Full wwPDB EM Validation Report ⓘ

Jan 24, 2024 – 04:59 PM EST

PDB ID	:	8FF4
EMDB ID	:	EMD-29039
Title	:	Cryo-EM structure of Cascade-DNA-TniQ-TnsC complex (composite) in type I-B CAST system
Authors	:	Chang, L.; Wang, S.
Deposited on	:	2022-12-07
Resolution	:	3.60 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:

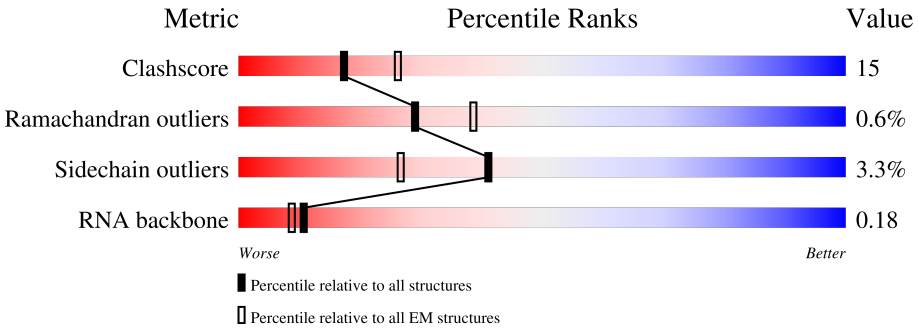
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	212	67% 31%
2	B	220	61% 34%
3	C	323	60% 27% 12%
3	D	323	59% 28% 12%
3	E	323	59% 27% 11%
3	F	323	59% 27% 12%
3	G	323	61% 27% 12%

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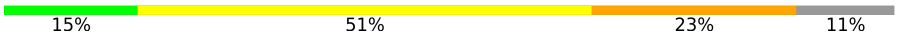
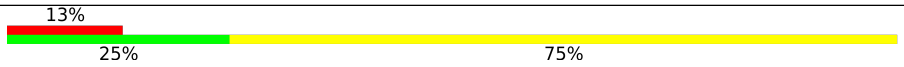
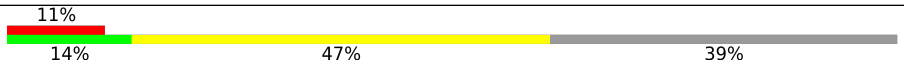
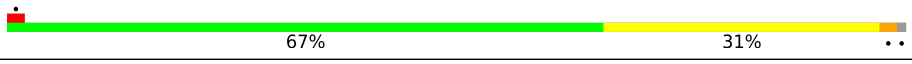
Mol	Chain	Length	Quality of chain
3	H	323	
4	I	534	
5	J	138	
5	K	138	
5	L	138	
6	M	71	
7	N	85	
8	O	85	
9	P	329	
10	Q	383	
10	R	383	
10	S	383	
10	T	383	
10	U	383	
10	V	383	
10	W	383	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 50322 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 Type I-B CRISPR-associated protein Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	212	Total	C	N	O	S	0	0
			1745	1116	313	305	11		

- Molecule 2 is a protein called Type I-B CRISPR-associated protein Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1702	1084	297	316	5		

- Molecule 3 is a protein called Type I-B CRISPR-associated protein Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	285	Total	C	N	O	S	0	0
			2323	1490	393	430	10		
3	D	285	Total	C	N	O	S	0	0
			2323	1490	393	430	10		
3	E	286	Total	C	N	O	S	0	0
			2330	1494	394	432	10		
3	F	285	Total	C	N	O	S	0	0
			2323	1490	393	430	10		
3	G	285	Total	C	N	O	S	0	0
			2323	1490	393	430	10		
3	H	285	Total	C	N	O	S	0	0
			2323	1490	393	430	10		

- Molecule 4 is a protein called Type I-B CRISPR-associated protein Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	494	Total	C	N	O	S	0	0
			4147	2689	698	748	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-7	MET	-	initiating methionine	UNP A0A235IGR9
I	-6	HIS	-	expression tag	UNP A0A235IGR9
I	-5	HIS	-	expression tag	UNP A0A235IGR9
I	-4	HIS	-	expression tag	UNP A0A235IGR9
I	-3	HIS	-	expression tag	UNP A0A235IGR9
I	-2	HIS	-	expression tag	UNP A0A235IGR9
I	-1	HIS	-	expression tag	UNP A0A235IGR9
I	0	HIS	-	expression tag	UNP A0A235IGR9
I	1	HIS	-	expression tag	UNP A0A235IGR9
I	2	ILE	-	expression tag	UNP A0A235IGR9

- Molecule 5 is a protein called Type I-B CRISPR-associated protein Cas11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	109	Total	C	N	O	S	0	0
			917	598	150	167	2		
5	K	109	Total	C	N	O	S	0	0
			917	598	150	167	2		
5	L	109	Total	C	N	O	S	0	0
			917	598	150	167	2		

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	63	Total	C	N	O	P	0	0
			1342	600	236	443	63		

- Molecule 7 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	85	Total	C	N	O	P	0	0
			1734	831	303	515	85		

- Molecule 8 is a DNA chain called Non-target DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	52	Total	C	N	O	P	0	0
			1070	510	198	310	52		

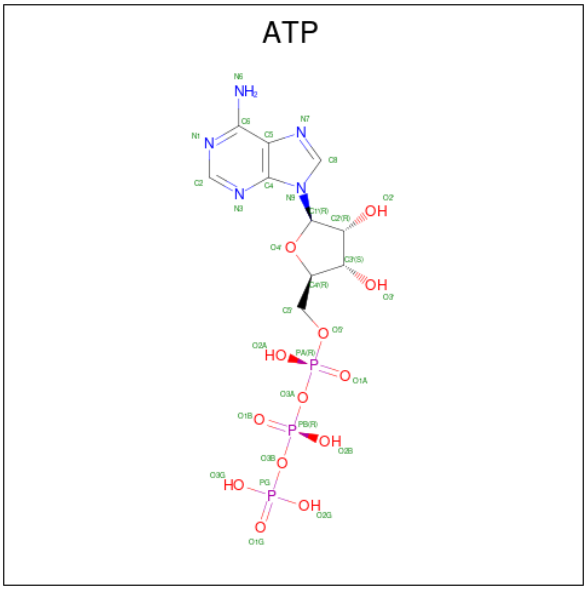
- Molecule 9 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	327	Total	C	N	O	S	0	0
			2618	1688	438	473	19		

- Molecule 10 is a protein called TnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	310	Total	C	N	O	S	0	0
			2508	1605	435	460	8		
10	R	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		
10	S	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		
10	T	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		
10	U	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		
10	V	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		
10	W	343	Total	C	N	O	S	0	0
			2756	1757	483	508	8		

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
11	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	S	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	V	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	W	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

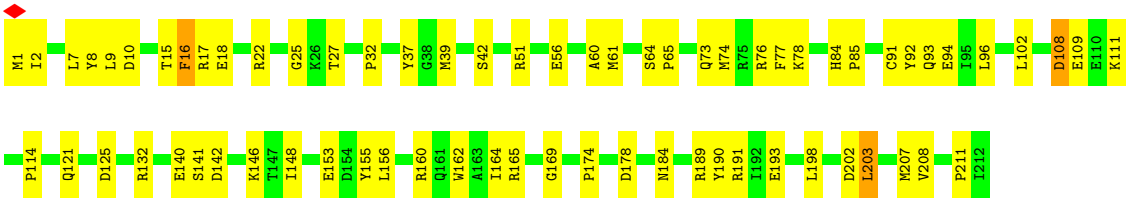
Mol	Chain	Residues	Atoms		AltConf
12	Q	1	Total	Mg	0
			1	1	
12	R	1	Total	Mg	0
			1	1	
12	S	1	Total	Mg	0
			1	1	
12	T	1	Total	Mg	0
			1	1	
12	U	1	Total	Mg	0
			1	1	
12	V	1	Total	Mg	0
			1	1	
12	W	1	Total	Mg	0
			1	1	

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.

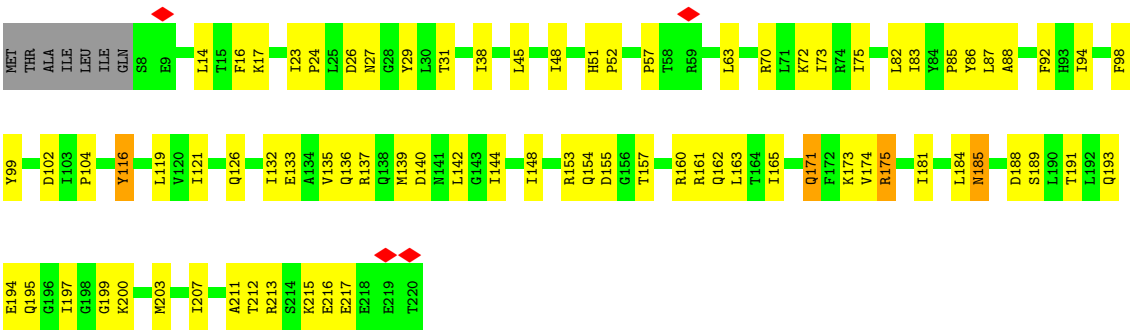
• Molecule 1: Type I-B CRISPR-associated protein Cas5

Chain A:



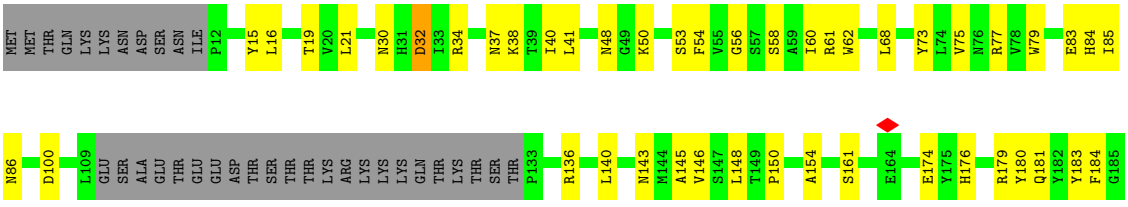
• Molecule 2: Type I-B CRISPR-associated protein Cas6

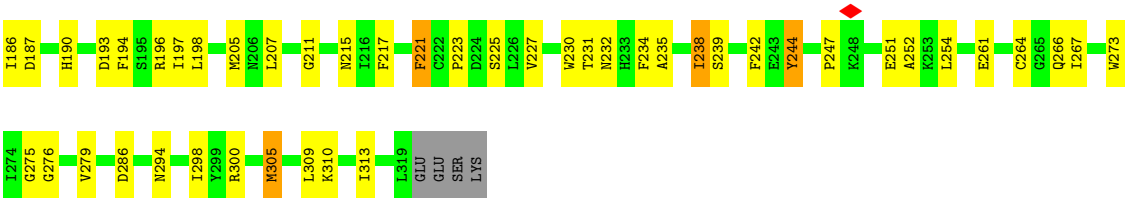
Chain B:



• Molecule 3: Type I-B CRISPR-associated protein Cas7

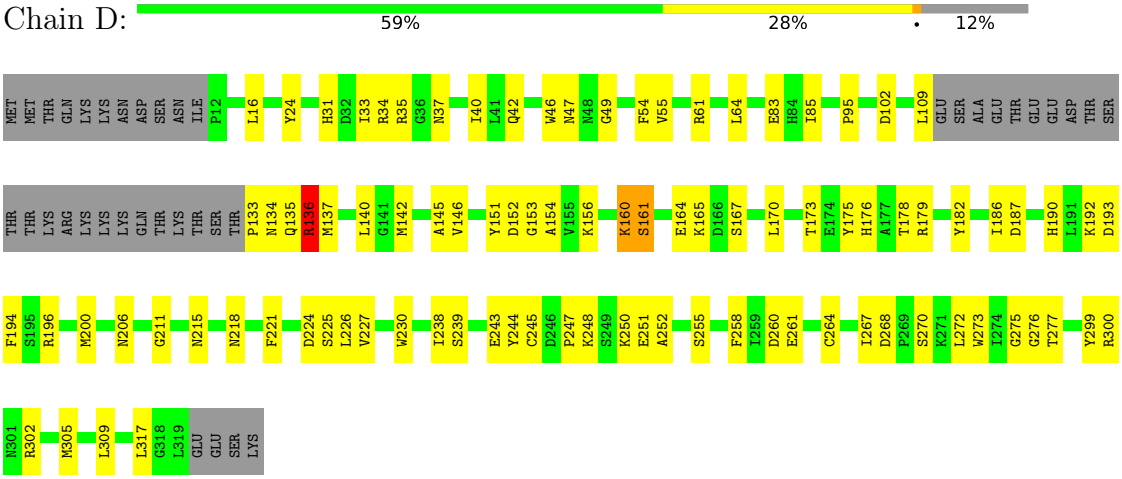
Chain C:





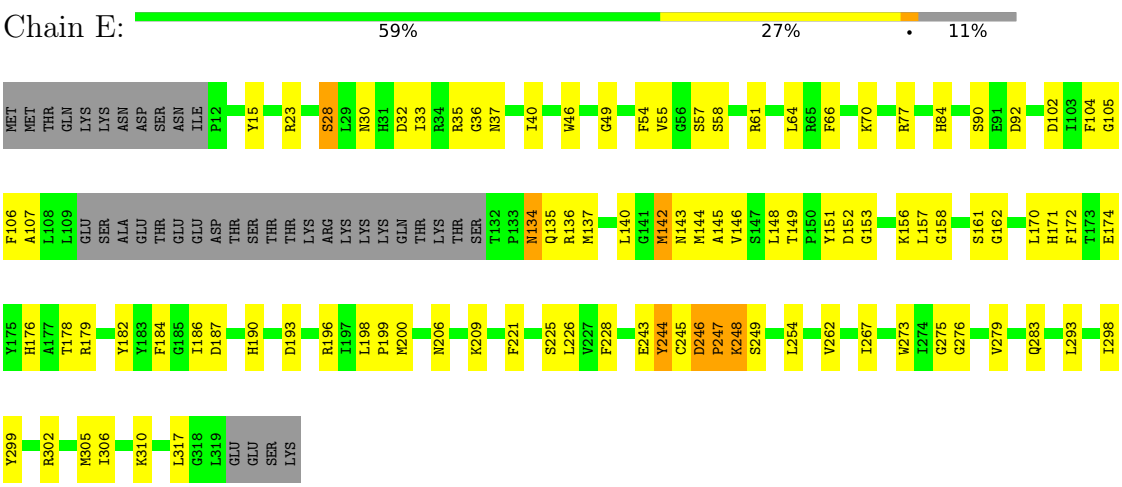
• Molecule 3: Type I-B CRISPR-associated protein Cas7

Chain D:



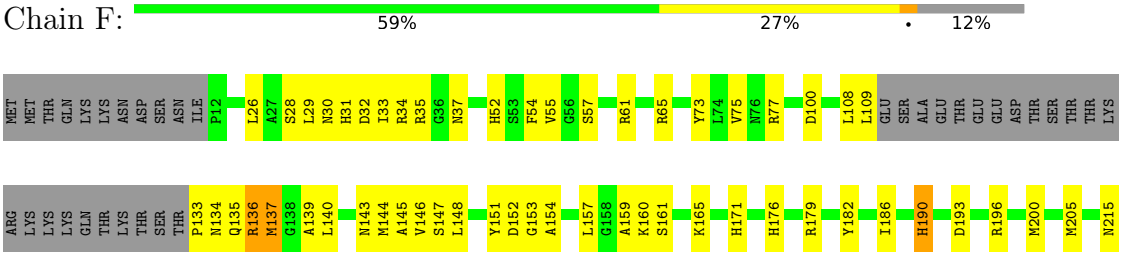
• Molecule 3: Type I-B CRISPR-associated protein Cas7

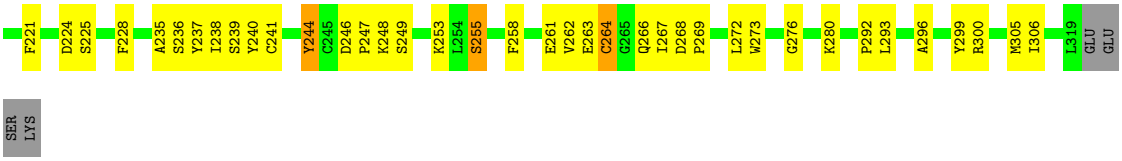
Chain E:



• Molecule 3: Type I-B CRISPR-associated protein Cas7

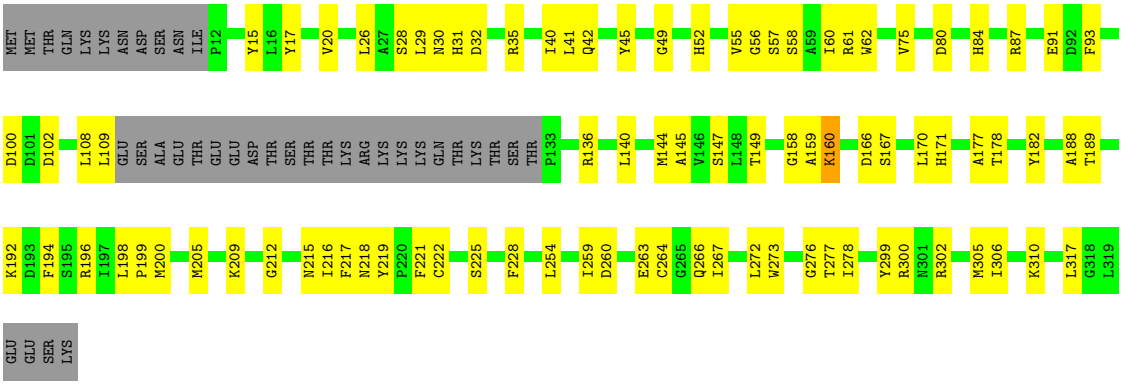
Chain F:





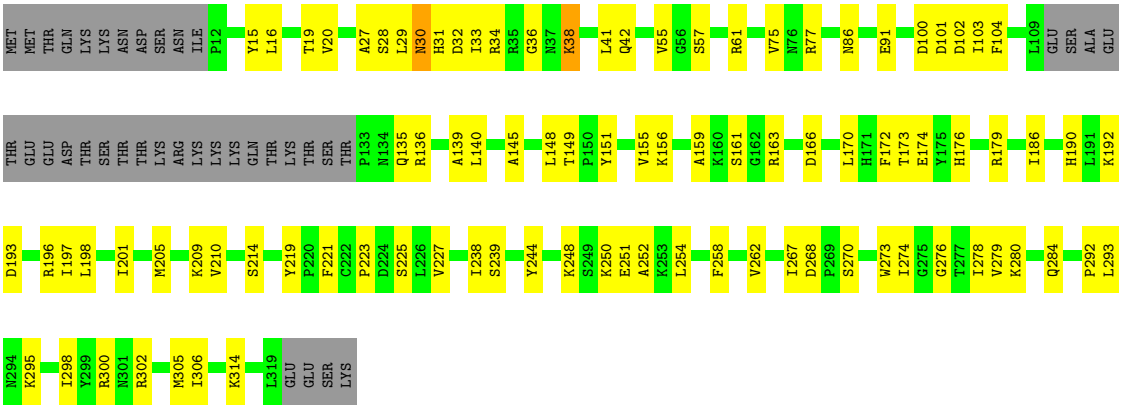
• Molecule 3: Type I-B CRISPR-associated protein Cas7

Chain G:



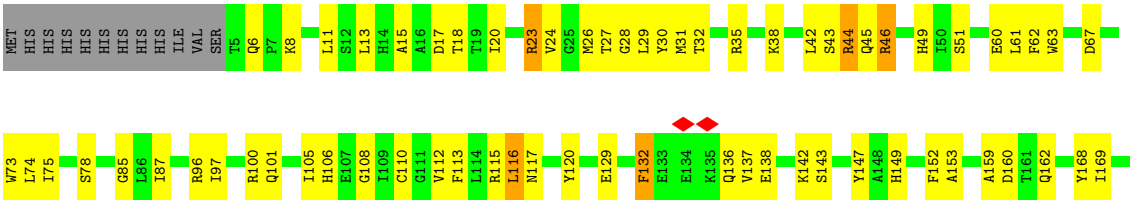
• Molecule 3: Type I-B CRISPR-associated protein Cas7

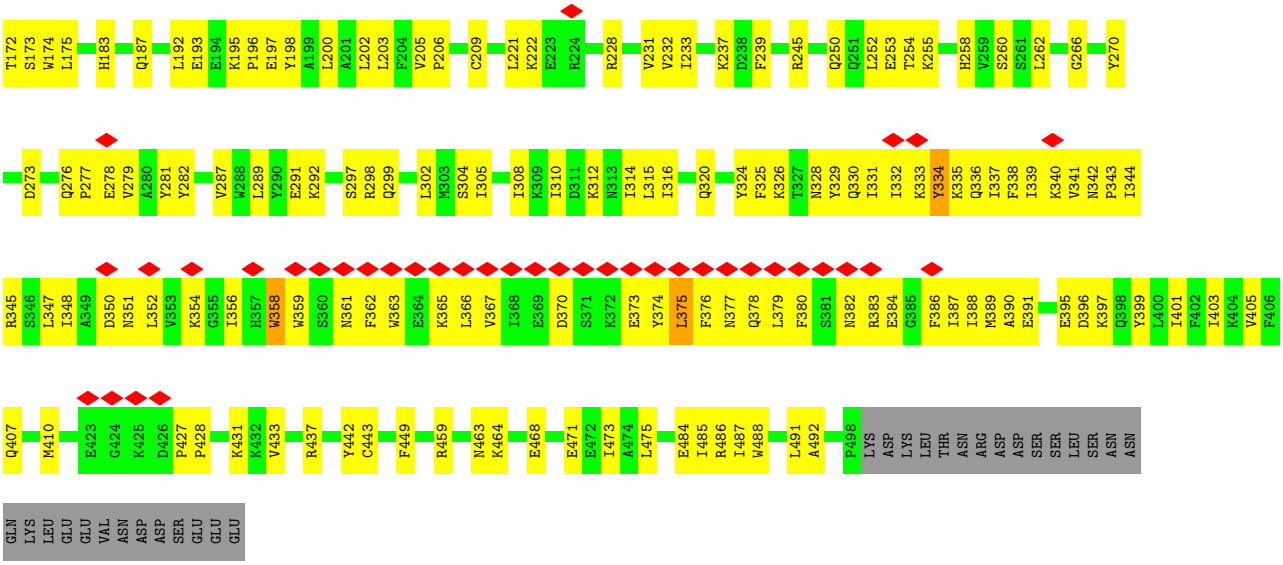
Chain H:



• Molecule 4: Type I-B CRISPR-associated protein Cas8

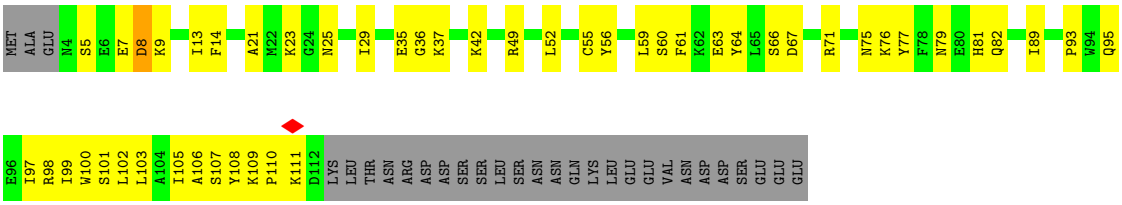
Chain I:





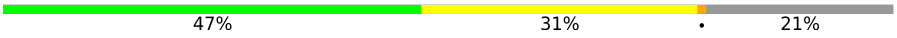
• Molecule 5: Type I-B CRISPR-associated protein Cas11

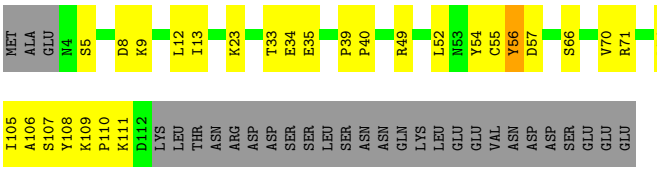
Chain J:



• Molecule 5: Type I-B CRISPR-associated protein Cas11

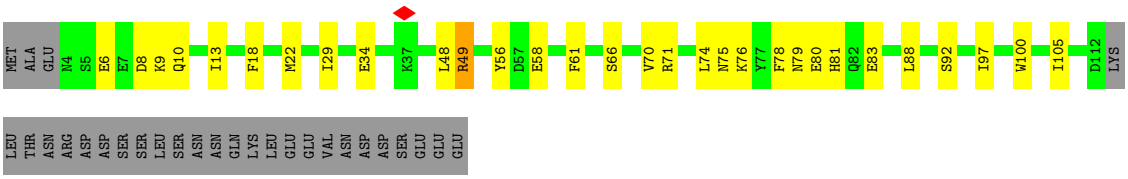
Chain K:





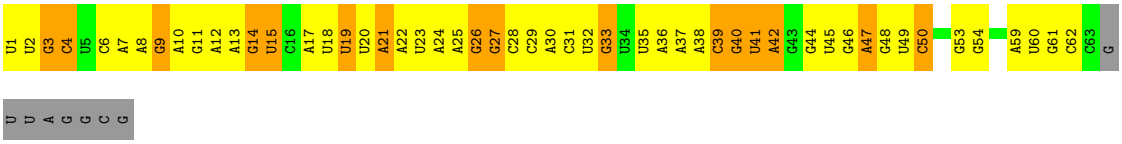
• Molecule 5: Type I-B CRISPR-associated protein Cas11

Chain L:

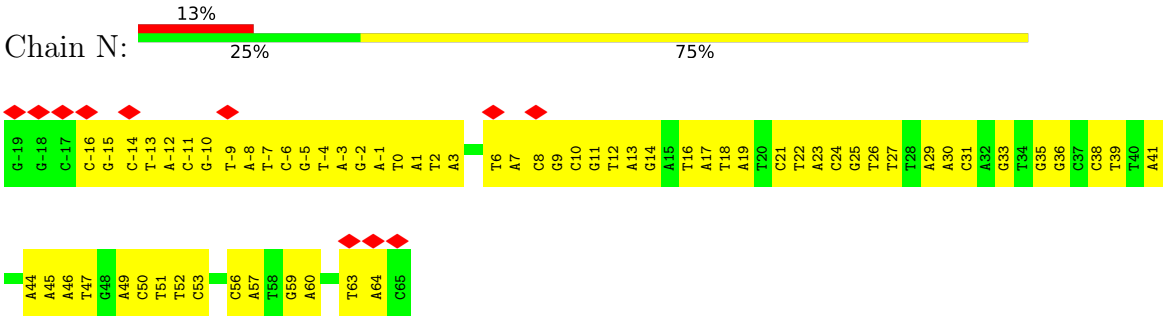


• Molecule 6: RNA

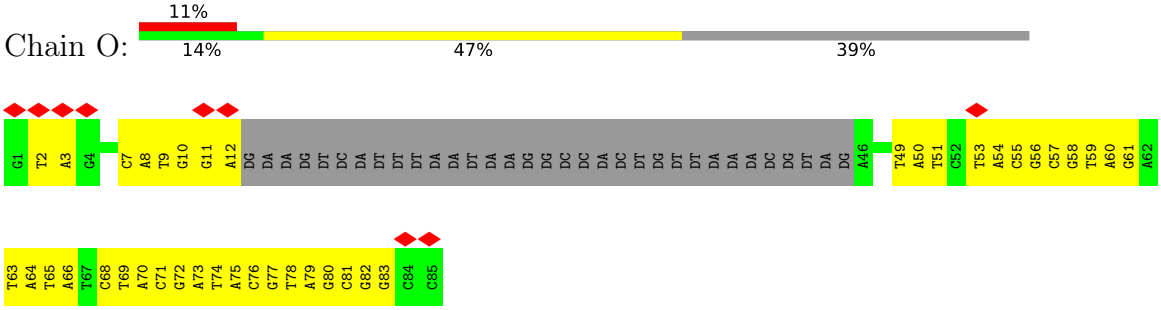
Chain M:



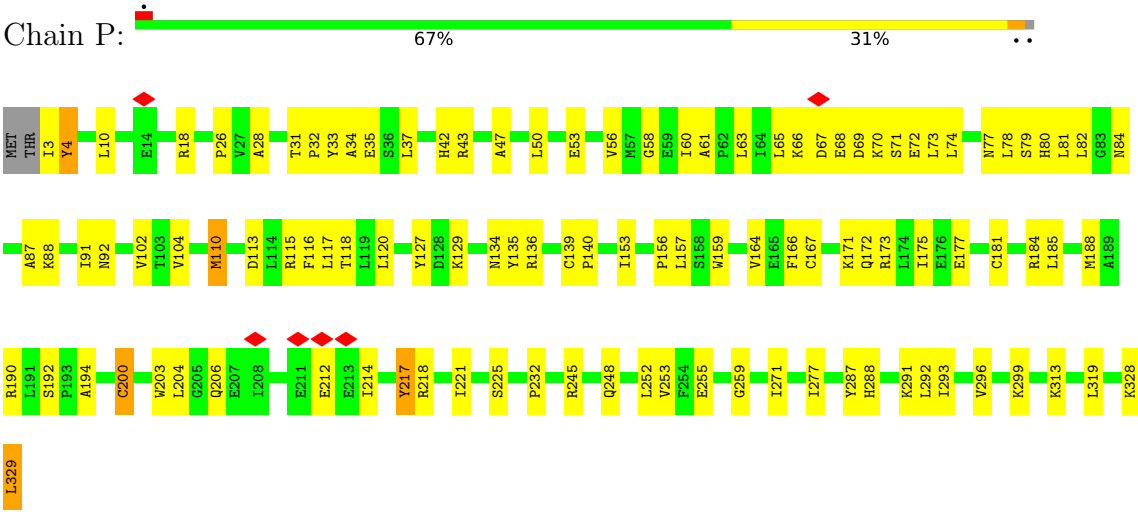
• Molecule 7: Target DNA strand



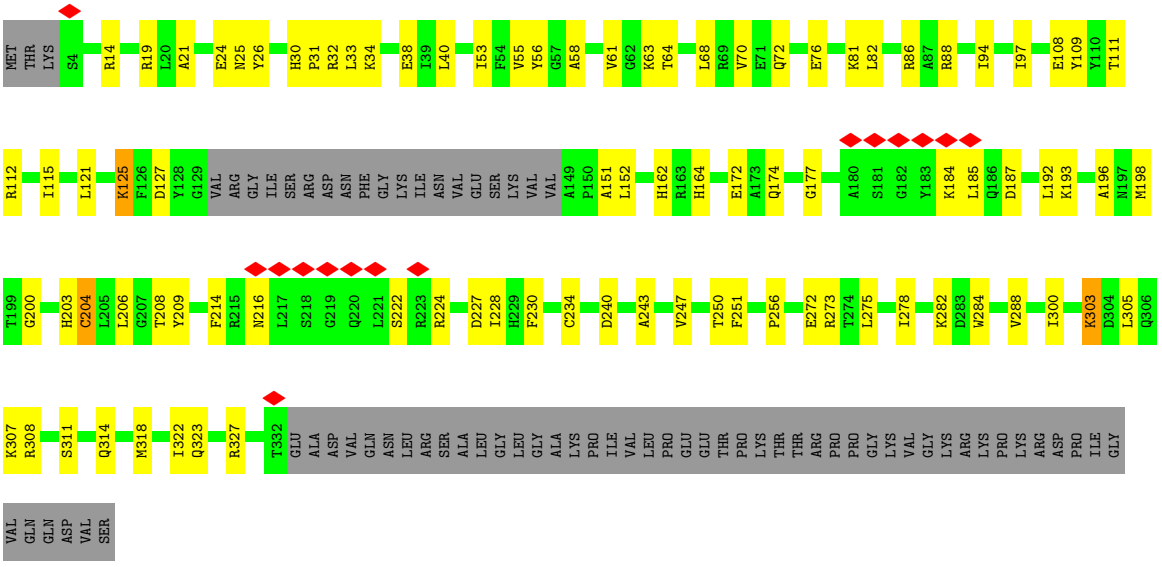
• Molecule 8: Non-target DNA strand



• Molecule 9: TniQ

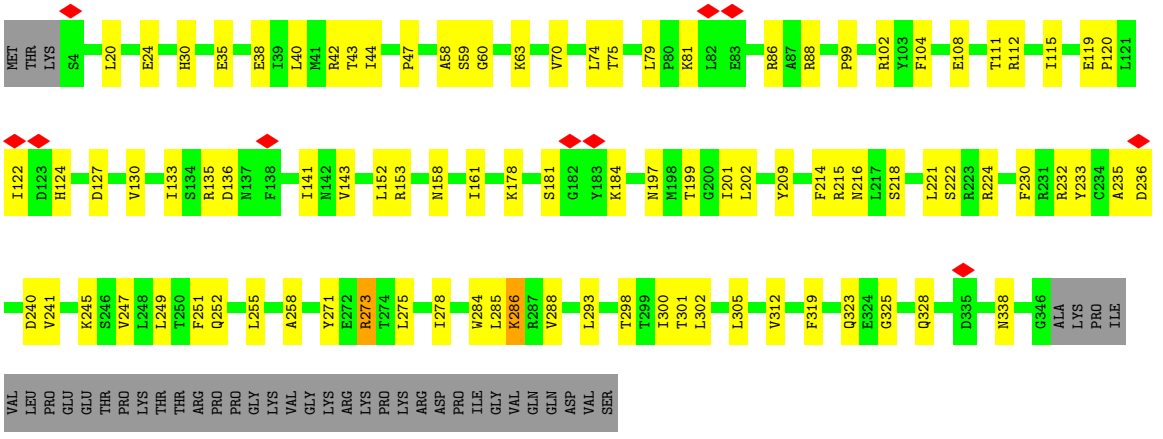


• Molecule 10: TnsC



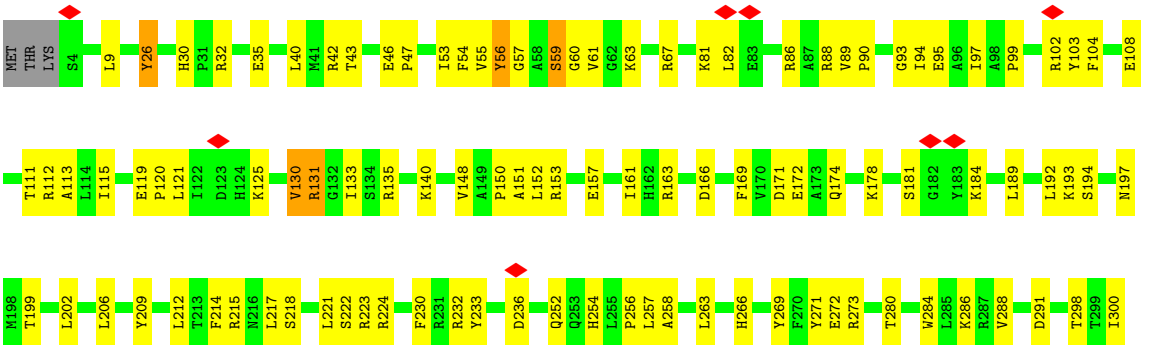
• Molecule 10: TnsC

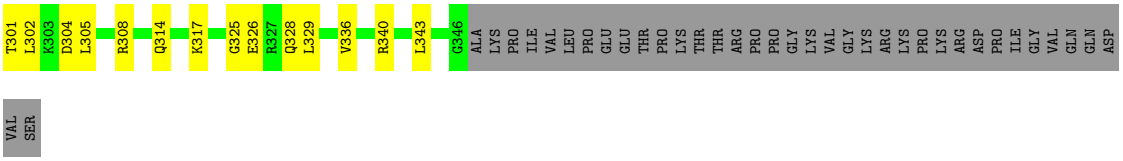
Chain R:



• Molecule 10: TnsC

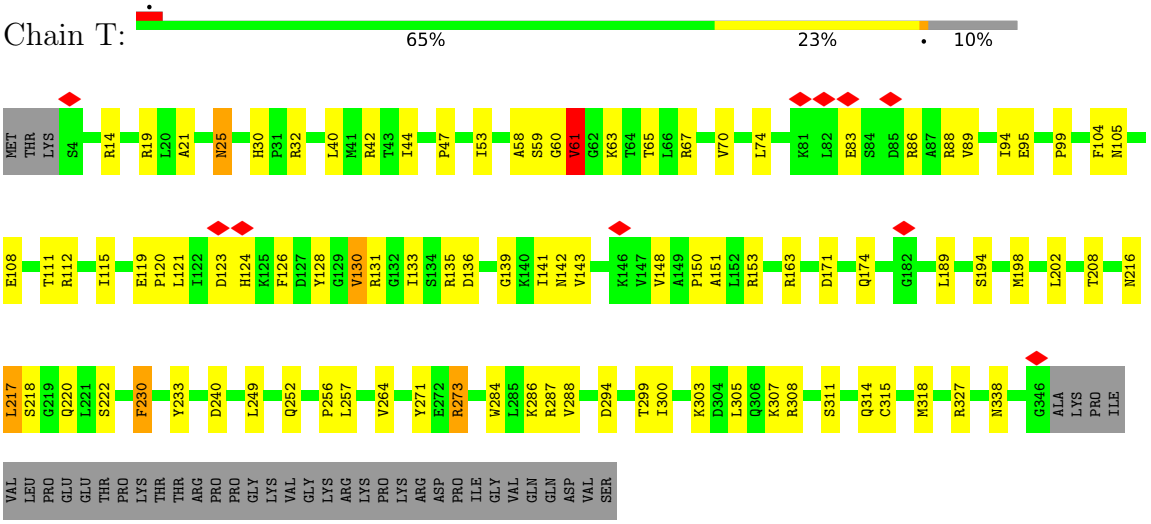
Chain S:





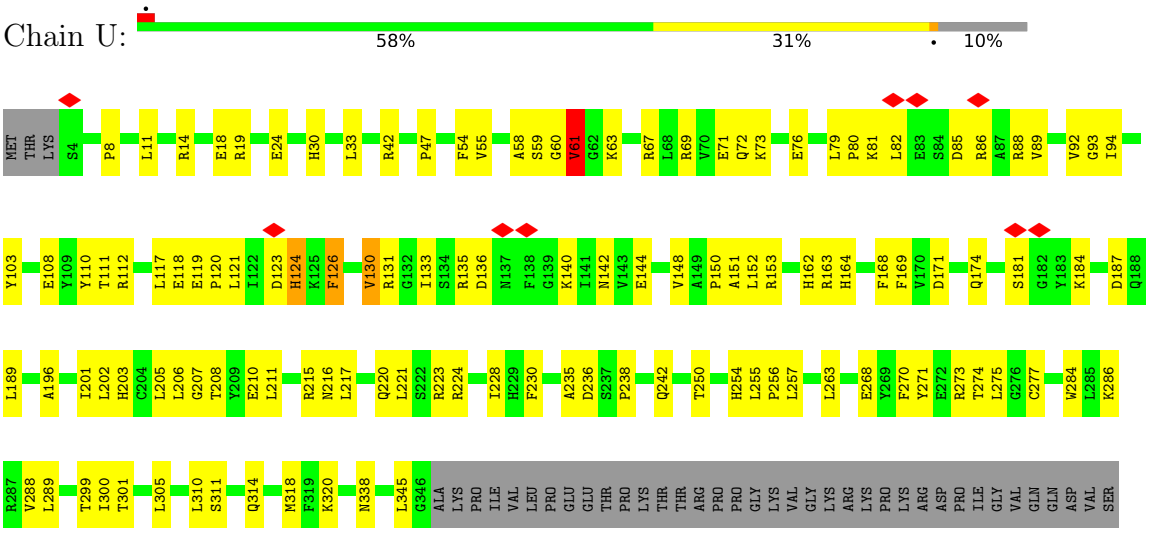
• Molecule 10: TnsC

Chain T:



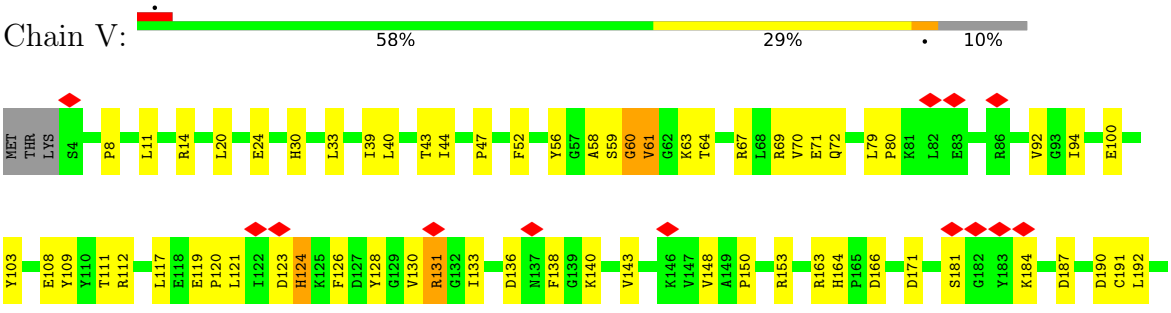
• Molecule 10: TnsC

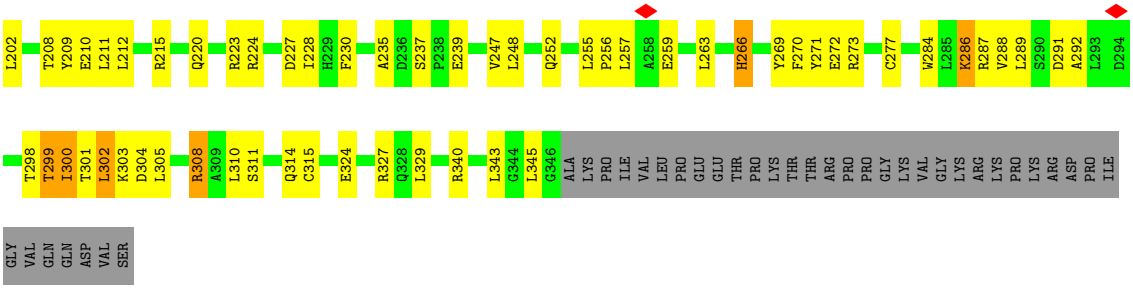
Chain U:



• Molecule 10: TnsC

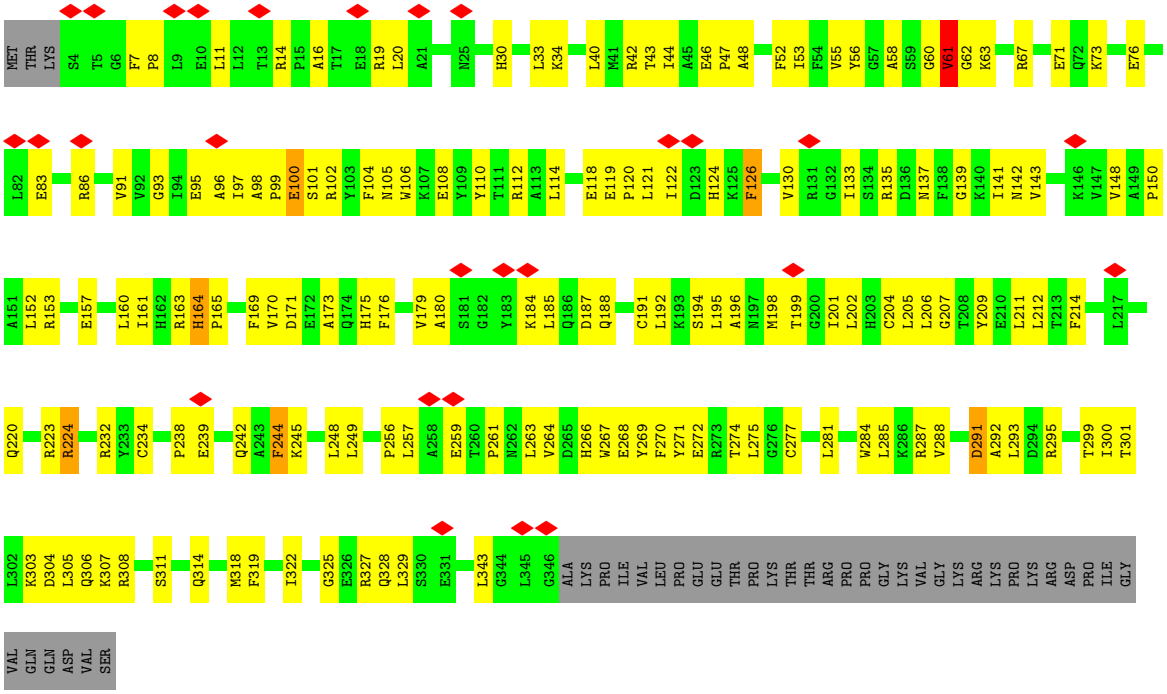
Chain V:





• Molecule 10: TnsC

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	35.722	Depositor
Minimum map value	-5.499	Depositor
Average map value	0.113	Depositor
Map value standard deviation	0.968	Depositor
Recommended contour level	4.6	Depositor
Map size (Å)	404.73602, 404.73602, 404.73602	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/1788	0.56	0/2422
2	B	0.26	0/1735	0.56	0/2341
3	C	0.26	0/2384	0.49	0/3220
3	D	0.26	0/2384	0.48	0/3220
3	E	0.25	0/2391	0.45	0/3231
3	F	0.25	0/2384	0.51	0/3220
3	G	0.25	0/2384	0.49	0/3220
3	H	0.26	0/2384	0.49	0/3220
4	I	0.26	0/4249	0.46	0/5741
5	J	0.28	0/938	0.49	0/1258
5	K	0.27	0/938	0.44	0/1258
5	L	0.27	0/938	0.44	0/1258
6	M	0.28	0/1500	0.86	0/2335
7	N	0.51	0/1941	0.93	0/2992
8	O	0.46	0/1200	0.89	0/1848
9	P	0.25	0/2673	0.51	0/3607
10	Q	0.24	0/2562	0.50	0/3468
10	R	0.25	0/2812	0.50	0/3805
10	S	0.25	0/2812	0.50	0/3805
10	T	0.25	0/2812	0.50	0/3805
10	U	0.25	0/2812	0.52	0/3805
10	V	0.25	0/2812	0.54	0/3805
10	W	0.26	0/2812	0.53	0/3805
All	All	0.28	0/51645	0.55	0/70689

There are no bond length outliers.

There are no bond angle outliers.

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	1745	0	1772	47	0
2	B	1702	0	1735	54	0
3	C	2323	0	2249	66	0
3	D	2323	0	2249	79	0
3	E	2330	0	2255	76	0
3	F	2323	0	2249	81	0
3	G	2323	0	2249	68	0
3	H	2323	0	2249	72	0
4	I	4147	0	4143	199	0
5	J	917	0	925	38	0
5	K	917	0	925	39	0
5	L	917	0	925	27	0
6	M	1342	0	675	59	0
7	N	1734	0	964	69	0
8	O	1070	0	588	37	0
9	P	2618	0	2687	78	0
10	Q	2508	0	2514	63	0
10	R	2756	0	2772	58	0
10	S	2756	0	2773	73	0
10	T	2756	0	2772	68	0
10	U	2756	0	2773	86	0
10	V	2756	0	2773	97	0
10	W	2756	0	2772	133	0
11	Q	31	0	12	1	0
11	R	31	0	12	1	0
11	S	31	0	12	1	0
11	T	31	0	12	2	0
11	U	31	0	12	2	0
11	V	31	0	12	4	0
11	W	31	0	12	1	0
12	Q	1	0	0	0	0
12	R	1	0	0	0	0
12	S	1	0	0	0	0
12	T	1	0	0	0	0
12	U	1	0	0	0	0
12	V	1	0	0	0	0
12	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50322	0	48072	1492	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 15.

All (1492) 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:I:366:LEU:HD13	4:I:379:LEU:HD12	1.35	1.08
4:I:366:LEU:HD22	4:I:379:LEU:HB2	1.48	0.96
5:J:49:ARG:HH12	5:K:71:ARG:HG3	1.34	0.93
4:I:137:VAL:HG13	4:I:335:LYS:HA	1.51	0.90
7:N:44:DA:H4'	7:N:45:DA:O5'	1.74	0.87
10:U:79:LEU:HG	10:U:80:PRO:HD3	1.60	0.83
3:H:279:VAL:HB	3:H:300:ARG:HD2	1.59	0.83
4:I:336:GLN:HB3	4:I:338:PHE:CE2	2.15	0.81
2:B:199:GLY:HA3	6:M:61:G:H5'	1.63	0.80
2:B:200:LYS:HB3	2:B:203:MET:HB2	1.62	0.80
10:V:292:ALA:HB2	10:V:300:ILE:HG23	1.63	0.80
10:R:24:GLU:HB3	10:R:286:LYS:HE3	1.64	0.80
9:P:32:PRO:HB3	9:P:225:SER:HB3	1.64	0.79
5:K:34:GLU:HG2	5:K:35:GLU:HG3	1.65	0.78
6:M:23:U:O4	6:M:24:A:N6	2.16	0.78
6:M:35:U:O4	6:M:36:A:N6	2.16	0.78
10:V:298:THR:HG23	10:V:299:THR:CG2	2.14	0.78
8:O:60:DA:H2'	8:O:61:DG:C8	2.18	0.77
4:I:377:ASN:HA	4:I:380:PHE:CD2	2.19	0.77
4:I:302:LEU:HD21	4:I:305:ILE:HD11	1.65	0.76
4:I:332:ILE:HG12	4:I:337:ILE:HG23	1.68	0.76
10:W:185:LEU:HB2	10:W:214:PHE:HE1	1.51	0.76
2:B:38:ILE:HD13	2:B:92:PHE:HB3	1.67	0.75
3:C:30:ASN:HD22	3:C:56:GLY:H	1.32	0.75
10:V:257:LEU:HD21	10:V:299:THR:HA	1.68	0.75
10:U:76:GLU:HA	10:U:79:LEU:HD23	1.69	0.75
5:J:55:CYS:SG	5:J:98:ARG:NH1	2.60	0.75
4:I:329:TYR:HB3	4:I:340:LYS:HB3	1.70	0.74
10:W:244:PHE:HE1	10:W:281:LEU:HD22	1.52	0.74
10:R:288:VAL:HG12	10:R:300:ILE:HD12	1.71	0.73
1:A:165:ARG:HG2	1:A:190:TYR:CE2	2.23	0.73
4:I:344:ILE:HD13	4:I:347:LEU:HD12	1.68	0.73
4:I:46:ARG:HH21	4:I:51:SER:HA	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ARG:NH1	6:M:37:A:OP1	2.22	0.73
9:P:58:GLY:HA3	10:Q:121:LEU:HD11	1.71	0.72
3:D:55:VAL:HB	3:D:145:ALA:HB3	1.70	0.72
9:P:77:ASN:O	9:P:80:HIS:ND1	2.21	0.72
4:I:344:ILE:HG13	4:I:386:PHE:HZ	1.55	0.72
4:I:348:ILE:HG12	4:I:362:PHE:CZ	2.25	0.72
5:K:110:PRO:HD3	5:L:79:ASN:HD22	1.54	0.72
1:A:76:ARG:NH1	7:N:57:DA:OP2	2.23	0.71
3:H:61:ARG:NH1	6:M:7:A:OP1	2.23	0.71
4:I:258:HIS:CG	4:I:339:ILE:HD12	2.24	0.71
3:D:165:LYS:HE3	6:M:40:G:H21	1.55	0.71
4:I:11:LEU:HD21	4:I:197:GLU:HB2	1.71	0.71
4:I:138:GLU:H	4:I:335:LYS:HG2	1.55	0.71
2:B:153:ARG:HD3	2:B:157:THR:HB	1.71	0.71
3:D:16:LEU:HD23	3:D:186:ILE:HD11	1.70	0.71
10:W:95:GLU:O	10:W:112:ARG:NH1	2.23	0.71
3:E:186:ILE:HG21	3:E:200:MET:HE1	1.72	0.71
3:H:55:VAL:HB	3:H:145:ALA:HB3	1.71	0.71
10:W:261:PRO:HB3	10:W:300:ILE:H	1.55	0.71
3:H:292:PRO:HA	3:H:295:LYS:HE3	1.73	0.71
10:Q:19:ARG:HG2	10:Q:256:PRO:HB2	1.73	0.71
10:V:259:GLU:OE1	10:V:299:THR:CG2	2.39	0.71
4:I:379:LEU:HA	4:I:386:PHE:HE2	1.55	0.70
10:U:174:GLN:HB2	10:U:210:GLU:HG2	1.72	0.70
3:G:149:THR:HB	3:G:178:THR:HG23	1.73	0.70
10:V:24:GLU:HB2	10:V:286:LYS:HE3	1.74	0.70
3:D:61:ARG:NH1	6:M:31:C:OP1	2.25	0.70
3:F:136:ARG:O	3:G:84:HIS:NE2	2.24	0.70
4:I:333:LYS:HB2	4:I:336:GLN:HB2	1.71	0.70
7:N:1:DA:OP2	9:P:190:ARG:NH1	2.26	0.69
10:W:248:LEU:HB3	10:W:264:VAL:HG12	1.74	0.69
3:H:155:VAL:HA	3:H:174:GLU:HA	1.74	0.69
3:H:251:GLU:N	3:H:251:GLU:OE2	2.26	0.69
9:P:84:ASN:HA	9:P:87:ALA:HB2	1.72	0.69
10:V:121:LEU:HD23	10:V:123:ASP:H	1.57	0.69
3:C:84:HIS:CE1	6:M:41:U:H4'	2.27	0.69
10:V:259:GLU:OE1	10:V:299:THR:HG21	1.92	0.69
8:O:11:DG:H2'	8:O:11:DG:N3	2.08	0.69
10:S:95:GLU:OE1	10:S:95:GLU:N	2.26	0.69
3:D:140:LEU:HA	3:D:186:ILE:HG22	1.75	0.69
10:R:124:HIS:O	10:R:135:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:60:GLY:C	10:V:277:CYS:HB3	2.13	0.68
5:J:21:ALA:HB2	5:J:75:ASN:HD21	1.58	0.68
9:P:79:SER:HB2	9:P:84:ASN:HB2	1.75	0.68
8:O:11:DG:H2"	8:O:12:DA:C8	2.29	0.68
3:F:215:ASN:ND2	6:M:25:A:OP2	2.27	0.68
10:T:153:ARG:NH2	10:T:194:SER:OG	2.25	0.68
3:G:61:ARG:NH1	6:M:13:A:OP1	2.27	0.67
3:G:136:ARG:HH21	3:G:192:LYS:HG2	1.59	0.67
4:I:373:GLU:HG2	4:I:376:PHE:HD2	1.59	0.67
4:I:13:LEU:HD22	4:I:23:ARG:HG3	1.75	0.67
9:P:18:ARG:HH21	10:Q:88:ARG:H	1.42	0.67
10:V:298:THR:HG23	10:V:299:THR:HG23	1.75	0.67
3:D:225:SER:HA	3:D:276:GLY:HA3	1.77	0.67
4:I:221:LEU:HG	4:I:338:PHE:HD1	1.60	0.67
3:C:309:LEU:O	3:C:313:ILE:HG12	1.95	0.66
4:I:142:LYS:HD2	8:O:11:DG:H3'	1.76	0.66
3:H:186:ILE:HD13	3:H:197:ILE:HD13	1.78	0.66
10:R:47:PRO:HB3	10:R:202:LEU:HD22	1.76	0.66
1:A:142:ASP:OD1	3:H:61:ARG:NE	2.27	0.66
3:C:48:ASN:HB2	3:C:50:LYS:HE2	1.77	0.66
4:I:222:LYS:HE2	4:I:333:LYS:HD2	1.77	0.66
3:E:198:LEU:HD22	3:E:310:LYS:HG2	1.77	0.66
3:H:102:ASP:OD2	3:H:196:ARG:NH1	2.26	0.66
10:W:288:VAL:HG21	10:W:305:LEU:HA	1.78	0.66
3:D:49:GLY:HA2	3:E:248:LYS:HB2	1.78	0.66
7:N:22:DT:H2"	7:N:23:DA:H5'	1.76	0.66
3:E:156:LYS:NZ	3:E:157:LEU:O	2.29	0.66
4:I:379:LEU:HA	4:I:386:PHE:CE2	2.31	0.66
1:A:109:GLU:O	1:A:111:LYS:NZ	2.29	0.65
3:E:61:ARG:NH1	6:M:25:A:OP1	2.29	0.65
9:P:56:VAL:HA	9:P:60:ILE:HD13	1.78	0.65
10:V:256:PRO:HD2	10:V:289:LEU:HD11	1.79	0.65
3:D:186:ILE:HG21	3:D:200:MET:HE1	1.78	0.65
3:E:148:LEU:HD11	3:E:243:GLU:HA	1.76	0.65
10:W:153:ARG:NH1	10:W:191:CYS:SG	2.69	0.65
5:K:109:LYS:HD3	5:L:74:LEU:HA	1.79	0.65
9:P:115:ARG:HB2	9:P:120:LEU:HD11	1.79	0.65
10:T:53:ILE:HD11	10:T:202:LEU:HD21	1.79	0.65
2:B:160:ARG:HB2	6:M:50:C:C4	2.32	0.65
10:T:115:ILE:HD13	10:T:141:ILE:HB	1.79	0.65
3:G:102:ASP:OD2	3:G:196:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:189:LEU:HD23	10:T:217:LEU:HD21	1.77	0.64
5:L:9:LYS:O	5:L:13:ILE:HG12	1.98	0.64
4:I:112:VAL:HG13	4:I:113:PHE:HD1	1.62	0.64
5:J:77:TYR:O	5:J:81:HIS:ND1	2.27	0.64
3:E:244:TYR:CE2	3:E:246:ASP:HB2	2.32	0.64
3:G:31:HIS:HA	3:G:41:LEU:HA	1.78	0.64
10:W:100:GLU:O	10:W:102:ARG:NH1	2.31	0.64
10:W:274:THR:HG21	10:W:281:LEU:HB2	1.80	0.64
3:C:37:ASN:ND2	9:P:255:GLU:OE1	2.29	0.64
3:F:246:ASP:OD2	3:F:253:LYS:NZ	2.29	0.64
3:G:147:SER:HB2	3:G:178:THR:HG21	1.78	0.64
3:E:49:GLY:HA2	3:F:248:LYS:HB2	1.80	0.64
10:W:153:ARG:NH2	10:W:194:SER:OG	2.31	0.64
4:I:75:ILE:HD12	4:I:153:ALA:HB2	1.79	0.64
10:R:215:ARG:NH1	10:R:328:GLN:O	2.29	0.64
10:V:187:ASP:HA	10:V:190:ASP:HB2	1.79	0.64
2:B:51:HIS:HB3	2:B:72:LYS:HB3	1.78	0.63
5:K:12:LEU:HD22	5:L:83:GLU:HG2	1.79	0.63
7:N:12:DT:H2"	7:N:13:DA:C8	2.33	0.63
3:C:161:SER:O	7:N:21:DC:N4	2.32	0.63
5:J:100:TRP:HA	5:J:103:LEU:HD12	1.79	0.63
10:W:311:SER:HB3	10:W:314:GLN:HG3	1.79	0.63
3:D:170:LEU:HD22	7:N:25:DG:C5	2.34	0.63
2:B:189:SER:O	2:B:193:GLN:HG3	1.98	0.63
4:I:366:LEU:O	4:I:370:ASP:HB3	1.98	0.63
10:W:153:ARG:CZ	10:W:195:LEU:HG	2.29	0.63
10:R:60:GLY:N	11:R:600:ATP:O2B	2.32	0.63
10:T:148:VAL:HG13	10:T:150:PRO:HD2	1.79	0.63
5:J:8:ASP:HB3	5:K:87:LEU:HD11	1.80	0.63
3:C:77:ARG:NH2	6:M:38:A:OP2	2.31	0.62
4:I:384:GLU:O	4:I:388:ILE:HG12	1.99	0.62
10:S:215:ARG:NH1	10:S:328:GLN:O	2.31	0.62
3:C:143:ASN:ND2	3:D:218:ASN:O	2.33	0.62
4:I:351:ASN:HA	4:I:354:LYS:HD2	1.79	0.62
10:Q:72:GLN:NE2	10:Q:76:GLU:OE2	2.32	0.62
10:T:47:PRO:HB3	10:T:202:LEU:HD22	1.81	0.62
10:R:181:SER:HB3	10:R:184:LYS:HB2	1.81	0.62
10:S:9:LEU:HD23	10:S:9:LEU:H	1.64	0.62
3:D:24:TYR:CD1	3:D:250:LYS:HB3	2.35	0.62
3:F:266:GLN:HE22	3:G:302:ARG:HH22	1.48	0.62
1:A:77:PHE:HB2	4:I:183:HIS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:239:SER:O	3:F:241:CYS:N	2.33	0.62
10:V:60:GLY:N	11:V:600:ATP:O2B	2.32	0.62
4:I:343:PRO:HG2	4:I:375:LEU:HD22	1.82	0.61
10:V:153:ARG:NH1	10:V:191:CYS:SG	2.73	0.61
3:D:42:GLN:HG3	3:D:54:PHE:HB2	1.80	0.61
3:H:159:ALA:HB2	3:H:170:LEU:HD23	1.82	0.61
5:J:102:LEU:HD22	5:K:70:VAL:HG21	1.81	0.61
10:S:99:PRO:HD2	10:S:178:LYS:HD2	1.83	0.61
3:C:181:GLN:NE2	3:C:242:PHE:O	2.31	0.61
3:F:143:ASN:OD1	3:G:218:ASN:N	2.33	0.61
10:Q:21:ALA:HA	10:Q:24:GLU:HG2	1.81	0.61
10:W:261:PRO:HG3	10:W:300:ILE:HG12	1.82	0.61
1:A:189:ARG:NH2	4:I:18:THR:OG1	2.32	0.61
4:I:358:TRP:CE3	4:I:359:TRP:HD1	2.19	0.61
10:W:209:TYR:HD2	10:W:325:GLY:HA3	1.65	0.61
3:D:215:ASN:ND2	6:M:37:A:OP2	2.34	0.61
10:T:294:ASP:OD2	10:U:42:ARG:NH1	2.33	0.61
10:U:144:GLU:N	10:U:144:GLU:OE2	2.33	0.61
3:C:16:LEU:HD23	3:C:186:ILE:HD12	1.82	0.61
3:F:33:ILE:HG13	4:I:442:TYR:CZ	2.35	0.61
10:Q:314:GLN:O	10:Q:318:MET:HG2	1.99	0.61
10:U:208:THR:HG23	10:U:210:GLU:H	1.66	0.61
5:L:48:LEU:HD22	5:L:105:ILE:HD11	1.82	0.61
10:S:153:ARG:NH2	10:S:194:SER:OG	2.34	0.61
10:V:298:THR:O	10:V:299:THR:HG22	2.01	0.61
3:D:40:ILE:H	3:D:40:ILE:HD12	1.66	0.61
4:I:348:ILE:HG23	4:I:358:TRP:HB3	1.82	0.61
10:W:47:PRO:HB3	10:W:202:LEU:HD22	1.82	0.61
3:G:205:MET:HG3	3:G:306:ILE:HG13	1.83	0.61
10:W:160:LEU:HD12	10:W:201:ILE:HD13	1.81	0.61
2:B:136:GLN:NE2	2:B:140:ASP:OD1	2.33	0.60
10:V:215:ARG:NH1	10:V:227:ASP:OD2	2.34	0.60
3:H:254:LEU:HD13	3:H:278:ILE:HG12	1.84	0.60
3:E:134:ASN:H	3:E:134:ASN:HD22	1.48	0.60
3:F:61:ARG:NH2	3:F:140:LEU:O	2.33	0.60
3:G:93:PHE:HE2	3:G:108:LEU:HB3	1.66	0.60
4:I:129:GLU:HB3	4:I:136:GLN:HB3	1.83	0.60
10:U:121:LEU:HB3	10:U:124:HIS:HE1	1.67	0.60
10:V:298:THR:C	10:V:299:THR:HG22	2.21	0.60
3:F:262:VAL:HG11	3:F:293:LEU:HD13	1.82	0.60
9:P:172:GLN:NE2	9:P:173:ARG:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:30:HIS:CD2	10:Q:33:LEU:H	2.19	0.60
10:Q:288:VAL:HG21	10:Q:305:LEU:HD23	1.83	0.60
10:V:184:LYS:HA	10:V:187:ASP:OD1	2.02	0.60
2:B:162:GLN:HE21	2:B:173:LYS:HD2	1.66	0.60
2:B:213:ARG:HH12	6:M:47:A:N6	2.00	0.60
4:I:168:TYR:HB3	4:I:193:GLU:HB3	1.84	0.60
4:I:232:VAL:HG12	4:I:287:VAL:HG22	1.84	0.60
5:J:9:LYS:O	5:J:13:ILE:HG23	2.02	0.60
10:S:214:PHE:HA	10:S:217:LEU:HD23	1.83	0.60
10:R:40:LEU:HD23	10:R:70:VAL:HG21	1.83	0.59
10:R:258:ALA:HB3	10:R:298:THR:HB	1.84	0.59
10:S:258:ALA:HB3	10:S:298:THR:HB	1.84	0.59
10:U:24:GLU:HG2	10:U:286:LYS:HD2	1.84	0.59
10:U:67:ARG:O	10:U:71:GLU:HG3	2.01	0.59
10:W:83:GLU:O	10:W:86:ARG:NH2	2.34	0.59
3:D:33:ILE:HG13	5:K:54:TYR:CE2	2.37	0.59
10:V:47:PRO:HB3	10:V:202:LEU:HD22	1.83	0.59
10:W:122:ILE:HD12	10:W:135:ARG:HH11	1.66	0.59
4:I:101:GLN:NE2	4:I:252:LEU:O	2.35	0.59
4:I:484:GLU:O	4:I:488:TRP:HD1	1.86	0.59
5:L:58:GLU:N	5:L:58:GLU:OE1	2.35	0.59
10:R:108:GLU:OE2	10:R:112:ARG:NH1	2.34	0.59
10:U:181:SER:HB3	10:U:184:LYS:HB2	1.84	0.59
10:V:59:SER:HA	11:V:600:ATP:O2B	2.02	0.59
5:K:9:LYS:O	5:K:13:ILE:HG23	2.03	0.59
3:C:62:TRP:CZ3	6:M:38:A:C2	2.90	0.59
3:D:261:GLU:OE1	3:E:302:ARG:NH2	2.35	0.59
3:F:108:LEU:H	3:F:135:GLN:HE21	1.51	0.59
4:I:112:VAL:HG21	4:I:231:VAL:HG21	1.83	0.59
3:C:154:ALA:H	9:P:328:LYS:HB2	1.66	0.59
5:K:101:SER:O	5:K:105:ILE:HG12	2.02	0.59
10:T:133:ILE:HG12	10:T:143:VAL:HG22	1.84	0.59
4:I:359:TRP:CZ2	4:I:386:PHE:HB3	2.38	0.59
10:S:93:GLY:HA2	10:S:169:PHE:HB2	1.84	0.59
10:W:269:TYR:CE2	10:W:284:TRP:HH2	2.20	0.59
2:B:85:PRO:O	9:P:245:ARG:NH1	2.35	0.59
3:D:61:ARG:NH2	3:D:140:LEU:O	2.36	0.59
5:K:57:ASP:OD1	5:K:94:TRP:NE1	2.36	0.59
3:H:29:LEU:HD12	3:H:55:VAL:HG21	1.85	0.59
10:U:196:ALA:HB2	10:U:203:HIS:HD2	1.68	0.59
3:D:136:ARG:O	3:E:84:HIS:NE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:255:LYS:NZ	4:I:328:ASN:O	2.32	0.58
4:I:266:GLY:HA3	4:I:308:ILE:HD12	1.85	0.58
7:N:6:DT:H3	8:O:60:DA:H2	1.51	0.58
10:S:172:GLU:OE1	10:S:174:GLN:NE2	2.31	0.58
3:E:28:SER:OG	3:E:174:GLU:O	2.21	0.58
3:E:134:ASN:HD22	3:E:134:ASN:N	2.02	0.58
7:N:23:DA:H4'	7:N:24:DC:OP1	2.03	0.58
4:I:379:LEU:O	4:I:383:ARG:N	2.37	0.58
10:V:121:LEU:O	10:V:124:HIS:ND1	2.32	0.58
10:R:275:LEU:HD22	10:S:343:LEU:HD11	1.86	0.58
10:T:288:VAL:HG21	10:T:305:LEU:HD13	1.86	0.58
10:W:165:PRO:HG2	10:W:201:ILE:HG12	1.85	0.58
3:E:225:SER:HA	3:E:276:GLY:HA3	1.85	0.58
9:P:287:TYR:HB2	9:P:293:ILE:HD11	1.85	0.58
10:U:82:LEU:O	10:U:86:ARG:NH1	2.35	0.58
9:P:113:ASP:OD1	9:P:113:ASP:N	2.36	0.58
10:Q:172:GLU:OE1	10:Q:174:GLN:NE2	2.36	0.58
3:C:193:ASP:HB3	3:C:196:ARG:HG3	1.85	0.58
4:I:35:ARG:HA	4:I:38:LYS:HD2	1.86	0.58
4:I:221:LEU:HG	4:I:338:PHE:CD1	2.39	0.58
10:R:252:GLN:HA	10:R:255:LEU:HD12	1.86	0.58
3:E:244:TYR:HE2	3:E:246:ASP:HB2	1.69	0.57
4:I:187:GLN:OE1	4:I:187:GLN:N	2.36	0.57
10:Q:303:LYS:HG3	10:Q:307:LYS:HE3	1.86	0.57
10:S:272:GLU:OE2	10:S:273:ARG:NH1	2.36	0.57
10:T:19:ARG:HG2	10:T:256:PRO:HB2	1.86	0.57
10:T:21:ALA:O	10:T:25:ASN:ND2	2.37	0.57
3:D:42:GLN:O	3:D:54:PHE:N	2.34	0.57
3:E:15:TYR:CE1	3:E:187:ASP:HB3	2.39	0.57
1:A:32:PRO:HB3	1:A:174:PRO:HD2	1.86	0.57
5:L:71:ARG:NH2	7:N:33:DG:OP1	2.38	0.57
10:W:19:ARG:HG2	10:W:256:PRO:HB2	1.86	0.57
3:E:152:ASP:OD1	3:E:153:GLY:N	2.34	0.57
3:H:179:ARG:NH1	3:H:250:LYS:O	2.38	0.57
4:I:344:ILE:O	4:I:348:ILE:HG13	2.04	0.57
1:A:146:LYS:HD3	3:H:239:SER:HB3	1.86	0.57
3:C:84:HIS:NE2	6:M:41:U:H4'	2.19	0.57
3:D:160:LYS:HD3	6:M:37:A:H1'	1.85	0.57
8:O:74:DT:H2"	8:O:75:DA:C8	2.39	0.57
10:V:181:SER:HB2	10:V:184:LYS:HB2	1.85	0.57
3:F:237:TYR:OH	3:G:302:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:112:ARG:NH2	10:S:157:GLU:OE1	2.38	0.57
10:R:232:ARG:NH1	10:R:233:TYR:O	2.38	0.57
10:T:14:ARG:O	10:T:19:ARG:NH2	2.38	0.57
2:B:142:LEU:HD22	2:B:195:GLN:HG3	1.87	0.57
3:D:226:LEU:N	3:D:275:GLY:O	2.37	0.57
3:G:299:TYR:HB2	3:G:305:MET:HB2	1.84	0.57
8:O:78:DT:H2"	8:O:79:DA:C8	2.40	0.57
1:A:73:GLN:N	6:M:9:G:OP2	2.32	0.57
3:E:33:ILE:HG22	3:E:40:ILE:HD11	1.85	0.56
3:H:16:LEU:HD21	3:H:201:ILE:HD11	1.85	0.56
3:H:198:LEU:HD21	3:H:314:LYS:HD2	1.87	0.56
6:M:11:G:O6	6:M:12:A:N6	2.38	0.56
10:U:271:TYR:CD1	10:V:345:LEU:HD21	2.40	0.56
2:B:135:VAL:O	2:B:139:MET:HB2	2.05	0.56
3:E:148:LEU:HG	3:E:244:TYR:HD1	1.70	0.56
7:N:-16:DC:H2"	7:N:-15:DG:C8	2.40	0.56
2:B:153:ARG:HB2	2:B:155:ASP:OD1	2.05	0.56
10:V:52:PHE:HZ	10:V:192:LEU:HB3	1.70	0.56
10:W:7:PHE:HD2	10:W:11:LEU:HD12	1.70	0.56
9:P:140:PRO:HG2	9:P:175:ILE:HD12	1.86	0.56
10:V:298:THR:HG23	10:V:299:THR:HG22	1.85	0.56
10:W:97:ILE:HD11	10:W:173:ALA:HA	1.88	0.56
3:E:54:PHE:HE1	3:E:146:VAL:HG23	1.69	0.56
4:I:159:ALA:O	4:I:162:GLN:NE2	2.38	0.56
7:N:18:DT:H2"	7:N:19:DA:C8	2.40	0.56
3:E:55:VAL:HB	3:E:145:ALA:HB3	1.88	0.56
3:E:158:GLY:HA3	3:E:171:HIS:CE1	2.40	0.56
3:F:37:ASN:HB3	3:F:171:HIS:HA	1.86	0.56
5:J:109:LYS:HD3	5:K:74:LEU:HA	1.88	0.56
10:R:273:ARG:HB2	10:R:284:TRP:CZ3	2.40	0.56
9:P:69:ASP:HB3	9:P:72:GLU:HB3	1.88	0.56
10:S:148:VAL:HG13	10:S:150:PRO:HD2	1.86	0.56
3:H:91:GLU:OE2	3:H:91:GLU:N	2.30	0.56
10:T:135:ARG:HD2	10:T:139:GLY:HA2	1.86	0.56
3:F:52:HIS:ND1	3:F:147:SER:O	2.36	0.56
4:I:292:LYS:HB3	4:I:297:SER:HB2	1.87	0.56
3:E:228:PHE:HB2	3:E:273:TRP:HB2	1.88	0.56
3:G:84:HIS:O	3:H:163:ARG:N	2.35	0.56
10:Q:111:THR:HB	10:Q:152:LEU:HD21	1.86	0.56
10:S:288:VAL:HG12	10:S:300:ILE:HD12	1.87	0.56
10:W:291:ASP:CG	10:W:308:ARG:HE	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:LEU:HD23	3:C:221:PHE:HB3	1.88	0.55
3:E:299:TYR:HB2	3:E:305:MET:HB2	1.88	0.55
6:M:38:A:O2'	6:M:39:C:H4'	2.06	0.55
10:V:311:SER:H	10:V:314:GLN:HE21	1.52	0.55
10:W:245:LYS:O	10:W:249:LEU:HG	2.06	0.55
3:H:136:ARG:HH21	3:H:192:LYS:HG2	1.72	0.55
2:B:203:MET:HE3	2:B:203:MET:HA	1.87	0.55
3:G:159:ALA:HA	3:G:170:LEU:HA	1.89	0.55
3:H:225:SER:HA	3:H:276:GLY:HA3	1.89	0.55
4:I:253:GLU:HG3	4:I:255:LYS:H	1.71	0.55
7:N:56:DC:H2"	7:N:57:DA:C8	2.41	0.55
3:E:137:MET:HB3	3:E:190:HIS:NE2	2.22	0.55
6:M:9:G:H1'	6:M:10:A:C8	2.42	0.55
7:N:2:DT:H2"	7:N:3:DA:C8	2.41	0.55
10:U:171:ASP:HA	10:U:206:LEU:HB2	1.89	0.55
10:W:58:ALA:O	10:W:63:LYS:NZ	2.40	0.55
2:B:116:TYR:HE2	2:B:213:ARG:HG3	1.72	0.55
3:D:194:PHE:HB3	3:D:317:LEU:HD13	1.87	0.55
10:R:236:ASP:OD1	10:R:236:ASP:N	2.38	0.55
4:I:142:LYS:NZ	8:O:11:DG:H5'	2.22	0.55
8:O:59:DT:H1'	8:O:60:DA:O4'	2.07	0.55
9:P:26:PRO:HB3	9:P:117:LEU:HD11	1.88	0.55
10:W:8:PRO:HD2	10:W:11:LEU:HD11	1.88	0.55
4:I:152:PHE:HD2	4:I:203:LEU:HG	1.72	0.55
10:R:197:ASN:OD1	10:R:224:ARG:NH2	2.39	0.55
1:A:132:ARG:NH1	3:H:15:TYR:OH	2.40	0.55
9:P:116:PHE:HB3	9:P:232:PRO:HG3	1.88	0.55
10:R:215:ARG:HG2	10:R:216:ASN:OD1	2.07	0.55
10:V:288:VAL:HG21	10:V:305:LEU:HD23	1.89	0.55
1:A:178:ASP:HB2	1:A:184:ASN:HB2	1.88	0.55
10:U:14:ARG:HB2	10:U:18:GLU:OE1	2.07	0.55
3:G:166:ASP:OD1	3:G:167:SER:N	2.34	0.55
5:J:23:LYS:HD2	5:J:111:LYS:HG2	1.89	0.55
5:K:71:ARG:NH2	7:N:27:DT:OP1	2.34	0.55
10:Q:64:THR:O	10:Q:68:LEU:HG	2.06	0.55
10:U:67:ARG:HB2	10:U:206:LEU:HD11	1.88	0.55
3:C:77:ARG:NE	3:C:86:ASN:OD1	2.38	0.54
3:C:83:GLU:HB2	3:C:85:ILE:HG22	1.89	0.54
4:I:24:VAL:HG11	4:I:233:ILE:HG22	1.89	0.54
4:I:475:LEU:HD11	5:L:8:ASP:HB3	1.89	0.54
10:W:106:TRP:NE1	10:W:188:GLN:OE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ARG:NH2	3:C:190:HIS:O	2.32	0.54
3:G:26:LEU:HD23	3:G:177:ALA:HB2	1.89	0.54
1:A:42:SER:HA	6:M:1:U:C2	2.43	0.54
4:I:117:ASN:ND2	8:O:9:DT:O3'	2.41	0.54
10:T:271:TYR:HD2	10:U:345:LEU:HD11	1.72	0.54
3:G:29:LEU:HD21	3:G:219:TYR:HB3	1.89	0.54
8:O:49:DT:H2"	8:O:50:DA:C8	2.42	0.54
10:V:308:ARG:HH12	10:W:43:THR:HG23	1.72	0.54
3:G:29:LEU:HD12	3:G:55:VAL:HG21	1.89	0.54
10:Q:14:ARG:O	10:Q:19:ARG:NH2	2.40	0.54
10:S:53:ILE:HD11	10:S:202:LEU:HD21	1.90	0.54
4:I:343:PRO:HD2	4:I:375:LEU:HB3	1.89	0.54
4:I:376:PHE:O	4:I:379:LEU:HB3	2.07	0.54
10:U:79:LEU:HA	10:U:82:LEU:HD12	1.90	0.54
2:B:119:LEU:HG	2:B:161:ARG:HB2	1.90	0.54
2:B:135:VAL:HG23	2:B:197:ILE:HG21	1.89	0.54
3:G:80:ASP:OD2	3:G:87:ARG:NH2	2.40	0.54
4:I:328:ASN:HA	4:I:340:LYS:O	2.08	0.54
2:B:48:ILE:HD12	2:B:75:ILE:HD13	1.89	0.54
3:D:35:ARG:H	3:D:40:ILE:HD11	1.73	0.54
3:F:193:ASP:HB3	3:F:196:ARG:HG3	1.90	0.54
4:I:18:THR:HG22	4:I:198:TYR:HE1	1.71	0.54
4:I:270:TYR:HD2	4:I:310:ILE:HD12	1.72	0.54
4:I:403:ILE:HD13	4:I:492:ALA:HB2	1.89	0.54
5:L:18:PHE:O	5:L:22:MET:HG3	2.08	0.54
2:B:184:LEU:O	2:B:185:ASN:HB3	2.08	0.54
6:M:60:U:H2'	6:M:61:G:H8	1.72	0.54
2:B:82:LEU:HD21	9:P:313:LYS:HB2	1.89	0.54
7:N:-11:DC:H2"	7:N:-10:DG:C8	2.42	0.54
10:S:88:ARG:NH2	10:S:166:ASP:OD1	2.41	0.54
10:U:120:PRO:HD2	10:U:135:ARG:HH22	1.71	0.54
10:U:126:PHE:HE2	10:U:162:HIS:ND1	2.06	0.54
10:V:59:SER:O	10:W:223:ARG:HD2	2.08	0.54
1:A:51:ARG:HH22	1:A:114:PRO:HD2	1.72	0.53
4:I:260:SER:HB3	4:I:341:VAL:HG21	1.90	0.53
10:S:288:VAL:HG21	10:S:305:LEU:HD23	1.90	0.53
3:F:28:SER:HB3	3:F:31:HIS:HE1	1.72	0.53
10:V:208:THR:HG23	10:V:210:GLU:H	1.73	0.53
3:E:245:CYS:O	3:E:246:ASP:C	2.46	0.53
4:I:334:TYR:O	4:I:336:GLN:HG3	2.09	0.53
5:K:95:GLN:O	5:K:99:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:110:PRO:HB3	5:L:79:ASN:O	2.08	0.53
10:S:314:GLN:NE2	10:T:222:SER:O	2.40	0.53
10:T:288:VAL:HG12	10:T:300:ILE:HD12	1.90	0.53
10:W:301:THR:N	10:W:304:ASP:OD2	2.41	0.53
10:W:319:PHE:HA	10:W:322:ILE:HG12	1.90	0.53
3:C:300:ARG:NH1	3:C:300:ARG:O	2.41	0.53
3:F:55:VAL:HB	3:F:145:ALA:HB3	1.91	0.53
3:F:153:GLY:HA3	5:L:56:TYR:HB2	1.91	0.53
4:I:222:LYS:HD2	4:I:338:PHE:CZ	2.43	0.53
4:I:344:ILE:HA	4:I:347:LEU:HD12	1.91	0.53
4:I:359:TRP:HZ2	4:I:386:PHE:HB3	1.73	0.53
4:I:401:ILE:HG22	4:I:473:ILE:HD11	1.90	0.53
10:T:303:LYS:HE3	10:T:307:LYS:HG3	1.90	0.53
10:W:148:VAL:HG13	10:W:150:PRO:HD2	1.91	0.53
3:G:52:HIS:ND1	3:G:147:SER:O	2.34	0.53
1:A:56:GLU:HG2	1:A:207:MET:HB2	1.90	0.53
3:F:151:TYR:HE1	3:F:154:ALA:HB3	1.73	0.53
3:H:31:HIS:HA	3:H:41:LEU:HA	1.89	0.53
10:Q:314:GLN:NE2	10:R:222:SER:O	2.40	0.53
10:R:241:VAL:O	10:R:245:LYS:HG2	2.08	0.53
10:V:298:THR:C	10:V:299:THR:CG2	2.77	0.53
10:W:266:HIS:HB2	10:W:270:PHE:CE2	2.44	0.53
4:I:172:THR:HG22	4:I:173:SER:H	1.73	0.53
10:Q:127:ASP:HB3	10:Q:151:ALA:HB2	1.91	0.53
10:R:209:TYR:HD2	10:R:325:GLY:HA3	1.74	0.53
10:S:189:LEU:HD23	10:S:221:LEU:HD13	1.89	0.53
10:V:255:LEU:HD22	10:V:289:LEU:HD12	1.91	0.53
3:F:28:SER:HB3	3:F:31:HIS:CE1	2.44	0.53
3:G:57:SER:HA	3:G:60:ILE:HD12	1.90	0.53
4:I:195:LYS:HD2	4:I:198:TYR:HE2	1.74	0.53
10:R:338:ASN:OD1	10:R:338:ASN:N	2.40	0.53
10:U:55:VAL:HG22	10:U:228:ILE:HB	1.89	0.53
10:V:79:LEU:HG	10:V:80:PRO:HD3	1.90	0.53
3:D:238:ILE:HG13	3:D:238:ILE:O	2.09	0.53
3:H:103:ILE:O	3:H:139:ALA:N	2.40	0.53
10:Q:127:ASP:OD1	10:Q:127:ASP:N	2.42	0.53
2:B:144:ILE:HD11	2:B:191:THR:HB	1.91	0.53
3:H:205:MET:HG3	3:H:306:ILE:HG13	1.91	0.53
10:U:94:ILE:HD12	10:U:168:PHE:CZ	2.43	0.53
3:C:16:LEU:HB2	3:C:230:TRP:HE3	1.74	0.52
3:D:244:TYR:HE2	3:D:247:PRO:HG3	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:35:ARG:HG2	3:G:40:ILE:HD11	1.90	0.52
4:I:172:THR:HB	4:I:174:TRP:CD1	2.44	0.52
10:W:126:PHE:O	10:W:126:PHE:CG	2.61	0.52
3:C:150:PRO:HD2	3:C:247:PRO:HG3	1.91	0.52
3:H:193:ASP:HB3	3:H:196:ARG:HG3	1.91	0.52
6:M:21:A:H1'	6:M:22:A:C8	2.43	0.52
8:O:59:DT:H2"	8:O:60:DA:C8	2.45	0.52
8:O:60:DA:H2"	8:O:61:DG:H5'	1.92	0.52
10:T:65:THR:HG23	11:T:600:ATP:H5'2	1.91	0.52
10:Q:311:SER:HB2	10:Q:314:GLN:HG3	1.91	0.52
10:T:273:ARG:HB2	10:T:284:TRP:CZ3	2.43	0.52
10:V:302:LEU:HD23	10:V:305:LEU:HD12	1.91	0.52
1:A:9:LEU:HD11	1:A:39:MET:HE1	1.91	0.52
3:F:264:CYS:SG	3:F:266:GLN:HG2	2.50	0.52
3:H:102:ASP:O	3:H:136:ARG:NH1	2.42	0.52
4:I:348:ILE:O	4:I:352:LEU:HG	2.10	0.52
10:S:54:PHE:HB3	10:S:56:TYR:CE1	2.43	0.52
10:S:181:SER:HB3	10:S:184:LYS:HB2	1.91	0.52
3:G:266:GLN:OE1	3:H:302:ARG:NH1	2.43	0.52
4:I:255:LYS:HA	4:I:339:ILE:HD13	1.92	0.52
7:N:35:DG:H2"	7:N:36:DG:C8	2.45	0.52
10:S:60:GLY:HA3	10:S:280:THR:HG23	1.91	0.52
1:A:91:CYS:SG	1:A:92:TYR:N	2.83	0.52
1:A:184:ASN:HB3	1:A:211:PRO:HG3	1.91	0.52
3:E:61:ARG:NH2	3:E:140:LEU:O	2.43	0.52
3:F:73:TYR:O	3:F:75:VAL:HG13	2.10	0.52
3:G:62:TRP:CE3	6:M:14:G:C2	2.97	0.52
4:I:85:GLY:HA3	4:I:143:SER:HB2	1.91	0.52
4:I:487:ILE:O	4:I:491:LEU:HG	2.09	0.52
7:N:16:DT:H2"	7:N:17:DA:C8	2.44	0.52
8:O:72:DG:H2"	8:O:73:DA:C8	2.44	0.52
9:P:35:GLU:OE1	9:P:43:ARG:NH2	2.43	0.52
10:U:121:LEU:HG	10:U:123:ASP:H	1.74	0.52
10:W:99:PRO:O	10:W:101:SER:N	2.43	0.52
10:W:287:ARG:NE	10:W:308:ARG:HB3	2.25	0.52
3:D:35:ARG:HG2	3:D:40:ILE:HD11	1.91	0.52
7:N:38:DC:H4'	7:N:39:DT:O5'	2.09	0.52
10:S:82:LEU:HD11	10:S:90:PRO:HG3	1.90	0.52
10:T:61:VAL:HG11	10:T:230:PHE:O	2.09	0.52
10:W:164:HIS:CG	10:W:164:HIS:O	2.63	0.52
10:W:209:TYR:CD2	10:W:325:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:227:VAL:HG22	3:H:274:ILE:HD12	1.92	0.52
7:N:-14:DC:H2"	7:N:-13:DT:C6	2.45	0.52
7:N:0:DT:H2"	7:N:1:DA:N7	2.25	0.52
8:O:81:DC:H2"	8:O:82:DG:C8	2.45	0.52
10:U:60:GLY:O	10:U:277:CYS:HB3	2.09	0.52
10:W:173:ALA:N	10:W:206:LEU:O	2.37	0.52
1:A:191:ARG:NH2	1:A:193:GLU:OE1	2.43	0.52
3:E:142:MET:HA	3:E:184:PHE:HA	1.92	0.52
3:E:161:SER:OG	3:E:162:GLY:N	2.43	0.52
3:F:159:ALA:N	6:M:27:G:OP2	2.37	0.52
8:O:69:DT:H2"	8:O:70:DA:C8	2.44	0.52
10:T:67:ARG:HH11	10:T:171:ASP:HB2	1.75	0.52
10:U:30:HIS:CE1	10:U:33:LEU:HB2	2.45	0.52
1:A:189:ARG:NH1	4:I:15:ALA:O	2.43	0.52
3:F:144:MET:HB2	3:G:26:LEU:HD13	1.91	0.52
3:H:151:TYR:HA	3:H:176:HIS:NE2	2.25	0.52
3:H:161:SER:H	6:M:14:G:H5"	1.75	0.52
4:I:101:GLN:O	4:I:105:ILE:HG22	2.10	0.52
6:M:3:G:H4'	6:M:4:C:O5'	2.10	0.52
10:T:121:LEU:HG	10:T:123:ASP:H	1.75	0.52
10:V:67:ARG:O	10:V:71:GLU:HG3	2.09	0.52
3:D:299:TYR:HB2	3:D:305:MET:HB3	1.92	0.51
3:H:170:LEU:HD11	7:N:49:DA:C5	2.46	0.51
4:I:312:LYS:O	4:I:316:ILE:HG12	2.10	0.51
7:N:22:DT:C2'	7:N:23:DA:H5'	2.40	0.51
10:U:300:ILE:HG22	10:U:301:THR:N	2.25	0.51
4:I:464:LYS:O	4:I:468:GLU:HG2	2.10	0.51
5:K:23:LYS:HB2	5:K:108:TYR:HE2	1.74	0.51
3:C:184:PHE:HE2	3:C:186:ILE:HD11	1.72	0.51
3:D:243:GLU:CD	3:D:255:SER:HA	2.29	0.51
3:E:106:PHE:CE2	3:E:136:ARG:HB2	2.46	0.51
5:L:61:PHE:HE2	5:L:97:ILE:HB	1.74	0.51
10:Q:193:LYS:HZ2	10:Q:224:ARG:HH21	1.57	0.51
3:E:105:GLY:HA2	3:E:136:ARG:HG2	1.91	0.51
3:H:61:ARG:NH2	3:H:140:LEU:O	2.43	0.51
4:I:205:VAL:HG13	4:I:206:PRO:HD3	1.93	0.51
8:O:76:DC:H2"	8:O:77:DG:C8	2.46	0.51
10:V:56:TYR:HE1	10:V:211:LEU:HB3	1.75	0.51
3:C:215:ASN:ND2	3:C:217:PHE:O	2.44	0.51
3:C:261:GLU:OE2	3:D:302:ARG:NH2	2.43	0.51
3:H:38:LYS:HA	3:H:172:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:142:LYS:HB2	8:O:12:DA:P	2.51	0.51
5:L:34:GLU:OE1	5:L:34:GLU:N	2.33	0.51
10:Q:34:LYS:O	10:Q:38:GLU:HG2	2.11	0.51
10:V:269:TYR:HE1	10:V:273:ARG:HE	1.58	0.51
8:O:65:DT:H2"	8:O:66:DA:C8	2.44	0.51
10:R:135:ARG:HD3	10:R:141:ILE:HG22	1.92	0.51
10:U:250:THR:O	10:U:254:HIS:ND1	2.42	0.51
10:W:20:LEU:CD2	10:W:293:LEU:HD23	2.40	0.51
4:I:396:ASP:O	4:I:397:LYS:C	2.49	0.51
7:N:52:DT:H2'	7:N:53:DC:C5	2.46	0.51
10:V:136:ASP:OD1	10:V:140:LYS:N	2.44	0.51
3:E:32:ASP:O	3:F:157:LEU:HD22	2.10	0.51
4:I:132:PHE:HE2	4:I:337:ILE:HD11	1.76	0.51
4:I:329:TYR:CD2	4:I:331:ILE:HG13	2.45	0.51
7:N:26:DT:H2"	7:N:27:DT:OP2	2.11	0.51
10:R:112:ARG:HA	10:R:115:ILE:HG22	1.93	0.51
9:P:37:LEU:HD23	9:P:118:THR:HB	1.92	0.51
10:V:117:LEU:HD21	10:V:163:ARG:HG3	1.93	0.51
10:W:110:TYR:HB3	10:W:152:LEU:HG	1.93	0.51
5:K:104:ALA:HA	5:K:107:SER:OG	2.11	0.51
10:S:153:ARG:NH1	10:S:157:GLU:OE2	2.42	0.51
10:W:67:ARG:NH1	10:W:71:GLU:OE1	2.43	0.51
10:W:114:LEU:O	10:W:118:GLU:HG2	2.11	0.51
3:D:227:VAL:HG12	3:D:238:ILE:HD12	1.93	0.50
3:G:30:ASN:ND2	3:G:56:GLY:H	2.09	0.50
5:L:92:SER:HB2	5:L:97:ILE:HD11	1.92	0.50
4:I:352:LEU:HD21	4:I:358:TRP:HD1	1.76	0.50
8:O:2:DT:H2"	8:O:3:DA:C8	2.46	0.50
8:O:49:DT:H5"	9:P:277:ILE:HG21	1.94	0.50
9:P:164:VAL:HG13	9:P:221:ILE:HG22	1.92	0.50
10:Q:55:VAL:HG22	10:Q:228:ILE:HB	1.93	0.50
10:U:47:PRO:HB3	10:U:202:LEU:HD22	1.94	0.50
10:U:268:GLU:HB3	10:V:340:ARG:HH12	1.77	0.50
3:E:30:ASN:N	3:E:30:ASN:OD1	2.44	0.50
3:E:193:ASP:HB3	3:E:196:ARG:HG3	1.93	0.50
6:M:60:U:H2'	6:M:61:G:C8	2.46	0.50
10:T:121:LEU:HB3	10:T:124:HIS:HE1	1.75	0.50
10:U:130:VAL:HG11	10:U:151:ALA:HB1	1.93	0.50
3:C:198:LEU:HD22	3:C:310:LYS:HE3	1.94	0.50
3:E:262:VAL:HG11	3:E:293:LEU:HG	1.93	0.50
8:O:59:DT:H2"	8:O:60:DA:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:140:PRO:HB3	9:P:206:GLN:H	1.74	0.50
2:B:51:HIS:HA	2:B:207:ILE:HG21	1.93	0.50
5:K:107:SER:O	5:K:110:PRO:HG2	2.11	0.50
10:V:237:SER:OG	10:V:239:GLU:OE1	2.23	0.50
10:W:96:ALA:HB3	10:W:170:VAL:HG13	1.93	0.50
10:W:268:GLU:O	10:W:272:GLU:HG2	2.12	0.50
3:F:161:SER:N	6:M:26:G:OP1	2.44	0.50
3:G:158:GLY:O	3:G:171:HIS:N	2.42	0.50
4:I:27:THR:O	4:I:31:MET:HG3	2.12	0.50
4:I:344:ILE:HG13	4:I:366:LEU:HD21	1.94	0.50
10:Q:208:THR:OG1	10:Q:209:TYR:N	2.45	0.50
10:V:52:PHE:CZ	10:V:192:LEU:HB3	2.45	0.50
10:W:207:GLY:HA3	10:W:211:LEU:HD22	1.92	0.50
2:B:181:ILE:HG22	2:B:184:LEU:HD11	1.93	0.50
3:E:243:GLU:OE1	3:E:244:TYR:N	2.44	0.50
3:F:108:LEU:HG	3:F:133:PRO:HG2	1.94	0.50
3:F:268:ASP:N	3:F:268:ASP:OD1	2.43	0.50
4:I:11:LEU:HB3	4:I:26:MET:SD	2.51	0.50
4:I:350:ASP:O	4:I:354:LYS:HG3	2.12	0.50
8:O:7:DC:H2"	8:O:8:DA:C8	2.47	0.50
10:U:130:VAL:HG21	10:U:151:ALA:HB1	1.94	0.50
10:U:196:ALA:HB2	10:U:203:HIS:CD2	2.46	0.50
10:W:97:ILE:HD13	10:W:176:PHE:HD1	1.77	0.50
3:D:33:ILE:HG13	5:K:54:TYR:CZ	2.46	0.50
3:F:143:ASN:HB3	3:F:240:TYR:OH	2.12	0.50
4:I:46:ARG:HA	4:I:73:TRP:CE2	2.47	0.50
3:F:137:MET:HB3	3:F:190:HIS:NE2	2.27	0.50
4:I:8:LYS:HB2	4:I:63:TRP:CH2	2.46	0.50
10:Q:247:VAL:HA	10:Q:250:THR:HG22	1.94	0.50
10:Q:322:ILE:HD12	10:Q:323:GLN:N	2.26	0.50
10:R:58:ALA:O	10:R:63:LYS:NZ	2.45	0.50
10:S:99:PRO:HG3	10:S:104:PHE:HA	1.93	0.50
10:W:14:ARG:NH1	10:W:14:ARG:HA	2.26	0.50
1:A:60:ALA:HB2	1:A:162:TRP:CZ3	2.47	0.49
3:H:31:HIS:H	3:H:41:LEU:HD23	1.77	0.49
4:I:342:ASN:HD22	4:I:343:PRO:HD2	1.76	0.49
10:U:275:LEU:HD22	10:V:343:LEU:HD11	1.93	0.49
10:V:30:HIS:CE1	10:V:33:LEU:HB2	2.47	0.49
3:H:155:VAL:HG21	3:H:172:PHE:HB3	1.93	0.49
7:N:41:DA:H5'	7:N:41:DA:C8	2.46	0.49
10:V:288:VAL:CG1	10:V:300:ILE:HG21	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:292:ALA:HA	10:W:295:ARG:NH2	2.27	0.49
3:D:154:ALA:HB1	3:D:175:TYR:CZ	2.47	0.49
3:E:226:LEU:N	3:E:275:GLY:O	2.34	0.49
3:G:225:SER:HA	3:G:276:GLY:HA3	1.94	0.49
4:I:373:GLU:HA	4:I:376:PHE:HB3	1.94	0.49
5:J:107:SER:HB3	5:K:82:GLN:NE2	2.26	0.49
7:N:29:DA:H2"	7:N:30:DA:C8	2.47	0.49
10:V:324:GLU:OE2	10:V:327:ARG:NH2	2.44	0.49
3:C:21:LEU:HD21	3:C:252:ALA:HB1	1.93	0.49
3:C:58:SER:OG	6:M:39:C:OP1	2.31	0.49
3:F:261:GLU:HB3	3:F:267:ILE:HD12	1.94	0.49
4:I:342:ASN:HB3	4:I:345:ARG:NE	2.26	0.49
9:P:177:GLU:HG2	9:P:184:ARG:HG3	1.93	0.49
8:O:55:DC:H2"	8:O:56:DG:C8	2.47	0.49
9:P:164:VAL:HA	9:P:221:ILE:HG22	1.95	0.49
10:V:148:VAL:HG13	10:V:150:PRO:HD2	1.95	0.49
10:W:120:PRO:HB2	10:W:124:HIS:CE1	2.47	0.49
4:I:28:GLY:O	4:I:32:THR:HG22	2.13	0.49
8:O:71:DC:H2"	8:O:72:DG:C8	2.48	0.49
10:Q:58:ALA:HB3	10:Q:61:VAL:HG13	1.95	0.49
10:U:164:HIS:CG	10:U:164:HIS:O	2.66	0.49
10:W:58:ALA:C	10:W:60:GLY:H	2.14	0.49
10:W:281:LEU:O	10:W:285:LEU:HG	2.11	0.49
10:W:287:ARG:HE	10:W:308:ARG:HB3	1.78	0.49
3:G:45:TYR:CD1	3:H:248:LYS:HD3	2.47	0.49
3:H:30:ASN:ND2	3:H:42:GLN:NE2	2.61	0.49
10:Q:193:LYS:O	10:Q:193:LYS:HD3	2.12	0.49
3:D:193:ASP:HB3	3:D:196:ARG:HG3	1.94	0.49
8:O:78:DT:H2"	8:O:79:DA:N7	2.26	0.49
9:P:313:LYS:HA	9:P:329:LEU:HD21	1.95	0.49
10:S:60:GLY:N	11:S:600:ATP:O2B	2.46	0.49
10:U:270:PHE:O	10:U:274:THR:OG1	2.23	0.49
3:D:136:ARG:HG2	3:D:137:MET:H	1.78	0.49
3:E:246:ASP:O	3:E:247:PRO:C	2.51	0.49
3:F:236:SER:O	3:F:236:SER:OG	2.30	0.49
3:G:215:ASN:ND2	6:M:18:U:OP2	2.40	0.49
4:I:108:GLY:O	4:I:112:VAL:HG12	2.12	0.49
10:R:158:ASN:O	10:R:161:ILE:HG13	2.13	0.49
10:U:60:GLY:N	11:U:600:ATP:O2B	2.44	0.49
2:B:126:GLN:OE1	2:B:175:ARG:NH2	2.40	0.49
3:C:279:VAL:HG13	3:C:298:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:SER:OG	6:M:27:G:OP1	2.31	0.49
4:I:137:VAL:HG13	4:I:335:LYS:CA	2.33	0.49
4:I:281:TYR:CE2	4:I:315:LEU:HD12	2.47	0.49
5:J:79:ASN:HA	5:J:82:GLN:HE21	1.78	0.49
5:L:75:ASN:O	5:L:79:ASN:N	2.46	0.49
9:P:287:TYR:HB3	9:P:292:LEU:HD23	1.93	0.49
1:A:8:TYR:HA	1:A:102:LEU:HD23	1.93	0.48
3:C:275:GLY:HA3	3:C:305:MET:HE2	1.94	0.48
3:G:32:ASP:HB3	3:G:42:GLN:HB2	1.95	0.48
4:I:195:LYS:HB2	4:I:198:TYR:HD2	1.78	0.48
4:I:324:TYR:HE2	4:I:388:ILE:HG21	1.78	0.48
10:T:136:ASP:HB3	10:T:142:ASN:HD21	1.77	0.48
1:A:10:ASP:OD1	1:A:146:LYS:HE3	2.13	0.48
3:C:235:ALA:HB2	3:D:206:ASN:HA	1.94	0.48
3:H:244:TYR:HB2	3:H:252:ALA:HA	1.96	0.48
9:P:53:GLU:HB2	9:P:190:ARG:HA	1.95	0.48
10:R:75:THR:O	10:R:79:LEU:HG	2.14	0.48
10:V:273:ARG:HB2	10:V:284:TRP:CZ3	2.48	0.48
4:I:331:ILE:HB	4:I:338:PHE:HB2	1.96	0.48
4:I:405:VAL:HA	4:I:463:ASN:HD21	1.78	0.48
4:I:428:PRO:HB2	4:I:431:LYS:HB3	1.95	0.48
5:K:106:ALA:HA	5:K:109:LYS:HZ2	1.77	0.48
10:R:199:THR:HB	10:R:201:ILE:HG12	1.95	0.48
10:R:273:ARG:HA	10:R:273:ARG:HD2	1.69	0.48
10:V:292:ALA:HB2	10:V:300:ILE:CG2	2.39	0.48
10:W:153:ARG:HH21	10:W:198:MET:HE2	1.78	0.48
3:H:156:LYS:HB3	3:H:173:THR:OG1	2.13	0.48
5:J:35:GLU:HG2	5:J:36:GLY:H	1.77	0.48
10:T:287:ARG:HD2	10:T:308:ARG:HD2	1.96	0.48
10:V:58:ALA:O	10:V:63:LYS:NZ	2.47	0.48
10:V:108:GLU:HA	10:V:111:THR:HG22	1.94	0.48
4:I:113:PHE:CE2	4:I:206:PRO:HG3	2.48	0.48
4:I:376:PHE:CE1	4:I:379:LEU:HD13	2.49	0.48
8:O:60:DA:H2'	8:O:61:DG:H8	1.75	0.48
9:P:60:ILE:HD12	9:P:60:ILE:H	1.79	0.48
10:T:59:SER:O	10:U:223:ARG:HD3	2.14	0.48
10:U:19:ARG:HG2	10:U:256:PRO:HB2	1.96	0.48
3:D:31:HIS:HA	3:D:40:ILE:O	2.14	0.48
3:F:34:ARG:HD2	7:N:39:DT:H73	1.95	0.48
4:I:378:GLN:O	4:I:382:ASN:N	2.46	0.48
9:P:156:PRO:HD2	9:P:159:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:133:ILE:HG22	10:W:143:VAL:HG23	1.94	0.48
2:B:52:PRO:C	6:M:47:A:H61	2.17	0.48
4:I:366:LEU:O	4:I:376:PHE:HB2	2.13	0.48
5:J:7:GLU:OE1	5:J:7:GLU:N	2.36	0.48
5:J:35:GLU:OE2	5:J:37:LYS:HG2	2.13	0.48
5:J:110:PRO:HG3	5:K:82:GLN:OE1	2.13	0.48
9:P:136:ARG:NH1	9:P:192:SER:OG	2.47	0.48
9:P:167:CYS:O	9:P:171:LYS:N	2.42	0.48
10:V:39:ILE:O	10:V:43:THR:OG1	2.29	0.48
10:W:153:ARG:HH22	10:W:194:SER:HG	1.62	0.48
3:E:92:ASP:N	3:E:92:ASP:OD1	2.46	0.48
4:I:17:ASP:OD1	4:I:17:ASP:N	2.47	0.48
5:K:23:LYS:HE3	5:K:111:LYS:HD3	1.94	0.48
9:P:80:HIS:CE1	9:P:81:LEU:HD22	2.49	0.48
9:P:153:ILE:HG23	9:P:194:ALA:HB3	1.96	0.48
10:T:89:VAL:HG22	10:T:163:ARG:HB3	1.96	0.48
2:B:116:TYR:CE2	2:B:213:ARG:HG3	2.47	0.48
3:D:16:LEU:HB2	3:D:230:TRP:HE3	1.79	0.48
4:I:387:ILE:O	4:I:391:GLU:HG3	2.13	0.48
10:T:287:ARG:NH1	10:T:308:ARG:O	2.46	0.48
10:U:58:ALA:O	10:U:61:VAL:HG22	2.14	0.48
10:U:288:VAL:HG12	10:U:300:ILE:HD12	1.94	0.48
3:D:187:ASP:OD2	3:D:190:HIS:HB2	2.14	0.48
3:G:49:GLY:HA2	3:H:248:LYS:HB2	1.95	0.48
3:G:272:LEU:HD12	3:G:272:LEU:HA	1.76	0.48
5:K:110:PRO:HD3	5:L:79:ASN:ND2	2.25	0.48
10:S:291:ASP:OD1	10:S:308:ARG:NH1	2.47	0.48
10:W:14:ARG:O	10:W:19:ARG:NH2	2.46	0.48
10:W:61:VAL:HG23	11:W:600:ATP:O1B	2.13	0.48
10:W:284:TRP:HA	10:W:287:ARG:NH2	2.29	0.48
3:E:77:ARG:NH2	6:M:26:G:OP2	2.47	0.47
3:F:109:LEU:HB3	7:N:47:DT:H5"	1.94	0.47
10:Q:63:LYS:HB3	10:Q:206:LEU:HD23	1.96	0.47
10:R:319:PHE:O	10:R:323:GLN:HG2	2.14	0.47
10:T:61:VAL:HG23	10:T:63:LYS:HG3	1.94	0.47
10:U:94:ILE:HD12	10:U:168:PHE:HZ	1.79	0.47
2:B:200:LYS:HD3	6:M:62:C:OP2	2.14	0.47
4:I:116:LEU:HD11	7:N:57:DA:N3	2.30	0.47
4:I:359:TRP:HE1	4:I:389:MET:HB2	1.79	0.47
7:N:50:DC:H4'	7:N:51:DT:O5'	2.13	0.47
10:R:20:LEU:HD12	10:R:286:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:291:ASP:OD1	10:W:291:ASP:N	2.47	0.47
3:H:161:SER:N	6:M:14:G:OP1	2.47	0.47
4:I:314:ILE:HD12	4:I:352:LEU:HB3	1.95	0.47
4:I:350:ASP:HB3	4:I:354:LYS:HE3	1.96	0.47
5:J:101:SER:O	5:J:105:ILE:HG12	2.14	0.47
10:Q:243:ALA:O	10:Q:247:VAL:HG13	2.13	0.47
10:S:130:VAL:HG21	10:S:151:ALA:HB1	1.95	0.47
10:T:108:GLU:HG3	10:U:150:PRO:HB3	1.95	0.47
10:V:20:LEU:HD12	10:V:286:LYS:HE2	1.96	0.47
1:A:164:ILE:HG23	1:A:203:LEU:HB3	1.96	0.47
3:D:95:PRO:O	3:D:102:ASP:HB2	2.14	0.47
3:F:151:TYR:HB2	3:F:176:HIS:CE1	2.49	0.47
4:I:29:LEU:HD21	4:I:200:LEU:HD23	1.96	0.47
5:K:13:ILE:HD12	5:K:81:HIS:ND1	2.29	0.47
7:N:59:DG:H2"	7:N:60:DA:C8	2.49	0.47
9:P:42:HIS:CE1	9:P:192:SER:HB3	2.49	0.47
10:Q:125:LYS:HA	10:Q:125:LYS:HD2	1.57	0.47
10:S:108:GLU:HA	10:S:111:THR:HG22	1.96	0.47
10:V:30:HIS:NE2	10:V:33:LEU:HB2	2.29	0.47
3:D:276:GLY:HA2	3:D:302:ARG:HH11	1.79	0.47
3:G:198:LEU:HD13	3:G:310:LYS:HG2	1.97	0.47
3:H:19:THR:OG1	3:H:239:SER:O	2.33	0.47
4:I:20:ILE:O	4:I:24:VAL:HG13	2.13	0.47
4:I:46:ARG:NH2	4:I:51:SER:HA	2.26	0.47
10:R:122:ILE:HA	10:R:135:ARG:HH12	1.79	0.47
10:S:26:TYR:HE2	10:S:254:HIS:ND1	2.12	0.47
10:T:58:ALA:O	10:T:63:LYS:NZ	2.48	0.47
10:U:59:SER:OG	10:V:220:GLN:HA	2.15	0.47
10:U:108:GLU:HA	10:U:111:THR:HG22	1.95	0.47
2:B:23:ILE:HD12	2:B:24:PRO:HD2	1.97	0.47
3:C:32:ASP:OD1	3:C:32:ASP:N	2.47	0.47
3:E:54:PHE:CE1	3:E:146:VAL:HG23	2.48	0.47
3:H:19:THR:OG1	3:H:238:ILE:O	2.23	0.47
4:I:6:GLN:OE1	4:I:6:GLN:N	2.32	0.47
4:I:343:PRO:O	4:I:347:LEU:HG	2.13	0.47
4:I:373:GLU:HA	4:I:376:PHE:CB	2.44	0.47
7:N:25:DG:H2"	7:N:26:DT:OP1	2.14	0.47
8:O:57:DC:H2"	8:O:58:DG:C2	2.49	0.47
9:P:248:GLN:O	9:P:252:LEU:HG	2.15	0.47
2:B:211:ALA:O	2:B:215:LYS:NZ	2.47	0.47
3:C:145:ALA:HB1	3:C:180:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:266:GLN:OE1	3:G:302:ARG:NH1	2.48	0.47
3:G:20:VAL:HG11	3:G:182:TYR:CZ	2.50	0.47
3:G:56:GLY:HA2	3:G:144:MET:SD	2.54	0.47
9:P:71:SER:HA	9:P:74:LEU:HG	1.96	0.47
10:R:81:LYS:HZ1	10:R:88:ARG:HH11	1.63	0.47
10:T:40:LEU:HD23	10:T:70:VAL:HG21	1.97	0.47
10:T:60:GLY:N	11:T:600:ATP:O2B	2.48	0.47
10:T:135:ARG:HG3	10:T:136:ASP:H	1.80	0.47
10:V:14:ARG:HA	10:V:14:ARG:CZ	2.45	0.47
10:V:212:LEU:HD11	10:V:329:LEU:HG	1.95	0.47
10:W:16:ALA:O	10:W:20:LEU:HG	2.15	0.47
10:W:249:LEU:HD23	10:W:264:VAL:HG11	1.96	0.47
1:A:84:HIS:ND1	1:A:85:PRO:HD2	2.29	0.47
2:B:116:TYR:OH	2:B:217:GLU:HG3	2.15	0.47
3:F:299:TYR:HB2	3:F:305:MET:HB2	1.96	0.47
3:G:259:ILE:O	3:G:263:GLU:HG2	2.15	0.47
9:P:50:LEU:HD11	10:Q:121:LEU:HB2	1.97	0.47
9:P:82:LEU:HD12	9:P:84:ASN:OD1	2.14	0.47
10:Q:32:ARG:NH2	10:Q:240:ASP:OD2	2.47	0.47
10:V:60:GLY:CA	10:V:277:CYS:HB3	2.45	0.47
10:V:64:THR:OG1	11:V:600:ATP:O1G	2.33	0.47
10:W:40:LEU:O	10:W:44:ILE:HG12	2.15	0.47
3:C:75:VAL:HG22	3:C:100:ASP:HB2	1.96	0.47
3:D:31:HIS:O	6:M:33:G:H2'	2.15	0.47
4:I:347:LEU:HD13	4:I:365:LYS:HG3	1.97	0.47
10:Q:308:ARG:HH12	10:R:43:THR:HA	1.80	0.47
10:V:133:ILE:HD12	10:V:143:VAL:HG22	1.96	0.47
1:A:16:PHE:CE2	1:A:96:LEU:HD12	2.50	0.47
3:F:148:LEU:HG	3:F:244:TYR:HD1	1.80	0.47
3:H:274:ILE:HB	3:H:298:ILE:HG12	1.97	0.47
5:L:61:PHE:CE2	5:L:97:ILE:HB	2.49	0.47
7:N:-2:DG:H2"	7:N:-1:DA:C8	2.50	0.47
10:W:303:LYS:NZ	10:W:306:GLN:HB2	2.30	0.47
3:D:152:ASP:OD1	3:D:153:GLY:N	2.46	0.46
3:D:245:CYS:CB	3:D:251:GLU:HG2	2.45	0.46
3:E:279:VAL:O	3:E:283:GLN:HG2	2.15	0.46
3:H:149:THR:HG21	3:H:248:LYS:H	1.80	0.46
9:P:34:ALA:O	9:P:156:PRO:HA	2.15	0.46
10:T:311:SER:HB2	10:T:314:GLN:HG3	1.96	0.46
10:U:61:VAL:HG23	11:U:600:ATP:O1B	2.16	0.46
10:V:8:PRO:HD2	10:V:11:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:266:GLN:HE22	3:D:302:ARG:HE	1.63	0.46
3:G:264:CYS:SG	3:G:266:GLN:HG2	2.55	0.46
4:I:74:LEU:O	4:I:78:SER:OG	2.25	0.46
4:I:278:GLU:HG2	4:I:279:VAL:HG23	1.97	0.46
10:S:197:ASN:HD21	10:S:224:ARG:NH1	2.13	0.46
10:S:317:LYS:HD2	10:T:216:ASN:HB2	1.97	0.46
10:T:315:CYS:HA	10:T:318:MET:HG3	1.96	0.46
10:U:311:SER:OG	10:U:314:GLN:HG2	2.16	0.46
10:V:248:LEU:HD21	10:V:263:LEU:HB3	1.98	0.46
3:G:254:LEU:HD13	3:G:278:ILE:HG12	1.97	0.46
5:J:59:LEU:HD22	5:J:59:LEU:H	1.80	0.46
10:S:89:VAL:HG22	10:S:163:ARG:HB3	1.98	0.46
10:W:73:LYS:O	10:W:76:GLU:HG3	2.15	0.46
1:A:121:GLN:NE2	1:A:125:ASP:OD1	2.45	0.46
3:H:34:ARG:HD2	3:H:36:GLY:H	1.81	0.46
4:I:342:ASN:HB3	4:I:345:ARG:CD	2.44	0.46
5:J:67:ASP:O	5:J:71:ARG:HG2	2.15	0.46
5:L:76:LYS:HA	5:L:79:ASN:OD1	2.15	0.46
10:Q:108:GLU:OE2	10:Q:112:ARG:NH2	2.46	0.46
10:S:94:ILE:HD13	10:S:113:ALA:HA	1.96	0.46
10:T:126:PHE:HD2	10:T:128:TYR:HD1	1.64	0.46
10:W:135:ARG:HA	10:W:141:ILE:HG13	1.96	0.46
2:B:14:LEU:N	2:B:73:ILE:O	2.42	0.46
3:C:275:GLY:HA2	3:C:279:VAL:HG21	1.98	0.46
4:I:147:TYR:CD1	4:I:149:HIS:HB2	2.50	0.46
7:N:8:DC:H2"	7:N:9:DG:N7	2.31	0.46
8:O:11:DG:C5	8:O:12:DA:C2	3.04	0.46
10:R:99:PRO:HG3	10:R:104:PHE:HA	1.97	0.46
10:S:232:ARG:NH1	10:S:271:TYR:OH	2.44	0.46
10:V:40:LEU:HD23	10:V:70:VAL:HG21	1.98	0.46
3:D:211:GLY:HA3	6:M:32:U:H6	1.81	0.46
3:H:238:ILE:HG22	3:H:258:PHE:HE1	1.81	0.46
9:P:10:LEU:HD13	10:Q:68:LEU:HB2	1.98	0.46
10:U:69:ARG:O	10:U:72:GLN:HG3	2.16	0.46
10:U:148:VAL:HG13	10:U:150:PRO:HD2	1.98	0.46
10:V:272:GLU:HA	10:W:343:LEU:HD13	1.97	0.46
3:C:244:TYR:HE2	3:C:251:GLU:H	1.62	0.46
3:E:149:THR:HG23	3:E:247:PRO:O	2.15	0.46
4:I:262:LEU:HD12	4:I:262:LEU:H	1.80	0.46
5:K:110:PRO:HA	5:L:79:ASN:HB3	1.96	0.46
10:S:47:PRO:HB3	10:S:202:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:291:ASP:HA	10:W:42:ARG:HH21	1.80	0.46
10:W:56:TYR:CD2	10:W:329:LEU:HD11	2.50	0.46
10:W:108:GLU:OE1	10:W:112:ARG:NH2	2.43	0.46
10:W:184:LYS:O	10:W:188:GLN:HG2	2.16	0.46
2:B:57:PRO:HA	2:B:63:LEU:HA	1.97	0.46
3:C:16:LEU:HB2	3:C:230:TRP:CE3	2.51	0.46
3:C:194:PHE:O	3:C:197:ILE:HG22	2.16	0.46
4:I:344:ILE:HD11	4:I:366:LEU:HG	1.97	0.46
9:P:37:LEU:HD11	9:P:91:ILE:HG22	1.97	0.46
10:Q:97:ILE:HD13	10:R:153:ARG:HH12	1.80	0.46
10:S:192:LEU:HD12	10:S:192:LEU:HA	1.83	0.46
10:T:83:GLU:O	10:T:86:ARG:NH2	2.49	0.46
2:B:132:ILE:O	2:B:135:VAL:HG12	2.16	0.46
3:C:225:SER:HA	3:C:276:GLY:HA3	1.96	0.46
3:D:109:LEU:HD22	7:N:35:DG:C4	2.50	0.46
3:E:157:LEU:HD12	3:E:158:GLY:H	1.80	0.46
3:F:75:VAL:HB	3:F:100:ASP:HB2	1.98	0.46
3:F:108:LEU:H	3:F:135:GLN:NE2	2.13	0.46
3:H:28:SER:HB3	3:H:31:HIS:NE2	2.31	0.46
4:I:97:ILE:HG23	4:I:101:GLN:HB2	1.98	0.46
5:K:52:LEU:HD23	5:K:52:LEU:HA	1.84	0.46
10:V:131:ARG:H	10:V:131:ARG:HD2	1.80	0.46
10:V:220:GLN:HE21	10:V:224:ARG:HH11	1.64	0.46
10:W:30:HIS:CE1	10:W:33:LEU:HB2	2.51	0.46
10:W:244:PHE:CE1	10:W:281:LEU:HD22	2.42	0.46
10:W:287:ARG:HG2	10:W:308:ARG:CG	2.46	0.46
10:W:303:LYS:HA	10:W:303:LYS:HD2	1.81	0.46
1:A:7:LEU:HD13	1:A:148:ILE:HD11	1.98	0.46
1:A:17:ARG:HG3	1:A:25:GLY:HA2	1.98	0.46
3:E:105:GLY:HA2	3:E:136:ARG:HB3	1.96	0.46
3:F:33:ILE:O	3:F:34:ARG:HG3	2.16	0.46
3:F:186:ILE:HD12	3:F:200:MET:HE1	1.97	0.46
3:F:266:GLN:HG3	3:F:267:ILE:HG13	1.97	0.46
3:G:15:TYR:HB2	3:G:17:TYR:CE2	2.51	0.46
4:I:276:GLN:NE2	4:I:278:GLU:OE2	2.34	0.46
5:J:61:PHE:HA	5:J:64:TYR:HB3	1.98	0.46
7:N:41:DA:H5'	7:N:41:DA:H8	1.81	0.46
9:P:166:PHE:HZ	9:P:212:GLU:HB2	1.81	0.46
10:Q:40:LEU:HD23	10:Q:70:VAL:HG21	1.98	0.46
10:S:301:THR:O	10:S:304:ASP:HB2	2.16	0.46
10:T:135:ARG:HG3	10:T:136:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:207:GLY:HA3	10:U:211:LEU:HD22	1.98	0.46
1:A:108:ASP:OD1	1:A:109:GLU:N	2.49	0.45
4:I:343:PRO:HB2	4:I:375:LEU:HD13	1.97	0.45
5:L:75:ASN:HB3	5:L:78:PHE:HB3	1.99	0.45
10:Q:56:TYR:OH	10:Q:227:ASP:OD2	2.32	0.45
10:R:247:VAL:HG11	10:R:278:ILE:HD12	1.98	0.45
10:V:40:LEU:O	10:V:44:ILE:HG23	2.16	0.45
10:V:69:ARG:O	10:V:72:GLN:HG3	2.16	0.45
10:W:97:ILE:HG21	10:W:176:PHE:CD1	2.51	0.45
10:W:239:GLU:CD	10:W:239:GLU:H	2.19	0.45
1:A:22:ARG:HD2	4:I:192:LEU:HD21	1.97	0.45
2:B:27:ASN:O	2:B:31:THR:HG22	2.16	0.45
3:C:53:SER:OG	3:C:176:HIS:ND1	2.29	0.45
3:D:160:LYS:O	3:D:161:SER:C	2.55	0.45
3:F:237:TYR:O	3:F:238:ILE:HG13	2.16	0.45
3:G:198:LEU:HB2	3:G:199:PRO:HD3	1.98	0.45
4:I:28:GLY:HA2	4:I:31:MET:HE2	1.98	0.45
4:I:100:ARG:HD2	4:I:132:PHE:CZ	2.52	0.45
4:I:390:ALA:HB1	4:I:396:ASP:OD2	2.17	0.45
5:J:95:GLN:O	5:J:99:ILE:HG13	2.16	0.45
7:N:-4:DT:H2"	7:N:-3:DA:C8	2.50	0.45
7:N:45:DA:H2"	7:N:46:DA:H5"	1.97	0.45
10:S:218:SER:HB3	10:S:221:LEU:HD12	1.97	0.45
10:T:121:LEU:HB3	10:T:124:HIS:CE1	2.51	0.45
10:V:94:ILE:HD11	10:V:109:TYR:HE1	1.81	0.45
10:W:122:ILE:HD13	10:W:139:GLY:H	1.81	0.45
4:I:61:LEU:HB3	4:I:63:TRP:HZ3	1.81	0.45
5:J:25:ASN:O	5:J:29:ILE:HG22	2.16	0.45
9:P:253:VAL:HG11	9:P:319:LEU:HB3	1.98	0.45
9:P:271:ILE:HG23	9:P:296:VAL:HG22	1.98	0.45
10:Q:94:ILE:HD11	10:Q:109:TYR:HE1	1.82	0.45
10:R:99:PRO:HD2	10:R:178:LYS:HD2	1.98	0.45
10:R:218:SER:OG	10:R:221:LEU:HD12	2.17	0.45
10:V:60:GLY:HA3	10:V:277:CYS:HB3	1.98	0.45
10:W:288:VAL:CG2	10:W:305:LEU:HA	2.46	0.45
3:F:54:PHE:CE1	3:F:146:VAL:HG12	2.51	0.45
3:F:151:TYR:CE1	3:F:154:ALA:HB3	2.50	0.45
4:I:348:ILE:HG12	4:I:362:PHE:HZ	1.75	0.45
5:J:60:SER:O	5:J:61:PHE:HB3	2.16	0.45
7:N:-7:DT:H2"	7:N:-6:DC:C6	2.51	0.45
10:Q:193:LYS:NZ	10:Q:224:ARG:HH21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:266:HIS:HB2	10:S:269:TYR:HB3	1.98	0.45
10:U:318:MET:SD	10:V:223:ARG:HB2	2.57	0.45
10:V:287:ARG:HG3	10:W:48:ALA:HB3	1.99	0.45
10:W:185:LEU:HD23	10:W:185:LEU:H	1.82	0.45
3:C:19:THR:OG1	3:C:239:SER:O	2.35	0.45
3:F:280:LYS:HE2	3:F:300:ARG:HE	1.82	0.45
3:G:109:LEU:HD22	7:N:53:DC:C2	2.51	0.45
4:I:363:TRP:CZ3	4:I:367:VAL:HG21	2.51	0.45
5:K:54:TYR:CZ	5:K:56:TYR:HE1	2.34	0.45
10:Q:185:LEU:HG	10:Q:214:PHE:CE2	2.52	0.45
1:A:169:GLY:N	1:A:189:ARG:HD3	2.32	0.45
2:B:163:LEU:HB3	2:B:174:VAL:HG23	1.98	0.45
3:F:179:ARG:NH2	3:F:224:ASP:OD2	2.49	0.45
3:G:58:SER:OG	6:M:15:U:OP1	2.34	0.45
3:H:57:SER:O	3:H:61:ARG:HG3	2.17	0.45
10:R:312:VAL:HG11	10:S:336:VAL:HG22	1.98	0.45
10:S:161:ILE:HG22	10:S:199:THR:HA	1.99	0.45
10:T:119:GLU:N	10:T:120:PRO:HD3	2.31	0.45
10:V:301:THR:OG1	10:V:303:LYS:HG2	2.16	0.45
10:W:98:ALA:HB3	10:W:175:HIS:CD2	2.52	0.45
3:D:151:TYR:HB2	3:D:176:HIS:CD2	2.52	0.45
3:D:156:LYS:N	3:D:173:THR:O	2.28	0.45
3:D:273:TRP:CD1	3:D:309:LEU:HD13	2.51	0.45
3:E:46:TRP:CE2	3:E:146:VAL:HG21	2.52	0.45
3:F:29:LEU:HD12	3:F:55:VAL:HG21	1.96	0.45
3:F:225:SER:HA	3:F:276:GLY:HA3	1.98	0.45
3:F:228:PHE:O	3:F:273:TRP:N	2.47	0.45
4:I:228:ARG:HG2	4:I:291:GLU:HB2	1.99	0.45
5:J:103:LEU:HD21	5:K:89:ILE:HG21	1.97	0.45
5:K:33:THR:HG21	5:K:39:PRO:HG3	1.98	0.45
9:P:117:LEU:O	9:P:157:LEU:HD11	2.16	0.45
1:A:61:MET:HE1	1:A:65:PRO:HD3	1.99	0.45
2:B:88:ALA:O	9:P:245:ARG:NH2	2.37	0.45
3:G:100:ASP:OD1	3:G:100:ASP:N	2.48	0.45
4:I:379:LEU:C	4:I:379:LEU:HD23	2.36	0.45
10:S:218:SER:O	10:S:222:SER:OG	2.24	0.45
10:U:136:ASP:OD1	10:U:140:LYS:N	2.49	0.45
10:V:273:ARG:NH1	10:V:310:LEU:O	2.48	0.45
10:W:99:PRO:HG3	10:W:112:ARG:CZ	2.47	0.45
2:B:121:ILE:HD11	2:B:200:LYS:HG3	1.98	0.45
4:I:142:LYS:HD2	8:O:11:DG:C3'	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:326:LYS:HD3	4:I:326:LYS:HA	1.78	0.45
5:J:5:SER:HB2	5:J:8:ASP:OD1	2.16	0.45
7:N:24:DC:C2	7:N:25:DG:C6	3.04	0.45
10:Q:177:GLY:HA3	10:Q:214:PHE:HZ	1.82	0.45
10:R:249:LEU:O	10:R:252:GLN:HG2	2.17	0.45
3:E:151:TYR:HB2	3:E:176:HIS:CE1	2.52	0.45
3:F:160:LYS:HB2	3:F:160:LYS:HE2	1.71	0.45
3:F:244:TYR:CE2	3:F:246:ASP:HB2	2.53	0.45
4:I:237:LYS:NZ	4:I:282:TYR:O	2.41	0.45
7:N:38:DC:H2"	7:N:39:DT:OP2	2.17	0.45
10:W:271:TYR:O	10:W:275:LEU:N	2.47	0.45
2:B:16:PHE:CE2	2:B:104:PRO:HB3	2.51	0.44
3:D:178:THR:OG1	3:D:179:ARG:N	2.50	0.44
3:D:238:ILE:HG22	3:D:258:PHE:HE1	1.83	0.44
3:E:90:SER:OG	3:E:92:ASP:OD1	2.34	0.44
3:G:209:LYS:HZ1	3:G:212:GLY:H	1.65	0.44
4:I:270:TYR:CD2	4:I:310:ILE:HD12	2.50	0.44
4:I:289:LEU:HD23	4:I:304:SER:HB3	1.98	0.44
4:I:449:PHE:CE2	4:I:485:ILE:HB	2.52	0.44
10:Q:288:VAL:HG12	10:Q:300:ILE:HD12	1.99	0.44
10:T:126:PHE:CG	10:T:126:PHE:O	2.69	0.44
10:U:189:LEU:HD23	10:U:221:LEU:HD13	1.97	0.44
10:W:55:VAL:HB	10:W:206:LEU:HA	1.99	0.44
10:W:318:MET:O	10:W:322:ILE:HG23	2.17	0.44
3:D:34:ARG:HG3	7:N:27:DT:H72	2.00	0.44
3:G:189:THR:HA	3:G:194:PHE:HE2	1.83	0.44
3:G:228:PHE:HB2	3:G:273:TRP:HB2	2.00	0.44
3:H:155:VAL:CG2	3:H:172:PHE:HB3	2.46	0.44
10:S:125:LYS:NZ	10:S:135:ARG:HG3	2.30	0.44
10:U:133:ILE:HD11	10:U:152:LEU:HD23	1.99	0.44
10:U:238:PRO:O	10:U:242:GLN:HG2	2.16	0.44
3:C:254:LEU:HD12	3:C:254:LEU:HA	1.87	0.44
3:E:145:ALA:HA	3:E:182:TYR:HB3	2.00	0.44
4:I:63:TRP:HE1	4:I:67:ASP:HA	1.82	0.44
8:O:9:DT:H2"	8:O:10:DG:C8	2.52	0.44
10:Q:94:ILE:HD11	10:Q:109:TYR:CE1	2.53	0.44
10:R:119:GLU:N	10:R:120:PRO:HD3	2.32	0.44
10:U:119:GLU:N	10:U:120:PRO:HD3	2.33	0.44
10:W:119:GLU:N	10:W:120:PRO:HD3	2.32	0.44
3:D:37:ASN:OD1	7:N:27:DT:H5"	2.18	0.44
3:D:61:ARG:HD3	6:M:31:C:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:136:ARG:HA	3:F:136:ARG:HD2	1.65	0.44
3:H:148:LEU:HD21	3:H:244:TYR:HB3	1.98	0.44
4:I:328:ASN:OD1	4:I:341:VAL:HA	2.18	0.44
5:J:79:ASN:HA	5:J:82:GLN:NE2	2.32	0.44
10:Q:216:ASN:O	10:Q:222:SER:OG	2.35	0.44
10:R:302:LEU:HD12	10:R:305:LEU:HD12	2.00	0.44
10:S:272:GLU:HG2	10:S:273:ARG:HG2	2.00	0.44
10:V:300:ILE:H	10:V:300:ILE:HG12	1.52	0.44
10:W:238:PRO:O	10:W:242:GLN:HG2	2.17	0.44
3:C:79:TRP:HE3	3:C:86:ASN:ND2	2.16	0.44
3:G:40:ILE:HD12	3:G:40:ILE:H	1.80	0.44
3:G:188:ALA:HB1	3:G:317:LEU:HD11	1.99	0.44
4:I:18:THR:HG22	4:I:198:TYR:CE1	2.51	0.44
4:I:255:LYS:HB2	4:I:330:GLN:OE1	2.17	0.44
4:I:277:PRO:HD2	4:I:278:GLU:OE1	2.18	0.44
4:I:343:PRO:HG2	4:I:375:LEU:HB3	1.99	0.44
7:N:47:DT:H6	7:N:47:DT:H2'	1.65	0.44
8:O:53:DT:H2"	8:O:54:DA:C8	2.52	0.44
10:S:119:GLU:N	10:S:120:PRO:HD3	2.33	0.44
10:S:133:ILE:HD11	10:S:152:LEU:HD23	2.00	0.44
10:T:130:VAL:HG21	10:T:151:ALA:HB1	1.99	0.44
10:T:249:LEU:O	10:T:252:GLN:HG2	2.18	0.44
10:W:93:GLY:HA2	10:W:169:PHE:HB2	2.00	0.44
10:W:184:LYS:O	10:W:188:GLN:N	2.36	0.44
3:E:178:THR:OG1	3:E:179:ARG:N	2.49	0.44
3:F:135:GLN:HB3	6:M:17:A:O2'	2.18	0.44
4:I:30:TYR:CD2	4:I:239:PHE:HB3	2.53	0.44
10:Q:82:LEU:HD11	10:Q:88:ARG:O	2.18	0.44
10:U:124:HIS:H	10:U:124:HIS:HD1	1.66	0.44
10:U:257:LEU:HD13	10:U:299:THR:HA	1.99	0.44
10:V:119:GLU:N	10:V:120:PRO:HD3	2.33	0.44
2:B:133:GLU:HG2	2:B:137:ARG:HH12	1.82	0.44
3:E:244:TYR:HE2	3:E:249:SER:HB2	1.83	0.44
3:F:139:ALA:O	3:F:186:ILE:HG13	2.17	0.44
4:I:46:ARG:HA	4:I:73:TRP:NE1	2.33	0.44
4:I:328:ASN:HB3	4:I:339:ILE:HG22	1.99	0.44
4:I:433:VAL:O	4:I:437:ARG:HG2	2.18	0.44
5:J:93:PRO:O	5:J:97:ILE:HD12	2.16	0.44
10:S:212:LEU:HD22	10:S:215:ARG:HD2	1.99	0.44
10:T:252:GLN:HE22	10:T:264:VAL:HG23	1.83	0.44
10:V:235:ALA:HB2	10:V:271:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:OE1	1:A:141:SER:N	2.51	0.44
3:C:187:ASP:OD2	3:C:190:HIS:HB2	2.17	0.44
3:D:133:PRO:HB2	3:D:134:ASN:H	1.58	0.44
3:E:54:PHE:HB3	3:E:144:MET:HE3	1.99	0.44
4:I:383:ARG:O	4:I:387:ILE:HG13	2.18	0.44
5:J:23:LYS:HB2	5:J:108:TYR:HE1	1.83	0.44
5:K:76:LYS:O	5:K:80:GLU:HG2	2.17	0.44
7:N:63:DT:H2"	7:N:64:DA:C8	2.53	0.44
9:P:110:MET:HG2	10:Q:86:ARG:HG3	1.99	0.44
10:R:235:ALA:HB2	10:R:271:TYR:CE2	2.53	0.44
10:R:288:VAL:HG21	10:R:305:LEU:HD23	1.99	0.44
10:S:209:TYR:HD2	10:S:325:GLY:HA3	1.81	0.44
10:T:108:GLU:HA	10:T:111:THR:HG22	2.00	0.44
10:W:304:ASP:OD1	10:W:307:LYS:NZ	2.47	0.44
3:D:239:SER:H	3:E:23:ARG:NH1	2.16	0.44
3:E:243:GLU:OE1	3:E:245:CYS:N	2.50	0.44
3:G:254:LEU:HD12	3:G:254:LEU:HA	1.81	0.44
3:G:277:THR:HA	3:G:300:ARG:NH1	2.33	0.44
5:J:42:LYS:HE2	5:J:42:LYS:HB3	1.89	0.44
10:Q:318:MET:O	10:Q:322:ILE:HG13	2.17	0.44
10:S:40:LEU:HA	10:S:43:THR:HG22	1.98	0.44
10:S:67:ARG:HH11	10:S:171:ASP:HB2	1.82	0.44
10:T:174:GLN:NE2	10:T:208:THR:OG1	2.51	0.44
10:V:314:GLN:H	10:V:314:GLN:HG2	1.64	0.44
10:W:195:LEU:O	10:W:196:ALA:C	2.55	0.44
10:W:220:GLN:O	10:W:224:ARG:HG3	2.18	0.44
3:C:61:ARG:NH2	3:C:140:LEU:O	2.51	0.43
3:C:211:GLY:O	6:M:38:A:C2	2.71	0.43
9:P:102:VAL:HG11	9:P:120:LEU:HD21	1.99	0.43
10:Q:53:ILE:HB	10:Q:204:CYS:HB2	2.00	0.43
10:S:32:ARG:O	10:S:35:GLU:HG2	2.18	0.43
10:T:99:PRO:HG3	10:T:104:PHE:HA	1.99	0.43
10:W:43:THR:HG21	10:W:53:ILE:HD11	2.00	0.43
10:W:98:ALA:HB3	10:W:175:HIS:CG	2.53	0.43
10:W:303:LYS:HZ3	10:W:306:GLN:HB2	1.82	0.43
3:G:260:ASP:CG	3:H:300:ARG:HH12	2.22	0.43
3:H:28:SER:HA	3:H:41:LEU:HD11	2.01	0.43
3:H:100:ASP:OD1	3:H:101:ASP:N	2.51	0.43
5:K:109:LYS:N	5:K:110:PRO:HD2	2.33	0.43
9:P:188:MET:HA	9:P:188:MET:HE2	2.00	0.43
10:T:88:ARG:NH1	10:T:163:ARG:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:8:PRO:HD2	10:U:11:LEU:HD11	2.01	0.43
10:U:88:ARG:HD3	10:U:89:VAL:N	2.33	0.43
3:D:83:GLU:HB2	3:D:85:ILE:HG22	2.00	0.43
3:F:35:ARG:HH22	4:I:442:TYR:HE2	1.66	0.43
3:F:65:ARG:HE	3:F:100:ASP:CG	2.22	0.43
3:H:77:ARG:HD3	3:H:86:ASN:HB3	2.00	0.43
5:J:66:SER:OG	9:P:259:GLY:HA2	2.18	0.43
5:J:102:LEU:HB3	5:K:66:SER:HB2	2.00	0.43
5:K:5:SER:O	5:K:8:ASP:N	2.50	0.43
6:M:29:C:N4	6:M:30:A:H62	2.16	0.43
9:P:203:TRP:HB2	10:W:137:ASN:OD1	2.18	0.43
10:R:255:LEU:HD21	10:R:285:LEU:HD12	1.99	0.43
10:S:56:TYR:CD2	10:S:329:LEU:HD11	2.53	0.43
10:T:142:ASN:HB3	10:U:131:ARG:HH22	1.84	0.43
10:W:97:ILE:HG22	10:W:104:PHE:CE1	2.53	0.43
3:F:32:ASP:OD2	4:I:442:TYR:OH	2.27	0.43
3:F:57:SER:O	3:F:61:ARG:HG3	2.17	0.43
3:F:109:LEU:HD21	6:M:17:A:C2	2.53	0.43
5:J:59:LEU:O	5:J:63:GLU:HG3	2.19	0.43
10:Q:30:HIS:ND1	10:Q:278:ILE:HG13	2.32	0.43
10:S:30:HIS:HB2	10:S:233:TYR:OH	2.19	0.43
10:U:320:LYS:HE3	10:U:320:LYS:HB2	1.90	0.43
10:V:215:ARG:HG3	10:V:215:ARG:HH11	1.82	0.43
10:V:252:GLN:HB2	10:V:263:LEU:HB2	1.99	0.43
3:C:41:LEU:N	3:C:174:GLU:OE1	2.41	0.43
3:G:40:ILE:HD12	3:G:40:ILE:N	2.34	0.43
3:H:268:ASP:OD2	3:H:270:SER:OG	2.34	0.43
3:H:280:LYS:O	3:H:284:GLN:HG2	2.19	0.43
6:M:59:A:H3'	6:M:60:U:O2	2.19	0.43
8:O:63:DT:H2"	8:O:64:DA:C8	2.54	0.43
8:O:68:DC:H2'	8:O:69:DT:H71	2.00	0.43
9:P:88:LYS:HG2	9:P:134:ASN:O	2.19	0.43
10:T:126:PHE:CD2	10:T:128:TYR:HD1	2.37	0.43
10:W:96:ALA:HA	10:W:112:ARG:HH12	1.82	0.43
1:A:189:ARG:HH21	4:I:23:ARG:CZ	2.31	0.43
3:C:68:LEU:O	3:C:73:TYR:HB2	2.19	0.43
3:E:37:ASN:HB3	3:E:171:HIS:HA	1.99	0.43
3:E:64:LEU:HB3	3:E:104:PHE:HZ	1.83	0.43
3:G:216:ILE:HG13	3:G:217:PHE:CD2	2.53	0.43
3:H:262:VAL:HG11	3:H:293:LEU:HD13	2.00	0.43
10:V:56:TYR:CE1	10:V:211:LEU:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:118:GLU:OE2	10:W:163:ARG:NH1	2.52	0.43
2:B:212:THR:O	2:B:216:GLU:HG3	2.19	0.43
3:E:102:ASP:OD2	3:E:196:ARG:NH1	2.41	0.43
3:E:157:LEU:HD13	3:E:172:PHE:CE2	2.53	0.43
4:I:87:ILE:HD12	4:I:87:ILE:HA	1.80	0.43
4:I:202:LEU:O	4:I:205:VAL:HG12	2.19	0.43
5:L:80:GLU:HB2	5:L:81:HIS:CE1	2.54	0.43
10:S:273:ARG:HB2	10:S:284:TRP:CZ3	2.54	0.43
10:W:287:ARG:HG2	10:W:308:ARG:HG3	2.00	0.43
1:A:27:THR:HG22	1:A:94:GLU:HB2	2.00	0.43
3:D:145:ALA:HA	3:D:182:TYR:HB3	2.01	0.43
3:D:211:GLY:HA3	6:M:32:U:C6	2.53	0.43
3:E:143:ASN:HD21	3:F:26:LEU:HB2	1.84	0.43
3:H:104:PHE:O	6:M:6:C:H5"	2.19	0.43
5:J:35:GLU:CG	5:J:36:GLY:H	2.31	0.43
10:U:81:LYS:NZ	10:U:85:ASP:OD2	2.39	0.43
10:U:270:PHE:HA	10:U:284:TRP:HZ3	1.84	0.43
2:B:194:GLU:OE1	2:B:195:GLN:N	2.52	0.43
3:C:205:MET:HE3	3:C:223:PRO:HD2	2.01	0.43
3:D:167:SER:HA	7:N:26:DT:OP1	2.19	0.43
3:E:279:VAL:HG13	3:E:298:ILE:HD11	2.01	0.43
4:I:115:ARG:HG3	4:I:299:GLN:HB2	2.00	0.43
6:M:24:A:H61	7:N:41:DA:N6	2.17	0.43
7:N:6:DT:H2"	7:N:7:DA:C8	2.53	0.43
7:N:11:DG:H5"	9:P:88:LYS:NZ	2.34	0.43
9:P:3:ILE:HB	10:Q:250:THR:HB	2.00	0.43
9:P:60:ILE:HG23	9:P:104:VAL:HG11	2.01	0.43
9:P:68:GLU:HB2	9:P:73:LEU:HD11	2.00	0.43
10:Q:58:ALA:O	10:Q:63:LYS:NZ	2.51	0.43
10:S:57:GLY:HA3	10:S:61:VAL:HG21	2.00	0.43
10:T:130:VAL:HG11	10:T:151:ALA:HB1	2.00	0.43
10:W:20:LEU:HD23	10:W:293:LEU:HD23	2.01	0.43
10:W:270:PHE:O	10:W:274:THR:HG23	2.19	0.43
3:C:50:LYS:HE3	3:C:50:LYS:HB2	1.82	0.43
3:D:200:MET:HE3	3:D:200:MET:HB3	1.73	0.43
3:E:134:ASN:ND2	3:E:135:GLN:HG2	2.34	0.43
3:E:170:LEU:HD22	7:N:31:DC:C2	2.53	0.43
3:F:186:ILE:HD12	3:F:200:MET:CE	2.49	0.43
3:F:272:LEU:HD12	3:F:272:LEU:HA	1.88	0.43
3:G:61:ARG:NH2	3:G:140:LEU:O	2.52	0.43
4:I:44:ARG:HG2	4:I:49:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:23:LYS:HD2	5:K:111:LYS:NZ	2.34	0.43
5:K:93:PRO:HD2	5:K:96:GLU:OE1	2.19	0.43
7:N:46:DA:N7	7:N:47:DT:H73	2.34	0.43
9:P:37:LEU:HD21	9:P:92:ASN:HA	2.01	0.43
9:P:166:PHE:CZ	9:P:212:GLU:HB2	2.54	0.43
10:R:133:ILE:HG12	10:R:143:VAL:HG22	2.01	0.43
10:S:46:GLU:N	10:S:46:GLU:OE1	2.52	0.43
10:S:252:GLN:NE2	10:S:263:LEU:HB2	2.34	0.43
10:V:100:GLU:HB3	10:W:106:TRP:CD1	2.53	0.43
2:B:184:LEU:O	2:B:188:ASP:HB2	2.19	0.42
3:D:170:LEU:HD22	7:N:25:DG:C4	2.53	0.42
3:H:306:ILE:HD13	3:H:306:ILE:HA	1.83	0.42
4:I:342:ASN:HD22	4:I:343:PRO:CD	2.31	0.42
7:N:-6:DC:H2"	7:N:-5:DG:C8	2.53	0.42
10:R:30:HIS:HB2	10:R:233:TYR:OH	2.19	0.42
10:S:42:ARG:HA	10:S:42:ARG:NE	2.34	0.42
10:S:55:VAL:HB	10:S:206:LEU:HD23	2.01	0.42
10:W:259:GLU:OE2	10:W:299:THR:HB	2.18	0.42
3:D:268:ASP:OD2	3:D:270:SER:OG	2.36	0.42
3:E:254:LEU:HD12	3:E:254:LEU:HA	1.84	0.42
3:F:135:GLN:O	6:M:17:A:O2'	2.34	0.42
3:G:55:VAL:HB	3:G:145:ALA:HB3	2.01	0.42
4:I:443:CYS:O	4:I:486:ARG:NH1	2.52	0.42
9:P:53:GLU:HA	9:P:78:LEU:HD13	2.01	0.42
10:Q:284:TRP:O	10:Q:288:VAL:HG23	2.19	0.42
10:U:93:GLY:HA2	10:U:169:PHE:HB2	2.00	0.42
10:V:220:GLN:O	10:V:224:ARG:HG3	2.19	0.42
10:V:287:ARG:HB3	10:V:308:ARG:HD2	2.00	0.42
3:C:183:TYR:CD1	3:C:239:SER:HA	2.54	0.42
3:C:286:ASP:OD1	3:C:286:ASP:N	2.53	0.42
4:I:63:TRP:NE1	4:I:67:ASP:OD1	2.51	0.42
4:I:359:TRP:CD2	4:I:362:PHE:HD2	2.37	0.42
7:N:8:DC:H2"	7:N:9:DG:C8	2.54	0.42
7:N:63:DT:H2"	7:N:64:DA:N7	2.34	0.42
10:R:81:LYS:HE2	10:R:88:ARG:HG2	2.01	0.42
10:V:39:ILE:HG22	10:V:228:ILE:HD13	2.01	0.42
10:V:300:ILE:HG22	10:V:304:ASP:OD2	2.20	0.42
1:A:37:TYR:CD2	1:A:208:VAL:HG11	2.54	0.42
2:B:29:TYR:CD1	2:B:165:ILE:HG13	2.54	0.42
3:E:57:SER:HB2	3:E:142:MET:HG3	2.02	0.42
4:I:333:LYS:O	4:I:335:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:50:DA:H2'	8:O:51:DT:H71	2.01	0.42
9:P:66:LYS:HA	9:P:66:LYS:HD2	1.69	0.42
9:P:185:LEU:HD11	9:P:204:LEU:HD11	2.01	0.42
10:Q:275:LEU:HD11	10:Q:318:MET:HG3	2.02	0.42
10:R:115:ILE:HD13	10:R:141:ILE:HG12	2.01	0.42
10:T:249:LEU:HD12	10:T:252:GLN:HE21	1.83	0.42
10:W:56:TYR:HE1	10:W:211:LEU:HB3	1.84	0.42
3:D:46:TRP:CG	3:D:47:ASN:N	2.86	0.42
3:E:57:SER:H	3:E:144:MET:HG2	1.84	0.42
3:F:165:LYS:HE2	7:N:36:DG:H21	1.84	0.42
3:F:205:MET:HG3	3:F:306:ILE:HG13	2.01	0.42
10:T:94:ILE:HD11	10:T:112:ARG:HB3	2.02	0.42
10:U:61:VAL:HG23	10:U:63:LYS:HG3	2.01	0.42
10:U:118:GLU:OE2	10:U:163:ARG:NE	2.49	0.42
10:U:255:LEU:HD22	10:U:289:LEU:HD21	2.02	0.42
10:V:248:LEU:HD11	10:V:270:PHE:CD2	2.55	0.42
10:W:67:ARG:NE	10:W:171:ASP:OD2	2.45	0.42
10:W:304:ASP:HA	10:W:307:LYS:HD2	2.01	0.42
3:C:148:LEU:HD12	3:C:148:LEU:HA	1.91	0.42
3:F:266:GLN:HE22	3:G:302:ARG:NH2	2.15	0.42
4:I:245:ARG:NE	4:I:273:ASP:OD2	2.40	0.42
4:I:395:GLU:CD	4:I:395:GLU:H	2.21	0.42
7:N:26:DT:H4'	7:N:27:DT:O5'	2.18	0.42
9:P:63:LEU:HD12	9:P:104:VAL:HG13	2.01	0.42
10:Q:282:LYS:HG2	11:Q:600:ATP:N3	2.34	0.42
10:T:60:GLY:O	10:T:61:VAL:HG13	2.20	0.42
10:U:73:LYS:O	10:U:76:GLU:HG3	2.18	0.42
10:U:189:LEU:HG	10:U:221:LEU:HD22	2.02	0.42
10:U:273:ARG:HB2	10:U:284:TRP:CZ3	2.54	0.42
10:U:288:VAL:HG21	10:U:305:LEU:HD22	2.01	0.42
10:V:108:GLU:OE2	10:V:112:ARG:NH2	2.52	0.42
2:B:86:TYR:C	2:B:87:LEU:HD22	2.40	0.42
3:D:192:LYS:HD3	3:D:192:LYS:HA	1.83	0.42
3:H:155:VAL:HG22	3:H:156:LYS:H	1.84	0.42
3:H:192:LYS:HA	3:H:192:LYS:HD3	1.88	0.42
4:I:44:ARG:O	4:I:45:GLN:C	2.55	0.42
9:P:47:ALA:HB1	10:Q:162:HIS:CE1	2.54	0.42
9:P:214:ILE:HB	9:P:218:ARG:NH2	2.34	0.42
9:P:217:TYR:O	9:P:221:ILE:HG12	2.19	0.42
9:P:288:HIS:CG	9:P:291:LYS:HD3	2.55	0.42
10:Q:111:THR:O	10:Q:115:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:189:LEU:HG	10:S:221:LEU:HD22	2.02	0.42
10:S:193:LYS:HE3	10:S:193:LYS:HB3	1.83	0.42
10:U:89:VAL:HG22	10:U:163:ARG:HB3	2.02	0.42
10:V:288:VAL:HG12	10:V:300:ILE:HG21	2.02	0.42
10:W:270:PHE:CZ	10:W:305:LEU:HD13	2.54	0.42
1:A:1:MET:HE2	1:A:2:ILE:O	2.20	0.42
1:A:155:TYR:HD1	1:A:156:LEU:HD23	1.85	0.42
2:B:45:LEU:HD22	2:B:83:ILE:HD11	2.01	0.42
3:E:134:ASN:H	3:E:134:ASN:ND2	2.17	0.42
4:I:320:GLN:HE21	4:I:324:TYR:HE2	1.66	0.42
5:L:6:GLU:O	5:L:10:GLN:HG2	2.19	0.42
9:P:28:ALA:HB1	9:P:31:THR:OG1	2.20	0.42
10:R:44:ILE:HG21	10:R:74:LEU:HD11	2.01	0.42
10:R:111:THR:HB	10:R:152:LEU:HD21	2.01	0.42
10:R:233:TYR:HD1	10:R:240:ASP:HB2	1.84	0.42
10:U:215:ARG:HG3	10:U:216:ASN:N	2.33	0.42
11:V:600:ATP:PG	10:W:220:GLN:HE22	2.43	0.42
10:W:220:GLN:OE1	10:W:224:ARG:NH1	2.49	0.42
4:I:160:ASP:N	4:I:160:ASP:OD1	2.53	0.42
4:I:221:LEU:HD21	4:I:339:ILE:H	1.83	0.42
4:I:331:ILE:H	4:I:331:ILE:HD12	1.85	0.42
7:N:-9:DT:H2"	7:N:-8:DA:N7	2.35	0.42
9:P:4:TYR:CE2	10:Q:31:PRO:HD3	2.55	0.42
10:T:273:ARG:HD2	10:T:273:ARG:HA	1.76	0.42
10:V:126:PHE:O	10:V:126:PHE:CD1	2.73	0.42
1:A:153:GLU:HB3	1:A:198:LEU:HB3	2.01	0.42
3:F:152:ASP:OD1	3:F:152:ASP:N	2.43	0.42
4:I:175:LEU:HG	4:I:202:LEU:HB3	2.01	0.42
4:I:326:LYS:HB2	4:I:378:GLN:OE1	2.19	0.42
4:I:340:LYS:HG3	4:I:374:TYR:CE1	2.55	0.42
4:I:344:ILE:HD13	4:I:344:ILE:HA	1.93	0.42
9:P:271:ILE:HD12	9:P:299:LYS:HG3	2.02	0.42
10:U:263:LEU:HD12	10:U:263:LEU:HA	1.87	0.42
3:C:60:ILE:HG23	3:C:207:LEU:HD21	2.01	0.41
3:F:280:LYS:HE2	3:F:280:LYS:HB2	1.86	0.41
7:N:24:DC:H6	7:N:24:DC:H2'	1.73	0.41
10:U:189:LEU:HD12	10:U:189:LEU:HA	1.88	0.41
10:U:217:LEU:O	10:U:221:LEU:HB2	2.20	0.41
10:U:220:GLN:OE1	10:U:224:ARG:NH1	2.51	0.41
10:W:71:GLU:HA	10:W:91:VAL:HG11	2.02	0.41
2:B:94:ILE:HD12	2:B:99:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:109:LYS:H	5:J:109:LYS:HG3	1.48	0.41
8:O:82:DG:H2"	8:O:83:DG:C8	2.55	0.41
10:R:35:GLU:O	10:R:38:GLU:HG2	2.20	0.41
10:V:67:ARG:NH1	10:V:171:ASP:HB2	2.35	0.41
10:W:52:PHE:HZ	10:W:192:LEU:HB3	1.86	0.41
3:C:227:VAL:HG12	3:C:238:ILE:HD12	2.01	0.41
3:F:263:GLU:OE1	3:F:292:PRO:HD2	2.20	0.41
3:H:159:ALA:HA	3:H:170:LEU:H	1.84	0.41
4:I:169:ILE:HD11	4:I:196:PRO:HG3	2.02	0.41
4:I:459:ARG:HH21	5:L:49:ARG:HH21	1.67	0.41
6:M:12:A:H2'	6:M:13:A:C8	2.55	0.41
9:P:118:THR:HG23	9:P:120:LEU:HG	2.02	0.41
10:Q:26:TYR:O	10:Q:282:LYS:NZ	2.45	0.41
10:W:153:ARG:NH2	10:W:195:LEU:HG	2.34	0.41
2:B:17:LYS:NZ	2:B:70:ARG:HH22	2.19	0.41
3:E:158:GLY:N	3:E:171:HIS:O	2.52	0.41
3:H:20:VAL:HG23	3:H:223:PRO:HB3	2.01	0.41
3:H:27:ALA:HB2	3:H:219:TYR:CD1	2.55	0.41
4:I:120:TYR:HA	4:I:147:TYR:HA	2.02	0.41
5:K:102:LEU:HD22	5:L:70:VAL:HG11	2.03	0.41
8:O:79:DA:H2"	8:O:80:DG:C8	2.55	0.41
9:P:61:ALA:O	9:P:65:LEU:N	2.47	0.41
9:P:134:ASN:O	9:P:135:TYR:HD1	2.04	0.41
10:Q:30:HIS:NE2	10:Q:33:LEU:HB2	2.35	0.41
10:W:157:GLU:O	10:W:161:ILE:HG12	2.20	0.41
10:W:179:VAL:HG22	10:W:180:ALA:H	1.84	0.41
10:W:267:TRP:CG	10:W:268:GLU:N	2.89	0.41
10:W:268:GLU:H	10:W:268:GLU:CD	2.24	0.41
2:B:171:GLN:HE21	2:B:171:GLN:HB3	1.62	0.41
3:C:38:LYS:HE2	3:C:40:ILE:HG22	2.01	0.41
3:C:54:PHE:CE1	3:C:146:VAL:HG22	2.55	0.41
4:I:100:ARG:HH22	4:I:254:THR:HB	1.86	0.41
4:I:325:PHE:HA	4:I:382:ASN:CG	2.40	0.41
4:I:427:PRO:HA	4:I:428:PRO:HD3	1.91	0.41
7:N:46:DA:C8	7:N:47:DT:H73	2.55	0.41
9:P:181:CYS:HB3	9:P:200:CYS:HB3	2.02	0.41
10:S:111:THR:O	10:S:115:ILE:HG12	2.20	0.41
10:T:44:ILE:HG21	10:T:74:LEU:HD11	2.03	0.41
10:T:327:ARG:HG2	10:T:327:ARG:HH11	1.86	0.41
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.88	0.41
2:B:135:VAL:HG13	2:B:148:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:TYR:HH	3:C:234:PHE:HE2	1.67	0.41
3:D:165:LYS:HE3	6:M:40:G:N2	2.31	0.41
3:D:224:ASP:O	3:D:277:THR:HG22	2.20	0.41
3:H:209:LYS:HD2	3:H:214:SER:OG	2.21	0.41
3:H:273:TRP:HB3	3:H:305:MET:SD	2.61	0.41
4:I:262:LEU:HB3	4:I:287:VAL:HG11	2.02	0.41
5:L:66:SER:O	5:L:70:VAL:HG12	2.20	0.41
9:P:139:CYS:HB3	9:P:159:TRP:CZ2	2.56	0.41
10:S:291:ASP:OD2	10:S:308:ARG:HD3	2.21	0.41
10:T:32:ARG:NH2	10:T:240:ASP:OD2	2.53	0.41
10:U:54:PHE:CE2	10:U:205:LEU:HD12	2.55	0.41
10:W:184:LYS:HA	10:W:187:ASP:OD2	2.20	0.41
3:C:85:ILE:HD13	3:D:164:GLU:OE1	2.21	0.41
3:C:273:TRP:HB3	3:C:305:MET:SD	2.60	0.41
3:D:245:CYS:HB2	3:D:251:GLU:HG2	2.02	0.41
3:D:251:GLU:O	3:D:252:ALA:HB3	2.21	0.41
3:E:248:LYS:H	3:E:248:LYS:HG2	1.63	0.41
3:F:235:ALA:HA	3:G:222:CYS:SG	2.60	0.41
3:F:266:GLN:HE22	3:G:302:ARG:HH12	1.69	0.41
3:G:160:LYS:HE3	3:G:160:LYS:HB2	1.83	0.41
3:G:306:ILE:HD13	3:G:306:ILE:HA	1.86	0.41
4:I:138:GLU:HB3	4:I:335:LYS:HD3	2.02	0.41
4:I:407:GLN:HA	4:I:410:MET:HG2	2.02	0.41
7:N:17:DA:H2'	7:N:18:DT:H71	2.03	0.41
10:U:121:LEU:HB3	10:U:124:HIS:CE1	2.52	0.41
10:W:170:VAL:HB	10:W:205:LEU:HD23	2.03	0.41
10:W:195:LEU:O	10:W:199:THR:N	2.52	0.41
1:A:64:SER:HA	1:A:65:PRO:HD3	1.93	0.41
1:A:74:MET:HE1	1:A:91:CYS:HB3	2.03	0.41
2:B:14:LEU:HD12	2:B:14:LEU:HA	1.81	0.41
3:D:135:GLN:OE1	3:D:135:GLN:N	2.54	0.41
3:D:161:SER:N	6:M:38:A:OP1	2.54	0.41
3:H:170:LEU:HD11	7:N:49:DA:C4	2.56	0.41
10:Q:196:ALA:HB2	10:Q:203:HIS:HD2	1.86	0.41
10:Q:307:LYS:HB3	10:R:42:ARG:HH22	1.85	0.41
10:T:94:ILE:HG12	10:T:95:GLU:N	2.36	0.41
10:V:92:VAL:HG21	10:V:117:LEU:HA	2.02	0.41
10:V:126:PHE:HD1	10:V:128:TYR:CD1	2.39	0.41
10:W:165:PRO:HD2	10:W:201:ILE:CD1	2.51	0.41
10:W:212:LEU:HD13	10:W:328:GLN:HB2	2.03	0.41
1:A:76:ARG:NH1	1:A:78:LYS:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TYR:CE2	3:H:33:ILE:HD12	2.56	0.41
2:B:173:LYS:O	2:B:175:ARG:NH1	2.54	0.41
3:C:73:TYR:O	3:C:75:VAL:HG23	2.20	0.41
3:D:272:LEU:HD12	3:D:272:LEU:HA	1.96	0.41
3:E:35:ARG:HG3	3:E:36:GLY:N	2.36	0.41
3:F:269:PRO:HB3	3:F:296:ALA:HB2	2.02	0.41
3:G:91:GLU:OE1	3:G:91:GLU:N	2.38	0.41
4:I:344:ILE:HG13	4:I:386:PHE:CZ	2.45	0.41
4:I:373:GLU:HG2	4:I:376:PHE:CD2	2.47	0.41
4:I:396:ASP:O	4:I:399:TYR:N	2.54	0.41
5:J:52:LEU:HD23	5:J:52:LEU:HA	1.82	0.41
5:J:106:ALA:HB1	5:J:109:LYS:HZ1	1.86	0.41
7:N:-13:DT:H2"	7:N:-12:DA:N7	2.36	0.41
7:N:-1:DA:H2'	7:N:0:DT:H71	2.03	0.41
7:N:10:DC:H2"	7:N:11:DG:C8	2.56	0.41
10:Q:184:LYS:HA	10:Q:187:ASP:HB2	2.03	0.41
10:R:293:LEU:HD13	10:R:293:LEU:HA	1.94	0.41
10:S:97:ILE:HD11	10:S:112:ARG:HD2	2.02	0.41
10:S:102:ARG:CZ	10:S:102:ARG:HB2	2.51	0.41
10:T:142:ASN:HB3	10:U:131:ARG:NH2	2.36	0.41
10:T:249:LEU:HA	10:T:252:GLN:HE21	1.84	0.41
10:T:257:LEU:HD13	10:T:299:THR:HA	2.01	0.41
10:U:273:ARG:NH1	10:U:310:LEU:O	2.53	0.41
10:V:30:HIS:HB3	10:V:247:VAL:HG21	2.03	0.41
10:V:67:ARG:HH12	10:V:171:ASP:HB2	1.86	0.41
10:W:52:PHE:CZ	10:W:192:LEU:HB3	2.56	0.41
10:W:58:ALA:C	10:W:60:GLY:N	2.73	0.41
10:W:60:GLY:O	10:W:277:CYS:HB3	2.21	0.41
10:W:121:LEU:O	10:W:124:HIS:ND1	2.48	0.41
10:W:232:ARG:NE	10:W:322:ILE:HD12	2.35	0.41
2:B:17:LYS:HB2	2:B:102:ASP:CG	2.40	0.41
3:E:66:PHE:O	3:E:70:LYS:HG2	2.20	0.41
3:E:148:LEU:HD12	3:E:148:LEU:HA	1.90	0.41
3:E:198:LEU:HB2	3:E:199:PRO:HD3	2.02	0.41
3:G:215:ASN:HD21	6:M:18:U:P	2.43	0.41
4:I:331:ILE:O	4:I:338:PHE:N	2.54	0.41
7:N:13:DA:H2"	7:N:14:DG:H8	1.86	0.41
10:S:61:VAL:CG2	10:S:63:LYS:HG3	2.51	0.41
10:S:131:ARG:H	10:S:131:ARG:HG2	1.63	0.41
10:T:30:HIS:HB2	10:T:233:TYR:OH	2.21	0.41
10:V:208:THR:OG1	10:V:209:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TYR:O	1:A:148:ILE:HA	2.21	0.40
3:E:107:ALA:HA	3:E:135:GLN:HE22	1.85	0.40
3:F:133:PRO:HB2	3:F:134:ASN:H	1.65	0.40
3:H:55:VAL:HG11	3:H:210:VAL:HG11	2.03	0.40
5:K:83:GLU:OE1	5:K:83:GLU:N	2.44	0.40
10:S:302:LEU:O	10:S:305:LEU:N	2.54	0.40
10:T:126:PHE:HD2	10:T:128:TYR:CD1	2.39	0.40
10:T:153:ARG:HH21	10:T:198:MET:HE2	1.86	0.40
10:V:266:HIS:ND1	10:V:266:HIS:N	2.69	0.40
10:W:263:LEU:HD12	10:W:263:LEU:N	2.36	0.40
1:A:15:THR:HG21	1:A:93:GLN:NE2	2.36	0.40
3:C:264:CYS:SG	3:D:300:ARG:HG3	2.61	0.40
3:D:40:ILE:HD12	3:D:40:ILE:N	2.34	0.40
3:D:154:ALA:HB1	3:D:175:TYR:CE2	2.56	0.40
3:F:190:HIS:O	3:F:190:HIS:ND1	2.54	0.40
3:F:244:TYR:HE2	3:F:249:SER:HB2	1.86	0.40
5:J:76:LYS:H	5:J:76:LYS:HG3	1.66	0.40
6:M:41:U:H3'	6:M:42:A:H2'	2.03	0.40
10:U:235:ALA:HB2	10:U:271:TYR:CZ	2.56	0.40
10:W:288:VAL:HG11	10:W:305:LEU:HD23	2.03	0.40
2:B:26:ASP:OD1	2:B:26:ASP:N	2.54	0.40
3:C:231:THR:OG1	3:C:232:ASN:N	2.54	0.40
3:F:255:SER:OG	3:F:258:PHE:HB3	2.21	0.40
3:G:45:TYR:CG	3:H:248:LYS:HD3	2.56	0.40
3:G:109:LEU:HD11	6:M:12:A:C2	2.56	0.40
3:G:192:LYS:HA	3:G:192:LYS:HD3	1.84	0.40
3:H:75:VAL:HG13	3:H:100:ASP:HB3	2.03	0.40
4:I:354:LYS:HB2	4:I:356:ILE:HG12	2.03	0.40
5:K:39:PRO:HA	5:K:40:PRO:HD3	1.92	0.40
6:M:18:U:H2'	6:M:19:U:C6	2.56	0.40
10:W:257:LEU:HD12	10:W:261:PRO:HD3	2.04	0.40
3:C:21:LEU:HD11	3:C:179:ARG:HB2	2.03	0.40
3:C:186:ILE:HG21	3:C:197:ILE:HD13	2.02	0.40
3:D:54:PHE:HD1	3:D:146:VAL:HA	1.87	0.40
3:E:306:ILE:HD13	3:E:306:ILE:HA	1.86	0.40
3:E:317:LEU:HD23	3:E:317:LEU:HA	1.88	0.40
3:F:109:LEU:HD22	7:N:47:DT:C2	2.56	0.40
3:F:253:LYS:HB3	3:F:253:LYS:HE3	1.85	0.40
4:I:96:ARG:NH1	4:I:250:GLN:HE21	2.19	0.40
4:I:358:TRP:HE3	4:I:359:TRP:HD1	1.68	0.40
5:J:14:PHE:CE1	5:J:89:ILE:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:196:ALA:O	10:Q:200:GLY:N	2.47	0.40
10:R:135:ARG:HG3	10:R:136:ASP:H	1.87	0.40
10:S:59:SER:OG	10:T:220:GLN:HA	2.21	0.40
10:S:256:PRO:O	10:S:257:LEU:HD23	2.22	0.40
10:U:92:VAL:HG21	10:U:117:LEU:HG	2.02	0.40
10:U:164:HIS:HA	10:U:201:ILE:HD11	2.03	0.40
10:W:314:GLN:O	10:W:318:MET:HG2	2.21	0.40
1:A:140:GLU:OE1	1:A:142:ASP:N	2.30	0.40
3:D:64:LEU:HD23	3:D:64:LEU:HA	1.83	0.40
3:F:65:ARG:NE	3:F:100:ASP:OD1	2.52	0.40
4:I:43:SER:O	4:I:46:ARG:HD3	2.22	0.40
4:I:198:TYR:O	4:I:202:LEU:HG	2.21	0.40
4:I:329:TYR:CE2	4:I:331:ILE:HG13	2.57	0.40
4:I:365:LYS:O	4:I:370:ASP:HB2	2.21	0.40
4:I:471:GLU:OE2	4:I:471:GLU:N	2.42	0.40
5:L:29:ILE:HD13	5:L:29:ILE:HA	1.89	0.40
5:L:88:LEU:HD11	5:L:100:TRP:CZ3	2.56	0.40
6:M:41:U:H5'	6:M:42:A:C8	2.57	0.40
9:P:78:LEU:O	9:P:81:LEU:HD23	2.21	0.40
10:Q:272:GLU:OE2	10:Q:273:ARG:NE	2.55	0.40
10:R:59:SER:OG	10:S:223:ARG:HD3	2.22	0.40
10:S:209:TYR:HE2	10:S:326:GLU:HG3	1.86	0.40
10:U:61:VAL:CG2	10:U:63:LYS:HG3	2.52	0.40
10:U:110:TYR:CZ	10:U:153:ARG:HG3	2.57	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	210/212 (99%)	202 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	211/220 (96%)	201 (95%)	9 (4%)	1 (0%)	29	68
3	C	281/323 (87%)	249 (89%)	30 (11%)	2 (1%)	22	61
3	D	281/323 (87%)	243 (86%)	35 (12%)	3 (1%)	14	53
3	E	282/323 (87%)	258 (92%)	22 (8%)	2 (1%)	22	61
3	F	281/323 (87%)	243 (86%)	36 (13%)	2 (1%)	22	61
3	G	281/323 (87%)	263 (94%)	16 (6%)	2 (1%)	22	61
3	H	281/323 (87%)	257 (92%)	22 (8%)	2 (1%)	22	61
4	I	492/534 (92%)	476 (97%)	14 (3%)	2 (0%)	34	71
5	J	107/138 (78%)	98 (92%)	9 (8%)	0	100	100
5	K	107/138 (78%)	98 (92%)	8 (8%)	1 (1%)	17	57
5	L	107/138 (78%)	105 (98%)	2 (2%)	0	100	100
9	P	325/329 (99%)	312 (96%)	13 (4%)	0	100	100
10	Q	306/383 (80%)	291 (95%)	15 (5%)	0	100	100
10	R	341/383 (89%)	325 (95%)	15 (4%)	1 (0%)	41	75
10	S	341/383 (89%)	329 (96%)	11 (3%)	1 (0%)	41	75
10	T	341/383 (89%)	326 (96%)	12 (4%)	3 (1%)	17	57
10	U	341/383 (89%)	323 (95%)	16 (5%)	2 (1%)	25	64
10	V	341/383 (89%)	323 (95%)	15 (4%)	3 (1%)	17	57
10	W	341/383 (89%)	318 (93%)	19 (6%)	4 (1%)	13	51
All	All	5598/6328 (88%)	5240 (94%)	327 (6%)	31 (1%)	29	64

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	136	ARG
3	E	247	PRO
3	F	247	PRO
10	V	61	VAL
10	W	61	VAL
4	I	334	TYR
10	R	130	VAL
10	S	130	VAL
10	T	61	VAL
10	T	130	VAL
10	U	61	VAL

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Mol	Chain	Res	Type
10	U	130	VAL
3	G	267	ILE
4	I	361	ASN
10	T	218	SER
10	V	130	VAL
10	W	100	GLU
3	F	136	ARG
10	W	62	GLY
10	W	130	VAL
2	B	185	ASN
3	D	161	SER
3	G	75	VAL
3	H	38	LYS
3	E	267	ILE
10	V	60	GLY
3	C	267	ILE
3	D	267	ILE
5	K	92	SER
3	H	267	ILE
3	C	238	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	193/193 (100%)	187 (97%)	6 (3%)	40	71
2	B	187/193 (97%)	182 (97%)	5 (3%)	44	73
3	C	250/287 (87%)	244 (98%)	6 (2%)	49	75
3	D	250/287 (87%)	243 (97%)	7 (3%)	43	72
3	E	251/287 (88%)	242 (96%)	9 (4%)	35	67
3	F	250/287 (87%)	241 (96%)	9 (4%)	35	67
3	G	250/287 (87%)	246 (98%)	4 (2%)	62	83
3	H	250/287 (87%)	244 (98%)	6 (2%)	49	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	449/489 (92%)	435 (97%)	14 (3%)	40	71
5	J	98/126 (78%)	96 (98%)	2 (2%)	55	79
5	K	98/126 (78%)	95 (97%)	3 (3%)	40	71
5	L	98/126 (78%)	97 (99%)	1 (1%)	76	88
9	P	292/294 (99%)	282 (97%)	10 (3%)	37	69
10	Q	269/332 (81%)	257 (96%)	12 (4%)	27	62
10	R	296/332 (89%)	287 (97%)	9 (3%)	41	71
10	S	296/332 (89%)	283 (96%)	13 (4%)	28	63
10	T	296/332 (89%)	286 (97%)	10 (3%)	37	69
10	U	296/332 (89%)	286 (97%)	10 (3%)	37	69
10	V	296/332 (89%)	281 (95%)	15 (5%)	24	58
10	W	296/332 (89%)	283 (96%)	13 (4%)	28	63
All	All	4961/5593 (89%)	4797 (97%)	164 (3%)	41	69

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PHE
1	A	18	GLU
1	A	108	ASP
1	A	160	ARG
1	A	202	ASP
1	A	203	LEU
2	B	98	PHE
2	B	116	TYR
2	B	154	GLN
2	B	171	GLN
2	B	175	ARG
3	C	32	ASP
3	C	34	ARG
3	C	221	PHE
3	C	244	TYR
3	C	294	ASN
3	C	305	MET
3	D	136	ARG
3	D	142	MET
3	D	160	LYS
3	D	221	PHE

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Mol	Chain	Res	Type
3	D	248	LYS
3	D	260	ASP
3	D	264	CYS
3	E	28	SER
3	E	134	ASN
3	E	142	MET
3	E	206	ASN
3	E	209	LYS
3	E	221	PHE
3	E	244	TYR
3	E	246	ASP
3	E	248	LYS
3	F	30	ASN
3	F	77	ARG
3	F	137	MET
3	F	182	TYR
3	F	190	HIS
3	F	221	PHE
3	F	244	TYR
3	F	255	SER
3	F	264	CYS
3	G	28	SER
3	G	160	LYS
3	G	200	MET
3	G	221	PHE
3	H	30	ASN
3	H	32	ASP
3	H	135	GLN
3	H	166	ASP
3	H	190	HIS
3	H	221	PHE
4	I	23	ARG
4	I	42	LEU
4	I	44	ARG
4	I	46	ARG
4	I	60	GLU
4	I	62	PHE
4	I	106	HIS
4	I	110	CYS
4	I	116	LEU
4	I	132	PHE
4	I	209	CYS

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Mol	Chain	Res	Type
4	I	298	ARG
4	I	358	TRP
4	I	375	LEU
5	J	8	ASP
5	J	56	TYR
5	K	49	ARG
5	K	55	CYS
5	K	56	TYR
5	L	49	ARG
9	P	4	TYR
9	P	33	TYR
9	P	67	ASP
9	P	70	LYS
9	P	110	MET
9	P	127	TYR
9	P	129	LYS
9	P	200	CYS
9	P	217	TYR
9	P	329	LEU
10	Q	25	ASN
10	Q	81	LYS
10	Q	125	LYS
10	Q	164	HIS
10	Q	192	LEU
10	Q	198	MET
10	Q	204	CYS
10	Q	230	PHE
10	Q	234	CYS
10	Q	251	PHE
10	Q	303	LYS
10	Q	327	ARG
10	R	86	ARG
10	R	102	ARG
10	R	127	ASP
10	R	214	PHE
10	R	230	PHE
10	R	251	PHE
10	R	273	ARG
10	R	286	LYS
10	R	301	THR
10	S	26	TYR
10	S	56	TYR

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Mol	Chain	Res	Type
10	S	59	SER
10	S	81	LYS
10	S	86	ARG
10	S	103	TYR
10	S	121	LEU
10	S	131	ARG
10	S	140	LYS
10	S	230	PHE
10	S	236	ASP
10	S	286	LYS
10	S	340	ARG
10	T	25	ASN
10	T	42	ARG
10	T	61	VAL
10	T	105	ASN
10	T	131	ARG
10	T	217	LEU
10	T	230	PHE
10	T	273	ARG
10	T	286	LYS
10	T	338	ASN
10	U	61	VAL
10	U	103	TYR
10	U	112	ARG
10	U	124	HIS
10	U	126	PHE
10	U	142	ASN
10	U	187	ASP
10	U	230	PHE
10	U	236	ASP
10	U	338	ASN
10	V	61	VAL
10	V	103	TYR
10	V	124	HIS
10	V	131	ARG
10	V	138	PHE
10	V	164	HIS
10	V	166	ASP
10	V	230	PHE
10	V	266	HIS
10	V	286	LYS
10	V	299	THR

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Mol	Chain	Res	Type
10	V	300	ILE
10	V	302	LEU
10	V	308	ARG
10	V	315	CYS
10	W	34	LYS
10	W	46	GLU
10	W	61	VAL
10	W	105	ASN
10	W	126	PHE
10	W	142	ASN
10	W	164	HIS
10	W	204	CYS
10	W	224	ARG
10	W	234	CYS
10	W	244	PHE
10	W	291	ASP
10	W	327	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
3	C	30	ASN
3	E	134	ASN
3	E	135	GLN
3	F	84	HIS
3	F	135	GLN
3	G	30	ASN
3	G	42	GLN
3	H	30	ASN
4	I	342	ASN
5	L	79	ASN
10	Q	30	HIS
10	Q	124	HIS
10	S	30	HIS
10	T	25	ASN
10	T	203	HIS
10	U	203	HIS
10	V	314	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	M	62/71 (87%)	26 (41%)	4 (6%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	M	2	U
6	M	3	G
6	M	4	C
6	M	8	A
6	M	9	G
6	M	15	U
6	M	19	U
6	M	20	U
6	M	21	A
6	M	26	G
6	M	27	G
6	M	28	C
6	M	33	G
6	M	39	C
6	M	40	G
6	M	41	U
6	M	42	A
6	M	44	G
6	M	45	U
6	M	46	G
6	M	47	A
6	M	48	G
6	M	49	U
6	M	50	C
6	M	53	G
6	M	54	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	M	3	G
6	M	14	G
6	M	26	G
6	M	41	U

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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ATP	V	600	12	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
11	ATP	W	600	12	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
11	ATP	R	600	12	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
11	ATP	T	600	12	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
11	ATP	S	600	12	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
11	ATP	U	600	12	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
11	ATP	Q	600	12	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	V	600	12	-	2/18/38/38	0/3/3/3
11	ATP	W	600	12	-	3/18/38/38	0/3/3/3
11	ATP	R	600	12	-	3/18/38/38	0/3/3/3
11	ATP	T	600	12	-	2/18/38/38	0/3/3/3
11	ATP	S	600	12	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ATP	U	600	12	-	3/18/38/38	0/3/3/3
11	ATP	Q	600	12	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	V	600	ATP	C5-C6-N6	2.30	123.85	120.35
11	S	600	ATP	C5-C6-N6	2.30	123.85	120.35
11	U	600	ATP	C5-C6-N6	2.30	123.84	120.35
11	T	600	ATP	C5-C6-N6	2.29	123.83	120.35
11	W	600	ATP	C5-C6-N6	2.28	123.82	120.35
11	R	600	ATP	C5-C6-N6	2.27	123.80	120.35
11	Q	600	ATP	C5-C6-N6	2.26	123.78	120.35
11	Q	600	ATP	PB-O3B-PG	2.05	139.86	132.83
11	W	600	ATP	PB-O3B-PG	2.04	139.82	132.83
11	R	600	ATP	PB-O3B-PG	2.03	139.81	132.83
11	U	600	ATP	PB-O3B-PG	2.03	139.78	132.83
11	T	600	ATP	PB-O3B-PG	2.03	139.78	132.83
11	V	600	ATP	PB-O3B-PG	2.02	139.75	132.83
11	S	600	ATP	PB-O3B-PG	2.02	139.75	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	600	ATP	PB-O3B-PG-O3G
11	U	600	ATP	C5'-O5'-PA-O1A
11	W	600	ATP	C5'-O5'-PA-O1A
11	W	600	ATP	C5'-O5'-PA-O3A
11	Q	600	ATP	C4'-C5'-O5'-PA
11	R	600	ATP	C4'-C5'-O5'-PA
11	S	600	ATP	C4'-C5'-O5'-PA
11	T	600	ATP	C4'-C5'-O5'-PA
11	U	600	ATP	C4'-C5'-O5'-PA
11	V	600	ATP	C4'-C5'-O5'-PA
11	T	600	ATP	PA-O3A-PB-O1B
11	W	600	ATP	C4'-C5'-O5'-PA
11	Q	600	ATP	PB-O3B-PG-O1G
11	Q	600	ATP	PG-O3B-PB-O2B
11	U	600	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
11	S	600	ATP	C3'-C4'-C5'-O5'
11	Q	600	ATP	PG-O3B-PB-O1B
11	S	600	ATP	PA-O3A-PB-O2B
11	Q	600	ATP	C5'-O5'-PA-O1A
11	S	600	ATP	C5'-O5'-PA-O1A
11	V	600	ATP	C5'-O5'-PA-O1A
11	R	600	ATP	C3'-C4'-C5'-O5'

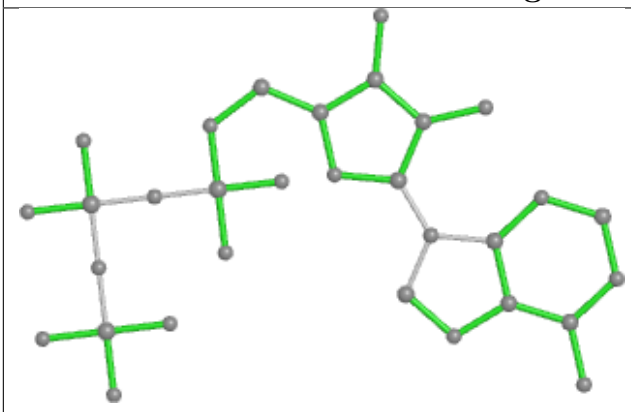
There are no ring outliers.

7 monomers are involved in 12 short contacts:

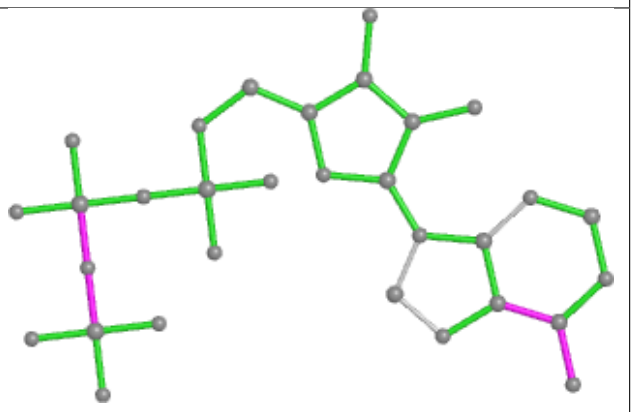
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	V	600	ATP	4	0
11	W	600	ATP	1	0
11	R	600	ATP	1	0
11	T	600	ATP	2	0
11	S	600	ATP	1	0
11	U	600	ATP	2	0
11	Q	600	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

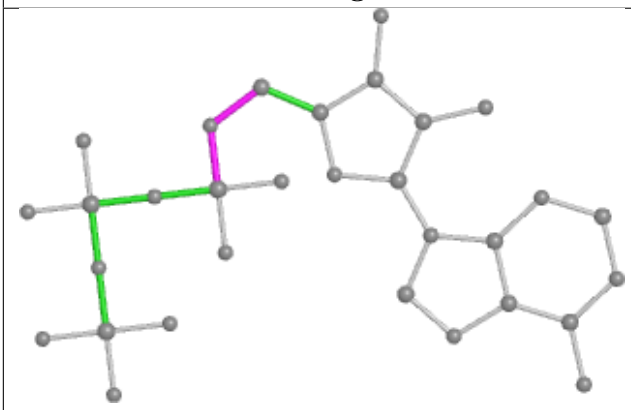
Ligand ATP V 600



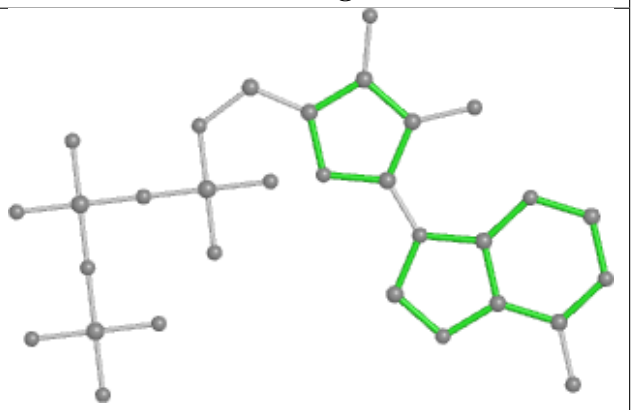
Bond lengths



Bond angles

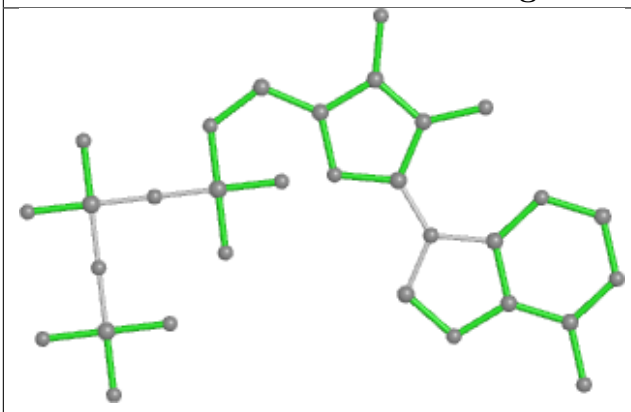


Torsions

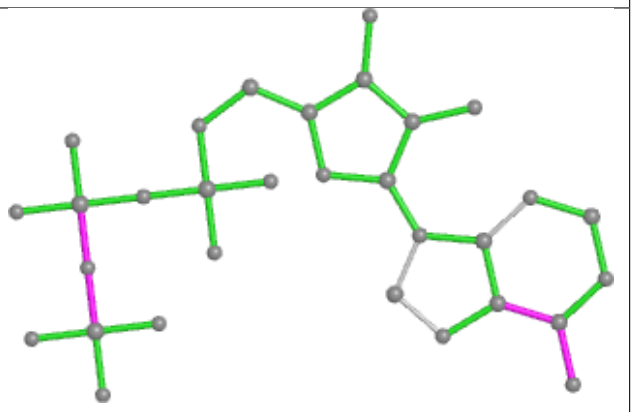


Rings

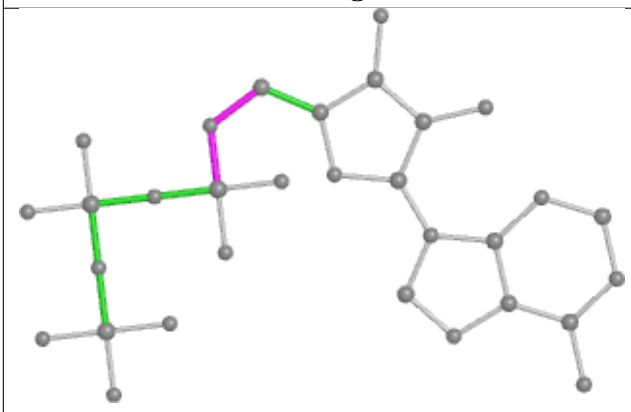
Ligand ATP W 600



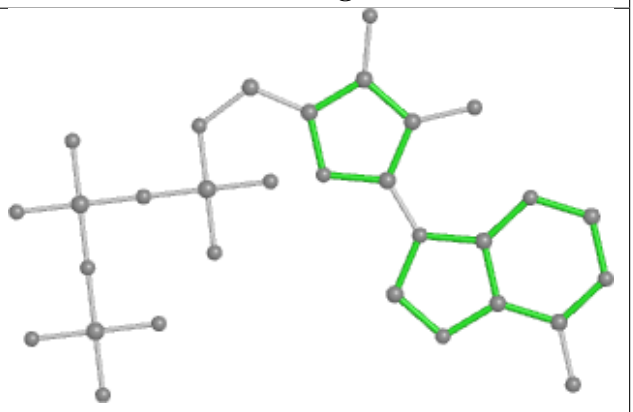
Bond lengths



Bond angles

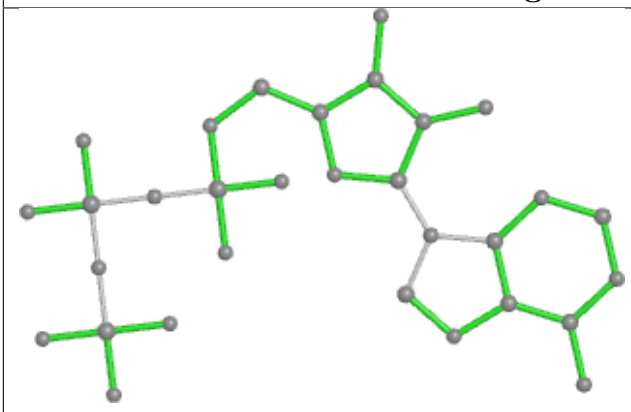


Torsions

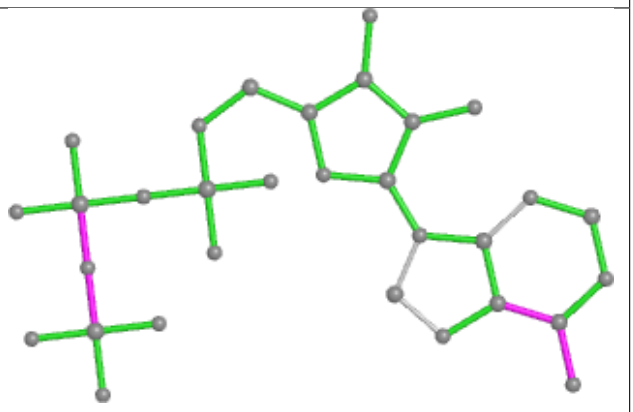


Rings

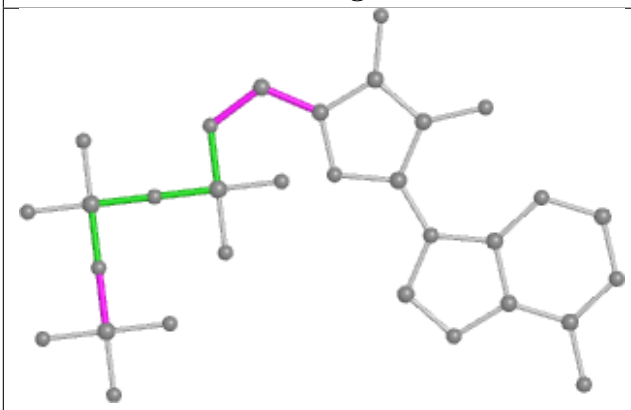
Ligand ATP R 600



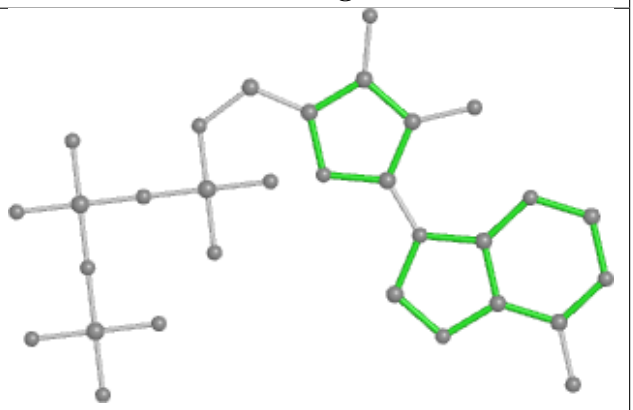
Bond lengths



Bond angles

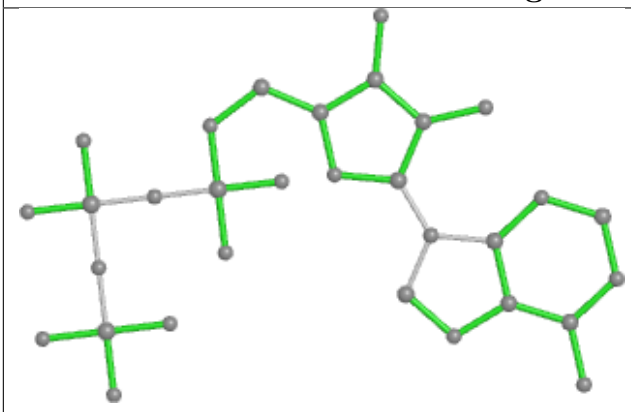


Torsions

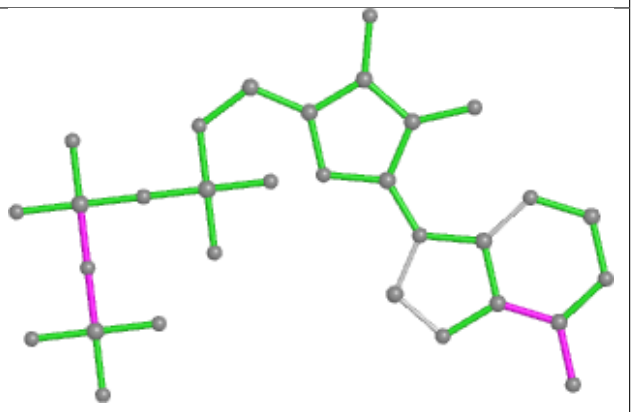


Rings

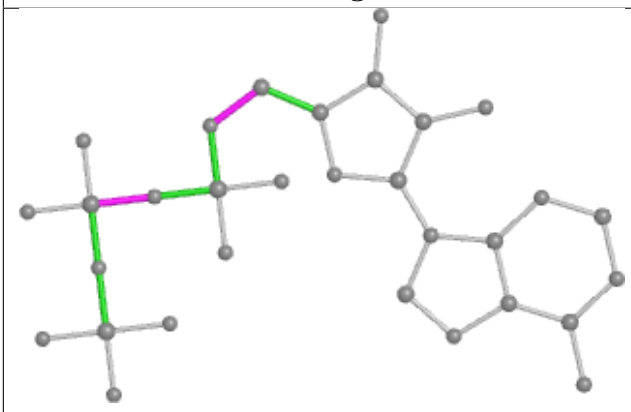
Ligand ATP T 600



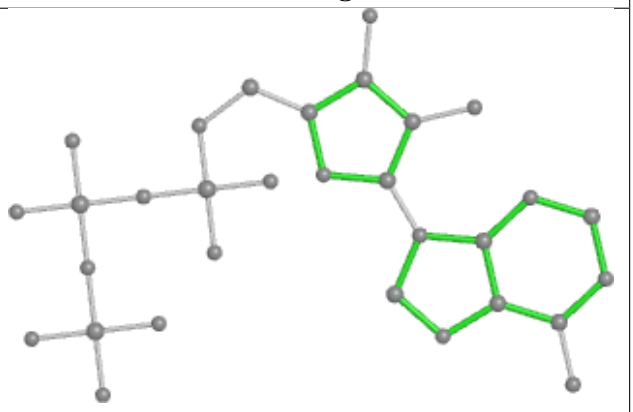
Bond lengths



Bond angles

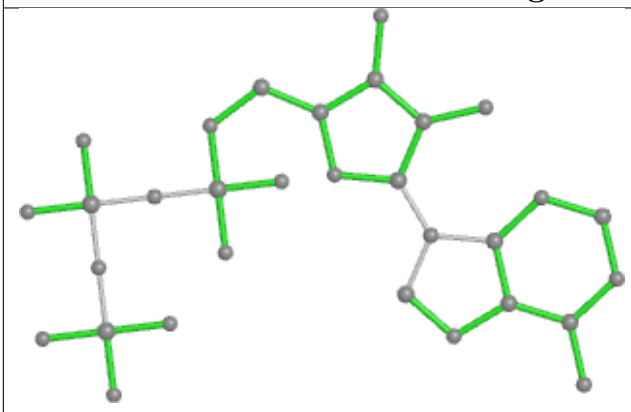


Torsions

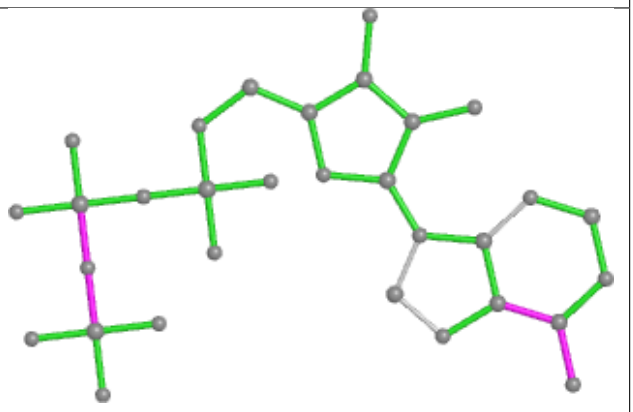


Rings

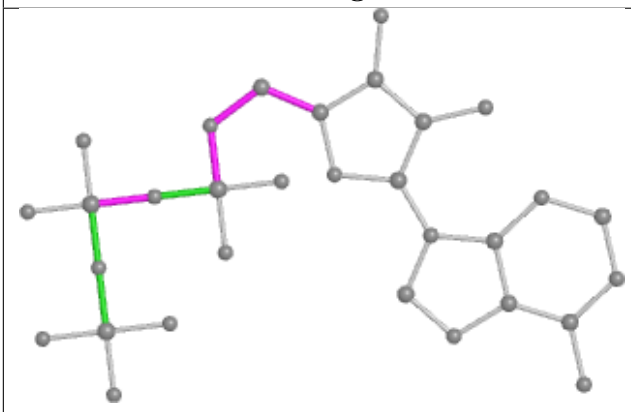
Ligand ATP S 600



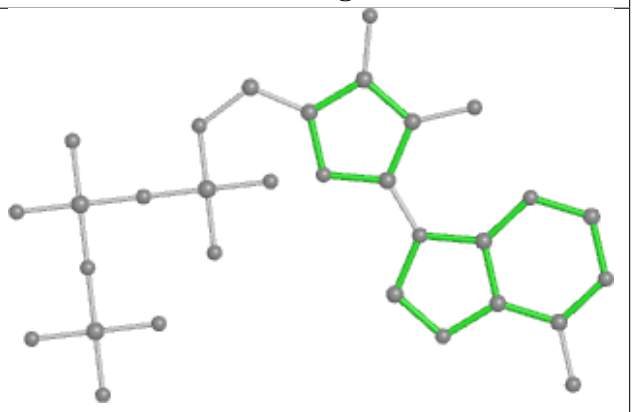
Bond lengths



Bond angles

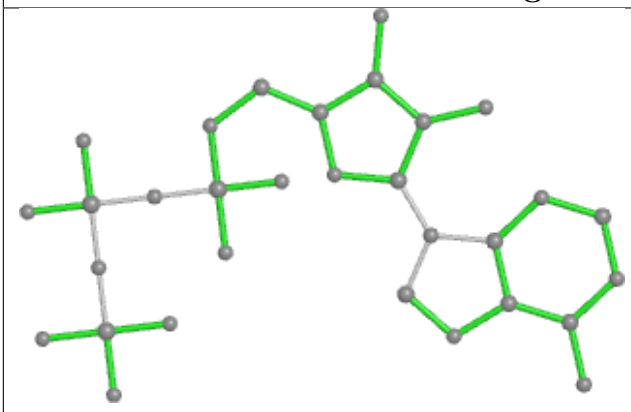


Torsions

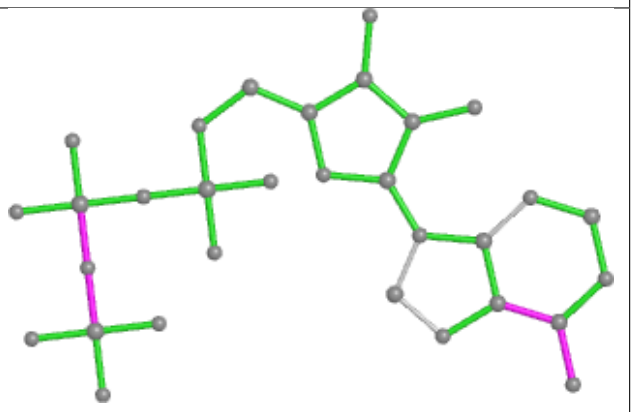


Rings

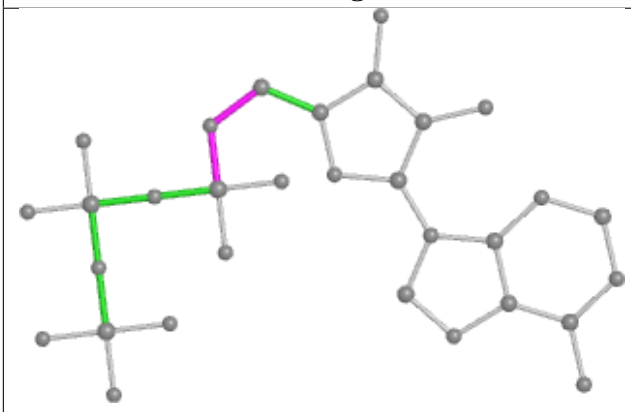
Ligand ATP U 600



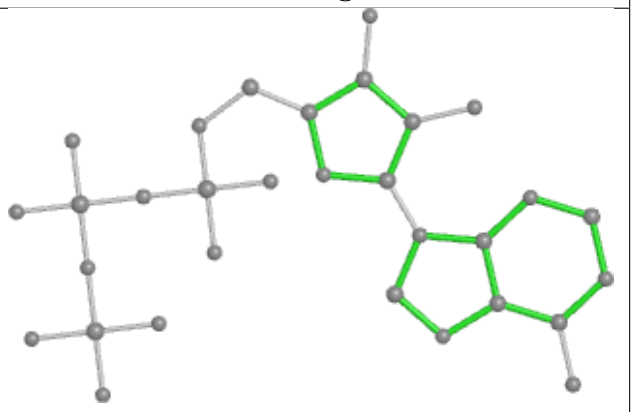
Bond lengths



Bond angles

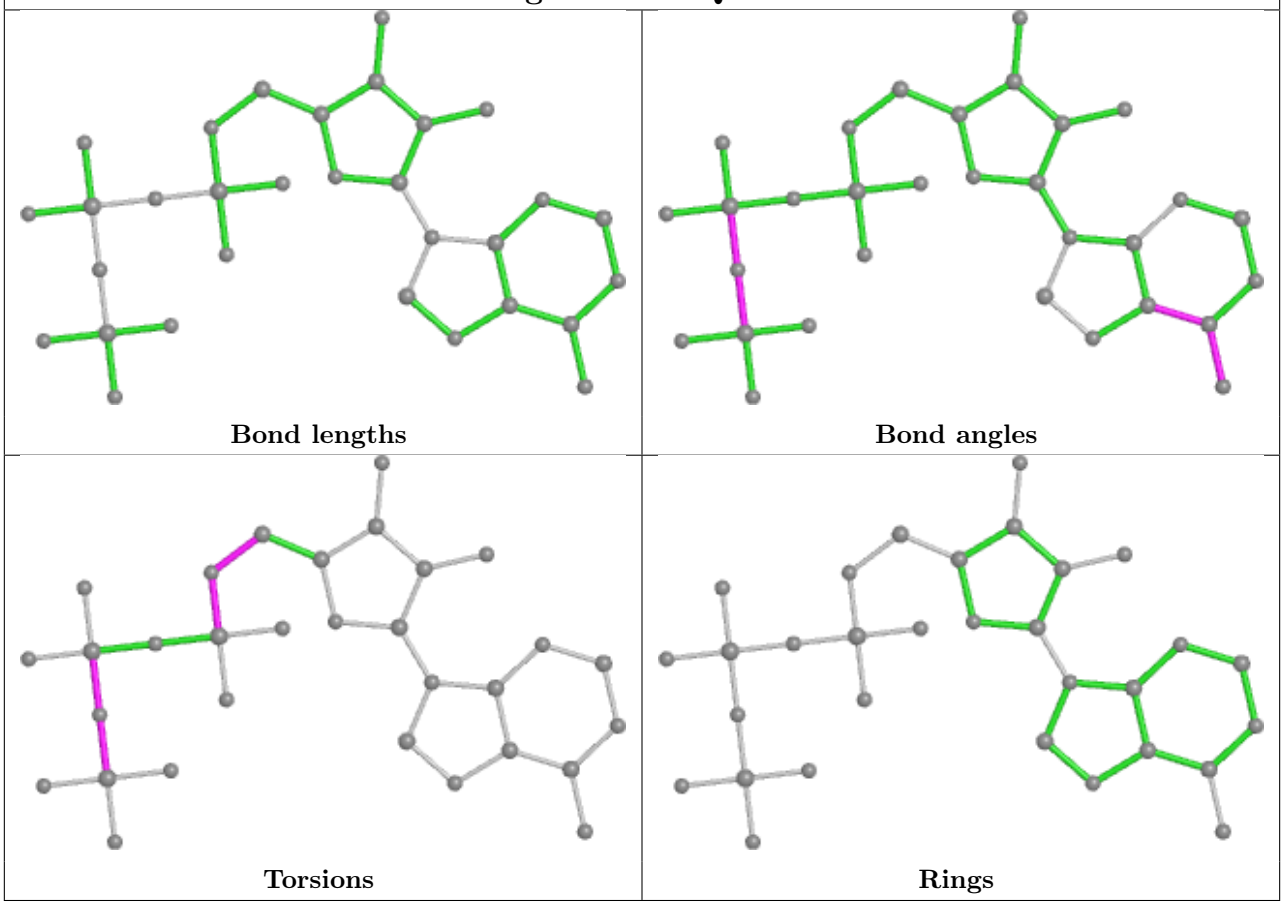


Torsions



Rings

Ligand ATP Q 600



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.

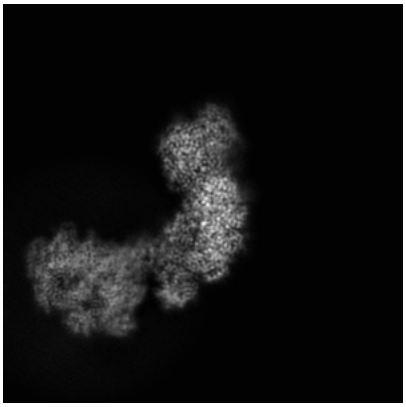
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29039. These allow visual inspection of the internal detail of the map and identification of artifacts.

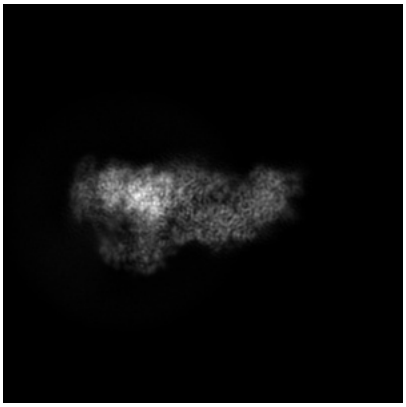
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

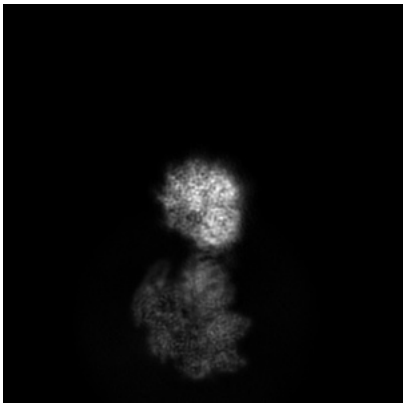
6.1.1 Primary map



X



Y

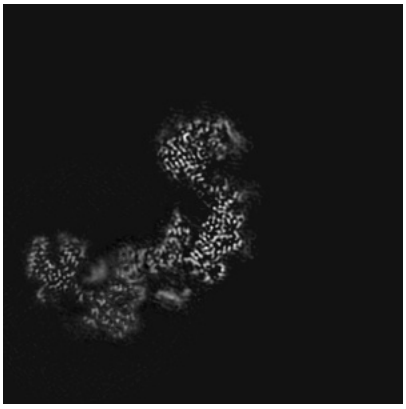


Z

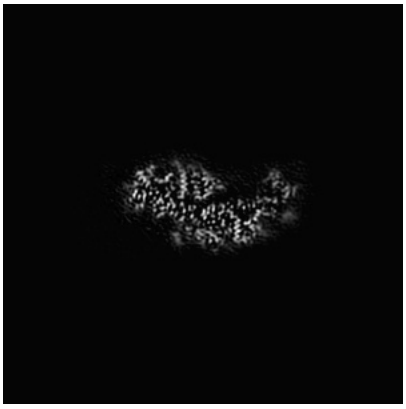
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 192



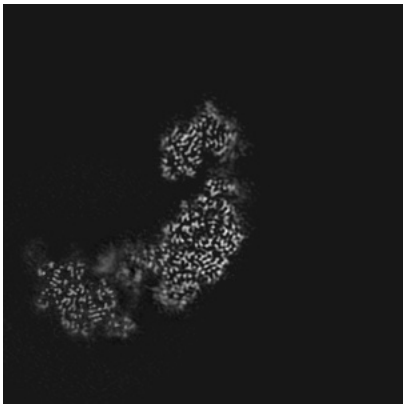
Y Index: 192

Z Index: 192

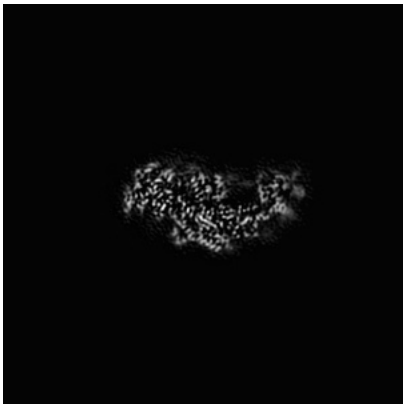
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 201



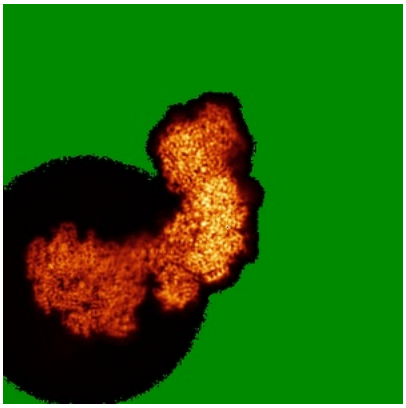
Y Index: 196

Z Index: 141

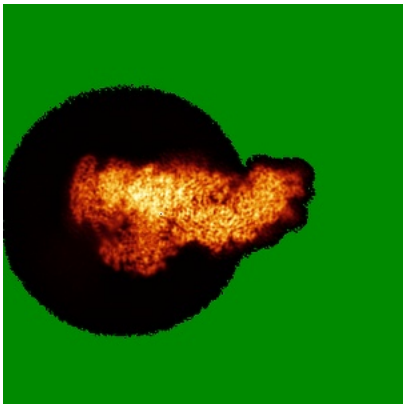
The images above show the largest variance slices of the map in three orthogonal directions.

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

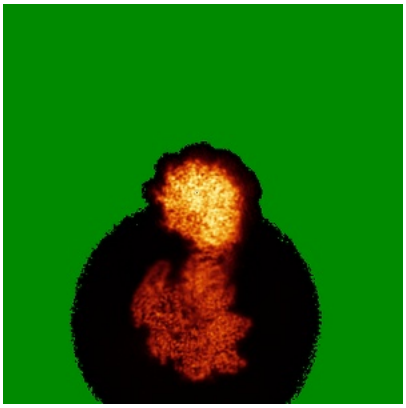
6.4.1 Primary map



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

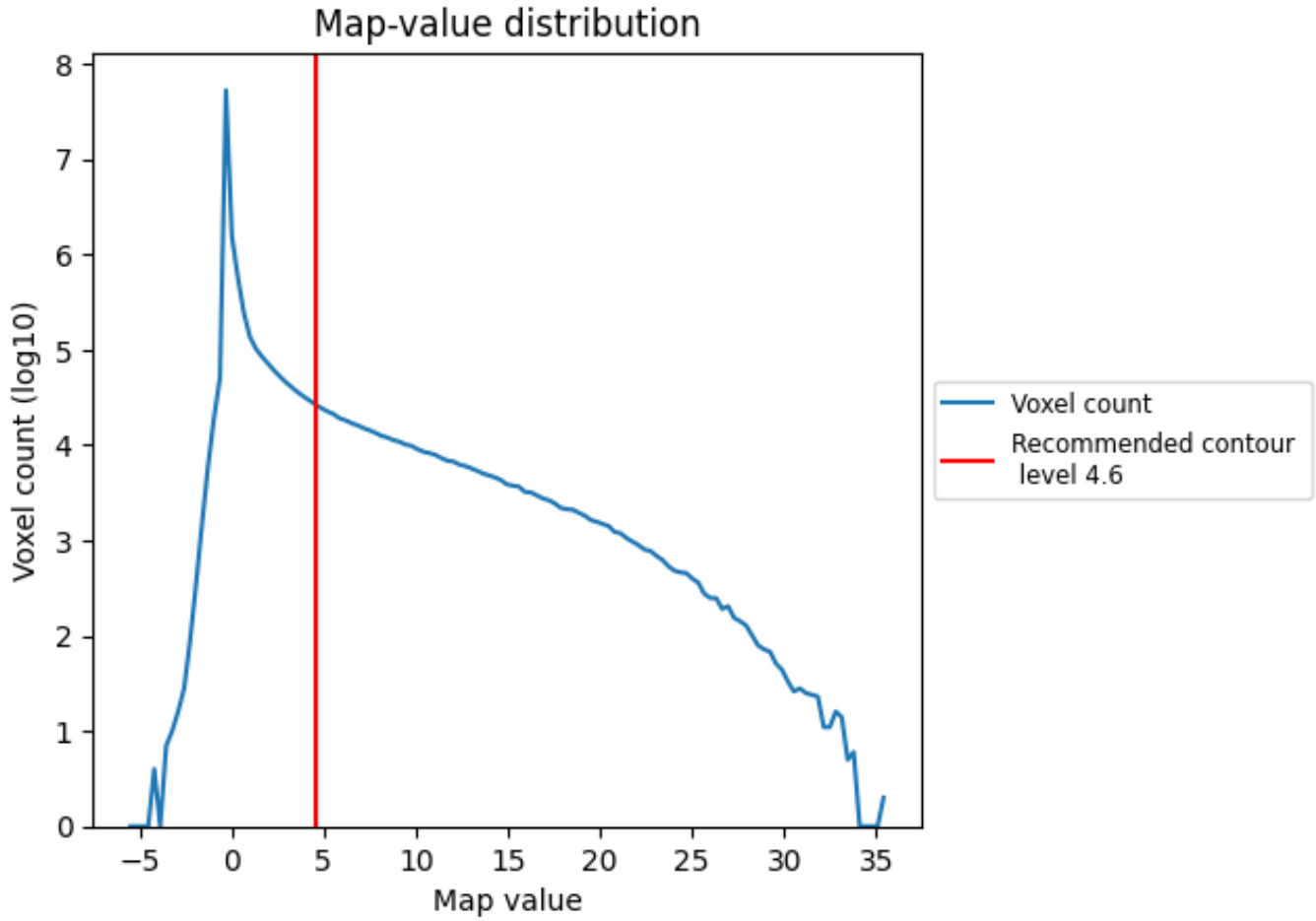
6.6 Mask visualisation (i)

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

7 Map analysis

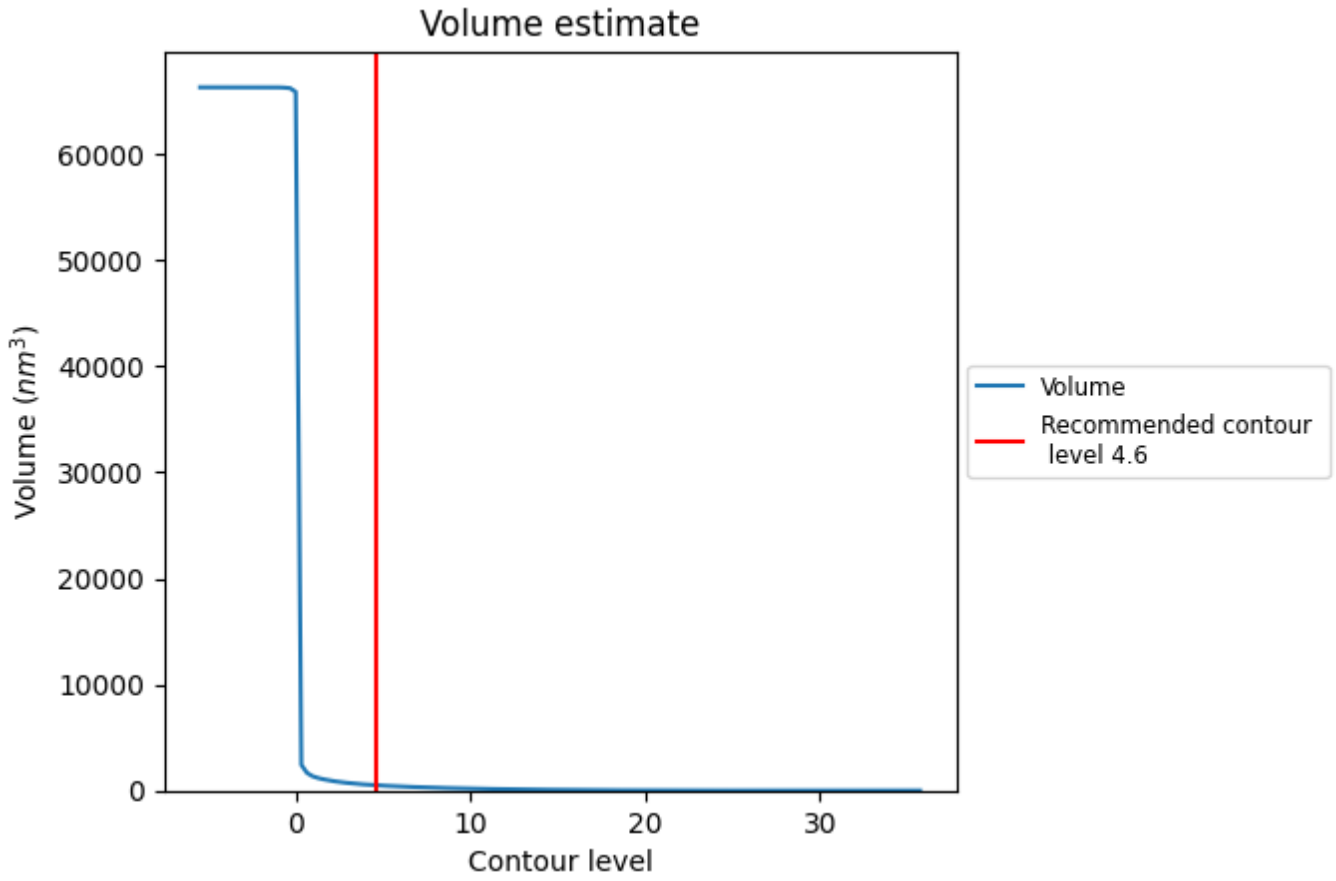
This section contains the results of statistical analysis of the map.

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.

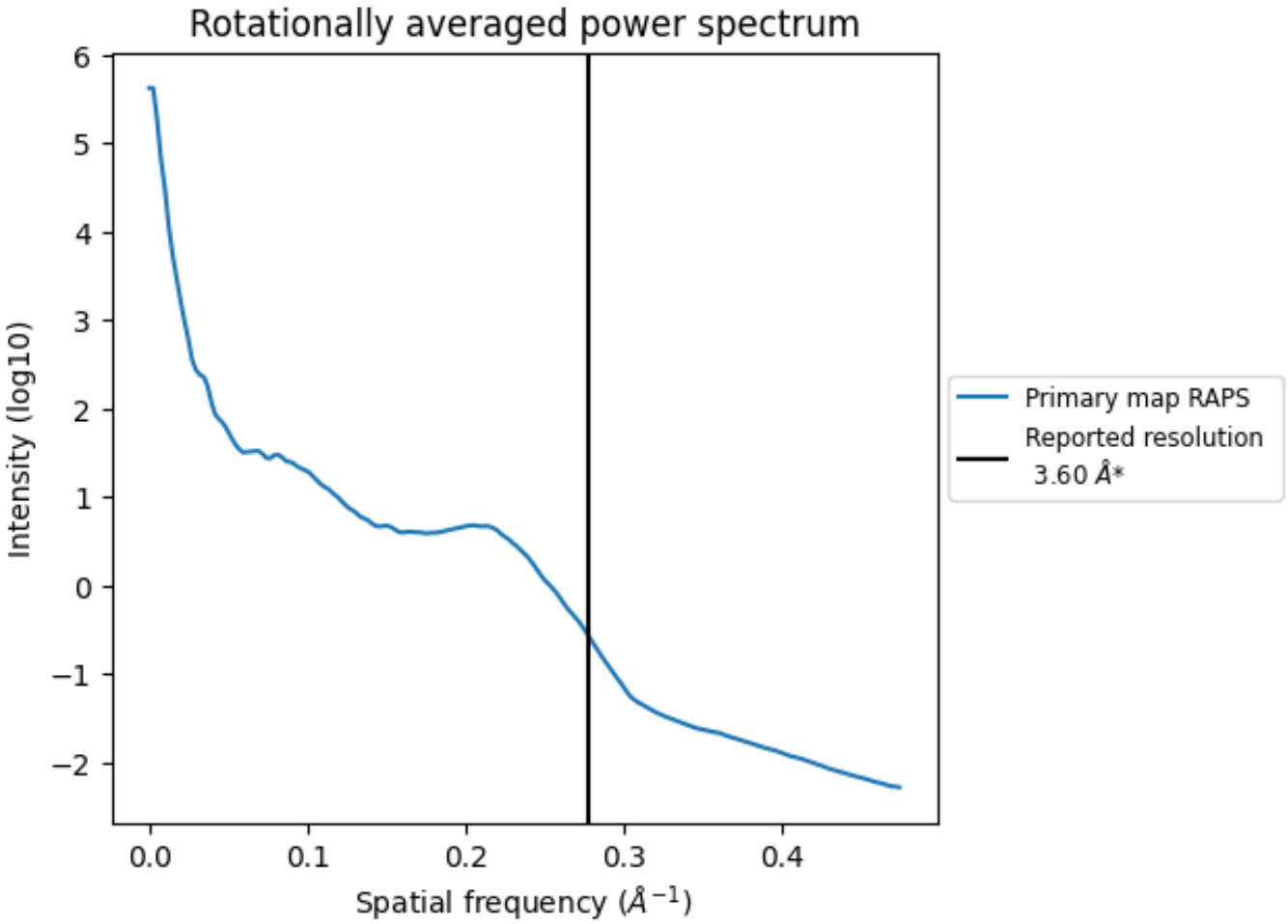
7.2 Volume estimate



The volume at the recommended contour level is 500 nm^3; this corresponds to an approximate mass of 452 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 0.278 Å^{-1}

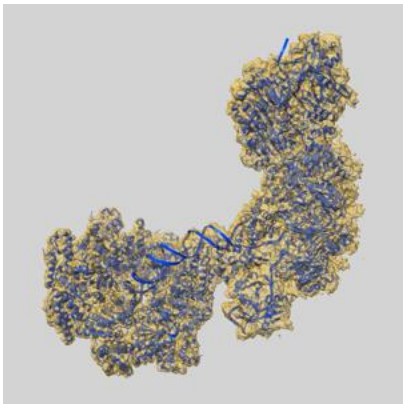
8 Fourier-Shell correlation

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

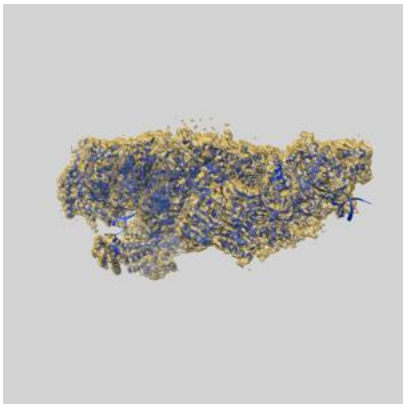
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29039 and PDB model 8FF4. Per-residue inclusion information can be found in section 3 on page 8.

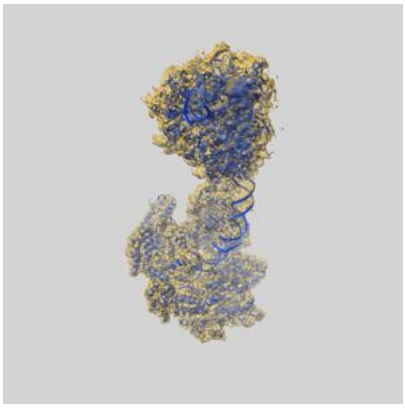
9.1 Map-model overlay



X



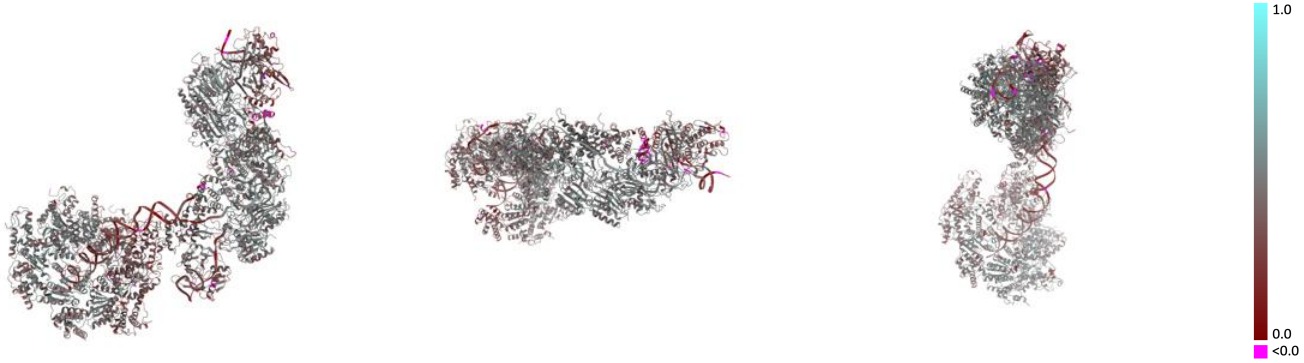
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.6 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.

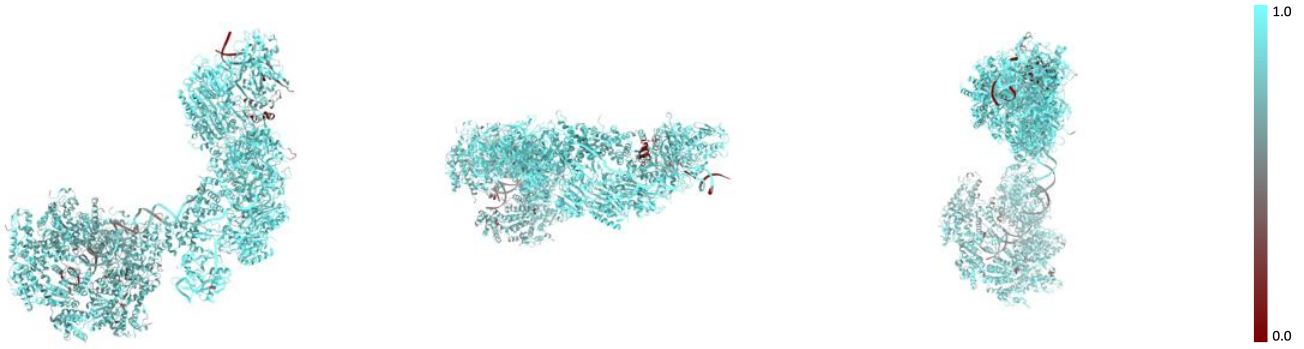
9.2 Q-score mapped to coordinate model (i)



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.

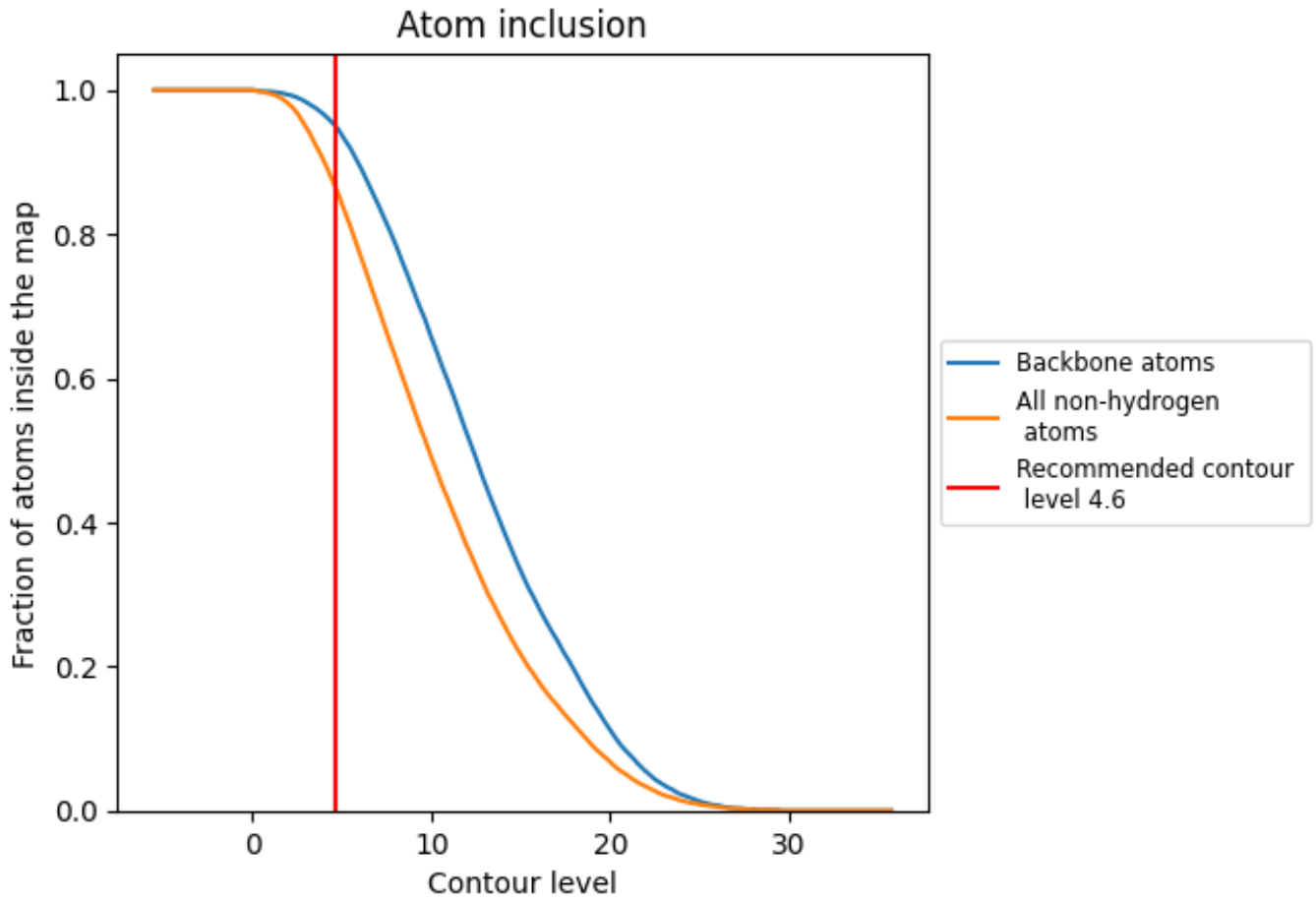
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.6).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.4170
A	0.9380	0.4670
B	0.9390	0.3850
C	0.9580	0.4590
D	0.9590	0.4770
E	0.9570	0.4800
F	0.9530	0.4780
G	0.9460	0.4840
H	0.9420	0.4720
I	0.8030	0.3320
J	0.9280	0.4060
K	0.9460	0.4320
L	0.9310	0.4370
M	0.9760	0.3950
N	0.7430	0.2910
O	0.5690	0.1840
P	0.8680	0.3520
Q	0.8200	0.3780
R	0.8320	0.4290
S	0.8420	0.4470
T	0.8400	0.4640
U	0.8350	0.4580
V	0.8050	0.4280
W	0.7390	0.3620