HE1	2:H:76:ALA:HB3	1.70	0.56
4:T:5:ILE:HD13	4:T:268:ALA:HB2	1.86	0.56
4:V:147:PHE:HE2	4:V:193:LEU:HD22	1.71	0.56
2:E:92:LYS:HA	2:E:95:VAL:HG22	1.87	0.56
4:T:156:LEU:HA	4:V:33:LYS:HE2	1.87	0.56
4:M:87:ARG:NH1	7:U:19:C:OP1	2.38	0.56
4:N:12:ASN:HB2	4:N:260:VAL:HB	1.87	0.56
4:O:161:LYS:HG3	7:U:39:A:H2	1.71	0.56
4:O:295:LYS:HB3	4:O:317:ILE:HD11	1.88	0.56
4:P:10:ARG:NH1	4:R:35:THR:OG1	2.29	0.56
6:S:171:ALA:HB3	6:S:251:LEU:HB3	1.88	0.56
4:T:143:PRO:HA	4:T:194:TYR:HA	1.87	0.56
1:A:149:ARG:NH2	5:Q:209:LEU:O	2.30	0.56
1:A:170:TYR:HA	1:A:176:TYR:HB2	1.88	0.56
1:A:201:THR:OG1	1:A:340:ASP:OD1	2.23	0.56
5:Q:142:LEU:HD21	5:Q:179:LEU:HB2	1.87	0.56
4:R:60:PHE:HE1	4:R:117:ASP:HB2	1.69	0.56
4:T:164:ARG:NH1	4:T:181:ALA:O	2.38	0.56
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.88	0.56
4:V:16:LEU:HG	4:V:251:GLY:HA3	1.88	0.56
9:Y:321:LEU:HD22	9:Y:324:LYS:HZ1	1.71	0.56
2:E:91:ARG:HA	2:E:91:ARG:HH11	1.70	0.55
4:L:65:ASP:HA	4:L:68:LYS:NZ	2.21	0.55
4:O:150:GLU:OE2	4:P:42:TRP:N	2.39	0.55
4:O:312:ASP:OD1	4:O:313:LEU:N	2.38	0.55
2:H:71:PRO:O	2:H:75:GLU:HG2	2.06	0.55
4:M:164:ARG:HE	4:M:183:MET:HB2	1.72	0.55
5:Q:95:ILE:O	5:Q:99:MET:HG2	2.05	0.55
4:R:97:LYS:HD2	4:R:114:GLU:HG3	1.88	0.55
1:A:177:MET:HG3	1:A:412:LYS:HD3	1.88	0.55
4:K:291:ARG:HG3	4:K:313:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:9:ILE:HD12	4:N:261:PHE:HE1	1.70	0.55
4:P:38:THR:O	4:P:39:GLU:HG3	2.07	0.55
1:A:429:GLU:OE2	1:A:431:LYS:HG2	2.06	0.55
4:L:314:GLY:O	4:L:315:GLU:HG3	2.06	0.55
4:N:326:GLU:HA	4:N:329:VAL:HG22	1.89	0.55
4:P:110:THR:HA	4:P:113:LYS:HG2	1.89	0.55
5:Q:122:MET:SD	5:Q:190:ARG:NE	2.76	0.55
4:R:66:TYR:HB3	4:R:240:LYS:HE3	1.88	0.55
4:W:123:PHE:HE1	4:W:130:ARG:HB3	1.70	0.55
1:A:199:SER:OG	1:A:207:ARG:NH2	2.34	0.55
4:M:267:VAL:HG13	4:M:278:LEU:HD21	1.88	0.55
5:Q:177:ASP:OD1	5:Q:178:VAL:N	2.38	0.55
6:S:4:LEU:HB3	6:S:123:TYR:HB2	1.88	0.55
4:V:295:LYS:HE2	4:V:317:ILE:HD11	1.87	0.55
9:Y:24:VAL:HB	9:Y:167:TYR:CE2	2.42	0.55
4:R:216:GLU:OE2	4:R:221:ARG:NE	2.39	0.55
9:Y:306:ALA:HB2	9:Y:314:GLY:HA3	1.88	0.55
4:O:9:ILE:HG22	4:O:263:VAL:HA	1.88	0.55
6:S:221:ILE:HB	6:S:232:TYR:HB3	1.89	0.55
4:T:187:ARG:HD3	4:T:189:TYR:HE1	1.71	0.55
4:V:35:THR:HG22	4:V:44:VAL:HG22	1.89	0.55
4:N:64:VAL:HG23	4:N:76:LEU:HD21	1.89	0.55
5:Q:68:VAL:O	5:Q:72:HIS:ND1	2.37	0.55
4:V:247:SER:HB2	4:W:277:ALA:H	1.71	0.55
1:A:201:THR:HG21	1:A:343:ILE:HD13	1.90	0.54
4:L:38:THR:H	4:L:149:LYS:HD3	1.71	0.54
4:L:326:GLU:OE2	4:M:296:ASN:HB2	2.07	0.54
4:R:139:SER:H	4:R:198:ILE:HG22	1.72	0.54
6:S:27:LEU:HG	6:S:86:ARG:NH2	2.21	0.54
4:V:24:THR:HG23	4:V:26:TYR:H	1.71	0.54
1:A:77:SER:OG	1:A:322:ALA:O	2.21	0.54
2:E:9:GLY:HA3	2:E:100:TRP:CD1	2.41	0.54
4:K:312:ASP:OD1	4:K:313:LEU:N	2.40	0.54
4:L:260:VAL:HG13	4:M:280:HIS:HB3	1.89	0.54
4:O:174:GLY:HA3	4:O:180:THR:HG21	1.89	0.54
4:T:16:LEU:HD22	4:T:251:GLY:HA3	1.88	0.54
4:K:306:VAL:HG23	4:K:319:ALA:HA	1.90	0.54
4:N:78:GLU:OE2	4:N:96:THR:HB	2.08	0.54
5:Q:188:LEU:HD12	5:Q:192:ARG:HE	1.71	0.54
4:T:271:SER:OG	4:T:272:GLU:N	2.39	0.54
9:Y:273:PHE:O	9:Y:277:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:275:TRP:O	9:Y:279:ARG:NH1	2.41	0.54
1:A:211:ALA:HB1	1:A:214:THR:HB	1.88	0.54
1:A:257:LYS:HE3	1:A:311:ALA:HA	1.89	0.54
6:S:130:GLN:HA	6:S:133:LYS:HB3	1.88	0.54
4:V:65:ASP:HA	4:V:68:LYS:NZ	2.22	0.54
9:Y:39:HIS:HB2	9:Y:42:SER:HB3	1.89	0.54
4:T:54:MET:HB3	4:T:58:TRP:HZ3	1.72	0.54
2:G:4:TRP:HH2	2:G:80:LYS:HE2	1.72	0.54
4:O:35:THR:HG22	4:O:44:VAL:HG12	1.89	0.54
6:S:145:VAL:HG21	6:S:149:THR:HA	1.88	0.54
9:Y:34:ALA:HB2	9:Y:47:THR:HG23	1.89	0.54
4:L:26:TYR:HD1	4:L:186:SER:HB2	1.72	0.54
4:R:6:SER:HA	4:R:196:PHE:O	2.07	0.54
4:O:158:THR:HG22	4:P:33:LYS:HG2	1.90	0.54
4:T:161:LYS:HA	4:T:186:SER:HA	1.89	0.54
4:T:285:ASP:HB2	4:T:288:GLU:OE2	2.08	0.54
4:V:313:LEU:HD23	4:V:313:LEU:O	2.08	0.54
9:Y:190:GLU:O	9:Y:191:GLU:HG2	2.08	0.54
1:A:132:THR:O	1:A:136:PHE:N	2.36	0.54
4:N:136:VAL:HG22	4:N:200:LEU:HB2	1.90	0.54
3:D:49:DG:H2'	3:D:50:DA:C8	2.43	0.53
2:I:5:ILE:HG23	2:I:8:ILE:HD11	1.90	0.53
4:K:26:TYR:HA	4:K:186:SER:HB2	1.90	0.53
4:L:322:VAL:HG11	4:L:328:LEU:HD12	1.88	0.53
4:P:271:SER:HB2	4:P:304:ILE:HD13	1.89	0.53
4:V:47:VAL:HG21	4:V:143:PRO:HG3	1.90	0.53
9:Y:221:ARG:HH22	9:Y:222:ARG:NH2	2.05	0.53
1:A:458:THR:OG1	1:A:459:THR:N	2.39	0.53
2:J:34:ALA:HB3	2:J:40:LEU:HD23	1.90	0.53
4:K:146:ASP:N	4:K:146:ASP:OD1	2.40	0.53
4:P:161:LYS:HG3	4:P:186:SER:HB3	1.90	0.53
5:Q:15:ILE:HA	5:Q:18:MET:HG2	1.90	0.53
6:S:235:ILE:HG23	6:S:237:PRO:HD3	1.90	0.53
4:T:38:THR:O	4:T:39:GLU:HG3	2.08	0.53
4:L:31:LYS:HG3	4:L:48:PRO:HA	1.90	0.53
4:L:266:LEU:HD23	4:L:309:TYR:HB3	1.90	0.53
4:N:155:ARG:NH1	4:N:157:ILE:O	2.42	0.53
4:W:243:ILE:HD11	4:W:329:VAL:HG21	1.89	0.53
1:A:26:LYS:HE2	1:A:217:ILE:HB	1.90	0.53
4:K:279:VAL:HG12	4:K:290:ASN:HD21	1.73	0.53
4:O:75:ASN:HA	4:O:97:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:35:THR:HG23	6:S:85:ILE:HD13	1.91	0.53
4:M:4:ARG:HG3	4:M:199:VAL:HG22	1.91	0.53
4:N:18:ALA:HA	4:N:29:ILE:HA	1.91	0.53
5:Q:188:LEU:HD12	5:Q:192:ARG:NE	2.24	0.53
4:T:11:LEU:HB3	4:T:14:HIS:CD2	2.44	0.53
4:T:323:SER:N	4:T:327:GLU:OE2	2.39	0.53
4:V:6:SER:HA	4:V:196:PHE:O	2.08	0.53
4:L:267:VAL:HG12	4:L:308:THR:HG22	1.91	0.53
9:Y:173:TYR:HD2	9:Y:218:LEU:HD12	1.74	0.53
4:L:326:GLU:HA	4:L:329:VAL:HG12	1.91	0.53
4:N:230:GLU:OE2	4:N:234:ARG:NH2	2.42	0.53
4:V:271:SER:HB3	4:V:304:ILE:HD13	1.91	0.53
1:A:444:PRO:HD2	1:A:484:TYR:H	1.73	0.53
4:L:271:SER:HB3	4:L:275:ILE:HG13	1.90	0.53
4:P:5:ILE:HG22	4:P:196:PHE:HE2	1.74	0.53
5:Q:166:VAL:HG23	5:Q:167:ILE:H	1.73	0.53
2:F:10:ARG:HG2	2:F:105:TRP:CD2	2.44	0.52
4:L:79:ARG:HB3	4:L:84:ASN:HB3	1.91	0.52
4:M:167:VAL:HG13	4:M:171:GLY:HA2	1.91	0.52
4:T:289:ALA:O	4:T:293:ILE:HG12	2.09	0.52
2:G:42:GLU:HB3	2:G:46:LYS:NZ	2.24	0.52
4:K:4:ARG:HG2	4:K:199:VAL:HG22	1.91	0.52
4:L:16:LEU:HD22	4:L:251:GLY:HA3	1.90	0.52
4:L:119:ASP:OD2	4:L:234:ARG:NH1	2.41	0.52
4:M:242:LEU:HA	4:M:245:MET:HE2	1.91	0.52
4:O:54:MET:HE1	7:U:32:U:O3'	2.09	0.52
1:A:179:ARG:NH1	9:Y:70:ILE:O	2.42	0.52
4:T:246:LEU:HD13	4:T:263:VAL:HG11	1.92	0.52
7:U:57:G:N2	4:V:19:GLN:O	2.43	0.52
2:G:77:LEU:O	2:G:80:LYS:HG3	2.10	0.52
4:K:45:VAL:HG21	4:K:148:ILE:HG21	1.92	0.52
4:P:279:VAL:HG12	4:P:290:ASN:OD1	2.10	0.52
4:T:35:THR:HG22	4:T:44:VAL:HG12	1.91	0.52
4:T:224:ILE:HD12	4:T:231:ARG:HD2	1.92	0.52
4:W:267:VAL:HG13	4:W:278:LEU:HD21	1.91	0.52
4:O:161:LYS:HA	4:O:186:SER:HA	1.91	0.52
4:R:295:LYS:HB2	4:R:317:ILE:HD11	1.91	0.52
4:V:4:ARG:HD3	4:V:199:VAL:HG23	1.91	0.52
2:C:89:ASP:HA	2:C:92:LYS:NZ	2.25	0.52
4:L:125:ALA:O	4:L:129:GLY:N	2.43	0.52
4:T:36:VAL:HG13	4:T:38:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:190:GLU:HG2	9:Y:191:GLU:N	2.24	0.52
1:A:338:PRO:O	1:A:340:ASP:N	2.42	0.52
1:A:492:ILE:HG22	1:A:493:VAL:HG13	1.91	0.52
4:M:167:VAL:H	4:N:84:ASN:HD21	1.57	0.52
4:N:291:ARG:HD2	4:N:314:GLY:HA3	1.91	0.52
4:R:164:ARG:HG2	4:R:185:PHE:HE1	1.74	0.52
9:Y:10:ILE:HD11	9:Y:150:ILE:HD11	1.92	0.52
4:L:308:THR:HG21	4:L:313:LEU:HD22	1.92	0.52
4:P:286:TYR:O	4:P:290:ASN:ND2	2.42	0.52
6:S:146:ILE:O	6:S:151:SER:OG	2.28	0.52
4:W:202:LEU:H	4:W:202:LEU:HD23	1.75	0.52
4:W:230:GLU:O	4:W:234:ARG:HG2	2.10	0.52
9:Y:222:ARG:HD3	9:Y:225:LEU:HD21	1.92	0.52
4:K:278:LEU:HB3	4:K:290:ASN:ND2	2.24	0.52
6:S:31:PRO:HG2	6:S:202:VAL:HA	1.92	0.52
6:S:7:CYS:HB3	6:S:120:LEU:HG	1.92	0.51
4:T:313:LEU:HD23	4:T:313:LEU:O	2.10	0.51
4:T:326:GLU:OE2	4:V:297:ALA:N	2.42	0.51
4:L:146:ASP:OD1	4:L:146:ASP:N	2.42	0.51
4:L:161:LYS:NZ	7:U:21:G:N7	2.58	0.51
4:N:133:VAL:HG12	7:U:23:C:H4'	1.93	0.51
4:R:34:VAL:O	4:R:44:VAL:HA	2.10	0.51
4:R:324:SER:HB2	4:T:293:ILE:HD13	1.92	0.51
4:V:138:ALA:HA	4:V:198:ILE:HD12	1.92	0.51
2:E:12:LEU:HA	2:E:15:LEU:HD23	1.93	0.51
4:K:32:THR:HG23	6:S:87:ASN:ND2	2.25	0.51
4:V:13:ALA:H	4:V:191:THR:HB	1.75	0.51
9:Y:126:ILE:HD11	9:Y:130:LEU:HB2	1.92	0.51
6:S:222:GLU:HB3	6:S:235:ILE:HD13	1.92	0.51
4:T:6:SER:HA	4:T:196:PHE:O	2.10	0.51
4:V:15:SER:OG	4:V:188:GLU:O	2.26	0.51
4:W:108:GLU:HA	4:W:111:ILE:HD13	1.92	0.51
4:L:131:ARG:HE	7:U:11:G:H1'	1.74	0.51
4:R:269:ILE:HD12	4:R:275:ILE:HD12	1.91	0.51
6:S:172:PHE:HD2	6:S:253:ILE:HD13	1.75	0.51
4:T:124:LEU:HD22	7:U:47:A:H2'	1.92	0.51
4:W:58:TRP:HA	4:W:61:VAL:HG12	1.91	0.51
4:M:227:ASP:OD1	4:M:227:ASP:N	2.44	0.51
4:W:97:LYS:NZ	4:W:115:LEU:HD22	2.25	0.51
9:Y:173:TYR:CE1	9:Y:175:LYS:HB2	2.45	0.51
2:C:103:ALA:HB3	2:C:105:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:267:VAL:HG21	4:O:290:ASN:HD22	1.76	0.51
5:Q:97:LYS:HZ3	5:Q:103:GLU:HA	1.76	0.51
5:Q:146:ASN:OD1	5:Q:147:GLY:N	2.41	0.51
4:W:200:LEU:HD11	4:W:242:LEU:HD21	1.91	0.51
1:A:94:LEU:HD22	1:A:99:LYS:HE3	1.91	0.51
1:A:138:TYR:HE1	1:A:431:LYS:HD3	1.75	0.51
4:K:217:GLU:H	4:K:221:ARG:HH12	1.56	0.51
4:N:38:THR:O	4:N:39:GLU:HG3	2.10	0.51
4:V:323:SER:N	4:V:327:GLU:OE2	2.43	0.51
4:W:231:ARG:O	4:W:235:ILE:HG12	2.10	0.51
1:A:94:LEU:HD11	1:A:107:LEU:HD11	1.93	0.51
2:C:5:ILE:HG23	2:C:97:LEU:HD13	1.93	0.51
2:G:52:PRO:HA	2:G:55:LYS:HG2	1.92	0.51
4:M:258:PHE:HD2	4:N:139:SER:HB3	1.76	0.51
4:O:87:ARG:HH12	4:O:121:HIS:HB2	1.76	0.51
4:O:117:ASP:OD1	4:O:117:ASP:N	2.44	0.51
9:Y:120:VAL:HB	9:Y:154:LEU:HD12	1.92	0.51
1:A:36:LYS:NZ	1:A:213:ASP:OD1	2.37	0.51
2:C:53:LYS:HE3	4:T:24:THR:HB	1.93	0.51
4:V:8:ARG:NH2	4:V:144:THR:HG21	2.25	0.51
4:V:231:ARG:O	4:V:235:ILE:HG12	2.11	0.51
2:C:3:GLY:O	2:C:5:ILE:HG12	2.11	0.50
2:H:77:LEU:HA	2:H:80:LYS:HZ3	1.76	0.50
5:Q:53:MET:O	5:Q:57:ILE:HG12	2.10	0.50
5:Q:159:MET:HA	5:Q:162:GLU:HG3	1.93	0.50
2:C:56:LYS:HD2	2:C:57:LYS:HD2	1.92	0.50
4:K:169:GLU:HG2	4:K:170:LYS:HD3	1.92	0.50
4:P:18:ALA:HA	4:P:29:ILE:HA	1.92	0.50
4:W:8:ARG:HB2	4:W:265:GLU:HG3	1.93	0.50
2:C:52:PRO:HG2	2:C:53:LYS:HZ2	1.75	0.50
3:D:49:DG:H1'	9:Y:96:ASN:HD21	1.76	0.50
2:H:56:LYS:HD3	4:O:24:THR:HG22	1.92	0.50
2:J:3:GLY:O	2:J:5:ILE:HG12	2.12	0.50
4:L:20:GLY:HA2	4:L:27:ILE:HG23	1.94	0.50
4:L:225:VAL:HG13	4:L:226:ILE:HG23	1.93	0.50
4:O:85:GLY:HA3	7:U:32:U:OP2	2.12	0.50
4:O:324:SER:OG	4:P:296:ASN:OD1	2.28	0.50
4:V:128:THR:OG1	4:V:130:ARG:NH1	2.45	0.50
4:V:135:LEU:HG	4:V:205:VAL:HG12	1.93	0.50
9:Y:140:LYS:HG3	9:Y:141:HIS:N	2.26	0.50
7:U:55:G:OP1	4:V:87:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:55:ARG:HH21	9:Y:114:LEU:HD23	1.75	0.50
2:G:57:LYS:HA	2:G:60:SER:HB3	1.94	0.50
2:I:38:GLU:OE1	2:J:88:LYS:NZ	2.31	0.50
4:L:4:ARG:HG3	4:L:199:VAL:HG23	1.93	0.50
4:R:16:LEU:HB3	4:R:251:GLY:HA3	1.92	0.50
1:A:118:LEU:HD23	1:A:480:LEU:HA	1.93	0.50
1:A:426:ARG:HB3	5:Q:190:ARG:NH1	2.22	0.50
2:F:4:TRP:HH2	2:F:80:LYS:HE2	1.76	0.50
4:P:217:GLU:HG2	4:P:217:GLU:O	2.11	0.50
2:J:45:TYR:HB3	2:J:49:ARG:NH2	2.27	0.50
4:M:97:LYS:HE3	4:M:114:GLU:HB2	1.93	0.50
4:O:50:ILE:HB	4:O:141:ILE:HB	1.92	0.50
4:R:20:GLY:HA2	4:R:27:ILE:HB	1.92	0.50
4:R:256:ARG:NH1	7:U:49:U:OP2	2.44	0.50
4:N:326:GLU:OE2	4:O:296:ASN:HB2	2.11	0.50
4:W:50:ILE:HB	4:W:141:ILE:HB	1.93	0.50
4:O:249:TYR:OH	4:P:4:ARG:NH2	2.44	0.50
4:O:327:GLU:O	4:O:331:ASN:ND2	2.32	0.50
4:T:197:SER:OG	4:T:280:HIS:HA	2.11	0.50
4:V:60:PHE:HE1	4:V:117:ASP:HB2	1.76	0.50
4:V:204:LEU:HD12	4:V:207:ILE:HB	1.93	0.50
1:A:87:ARG:HE	1:A:109:ARG:HA	1.76	0.49
2:E:5:ILE:HG22	2:E:100:TRP:HE1	1.77	0.49
1:A:183:LEU:HD11	1:A:421:ILE:HD11	1.95	0.49
1:A:272:TYR:HB2	1:A:315:VAL:HG11	1.93	0.49
2:F:36:THR:N	2:F:39:GLU:OE2	2.40	0.49
2:J:35:ARG:N	2:J:39:GLU:OE2	2.45	0.49
4:O:330:ALA:HA	4:O:333:VAL:HG22	1.93	0.49
4:R:328:LEU:O	4:R:332:LEU:HG	2.12	0.49
4:V:14:HIS:O	4:V:190:ALA:N	2.39	0.49
9:Y:167:TYR:CE1	9:Y:201:LYS:HB2	2.47	0.49
2:H:42:GLU:O	2:H:46:LYS:HG3	2.13	0.49
4:R:12:ASN:HD21	4:T:34:VAL:HB	1.77	0.49
4:W:58:TRP:NE1	4:W:251:GLY:O	2.40	0.49
4:L:11:LEU:HD12	4:L:12:ASN:H	1.76	0.49
4:M:105:LEU:HA	4:M:111:ILE:HD11	1.94	0.49
4:T:108:GLU:HA	4:T:111:ILE:HD12	1.94	0.49
1:A:272:TYR:HB2	1:A:315:VAL:HG21	1.94	0.49
4:N:131:ARG:HE	7:U:23:C:H1'	1.76	0.49
4:P:262:LYS:HB2	4:R:283:TYR:CE2	2.47	0.49
5:Q:134:THR:CG2	5:Q:136:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:21:GLY:HA3	4:R:24:THR:HG22	1.93	0.49
4:R:330:ALA:HA	4:R:333:VAL:HG22	1.93	0.49
4:T:16:LEU:HD11	4:T:259:PRO:HG3	1.93	0.49
4:V:25:ASN:HB3	4:V:184:LEU:HB2	1.93	0.49
4:V:94:THR:OG1	4:V:103:VAL:O	2.24	0.49
4:W:4:ARG:HE	4:W:277:ALA:HA	1.78	0.49
2:F:48:LEU:HD21	2:G:99:LEU:HG	1.94	0.49
2:I:36:THR:OG1	2:J:88:LYS:NZ	2.34	0.49
4:N:156:LEU:HD13	4:N:191:THR:H	1.77	0.49
4:V:242:LEU:HD13	4:V:245:MET:HG3	1.94	0.49
9:Y:194:MET:O	9:Y:198:LEU:HG	2.12	0.49
4:K:119:ASP:OD2	4:K:234:ARG:NH1	2.46	0.49
9:Y:11:ASP:OD1	9:Y:12:PRO:HD2	2.13	0.49
2:J:9:GLY:HA3	2:J:100:TRP:HB3	1.94	0.49
4:K:120:VAL:HG13	4:K:121:HIS:HD2	1.76	0.49
4:K:269:ILE:HG22	4:K:306:VAL:HG12	1.95	0.49
4:O:22:GLY:HA2	7:U:33:G:N2	2.28	0.49
5:Q:83:ARG:NH1	5:Q:132:GLU:HG3	2.27	0.49
6:S:170:LEU:O	6:S:237:PRO:HD2	2.13	0.49
9:Y:3:ASN:N	9:Y:47:THR:O	2.35	0.49
9:Y:175:LYS:HB3	9:Y:180:TRP:HZ3	1.78	0.49
1:A:321:GLU:O	1:A:348:ARG:NH2	2.45	0.49
1:A:403:VAL:HG22	1:A:407:HIS:HD2	1.78	0.49
4:M:165:VAL:HA	4:M:182:GLN:HG2	1.95	0.49
1:A:90:VAL:HA	1:A:93:LEU:HG	1.95	0.49
1:A:425:ARG:N	5:Q:199:ARG:HH21	2.10	0.49
4:K:298:ARG:NH2	4:K:304:ILE:O	2.38	0.49
4:O:58:TRP:CD1	4:O:250:ILE:HA	2.48	0.49
2:I:49:ARG:NH2	2:J:29:ASP:OD1	2.44	0.48
4:R:173:ILE:HD11	4:R:182:GLN:HG3	1.94	0.48
4:T:227:ASP:OD1	4:T:227:ASP:N	2.46	0.48
4:T:266:LEU:HG	4:T:309:TYR:HB3	1.96	0.48
1:A:137:LEU:HD22	1:A:440:LEU:HD11	1.95	0.48
2:H:75:GLU:O	2:H:79:GLU:HG2	2.12	0.48
4:K:164:ARG:O	4:K:182:GLN:HB3	2.13	0.48
4:K:283:TYR:CZ	6:S:9:ARG:HG2	2.48	0.48
4:L:246:LEU:HD12	4:L:325:VAL:HG21	1.95	0.48
4:P:60:PHE:CE1	4:P:117:ASP:HB2	2.48	0.48
5:Q:66:SER:O	5:Q:67:GLU:HG2	2.13	0.48
4:R:246:LEU:HB2	4:R:325:VAL:HG11	1.95	0.48
9:Y:182:HIS:CG	9:Y:221:ARG:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:222:ARG:NH1	9:Y:265:GLU:OE2	2.46	0.48
1:A:177:MET:HG2	1:A:415:PHE:CD1	2.49	0.48
4:K:307:PHE:HB3	4:K:322:VAL:HG21	1.94	0.48
4:N:16:LEU:HD11	4:N:259:PRO:HG3	1.96	0.48
4:N:265:GLU:HA	4:N:309:TYR:HD2	1.78	0.48
4:O:4:ARG:NH1	4:O:275:ILE:O	2.47	0.48
4:P:200:LEU:HD11	4:P:242:LEU:HD11	1.95	0.48
6:S:197:ILE:HG23	6:S:216:ILE:HG23	1.95	0.48
9:Y:126:ILE:HD12	9:Y:127:PRO:HD2	1.94	0.48
9:Y:182:HIS:HB3	9:Y:221:ARG:HG3	1.96	0.48
2:I:12:LEU:HD13	2:I:15:LEU:HD21	1.96	0.48
4:K:117:ASP:N	4:K:117:ASP:OD1	2.45	0.48
4:O:55:LEU:CD2	4:O:198:ILE:HD12	2.44	0.48
6:S:7:CYS:SG	6:S:157:TRP:HB3	2.53	0.48
1:A:419:GLY:O	1:A:423:THR:OG1	2.25	0.48
4:O:243:ILE:HD11	4:O:329:VAL:HG11	1.96	0.48
4:W:66:TYR:HE2	4:W:244:PRO:HD3	1.78	0.48
1:A:326:LEU:HD12	1:A:327:PRO:HD2	1.95	0.48
5:Q:91:TYR:HA	5:Q:171:PRO:HG2	1.96	0.48
9:Y:236:GLU:HG3	9:Y:275:TRP:CE2	2.48	0.48
1:A:206:LEU:O	1:A:210:ILE:HG12	2.14	0.48
4:R:16:LEU:HD11	4:R:259:PRO:HG3	1.95	0.48
4:T:164:ARG:NH2	4:V:86:THR:OG1	2.47	0.48
2:E:39:GLU:O	2:E:42:GLU:HG3	2.14	0.48
2:I:49:ARG:HH22	2:J:29:ASP:CG	2.17	0.48
4:L:16:LEU:HD11	4:L:259:PRO:HG3	1.96	0.48
4:M:8:ARG:HB3	4:M:193:LEU:HD21	1.95	0.48
4:N:249:TYR:OH	4:O:4:ARG:NH2	2.46	0.48
4:N:269:ILE:HG22	4:N:306:VAL:HG22	1.96	0.48
4:P:291:ARG:HH12	4:P:314:GLY:HA3	1.79	0.48
5:Q:108:ILE:O	5:Q:112:VAL:HG23	2.14	0.48
6:S:24:THR:HA	6:S:112:GLU:OE2	2.13	0.48
4:T:75:ASN:HA	4:T:97:LYS:HE3	1.95	0.48
9:Y:88:ASP:HB3	9:Y:165:HIS:ND1	2.28	0.48
9:Y:137:TYR:HB3	9:Y:144:VAL:HB	1.95	0.48
2:F:103:ALA:HB3	2:F:105:TRP:CD1	2.48	0.48
4:M:38:THR:OG1	4:M:41:GLY:O	2.32	0.48
4:O:16:LEU:HD21	4:O:259:PRO:HG3	1.94	0.48
5:Q:34:ILE:HA	5:Q:37:MET:HG2	1.95	0.48
5:Q:203:GLY:O	5:Q:207:ILE:HG12	2.14	0.48
4:R:89:GLY:N	4:R:92:GLU:OE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:113:LYS:HD3	4:R:225:VAL:HG12	1.95	0.48
6:S:112:GLU:N	6:S:112:GLU:OE1	2.47	0.48
4:T:330:ALA:HA	4:T:333:VAL:HG22	1.95	0.48
4:W:236:GLU:O	4:W:240:LYS:HG2	2.14	0.48
1:A:463:LEU:HD23	1:A:473:THR:HB	1.95	0.47
2:J:68:ILE:HD12	2:J:68:ILE:H	1.79	0.47
4:L:269:ILE:HG22	4:L:306:VAL:HG22	1.96	0.47
4:N:6:SER:HA	4:N:196:PHE:O	2.14	0.47
4:T:322:VAL:HB	4:T:327:GLU:OE2	2.14	0.47
4:W:108:GLU:HG3	4:W:123:PHE:HZ	1.79	0.47
4:M:16:LEU:HD11	4:M:259:PRO:HG3	1.96	0.47
4:O:192:GLY:HA2	4:P:35:THR:HG21	1.96	0.47
6:S:173:SER:HA	6:S:220:PRO:HG3	1.96	0.47
9:Y:24:VAL:HB	9:Y:167:TYR:HE2	1.77	0.47
2:E:90:LEU:O	2:E:93:LEU:HB2	2.14	0.47
2:F:38:GLU:HG3	2:G:92:LYS:HB3	1.97	0.47
2:H:11:TYR:HA	2:H:14:TYR:HD2	1.78	0.47
4:K:90:GLN:HA	4:K:127:LYS:HE3	1.96	0.47
4:K:177:LYS:HG3	4:K:178:GLU:N	2.29	0.47
6:S:111:ARG:HG3	6:S:112:GLU:N	2.29	0.47
6:S:224:ARG:NH1	6:S:231:TYR:OH	2.46	0.47
4:T:28:GLU:HA	4:T:188:GLU:HG2	1.96	0.47
1:A:251:ILE:HD11	1:A:258:VAL:HB	1.97	0.47
2:C:39:GLU:HA	2:C:42:GLU:HG2	1.95	0.47
4:M:143:PRO:HA	4:M:194:TYR:HA	1.96	0.47
4:N:269:ILE:HD12	4:N:275:ILE:HD12	1.96	0.47
4:O:16:LEU:HD22	4:O:251:GLY:HA3	1.96	0.47
5:Q:83:ARG:HB3	5:Q:86:LEU:HD13	1.95	0.47
4:W:242:LEU:HD13	4:W:245:MET:HG3	1.95	0.47
9:Y:173:TYR:HE1	9:Y:175:LYS:HB2	1.78	0.47
1:A:73:LEU:HD23	1:A:77:SER:HB3	1.96	0.47
1:A:425:ARG:NH2	5:Q:190:ARG:O	2.46	0.47
2:F:6:ARG:O	2:F:10:ARG:HG3	2.13	0.47
2:H:37:GLN:N	2:H:90:LEU:HD11	2.30	0.47
2:J:91:ARG:O	2:J:95:VAL:HG12	2.14	0.47
5:Q:83:ARG:HH12	5:Q:132:GLU:HG3	1.79	0.47
4:R:287:ILE:HD12	4:R:311:VAL:HG11	1.95	0.47
6:S:202:VAL:HG22	6:S:217:PHE:CZ	2.50	0.47
2:I:17:ASP:OD2	2:I:107:ASN:ND2	2.47	0.47
4:K:169:GLU:HG2	4:K:170:LYS:N	2.30	0.47
4:L:79:ARG:HD3	4:L:86:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:134:THR:HG22	5:Q:136:GLU:HG2	1.95	0.47
4:R:263:VAL:HG11	4:R:266:LEU:HD23	1.97	0.47
2:C:89:ASP:HA	2:C:92:LYS:HZ3	1.79	0.47
2:H:17:ASP:N	2:H:17:ASP:OD1	2.47	0.47
4:L:292:SER:HA	4:L:295:LYS:HG2	1.96	0.47
4:N:90:GLN:OE1	4:N:91:GLY:N	2.47	0.47
4:O:55:LEU:HD21	4:O:198:ILE:HD12	1.97	0.47
4:O:187:ARG:HD2	4:O:188:GLU:H	1.80	0.47
4:O:329:VAL:O	4:O:333:VAL:HG13	2.15	0.47
5:Q:33:ILE:HD12	5:Q:205:LEU:HD13	1.96	0.47
5:Q:55:THR:HG22	5:Q:163:LYS:HE3	1.97	0.47
6:S:223:GLU:N	6:S:223:GLU:OE1	2.47	0.47
6:S:228:ARG:NH1	9:Y:269:LYS:HB2	2.29	0.47
6:S:228:ARG:HH11	9:Y:269:LYS:HB2	1.80	0.47
4:T:91:GLY:HA2	4:T:127:LYS:NZ	2.29	0.47
4:W:4:ARG:HB2	4:W:269:ILE:HG22	1.97	0.47
4:W:63:PHE:CE2	4:W:120:VAL:HG11	2.49	0.47
1:A:491:ASN:O	1:A:493:VAL:N	2.47	0.47
4:L:262:LYS:HB2	4:M:283:TYR:CE2	2.50	0.47
4:R:174:GLY:HA3	4:R:180:THR:HG21	1.96	0.47
4:T:14:HIS:CE1	4:T:190:ALA:HB3	2.50	0.47
4:T:138:ALA:HA	4:T:198:ILE:HD12	1.97	0.47
1:A:78:LEU:HD21	1:A:292:ILE:HG22	1.97	0.47
1:A:261:VAL:HG21	1:A:345:ARG:HD3	1.97	0.47
1:A:503:PHE:O	1:A:504:LYS:HG2	2.15	0.47
4:W:16:LEU:HD22	4:W:251:GLY:HA3	1.96	0.47
1:A:251:ILE:HB	1:A:256:LYS:HB2	1.97	0.47
2:E:7:ASN:OD1	2:E:8:ILE:N	2.46	0.47
5:Q:30:ILE:O	5:Q:34:ILE:HG12	2.15	0.47
4:T:8:ARG:HH22	4:T:284:GLU:HA	1.80	0.47
4:W:113:LYS:HG2	4:W:226:ILE:HG22	1.95	0.47
4:W:117:ASP:N	4:W:117:ASP:OD1	2.47	0.47
2:C:67:ARG:HH22	2:C:70:SER:H	1.61	0.46
2:E:17:ASP:OD1	2:E:17:ASP:N	2.48	0.46
2:H:74:ILE:HG23	2:H:75:GLU:OE2	2.16	0.46
5:Q:111:LEU:HB3	5:Q:202:VAL:HG21	1.98	0.46
4:V:59:HIS:CD2	4:V:136:VAL:HG11	2.50	0.46
4:M:151:VAL:O	4:M:152:GLU:HG3	2.16	0.46
4:M:155:ARG:HG2	4:M:157:ILE:HG12	1.97	0.46
4:T:130:ARG:N	4:T:130:ARG:HD3	2.30	0.46
9:Y:140:LYS:HB3	9:Y:145:GLN:HE22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:LYS:NZ	2:J:60:SER:HB2	2.31	0.46
2:J:70:SER:O	2:J:73:ASP:HB2	2.16	0.46
5:Q:159:MET:O	5:Q:163:LYS:HG2	2.15	0.46
4:T:147:PHE:HE1	4:T:192:GLY:HA2	1.81	0.46
7:U:53:C:H4'	4:V:131:ARG:NH1	2.30	0.46
1:A:77:SER:OG	1:A:78:LEU:N	2.47	0.46
4:O:331:ASN:HA	4:O:334:LYS:HE2	1.98	0.46
1:A:11:LEU:HD23	1:A:11:LEU:H	1.80	0.46
2:C:11:TYR:CE2	2:C:48:LEU:HA	2.50	0.46
4:K:32:THR:HG21	4:K:142:LEU:HD11	1.98	0.46
4:P:56:LYS:NZ	4:P:134:SER:OG	2.45	0.46
1:A:250:LYS:HD2	1:A:251:ILE:HG23	1.98	0.46
2:I:78:GLU:O	2:I:81:VAL:HG12	2.15	0.46
4:R:330:ALA:HB2	4:T:300:LEU:HD21	1.98	0.46
4:V:330:ALA:HA	4:V:333:VAL:HG12	1.97	0.46
2:F:28:VAL:HA	2:F:31:ILE:HG22	1.98	0.46
4:O:15:SER:OG	4:O:187:ARG:NE	2.44	0.46
1:A:337:ALA:HB3	1:A:342:LEU:HB2	1.98	0.46
2:H:4:TRP:HH2	2:H:80:LYS:HD3	1.80	0.46
2:H:70:SER:OG	2:H:73:ASP:OD2	2.28	0.46
4:N:167:VAL:O	4:O:82:ARG:NH1	2.46	0.46
5:Q:163:LYS:HG3	5:Q:164:LEU:N	2.31	0.46
4:R:55:LEU:HD11	4:R:141:ILE:HD11	1.98	0.46
4:R:260:VAL:HG22	4:T:280:HIS:CD2	2.51	0.46
2:F:11:TYR:HE2	2:F:48:LEU:HA	1.81	0.46
4:N:15:SER:OG	4:N:187:ARG:NE	2.49	0.46
4:N:255:ALA:HA	4:O:137:LYS:HA	1.98	0.46
4:R:124:LEU:HD23	7:U:42:U:C6	2.51	0.46
4:V:79:ARG:HA	4:V:82:ARG:HH21	1.81	0.46
4:V:111:ILE:O	4:V:115:LEU:HB2	2.15	0.46
4:V:322:VAL:HG11	4:V:328:LEU:HD13	1.98	0.46
1:A:149:ARG:NH1	1:A:150:PHE:O	2.48	0.46
2:E:26:ASP:N	2:E:26:ASP:OD1	2.48	0.46
4:N:17:ASN:HB3	4:N:50:ILE:HG22	1.97	0.46
4:P:266:LEU:HG	4:P:309:TYR:HB3	1.97	0.46
4:R:18:ALA:HA	4:R:29:ILE:HA	1.98	0.46
4:T:12:ASN:OD1	4:T:191:THR:OG1	2.27	0.46
1:A:37:VAL:HB	1:A:196:VAL:HG12	1.96	0.45
1:A:133:TRP:HA	1:A:136:PHE:HB3	1.98	0.45
2:C:22:GLU:O	2:C:22:GLU:HG2	2.15	0.45
4:P:263:VAL:HG11	4:P:266:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:75:ASN:HA	4:R:97:LYS:HE3	1.97	0.45
4:R:90:GLN:HA	4:R:126:PRO:HG2	1.98	0.45
4:T:146:ASP:OD1	4:T:146:ASP:N	2.48	0.45
4:W:118:ALA:HB1	4:W:123:PHE:CD2	2.51	0.45
1:A:49:GLU:HB2	1:A:53:MET:HE3	1.99	0.45
1:A:336:ILE:HB	1:A:363:ILE:HG21	1.98	0.45
2:F:3:GLY:O	2:F:5:ILE:HG12	2.16	0.45
4:K:59:HIS:CE1	4:K:136:VAL:HG21	2.51	0.45
4:M:205:VAL:HG23	4:M:231:ARG:HG3	1.97	0.45
4:N:9:ILE:HD12	4:N:261:PHE:CE1	2.51	0.45
4:N:48:PRO:HD3	4:N:157:ILE:HD11	1.98	0.45
4:P:323:SER:HG	4:R:292:SER:HG	1.59	0.45
4:V:7:GLY:HA3	4:V:265:GLU:O	2.15	0.45
4:V:36:VAL:HG23	4:V:38:THR:HG23	1.98	0.45
9:Y:51:ASN:OD1	9:Y:52:GLU:N	2.49	0.45
1:A:444:PRO:HG2	1:A:484:TYR:HB2	1.99	0.45
4:M:18:ALA:HA	4:M:29:ILE:HD12	1.98	0.45
4:R:53:ASN:ND2	7:U:43:C:O2'	2.30	0.45
4:V:143:PRO:HB2	4:V:148:ILE:HD11	1.97	0.45
9:Y:226:LEU:HD13	9:Y:270:LEU:HD11	1.97	0.45
2:E:103:ALA:HB3	2:E:105:TRP:CD1	2.51	0.45
4:K:14:HIS:HB2	4:K:16:LEU:HG	1.98	0.45
6:S:37:ALA:HB1	6:S:143:ILE:HD12	1.97	0.45
6:S:141:MET:HG3	6:S:142:LEU:HD12	1.98	0.45
4:W:61:VAL:HA	4:W:64:VAL:HG12	1.99	0.45
4:K:177:LYS:HG3	4:K:178:GLU:H	1.81	0.45
4:L:89:GLY:N	4:L:92:GLU:OE2	2.50	0.45
4:L:147:PHE:HE2	4:L:156:LEU:HD11	1.81	0.45
4:M:326:GLU:OE2	4:N:296:ASN:HB2	2.16	0.45
4:N:312:ASP:OD1	4:N:312:ASP:N	2.49	0.45
4:O:88:PHE:HE1	4:O:95:ALA:HB2	1.80	0.45
5:Q:134:THR:HG22	5:Q:136:GLU:H	1.82	0.45
4:T:120:VAL:HG13	4:T:121:HIS:HD2	1.81	0.45
4:N:244:PRO:HB2	4:N:249:TYR:HB2	1.99	0.45
6:S:111:ARG:HG3	6:S:112:GLU:H	1.80	0.45
4:W:87:ARG:HD3	4:W:123:PHE:HA	1.98	0.45
4:W:291:ARG:HH11	4:W:291:ARG:HG3	1.81	0.45
1:A:338:PRO:HD2	1:A:341:ALA:HB3	1.98	0.45
4:K:25:ASN:HB3	4:K:185:PHE:HA	1.98	0.45
4:M:24:THR:HG22	4:M:26:TYR:H	1.82	0.45
4:M:167:VAL:H	4:N:84:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:331:ASN:O	4:P:334:LYS:HG2	2.16	0.45
4:T:67:PHE:O	4:T:70:THR:OG1	2.33	0.45
9:Y:66:LEU:O	9:Y:70:ILE:HG12	2.17	0.45
9:Y:222:ARG:HD3	9:Y:222:ARG:HA	1.64	0.45
2:E:4:TRP:HH2	2:E:80:LYS:HG2	1.81	0.45
2:F:78:GLU:HA	2:F:81:VAL:HG12	1.98	0.45
4:M:245:MET:HB3	4:M:250:ILE:HD11	1.99	0.45
6:S:225:ARG:HH22	9:Y:269:LYS:HE3	1.82	0.45
4:T:9:ILE:O	4:T:193:LEU:HD12	2.16	0.45
2:C:46:LYS:HA	2:C:49:ARG:NH1	2.32	0.45
2:I:15:LEU:HD12	2:I:16:VAL:HG23	1.99	0.45
4:N:87:ARG:HH21	4:N:121:HIS:HB2	1.81	0.45
4:P:307:PHE:HD1	4:P:320:THR:HB	1.82	0.45
5:Q:19:LEU:O	5:Q:23:GLU:HG2	2.17	0.45
4:V:316:ASP:OD1	4:V:316:ASP:N	2.50	0.45
4:W:118:ALA:HB1	4:W:123:PHE:HD2	1.82	0.45
9:Y:23:VAL:HG11	9:Y:197:ILE:HD13	1.99	0.45
1:A:257:LYS:HD2	1:A:326:LEU:HD21	1.98	0.45
2:C:28:VAL:HA	2:C:31:ILE:HG12	1.98	0.45
2:C:103:ALA:HB3	2:C:105:TRP:CE3	2.51	0.45
2:E:73:ASP:O	2:E:77:LEU:HG	2.17	0.45
2:J:27:VAL:O	2:J:31:ILE:HG12	2.17	0.45
4:L:246:LEU:HD13	4:L:263:VAL:HG11	1.98	0.45
4:M:16:LEU:HD22	4:M:251:GLY:HA3	1.98	0.45
5:Q:196:GLY:O	5:Q:200:MET:HG2	2.17	0.45
4:T:255:ALA:O	4:V:138:ALA:N	2.31	0.45
4:V:103:VAL:HG11	4:V:114:GLU:HG3	1.99	0.45
4:L:143:PRO:HA	4:L:194:TYR:HA	1.99	0.44
4:W:2:TYR:HB3	4:W:4:ARG:HH12	1.82	0.44
2:C:5:ILE:HG22	2:C:100:TRP:HE1	1.82	0.44
2:C:99:LEU:HD12	2:J:45:TYR:CE1	2.51	0.44
4:M:255:ALA:HA	4:N:137:LYS:HA	1.99	0.44
4:P:93:THR:OG1	4:P:127:LYS:NZ	2.30	0.44
4:P:183:MET:SD	4:P:183:MET:N	2.90	0.44
4:W:227:ASP:HB3	4:W:230:GLU:OE1	2.17	0.44
9:Y:55:ARG:NH2	9:Y:114:LEU:HD23	2.32	0.44
9:Y:190:GLU:OE1	9:Y:190:GLU:N	2.50	0.44
2:C:67:ARG:HH22	2:C:70:SER:N	2.15	0.44
2:C:91:ARG:O	2:C:95:VAL:HG12	2.18	0.44
2:H:20:PHE:HA	2:H:57:LYS:NZ	2.32	0.44
2:J:63:CYS:HB2	2:J:108:CYS:HB2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:26:TYR:HD1	4:P:186:SER:HG	1.66	0.44
2:C:25:TYR:CZ	4:R:26:TYR:HB3	2.52	0.44
2:G:76:ALA:O	2:G:79:GLU:HG3	2.18	0.44
2:G:78:GLU:O	2:G:82:GLU:OE1	2.36	0.44
4:M:269:ILE:HG22	4:M:306:VAL:HG22	1.99	0.44
4:P:151:VAL:HG22	4:P:154:GLU:HB2	1.99	0.44
4:V:67:PHE:HB2	4:V:237:SER:CB	2.48	0.44
9:Y:191:GLU:O	9:Y:241:LYS:NZ	2.50	0.44
2:J:67:ARG:NH1	2:J:68:ILE:O	2.49	0.44
4:K:255:ALA:HB1	4:L:56:LYS:HE2	1.99	0.44
1:A:326:LEU:HD23	1:A:329:VAL:HG22	2.00	0.44
2:F:11:TYR:CE2	2:F:48:LEU:HA	2.52	0.44
4:K:316:ASP:N	4:K:316:ASP:OD1	2.50	0.44
4:K:326:GLU:HA	4:K:329:VAL:HG22	2.00	0.44
4:P:8:ARG:HB3	4:P:193:LEU:HD21	1.99	0.44
4:P:290:ASN:O	4:P:294:ILE:HG12	2.17	0.44
4:R:35:THR:HG22	4:R:44:VAL:HG12	2.00	0.44
4:R:60:PHE:CE1	4:R:117:ASP:HB2	2.51	0.44
4:V:239:LEU:HD21	4:V:333:VAL:HG23	2.00	0.44
9:Y:173:TYR:CD2	9:Y:218:LEU:HD12	2.52	0.44
4:M:19:GLN:HG3	4:M:30:THR:HG22	2.00	0.44
4:M:147:PHE:HE2	4:M:156:LEU:HD11	1.82	0.44
4:N:5:ILE:HG22	4:N:268:ALA:HB2	1.99	0.44
4:O:87:ARG:HA	4:O:87:ARG:HD3	1.85	0.44
4:R:316:ASP:N	4:R:316:ASP:OD1	2.51	0.44
9:Y:158:ALA:O	9:Y:162:VAL:HG23	2.17	0.44
2:E:7:ASN:ND2	2:E:73:ASP:OD2	2.50	0.44
2:F:33:LYS:HB2	2:F:33:LYS:NZ	2.33	0.44
4:R:25:ASN:HB3	4:R:185:PHE:HA	1.98	0.44
4:W:4:ARG:HD3	4:W:278:LEU:H	1.82	0.44
4:W:29:ILE:HG23	4:W:31:LYS:NZ	2.33	0.44
4:K:35:THR:HG22	4:K:44:VAL:HG12	2.00	0.44
4:L:65:ASP:HA	4:L:68:LYS:HZ3	1.83	0.44
2:C:96:SER:HA	2:J:45:TYR:OH	2.18	0.43
2:C:100:TRP:CH2	2:J:75:GLU:HG3	2.53	0.43
4:K:64:VAL:HG21	4:K:80:ALA:HB1	2.00	0.43
4:K:166:ASP:HB3	4:K:182:GLN:HG2	2.00	0.43
4:P:88:PHE:HE1	4:P:95:ALA:HB2	1.83	0.43
4:R:27:ILE:HG12	4:R:186:SER:O	2.18	0.43
4:V:3:VAL:HB	4:V:200:LEU:HB2	1.99	0.43
4:V:34:VAL:HG11	4:V:282:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:149:LYS:NZ	4:W:150:GLU:OE2	2.51	0.43
9:Y:105:ARG:O	9:Y:108:GLU:HG3	2.18	0.43
9:Y:165:HIS:O	9:Y:204:LYS:HE3	2.18	0.43
2:C:17:ASP:OD2	2:C:107:ASN:ND2	2.40	0.43
4:K:211:LEU:HB3	4:K:223:ASN:HD22	1.84	0.43
4:P:6:SER:HA	4:P:196:PHE:O	2.18	0.43
4:V:5:ILE:HD12	4:V:267:VAL:O	2.18	0.43
4:W:146:ASP:HA	4:W:149:LYS:HG2	1.99	0.43
2:F:36:THR:OG1	2:F:37:GLN:N	2.51	0.43
4:K:308:THR:HB	4:K:311:VAL:HG13	2.00	0.43
4:O:183:MET:SD	4:O:183:MET:N	2.91	0.43
4:P:271:SER:HB3	4:P:275:ILE:HD13	2.00	0.43
4:R:145:GLU:HA	4:R:148:ILE:HG22	2.00	0.43
4:W:287:ILE:HD12	4:W:287:ILE:H	1.83	0.43
1:A:194:PRO:HD3	5:Q:35:ARG:HH22	1.83	0.43
1:A:416:VAL:HG12	1:A:436:LEU:HD13	2.00	0.43
2:H:63:CYS:HB2	2:H:108:CYS:HB2	1.65	0.43
4:K:53:ASN:ND2	7:U:7:A:O2'	2.50	0.43
4:K:239:LEU:HD23	4:K:239:LEU:HA	1.89	0.43
4:K:246:LEU:HD12	4:K:325:VAL:HG11	2.00	0.43
4:L:107:ASP:OD1	4:L:107:ASP:N	2.50	0.43
4:V:112:ILE:HG21	4:V:132:ARG:HH21	1.82	0.43
4:V:183:MET:SD	4:V:185:PHE:HB2	2.58	0.43
4:W:47:VAL:HB	4:W:143:PRO:HG2	2.00	0.43
9:Y:195:ILE:HD12	9:Y:195:ILE:H	1.83	0.43
9:Y:289:ILE:HD13	9:Y:292:LEU:HD21	2.00	0.43
1:A:410:GLU:HB2	1:A:412:LYS:NZ	2.34	0.43
4:K:33:LYS:HB2	6:S:85:ILE:HD12	2.01	0.43
4:K:276:PRO:HB3	6:S:142:LEU:H	1.82	0.43
4:M:291:ARG:HH21	4:M:314:GLY:N	2.17	0.43
4:R:257:SER:HA	4:T:140:PHE:CE1	2.53	0.43
6:S:161:VAL:HG23	6:S:244:LEU:HD11	2.00	0.43
4:L:50:ILE:HB	4:L:141:ILE:HB	2.00	0.43
4:L:286:TYR:HD2	4:L:290:ASN:HD21	1.66	0.43
4:N:60:PHE:HE1	4:N:117:ASP:HB2	1.83	0.43
4:N:191:THR:HG21	4:O:34:VAL:HA	2.00	0.43
4:P:187:ARG:NH2	4:P:253:ASN:HD22	2.17	0.43
6:S:225:ARG:HG3	6:S:230:VAL:HG22	2.01	0.43
9:Y:320:LYS:HG2	9:Y:324:LYS:NZ	2.34	0.43
2:C:75:GLU:HG3	2:E:100:TRP:HH2	1.82	0.43
4:K:245:MET:HG3	4:K:250:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:54:MET:SD	4:M:58:TRP:HD1	2.41	0.43
5:Q:57:ILE:HA	5:Q:60:HIS:HD2	1.83	0.43
4:R:140:PHE:HB3	4:R:142:LEU:CD1	2.49	0.43
6:S:144:ASP:OD1	6:S:145:VAL:N	2.52	0.43
6:S:202:VAL:HG22	6:S:217:PHE:HZ	1.83	0.43
4:V:241:ALA:O	4:V:244:PRO:HD2	2.19	0.43
2:F:35:ARG:HH22	2:F:91:ARG:NH1	2.17	0.43
2:G:38:GLU:HG3	2:H:92:LYS:HB3	2.01	0.43
4:M:156:LEU:HD23	4:M:156:LEU:HA	1.90	0.43
4:M:226:ILE:HD12	4:M:230:GLU:HB3	2.00	0.43
4:M:262:LYS:HB2	4:N:283:TYR:CZ	2.54	0.43
4:N:163:ASN:HA	4:N:184:LEU:HA	2.01	0.43
4:O:232:LYS:O	4:O:236:GLU:HG2	2.18	0.43
6:S:4:LEU:HD12	6:S:160:PHE:HE1	1.83	0.43
4:T:291:ARG:HA	4:T:294:ILE:HG12	2.01	0.43
1:A:500:TYR:HB2	1:A:507:LYS:HE3	2.01	0.43
2:C:100:TRP:HH2	2:J:75:GLU:HG3	1.84	0.43
2:I:35:ARG:HH22	2:I:91:ARG:NH1	2.16	0.43
4:K:9:ILE:HD12	4:K:261:PHE:CE1	2.53	0.43
4:L:37:ARG:NH2	4:L:40:ASN:O	2.50	0.43
4:L:130:ARG:HA	4:L:130:ARG:HD2	1.87	0.43
4:N:33:LYS:HE3	4:N:44:VAL:HG21	2.01	0.43
4:V:57:HIS:CD2	4:V:85:GLY:HA3	2.54	0.43
4:W:14:HIS:O	4:W:190:ALA:N	2.52	0.43
1:A:302:ARG:O	1:A:306:ARG:NE	2.52	0.43
2:H:92:LYS:HA	2:H:95:VAL:HG12	2.01	0.43
4:K:55:LEU:HD13	4:K:250:ILE:HD12	2.01	0.43
5:Q:34:ILE:HG22	5:Q:38:LYS:NZ	2.34	0.43
4:R:161:LYS:NZ	4:R:184:LEU:HD12	2.34	0.43
6:S:81:LEU:HD12	6:S:120:LEU:HD13	2.00	0.43
2:F:77:LEU:HD12	2:F:80:LYS:HE3	2.00	0.42
4:K:243:ILE:HB	4:K:244:PRO:HD3	2.01	0.42
4:L:331:ASN:O	4:L:334:LYS:HG2	2.19	0.42
4:M:214:LYS:HA	4:M:214:LYS:HD2	1.77	0.42
4:R:159:ALA:HA	4:R:188:GLU:HA	2.01	0.42
4:V:181:ALA:HB2	4:W:90:GLN:H	1.84	0.42
1:A:56:PHE:CE2	1:A:89:LEU:HB3	2.54	0.42
1:A:287:SER:HB2	1:A:312:ARG:HG3	2.01	0.42
2:H:34:ALA:HB1	2:H:39:GLU:HB3	2.00	0.42
2:H:49:ARG:NH1	2:I:29:ASP:OD1	2.33	0.42
4:M:50:ILE:HB	4:M:141:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:241:ALA:O	4:N:244:PRO:HD2	2.19	0.42
4:P:91:GLY:HA2	4:P:127:LYS:HD2	2.00	0.42
5:Q:35:ARG:HA	5:Q:38:LYS:HE2	2.00	0.42
6:S:40:LYS:HA	6:S:43:ILE:HG12	2.01	0.42
4:W:111:ILE:HG23	4:W:115:LEU:HD12	2.00	0.42
9:Y:106:ASN:O	9:Y:110:LEU:HD23	2.19	0.42
2:E:61:LYS:HB3	2:E:61:LYS:HE2	1.81	0.42
2:G:77:LEU:HG	2:G:80:LYS:HE3	2.00	0.42
2:J:38:GLU:HG2	2:J:39:GLU:N	2.33	0.42
4:K:17:ASN:ND2	4:K:51:THR:H	2.16	0.42
4:M:137:LYS:HB2	4:M:199:VAL:HB	2.01	0.42
4:N:110:THR:HA	4:N:113:LYS:HG2	1.99	0.42
4:N:137:LYS:HB2	4:N:199:VAL:HG13	2.00	0.42
6:S:34:LEU:HD11	6:S:121:VAL:HG11	2.01	0.42
9:Y:69:HIS:HB2	9:Y:89:PHE:HZ	1.84	0.42
1:A:425:ARG:HH21	5:Q:191:HIS:HA	1.84	0.42
2:F:104:SER:HB3	9:Y:330:SER:HA	2.01	0.42
2:G:67:ARG:HA	2:G:67:ARG:HD2	1.79	0.42
2:I:36:THR:HG23	2:I:39:GLU:H	1.84	0.42
4:L:295:LYS:HG3	4:L:296:ASN:N	2.35	0.42
4:N:117:ASP:OD1	4:N:117:ASP:N	2.53	0.42
5:Q:136:GLU:HG3	5:Q:137:VAL:N	2.33	0.42
6:S:17:LYS:HG2	6:S:26:PHE:HE1	1.84	0.42
4:V:290:ASN:O	4:V:294:ILE:HG12	2.19	0.42
4:W:123:PHE:CE1	4:W:130:ARG:HB3	2.52	0.42
1:A:506:LEU:O	1:A:507:LYS:HG3	2.19	0.42
2:H:38:GLU:OE2	2:I:92:LYS:HB2	2.19	0.42
4:N:9:ILE:HG22	4:N:263:VAL:HA	2.01	0.42
4:N:78:GLU:HA	4:N:81:LEU:HD23	2.02	0.42
4:P:260:VAL:HG12	4:R:283:TYR:CZ	2.55	0.42
4:R:291:ARG:HH12	4:R:295:LYS:HE3	1.83	0.42
6:S:199:LYS:HE2	6:S:214:GLU:HB3	2.02	0.42
4:T:246:LEU:HA	4:T:261:PHE:CE1	2.54	0.42
4:W:97:LYS:HZ2	4:W:115:LEU:HD22	1.84	0.42
9:Y:207:LEU:N	9:Y:208:PRO:HD3	2.34	0.42
2:J:59:GLU:H	2:J:59:GLU:CD	2.21	0.42
4:L:38:THR:O	4:L:39:GLU:HG3	2.20	0.42
4:M:77:THR:HG22	4:M:79:ARG:H	1.84	0.42
4:N:246:LEU:HD12	4:N:325:VAL:HG21	2.02	0.42
4:O:121:HIS:CE1	4:O:136:VAL:HG11	2.55	0.42
4:P:117:ASP:OD1	4:P:118:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:113:LYS:HA	4:R:226:ILE:HG22	2.01	0.42
6:S:170:LEU:HB3	6:S:237:PRO:HB2	2.01	0.42
4:V:58:TRP:CA	4:V:61:VAL:HG12	2.43	0.42
4:W:155:ARG:O	4:W:157:ILE:N	2.51	0.42
9:Y:194:MET:SD	9:Y:194:MET:N	2.92	0.42
1:A:152:PHE:CE2	1:A:154:ALA:HB3	2.54	0.42
2:F:95:VAL:HG11	9:Y:312:LEU:HD12	2.02	0.42
2:J:10:ARG:HD2	2:J:105:TRP:CE2	2.55	0.42
4:K:295:LYS:NZ	4:K:317:ILE:HD11	2.34	0.42
4:M:260:VAL:HG12	4:N:283:TYR:CE2	2.55	0.42
4:P:150:GLU:OE2	4:R:42:TRP:N	2.53	0.42
4:P:309:TYR:HB2	4:P:322:VAL:HG23	2.01	0.42
4:V:225:VAL:HG23	4:V:226:ILE:HG23	2.01	0.42
2:C:40:LEU:HD12	2:C:41:LEU:N	2.35	0.42
4:K:94:THR:HG23	4:K:102:THR:HG23	2.02	0.42
4:L:11:LEU:HD13	4:L:261:PHE:CE1	2.55	0.42
4:M:258:PHE:HB3	4:N:139:SER:HB3	2.00	0.42
4:M:330:ALA:HA	4:M:333:VAL:HG12	2.01	0.42
4:P:12:ASN:OD1	4:P:13:ALA:N	2.53	0.42
6:S:63:ILE:HD13	6:S:204:PRO:HG2	2.02	0.42
4:T:33:LYS:HA	4:T:45:VAL:O	2.20	0.42
4:T:269:ILE:HD12	4:T:275:ILE:HD12	2.02	0.42
9:Y:95:ILE:CG1	9:Y:252:ARG:HD3	2.50	0.42
2:E:7:ASN:O	2:E:67:ARG:NH2	2.41	0.42
2:F:93:LEU:HD23	2:F:97:LEU:HD23	2.02	0.42
2:H:77:LEU:O	2:H:81:VAL:HG23	2.20	0.42
2:I:93:LEU:O	2:I:97:LEU:HG	2.20	0.42
2:J:44:VAL:HG12	2:J:48:LEU:HD23	2.01	0.42
2:J:95:VAL:O	2:J:99:LEU:HD23	2.20	0.42
4:K:143:PRO:HG2	4:K:148:ILE:HD11	2.02	0.42
4:L:233:ALA:HA	4:L:236:GLU:HG2	2.01	0.42
4:P:192:GLY:HA2	4:R:35:THR:HG21	2.02	0.42
5:Q:51:LYS:HG3	5:Q:164:LEU:HD11	2.02	0.42
6:S:18:ARG:HD2	6:S:18:ARG:O	2.19	0.42
4:V:8:ARG:CZ	4:V:286:TYR:HE1	2.33	0.42
9:Y:69:HIS:HB2	9:Y:89:PHE:CZ	2.54	0.42
9:Y:184:TYR:CZ	9:Y:225:LEU:HB3	2.55	0.42
4:K:37:ARG:NH1	4:K:41:GLY:O	2.53	0.42
4:O:313:LEU:HD23	4:O:313:LEU:HA	1.89	0.42
4:R:59:HIS:CE1	4:R:136:VAL:HG21	2.52	0.42
4:V:66:TYR:CZ	4:V:244:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:5:ILE:HG22	4:W:196:PHE:HE2	1.85	0.42
4:W:67:PHE:O	4:W:70:THR:HG22	2.20	0.42
9:Y:185:GLN:CG	9:Y:246:HIS:HB2	2.50	0.42
1:A:282:THR:OG1	1:A:312:ARG:NH2	2.52	0.41
2:H:7:ASN:OD1	2:H:8:ILE:N	2.51	0.41
2:J:91:ARG:HA	2:J:91:ARG:NE	2.34	0.41
4:K:263:VAL:HG11	4:K:266:LEU:HD23	2.02	0.41
4:O:9:ILE:HG23	4:O:196:PHE:HE2	1.84	0.41
4:O:241:ALA:O	4:O:245:MET:HG3	2.19	0.41
6:S:169:PRO:HA	6:S:239:GLU:HA	2.01	0.41
4:T:244:PRO:HB2	4:T:249:TYR:CD2	2.55	0.41
7:U:26:U:C2	7:U:28:C:H4'	2.54	0.41
4:V:2:TYR:HE1	4:V:203:GLY:HA3	1.85	0.41
4:V:9:ILE:HD12	4:V:261:PHE:HE1	1.85	0.41
4:V:75:ASN:O	4:V:76:LEU:HD22	2.20	0.41
9:Y:320:LYS:HG2	9:Y:324:LYS:HZ2	1.85	0.41
2:E:55:LYS:HE3	2:E:55:LYS:HB3	1.88	0.41
2:E:99:LEU:HD22	2:E:100:TRP:CE2	2.55	0.41
4:M:16:LEU:HD21	4:M:259:PRO:HD3	2.02	0.41
4:N:9:ILE:O	4:N:193:LEU:HD12	2.20	0.41
4:O:267:VAL:HG21	4:O:290:ASN:ND2	2.35	0.41
4:V:207:ILE:CD1	4:V:231:ARG:HH12	2.33	0.41
4:W:31:LYS:HA	4:W:31:LYS:HD3	1.85	0.41
9:Y:168:THR:HB	9:Y:184:TYR:O	2.20	0.41
9:Y:219:ILE:HG22	9:Y:220:ASN:H	1.85	0.41
4:K:51:THR:HG23	4:K:54:MET:H	1.83	0.41
4:M:308:THR:O	4:M:322:VAL:HG12	2.21	0.41
4:N:59:HIS:CE1	4:N:136:VAL:HG21	2.55	0.41
4:N:246:LEU:HB3	4:N:263:VAL:HG21	2.02	0.41
4:O:16:LEU:HB3	4:O:251:GLY:HA3	2.02	0.41
4:O:145:GLU:O	4:O:149:LYS:HG2	2.20	0.41
4:O:162:HIS:HB2	7:U:39:A:OP2	2.20	0.41
4:P:298:ARG:NH2	4:P:304:ILE:O	2.52	0.41
4:R:260:VAL:HG13	4:T:280:HIS:HB3	2.01	0.41
6:S:175:PRO:HA	6:S:217:PHE:HD1	1.85	0.41
4:T:5:ILE:HD12	4:T:267:VAL:O	2.20	0.41
4:V:10:ARG:HD2	4:W:283:TYR:HE1	1.86	0.41
9:Y:13:ILE:HG12	9:Y:185:GLN:HE22	1.85	0.41
1:A:445:TYR:O	1:A:520:ARG:N	2.53	0.41
2:E:4:TRP:CH2	2:E:80:LYS:HG2	2.56	0.41
2:G:42:GLU:HB3	2:G:46:LYS:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:14:HIS:NE2	4:K:190:ALA:HB3	2.35	0.41
4:K:87:ARG:HB2	7:U:6:A:O2'	2.21	0.41
4:P:10:ARG:HE	4:R:283:TYR:HE1	1.69	0.41
5:Q:159:MET:HA	5:Q:162:GLU:CG	2.51	0.41
4:T:107:ASP:O	4:T:110:THR:HG22	2.20	0.41
4:V:73:GLY:O	4:V:76:LEU:HD23	2.20	0.41
4:V:254:LEU:HD13	4:V:258:PHE:HA	2.02	0.41
4:W:106:ASN:HA	4:W:130:ARG:NH1	2.36	0.41
4:M:232:LYS:O	4:M:236:GLU:OE1	2.37	0.41
6:S:8:LEU:HD23	6:S:153:ALA:HB1	2.02	0.41
1:A:334:THR:O	1:A:361:ILE:HA	2.21	0.41
2:C:58:ALA:HB2	2:C:66:PRO:HD3	2.02	0.41
2:F:87:PRO:O	2:F:91:ARG:HG2	2.20	0.41
2:I:7:ASN:OD1	2:I:8:ILE:N	2.51	0.41
2:J:30:GLY:O	2:J:34:ALA:HB2	2.21	0.41
4:K:84:ASN:ND2	6:S:104:GLU:OE2	2.52	0.41
4:K:120:VAL:HG13	4:K:121:HIS:CD2	2.55	0.41
4:K:335:MET:SD	4:K:335:MET:N	2.94	0.41
4:L:165:VAL:HG21	7:U:20:G:C8	2.55	0.41
4:N:64:VAL:HG21	4:N:80:ALA:HB1	2.02	0.41
4:O:271:SER:OG	4:O:272:GLU:N	2.54	0.41
4:P:19:GLN:N	4:P:28:GLU:O	2.43	0.41
4:P:260:VAL:HG22	4:R:280:HIS:CD2	2.54	0.41
4:T:113:LYS:HD2	4:T:226:ILE:HG22	2.03	0.41
4:V:4:ARG:HB2	4:V:269:ILE:CG1	2.51	0.41
1:A:201:THR:HG22	1:A:394:VAL:HG21	2.01	0.41
2:E:10:ARG:HD3	2:E:105:TRP:CD2	2.56	0.41
2:F:63:CYS:HB3	2:F:108:CYS:HB3	1.93	0.41
2:F:99:LEU:HD22	9:Y:337:LEU:HD22	2.02	0.41
2:I:14:TYR:CE2	2:I:66:PRO:HB3	2.55	0.41
2:J:71:PRO:O	2:J:74:ILE:N	2.51	0.41
5:Q:34:ILE:C	5:Q:38:LYS:HZ3	2.24	0.41
5:Q:134:THR:HG23	5:Q:135:PRO:HD2	2.02	0.41
5:Q:178:VAL:O	5:Q:182:VAL:HG12	2.21	0.41
4:R:46:GLU:HA	4:R:46:GLU:OE2	2.21	0.41
4:R:107:ASP:H	4:R:130:ARG:HE	1.68	0.41
6:S:86:ARG:HH12	6:S:232:TYR:HE2	1.68	0.41
4:T:154:GLU:O	4:T:156:LEU:HG	2.21	0.41
4:W:111:ILE:HD12	4:W:111:ILE:H	1.86	0.41
9:Y:49:VAL:HG22	9:Y:50:SER:O	2.21	0.41
1:A:293:HIS:CD2	1:A:301:ARG:HE	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:ILE:HB	2:I:104:SER:HB2	2.03	0.41
4:K:77:THR:HG22	4:K:115:LEU:HD22	2.03	0.41
4:L:113:LYS:HG3	4:L:226:ILE:HG22	2.03	0.41
4:L:287:ILE:H	4:L:287:ILE:HD12	1.86	0.41
4:M:2:TYR:HB3	4:M:4:ARG:NH1	2.35	0.41
4:M:17:ASN:ND2	4:M:51:THR:OG1	2.53	0.41
4:M:231:ARG:O	4:M:235:ILE:HG12	2.21	0.41
4:N:262:LYS:NZ	4:N:264:GLU:OE2	2.40	0.41
4:P:76:LEU:O	4:P:98:ALA:N	2.54	0.41
5:Q:140:ASP:OD2	5:Q:143:ARG:NH1	2.53	0.41
4:R:239:LEU:HD23	4:R:333:VAL:HG12	2.03	0.41
6:S:107:ASP:O	6:S:109:MET:HG2	2.21	0.41
4:V:307:PHE:CE2	4:V:331:ASN:HB3	2.55	0.41
9:Y:13:ILE:HG21	9:Y:132:PRO:HD2	2.03	0.41
2:E:20:PHE:O	2:E:22:GLU:N	2.53	0.41
2:G:16:VAL:HG11	2:G:102:PHE:CE2	2.56	0.41
2:H:38:GLU:O	2:H:42:GLU:OE1	2.39	0.41
2:I:6:ARG:HA	2:I:100:TRP:HZ2	1.86	0.41
4:K:43:THR:HA	6:S:227:LYS:HG3	2.02	0.41
4:L:11:LEU:HD11	4:L:14:HIS:HB3	2.03	0.41
4:L:135:LEU:HD11	4:L:204:LEU:HB3	2.02	0.41
4:L:242:LEU:HA	4:L:245:MET:HB2	2.02	0.41
4:M:294:ILE:HG21	4:M:306:VAL:HG21	2.03	0.41
4:P:106:ASN:HA	4:P:130:ARG:HH11	1.85	0.41
4:P:247:SER:HB2	4:R:277:ALA:H	1.85	0.41
5:Q:21:ALA:O	5:Q:25:VAL:HG23	2.21	0.41
6:S:233:ALA:HA	6:S:234:ARG:NH2	2.36	0.41
4:T:2:TYR:HD2	4:T:274:PRO:HA	1.85	0.41
4:V:14:HIS:ND1	4:V:190:ALA:O	2.54	0.41
4:W:4:ARG:HG2	4:W:199:VAL:HG22	2.02	0.41
4:W:9:ILE:HG21	4:W:261:PHE:CZ	2.56	0.41
4:W:66:TYR:CE2	4:W:244:PRO:HD3	2.55	0.41
1:A:457:LEU:HD21	1:A:497:PHE:HD1	1.86	0.41
2:E:87:PRO:O	2:E:90:LEU:HG	2.20	0.41
2:J:67:ARG:HH22	2:J:70:SER:HB3	1.85	0.41
4:P:216:GLU:OE2	4:P:216:GLU:N	2.54	0.41
4:R:88:PHE:CD1	4:R:105:LEU:HD21	2.56	0.41
4:R:239:LEU:HD21	4:R:332:LEU:HB2	2.02	0.41
4:V:155:ARG:NH1	4:V:157:ILE:HD11	2.36	0.41
4:V:255:ALA:HB1	4:W:134:SER:HB3	2.02	0.41
9:Y:26:LEU:HD21	9:Y:49:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASP:HA	1:A:504:LYS:HD3	2.02	0.40
2:G:26:ASP:OD1	4:M:155:ARG:NH1	2.54	0.40
4:L:150:GLU:OE2	4:M:41:GLY:HA3	2.21	0.40
4:N:253:ASN:HD22	4:N:257:SER:HB3	1.84	0.40
4:P:45:VAL:HG21	4:P:148:ILE:HD12	2.03	0.40
4:P:127:LYS:HE3	4:P:127:LYS:HB2	1.91	0.40
4:V:60:PHE:CE1	4:V:117:ASP:HB2	2.55	0.40
4:W:224:ILE:HD13	4:W:231:ARG:HD2	2.01	0.40
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.88	0.40
1:A:333:VAL:HG12	1:A:360:ILE:HG13	2.03	0.40
2:I:64:PRO:HA	2:I:65:PRO:HD3	1.89	0.40
4:N:146:ASP:N	4:N:146:ASP:OD1	2.55	0.40
4:R:262:LYS:HB3	4:T:283:TYR:CE2	2.56	0.40
4:V:55:LEU:HD11	4:V:141:ILE:HD11	2.03	0.40
4:V:298:ARG:NH1	4:V:304:ILE:O	2.54	0.40
4:W:232:LYS:O	4:W:235:ILE:N	2.54	0.40
1:A:507:LYS:HD2	1:A:508:LEU:N	2.36	0.40
4:K:217:GLU:HG2	4:K:217:GLU:O	2.22	0.40
4:M:160:ILE:HG21	4:N:51:THR:HG21	2.03	0.40
4:O:119:ASP:OD2	4:O:234:ARG:NH1	2.54	0.40
4:T:33:LYS:HB3	4:T:46:GLU:OE2	2.22	0.40
4:T:279:VAL:HG22	4:T:290:ASN:OD1	2.20	0.40
4:V:12:ASN:ND2	4:V:191:THR:OG1	2.54	0.40
9:Y:236:GLU:HG3	9:Y:275:TRP:CD2	2.57	0.40
2:E:56:LYS:HE2	2:E:56:LYS:HB2	1.93	0.40
2:F:89:ASP:HA	2:F:92:LYS:HE2	2.03	0.40
2:J:57:LYS:HZ2	2:J:60:SER:HB2	1.86	0.40
4:K:9:ILE:HD12	4:K:261:PHE:HE1	1.86	0.40
4:O:165:VAL:HG11	7:U:40:C:H6	1.87	0.40
4:R:87:ARG:HH12	4:R:121:HIS:HB3	1.87	0.40
6:S:72:ASP:HB2	6:S:256:PRO:HG2	2.02	0.40
4:T:25:ASN:HD22	4:T:184:LEU:HB2	1.87	0.40
4:T:298:ARG:HH12	4:T:318:GLU:HB2	1.86	0.40
4:V:52:GLY:HA2	4:V:55:LEU:HD23	2.03	0.40
4:V:112:ILE:HG21	4:V:132:ARG:NH2	2.37	0.40
3:D:44:DC:H2"	3:D:45:DA:C8	2.57	0.40
4:L:10:ARG:HD3	4:M:283:TYR:HE1	1.87	0.40
4:L:65:ASP:HA	4:L:68:LYS:HZ1	1.87	0.40
4:M:175:SER:H	4:M:177:LYS:HZ3	1.70	0.40
5:Q:38:LYS:CD	5:Q:43:LYS:HG3	2.51	0.40
6:S:38:LEU:HD22	6:S:123:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:170:LEU:HA	6:S:252:GLY:HA3	2.03	0.40
9:Y:220:ASN:O	9:Y:223:LEU:N	2.53	0.40
9:Y:273:PHE:CD2	9:Y:307:ILE:HG23	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
1	A	568/651 (87%)	479 (84%)	79 (14%)	10 (2%)	8 35
2	C	105/108 (97%)	102 (97%)	3 (3%)	0	100 100
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100 100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100 100
2	G	106/108 (98%)	103 (97%)	3 (3%)	0	100 100
2	H	105/108 (97%)	96 (91%)	9 (9%)	0	100 100
2	I	105/108 (97%)	95 (90%)	10 (10%)	0	100 100
2	J	105/108 (97%)	99 (94%)	6 (6%)	0	100 100
4	K	333/336 (99%)	304 (91%)	27 (8%)	2 (1%)	25 57
4	L	334/336 (99%)	306 (92%)	28 (8%)	0	100 100
4	M	334/336 (99%)	317 (95%)	17 (5%)	0	100 100
4	N	334/336 (99%)	317 (95%)	17 (5%)	0	100 100
4	O	334/336 (99%)	310 (93%)	24 (7%)	0	100 100
4	P	334/336 (99%)	311 (93%)	23 (7%)	0	100 100
4	R	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	41 71
4	T	334/336 (99%)	314 (94%)	20 (6%)	0	100 100
4	V	334/336 (99%)	309 (92%)	25 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	W	300/336 (89%)	282 (94%)	18 (6%)	0	100 100
5	Q	235/238 (99%)	219 (93%)	14 (6%)	2 (1%)	17 48
6	S	234/256 (91%)	216 (92%)	18 (8%)	0	100 100
9	Y	329/341 (96%)	299 (91%)	30 (9%)	0	100 100
All	All	5407/5602 (96%)	4990 (92%)	402 (7%)	15 (0%)	44 71

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	PRO
1	A	593	ILE
1	A	595	PRO
4	K	152	GLU
4	R	185	PHE
1	A	455	VAL
1	A	521	PRO
1	A	613	ILE
5	Q	175	GLN
1	A	507	LYS
4	K	154	GLU
1	A	458	THR
1	A	518	ARG
5	Q	117	HIS
1	A	492	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	422/577 (73%)	417 (99%)	5 (1%)	71 83
2	C	91/91 (100%)	90 (99%)	1 (1%)	73 85
2	E	91/91 (100%)	90 (99%)	1 (1%)	73 85
2	F	91/91 (100%)	89 (98%)	2 (2%)	52 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	91/91 (100%)	89 (98%)	2 (2%)	52 74
2	H	91/91 (100%)	90 (99%)	1 (1%)	73 85
2	I	91/91 (100%)	90 (99%)	1 (1%)	73 85
2	J	91/91 (100%)	90 (99%)	1 (1%)	73 85
4	K	275/277 (99%)	274 (100%)	1 (0%)	91 95
4	L	276/277 (100%)	276 (100%)	0	100 100
4	M	274/277 (99%)	274 (100%)	0	100 100
4	N	275/277 (99%)	274 (100%)	1 (0%)	91 95
4	O	275/277 (99%)	275 (100%)	0	100 100
4	P	275/277 (99%)	275 (100%)	0	100 100
4	R	275/277 (99%)	273 (99%)	2 (1%)	84 90
4	T	275/277 (99%)	270 (98%)	5 (2%)	59 78
4	V	275/277 (99%)	273 (99%)	2 (1%)	84 90
4	W	249/277 (90%)	249 (100%)	0	100 100
5	Q	191/210 (91%)	191 (100%)	0	100 100
6	S	211/224 (94%)	210 (100%)	1 (0%)	88 93
9	Y	282/292 (97%)	280 (99%)	2 (1%)	84 90
All	All	4467/4710 (95%)	4439 (99%)	28 (1%)	86 91

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LYS
1	A	221	LYS
1	A	250	LYS
1	A	306	ARG
1	A	507	LYS
2	C	56	LYS
2	E	92	LYS
2	F	49	ARG
2	F	80	LYS
2	G	33	LYS
2	G	80	LYS
2	H	33	LYS
2	I	33	LYS
2	J	67	ARG

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Mol	Chain	Res	Type
4	K	221	ARG
4	N	17	ASN
4	R	17	ASN
4	R	229	ASN
6	S	225	ARG
4	T	17	ASN
4	T	68	LYS
4	T	149	LYS
4	T	223	ASN
4	T	262	LYS
4	V	149	LYS
4	V	221	ARG
9	Y	98	VAL
9	Y	125	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	168	GLN
1	A	407	HIS
4	K	17	ASN
4	K	290	ASN
4	M	17	ASN
4	O	12	ASN
4	T	14	HIS
4	T	17	ASN
4	T	219	GLN
4	T	223	ASN
4	T	331	ASN
4	V	17	ASN
4	V	53	ASN
4	V	59	HIS
9	Y	185	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	U	56/57 (98%)	15 (26%)	1 (1%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	U	2	U
7	U	3	U
7	U	4	G
7	U	7	A
7	U	8	G
7	U	9	U
7	U	15	U
7	U	19	C
7	U	27	G
7	U	32	U
7	U	39	A
7	U	45	G
7	U	51	G
7	U	52	C
7	U	57	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	U	18	G

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

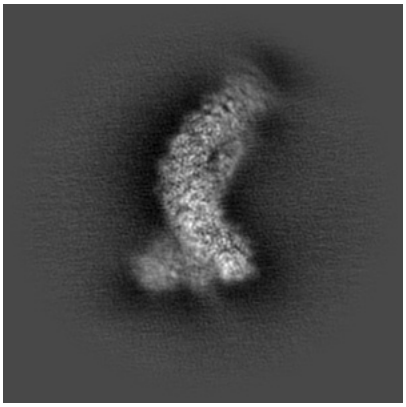
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14245. These allow visual inspection of the internal detail of the map and identification of artifacts.

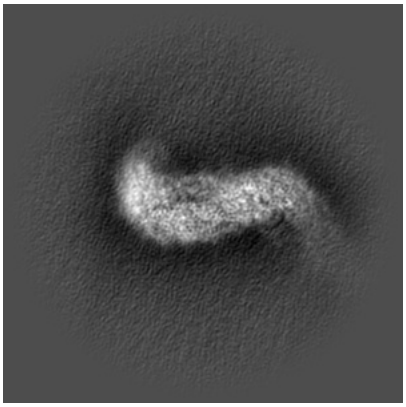
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

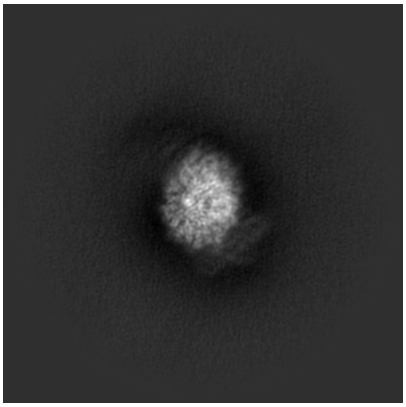
6.1.1 Primary map



X



Y

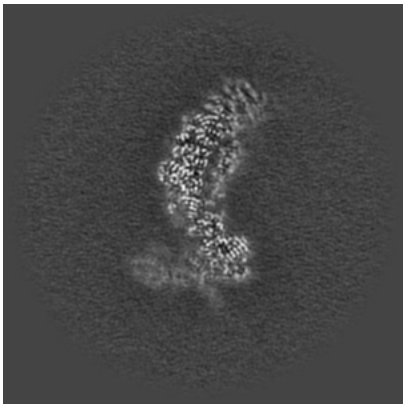


Z

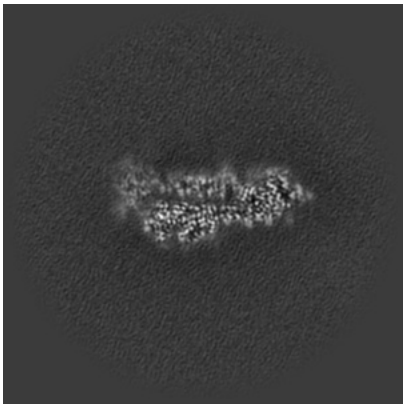
The images above show the map projected in three orthogonal directions.

6.2 Central slices

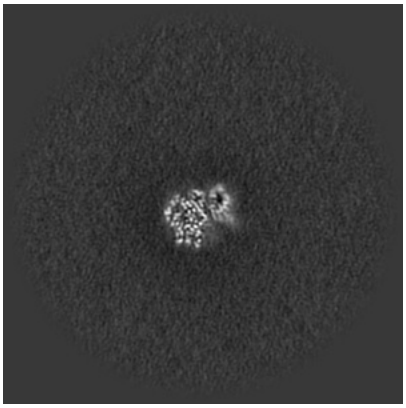
6.2.1 Primary map



X Index: 160



Y Index: 160

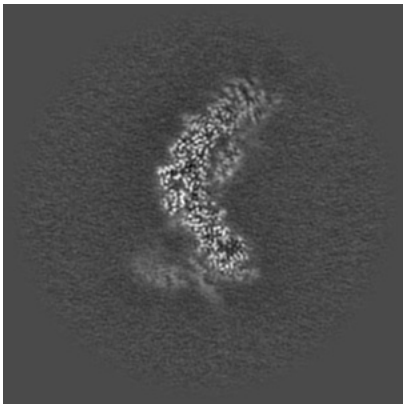


Z Index: 160

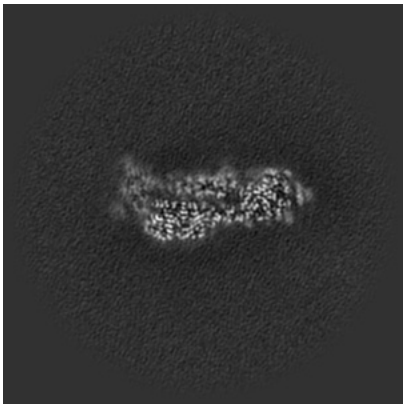
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 157



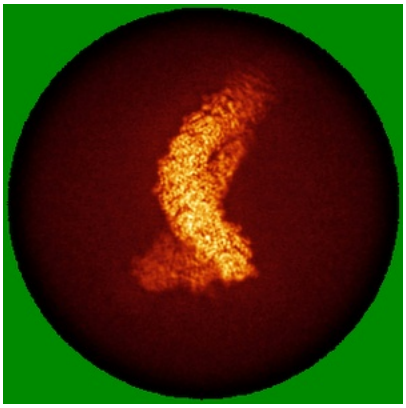
Y Index: 162

Z Index: 143

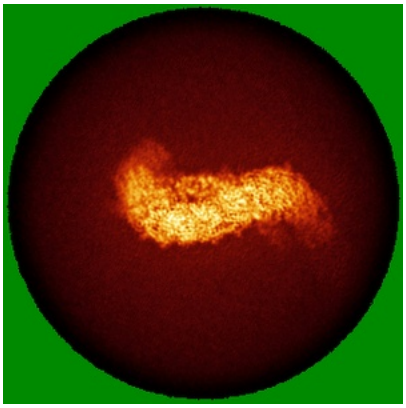
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

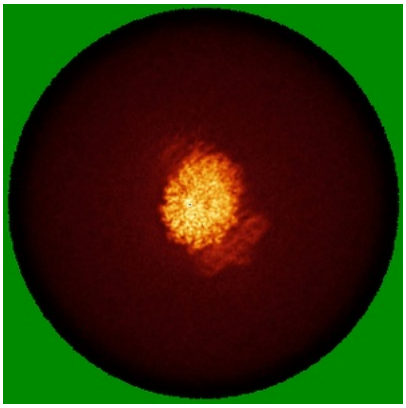
6.4.1 Primary map



X



Y

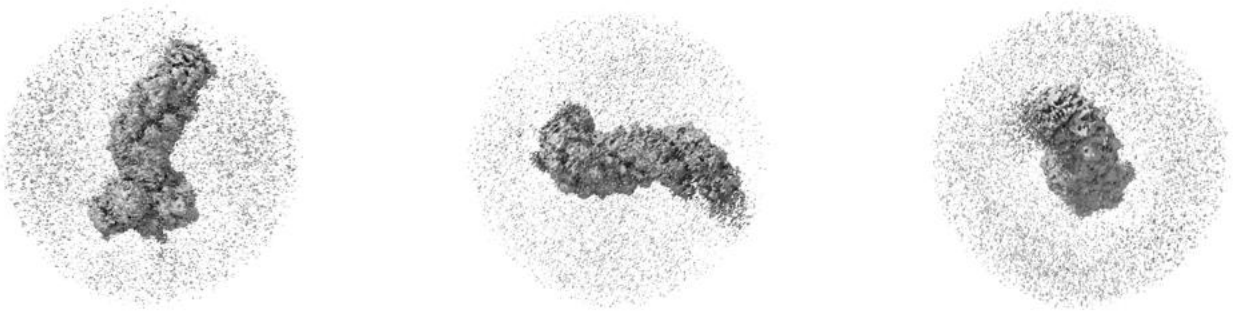


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

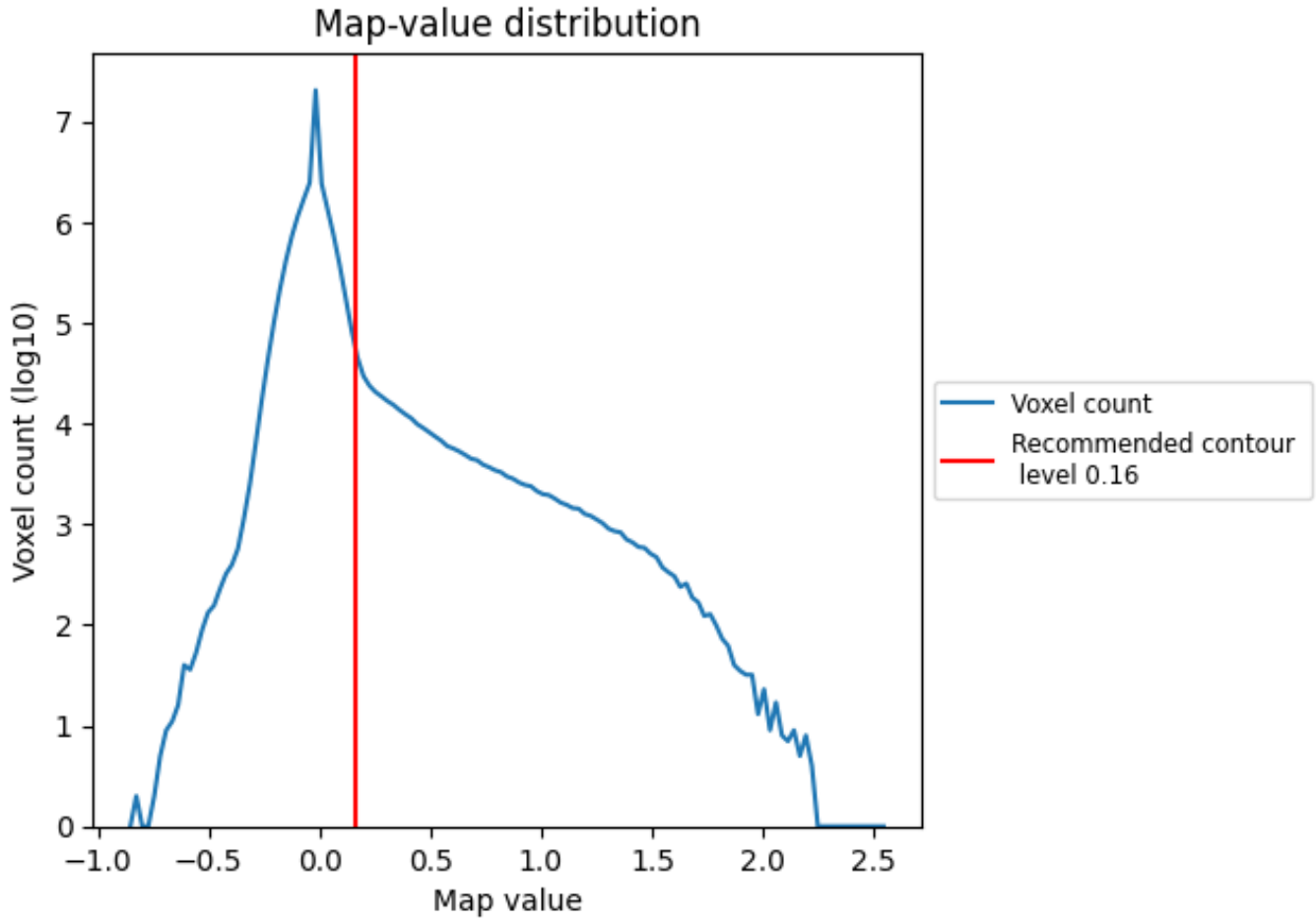
6.6 Mask visualisation (i)

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

7 Map analysis

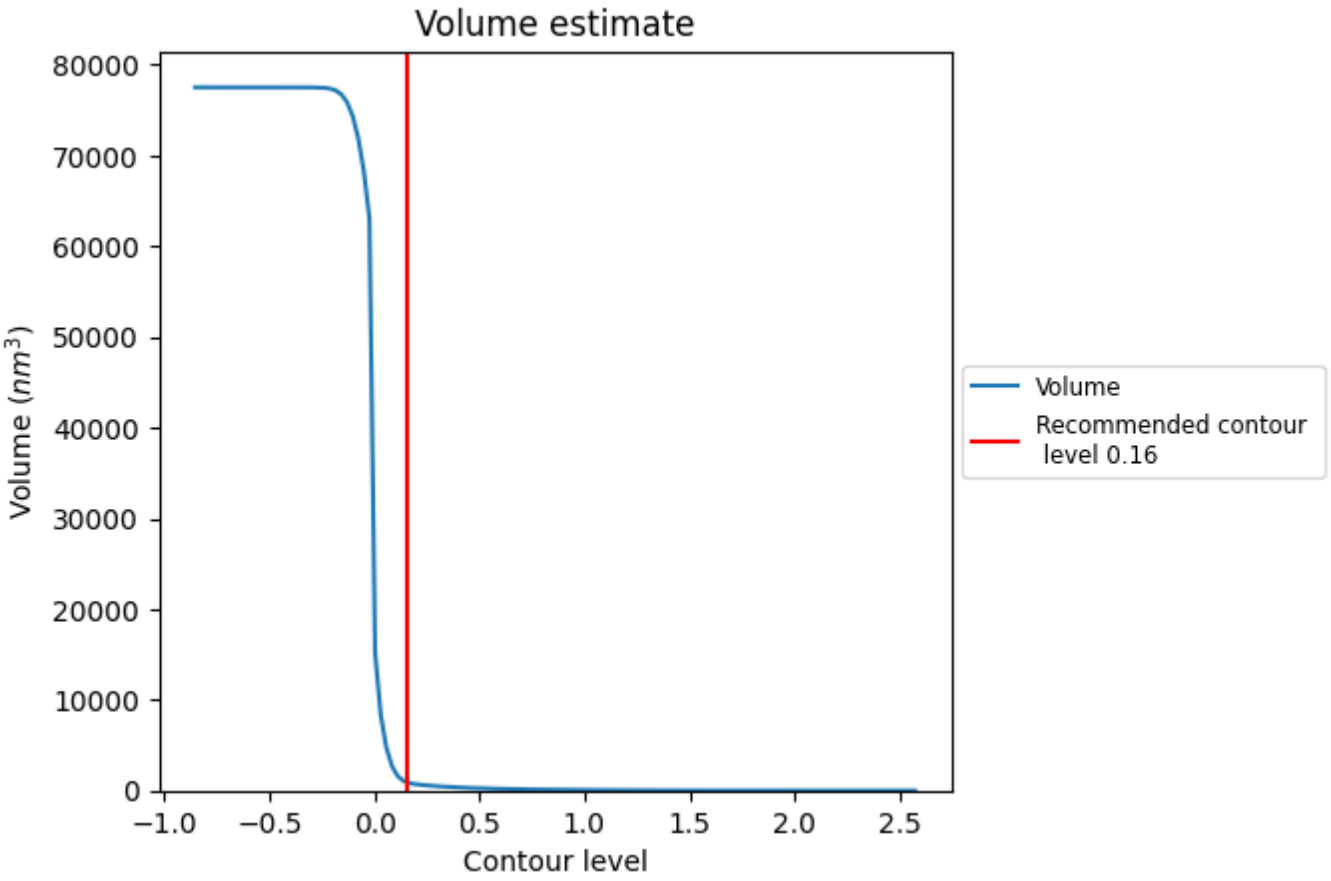
This section contains the results of statistical analysis of the map.

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.

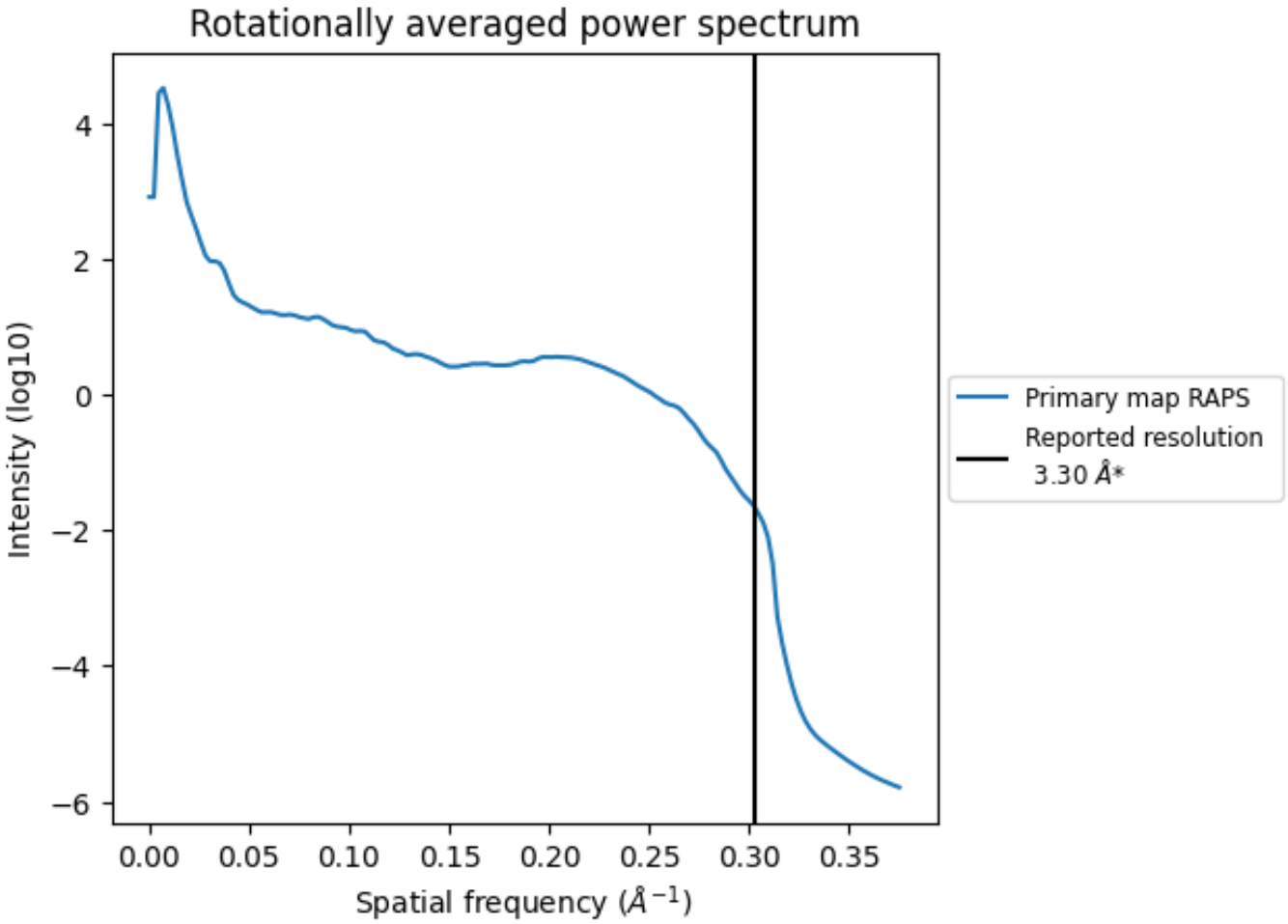
7.2 Volume estimate



The volume at the recommended contour level is 876 nm^3; this corresponds to an approximate mass of 791 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)

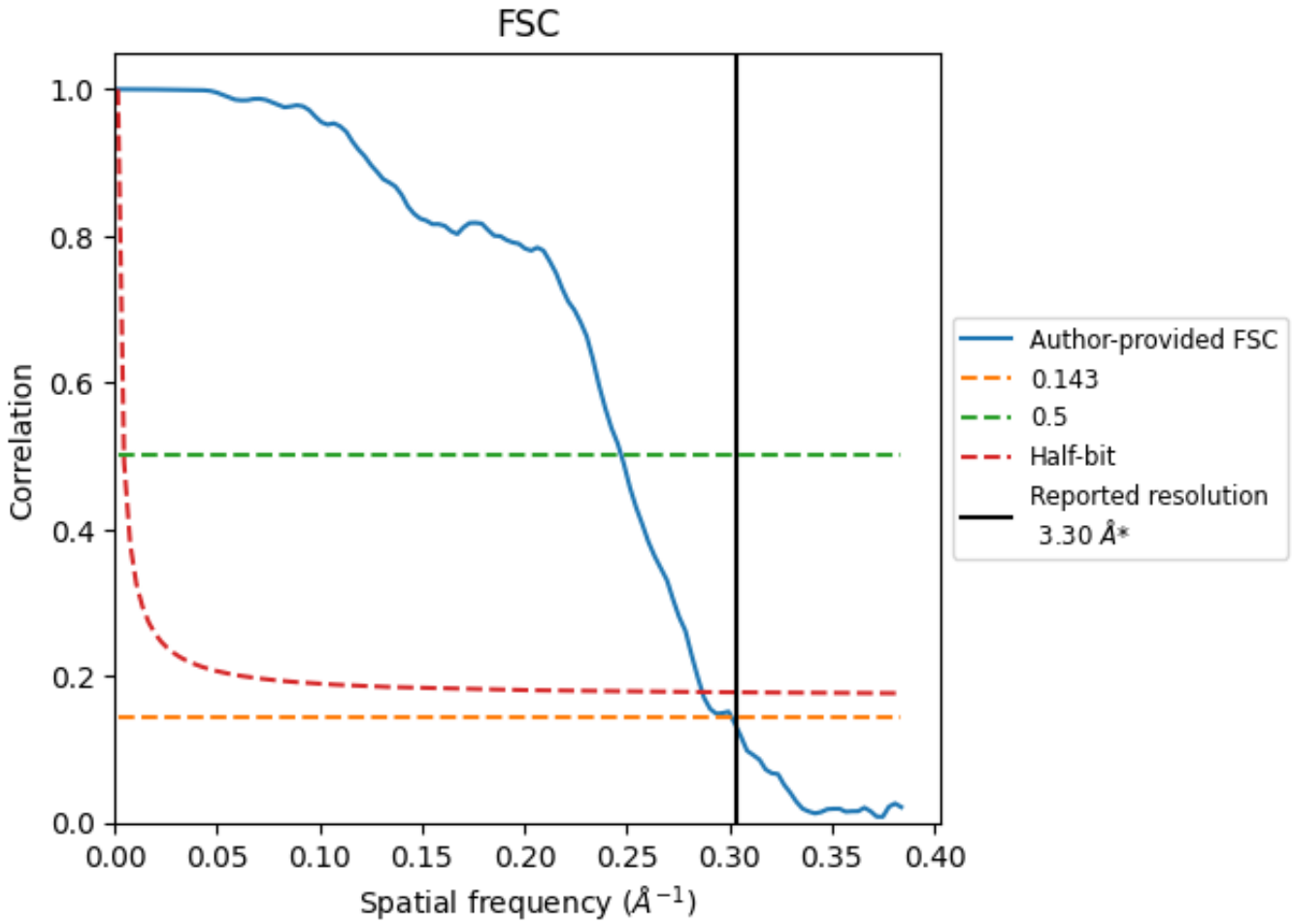


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

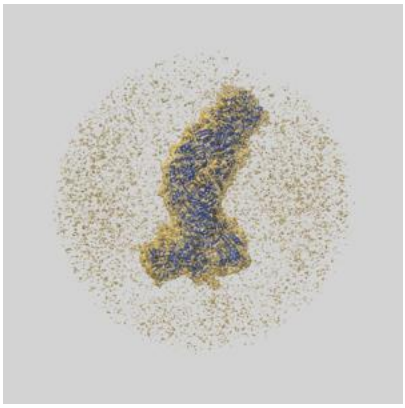
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	4.04	3.49
Unmasked-calculated*	-	-	-

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

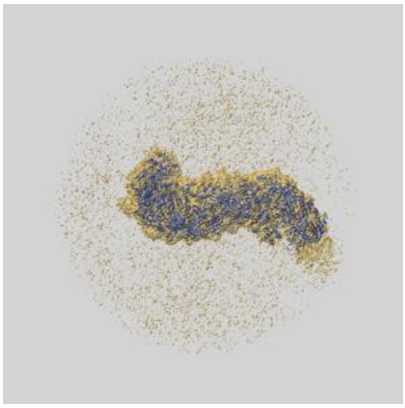
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14245 and PDB model 7R2K. Per-residue inclusion information can be found in section 3 on page 7.

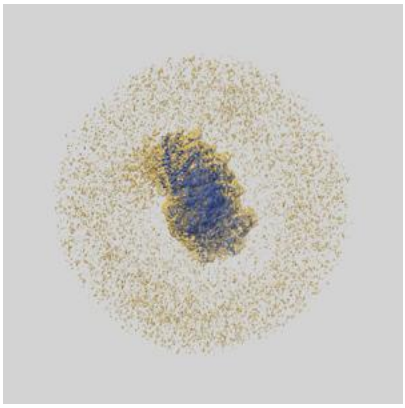
9.1 Map-model overlay



X



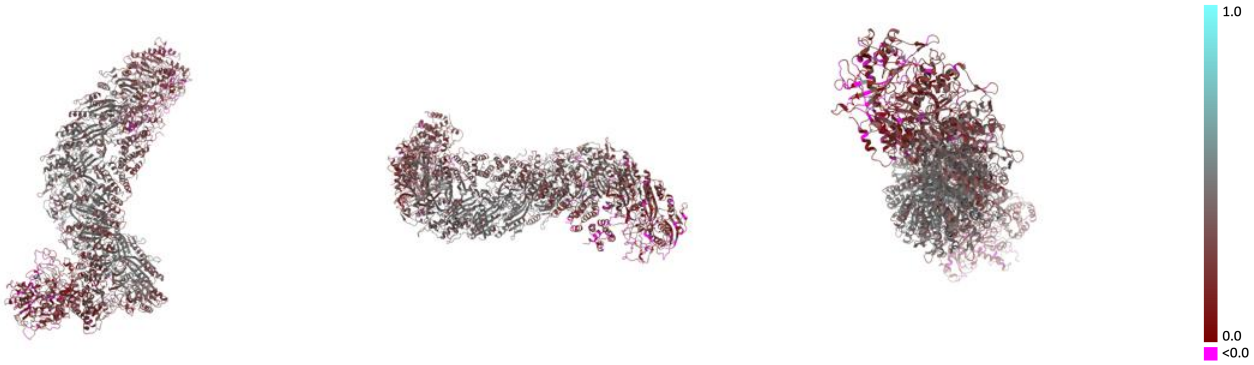
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

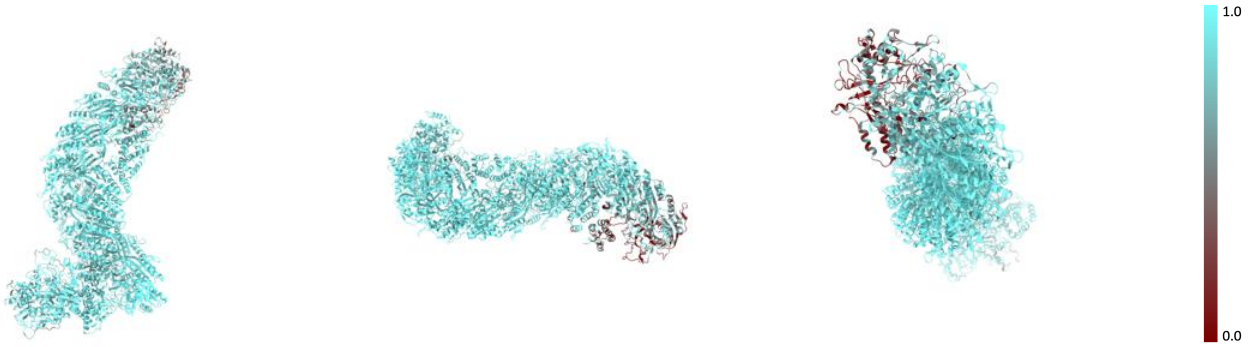
9.2 Q-score mapped to coordinate model



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.

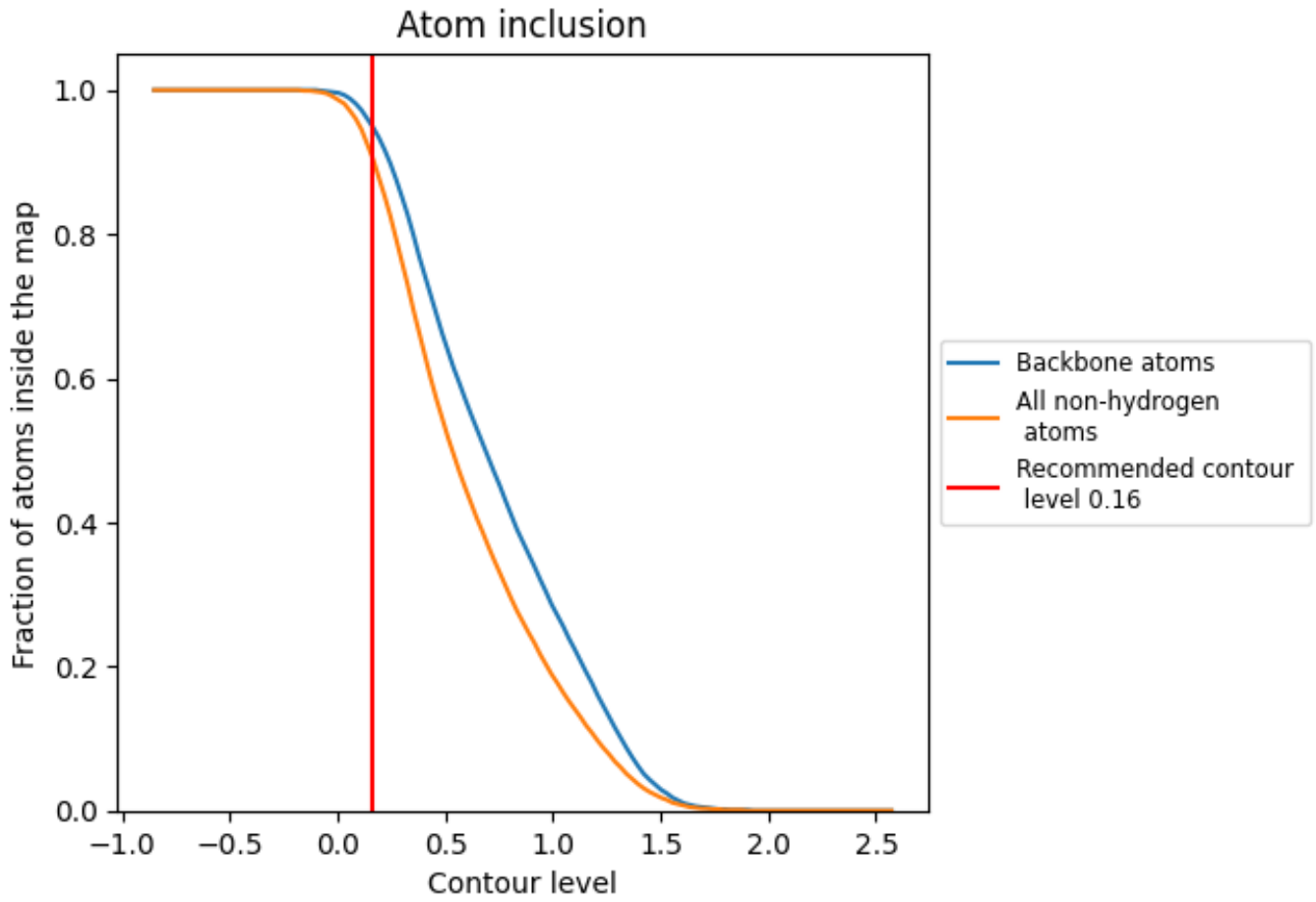
9.3 Atom inclusion mapped to coordinate model



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.3240
A	0.8880	0.1780
C	0.8330	0.2250
D	0.9520	0.2800
E	0.4250	0.1410
F	0.9860	0.3310
G	0.9960	0.3550
H	0.9880	0.3460
I	0.9810	0.3410
J	0.9500	0.2920
K	0.9910	0.3980
L	0.9890	0.4130
M	0.9930	0.4270
N	0.9880	0.4280
O	0.9840	0.4270
P	0.9770	0.4090
Q	0.9070	0.2470
R	0.9510	0.3880
S	0.9860	0.3180
T	0.8830	0.3220
U	0.9650	0.3890
V	0.7390	0.2340
W	0.5120	0.1750
X	0.7270	0.0590
Y	0.9470	0.2930