



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:45 AM UTC

PDB ID : 6QDV / pdb_00006qdv
EMDB ID : EMD-4525
Title : Human post-catalytic P complex spliceosome
Authors : Fica, S.M.; Oubridge, C.; Wilkinson, M.E.; Newman, A.J.; Nagai, K.
Deposited on : 2019-01-03
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

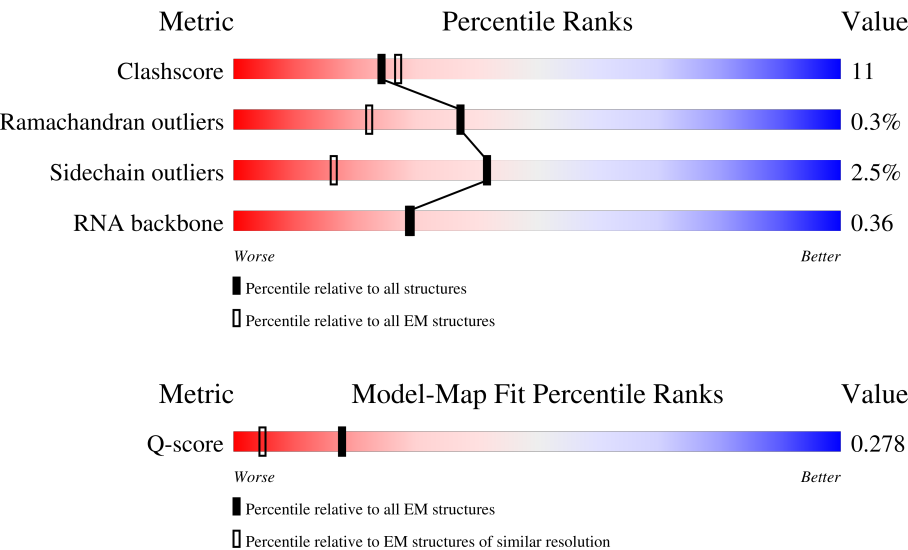
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	189	
2	5	116	
3	6	106	

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Mol	Chain	Length	Quality of chain
4	7	390	
5	8	91	
6	9	144	
7	A	2335	
8	B	1722	
9	C	899	
10	D	123	
11	E	14	
12	F	122	
13	G	60	
14	H	908	
15	I	113	
16	J	320	
17	K	295	
18	L	144	
19	M	289	
20	N	306	
21	O	802	
22	P	229	
23	R	26	
24	S	848	
25	T	855	
26	U	1485	
27	V	1220	
28	W	162	

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Mol	Chain	Length	Quality of chain
29	Y	92	
30	Z	30	
31	b	82	
31	k	82	
32	c	586	
33	d	84	
33	n	84	
34	e	81	
34	p	81	
35	f	72	
35	q	72	
36	g	73	
36	r	73	
37	h	80	
37	l	80	
38	i	164	
39	j	118	
39	m	118	
40	o	513	
41	s	225	
42	t	504	
42	u	504	
42	v	504	
42	w	504	
43	y	144	

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Mol	Chain	Length	Quality of chain
44	z	34	100% 82% 18%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 121152 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	120	Total	C	N	O	P	0	0
			2535	1135	428	852	120		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	75	Total	C	N	O	P	0	0
			1579	708	264	532	75		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 4 is a protein called Eukaryotic initiation factor 4A-III, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	390	Total	C	N	O	S	0	0
			3130	1976	546	589	19		

- Molecule 5 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 6 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2250	Total	C	N	O	S	0	0
			18655	12009	3256	3309	81		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	1722	Total	C	N	O	S	0	0
			13846	8848	2369	2557	72		

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	899	Total	C	N	O	S	0	0
			7116	4553	1184	1345	34		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q15029

- Molecule 10 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 11 is a RNA chain called Ligated exons: MINX mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	14	Total	C	N	O	P	0	0
			296	132	52	98	14		

- Molecule 12 is a protein called Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	122	Total	C	N	O	S	0	0
			1084	712	197	173	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	654	ALA	GLU	conflict	UNP Q8WUQ7

- Molecule 13 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	60	Total	C	N	O	S	0	0
			504	314	96	92	2		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	459	Total	C	N	O	S	0	0
			3713	2380	634	678	21		

- Molecule 15 is a RNA chain called Intron lariat: MINX RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	42	Total	C	N	O	P	0	0
			872	390	148	292	42		

- Molecule 16 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	320	Total	C	N	O	S	0	0
			2523	1594	457	464	8		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	K	295	Total	C	N	O	P	S	0	0
			2360	1479	431	435	2	13		

- Molecule 18 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	144	Total	C	N	O	S	0	0
			1188	748	218	210	12		

- Molecule 19 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	289	Total	C	N	O	S	0	0
			2318	1455	416	428	19		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	143	ALA	THR	conflict	UNP Q9NW64
M	144	ALA	SER	conflict	UNP Q9NW64
M	145	ALA	ASP	conflict	UNP Q9NW64
M	146	ALA	MET	conflict	UNP Q9NW64

- Molecule 20 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ALA	deletion	UNP Q96DI7

- Molecule 21 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	441	Total	C	N	O	S	0	0
			3416	2116	648	639	13		

- Molecule 22 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	106	Total	C	N	O	S	0	0
			888	544	174	168	2		

- Molecule 23 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 24 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	570	Total	C	N	O	S	0	0
			3965	2482	740	737	6		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	639	Total	C	N	O	S	0	0
			4003	2479	748	763	13		

- Molecule 26 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	1322	Total	C	N	O	S	4	0
			10885	6989	1879	1963	54		

- Molecule 27 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	713	Total	C	N	O	S	0	0
			2995	1538	722	734	1		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	92	Total	C	N	O	S	0	0
			745	480	130	130	5		

- Molecule 30 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	30	Total	C	N	O	S	0	0
			230	140	43	45	2		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	68	Total	C	N	O	S	0	0
			545	347	95	96	7		
31	k	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	269	Total	C	N	O	S	0	0
			2215	1392	397	418	8		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
33	n	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	79	Total	C	N	O	S	0	0
			651	413	115	118	5		
34	p	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
35	q	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
36	r	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
37	l	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	164	Total	C	N	O	S	0	0
			1270	810	220	233	7		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	95	Total	C	N	O	S	0	0
			774	486	141	142	5		
39	m	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 40 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	513	Total	C	N	O	S	0	0
			4157	2643	719	771	24		

- Molecule 41 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	169	Total	C	N	O	S	0	0
			1402	872	257	264	9		

- Molecule 42 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
42	u	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
42	v	125	Total	C	N	O	S	0	0
			988	618	176	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	118	Total	C	N	O	S	0	0
			938	586	167	181	4		

- Molecule 43 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	144	Total	C	N	O	S	0	0
			1218	758	225	233	2		

- Molecule 44 is a protein called Replication stress response regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	34	Total	C	N	O	S	0	0
			280	166	59	53	2		

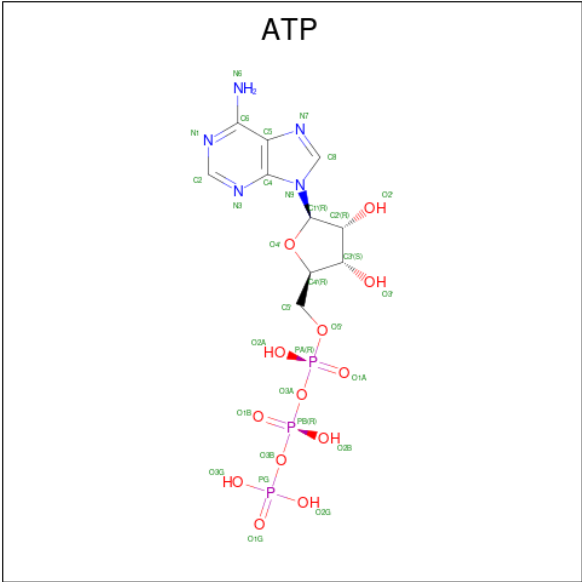
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	6	5	Total	Mg	0
			5	5	
45	7	1	Total	Mg	0
			1	1	
45	C	1	Total	Mg	0
			1	1	

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

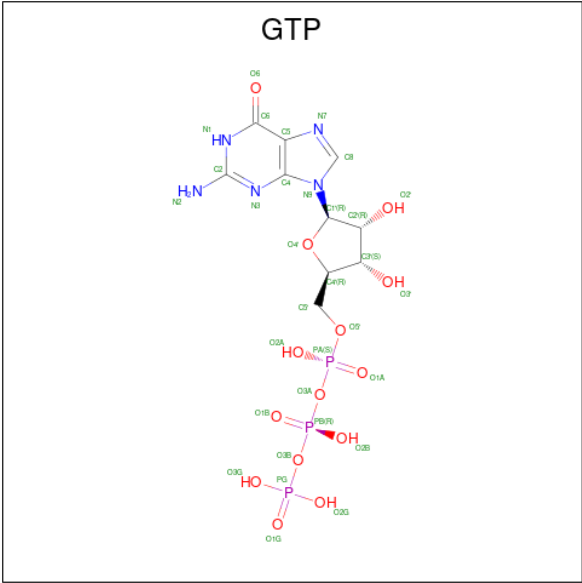
Mol	Chain	Residues	Atoms		AltConf
46	6	1	Total	K	0
			1	1	

- Molecule 47 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
47	7	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

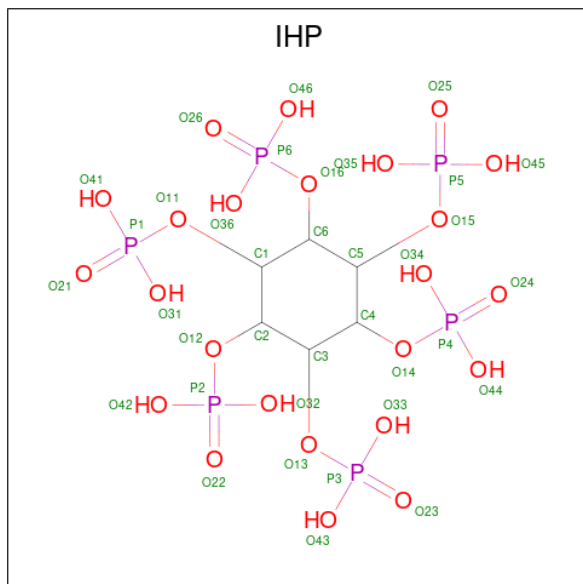


Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	L	3	Total	Zn	0
			3	3	
49	M	3	Total	Zn	0
			3	3	
49	c	1	Total	Zn	0
			1	1	

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

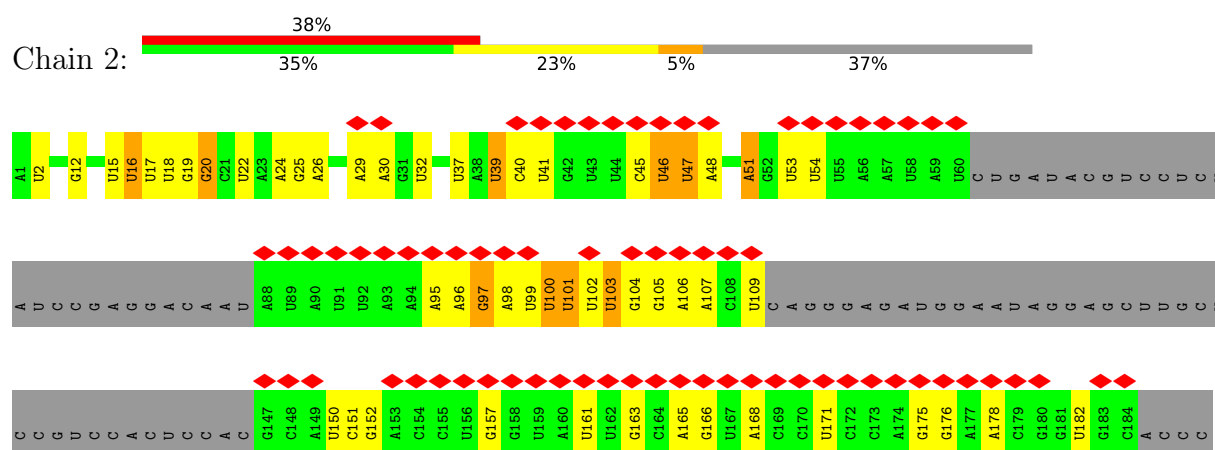


Mol	Chain	Residues	Atoms				AltConf
50	c	1	Total	C	O	P	0
			36	6	24	6	

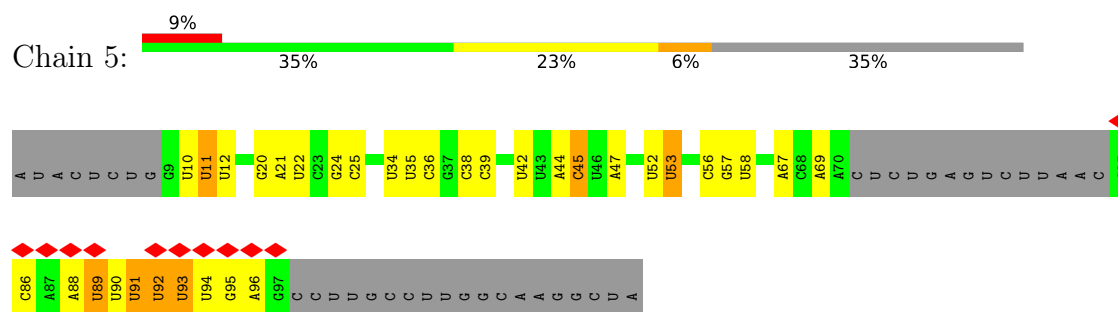
3 Residue-property plots [i](#)

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.

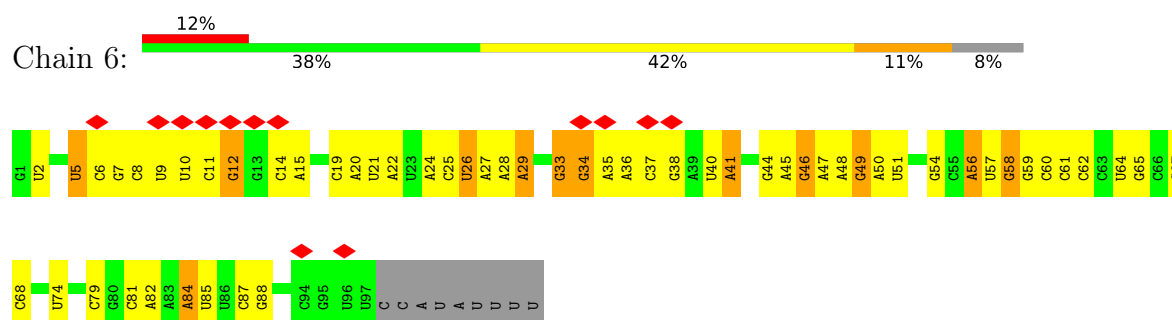
- Molecule 1: U2 snRNA



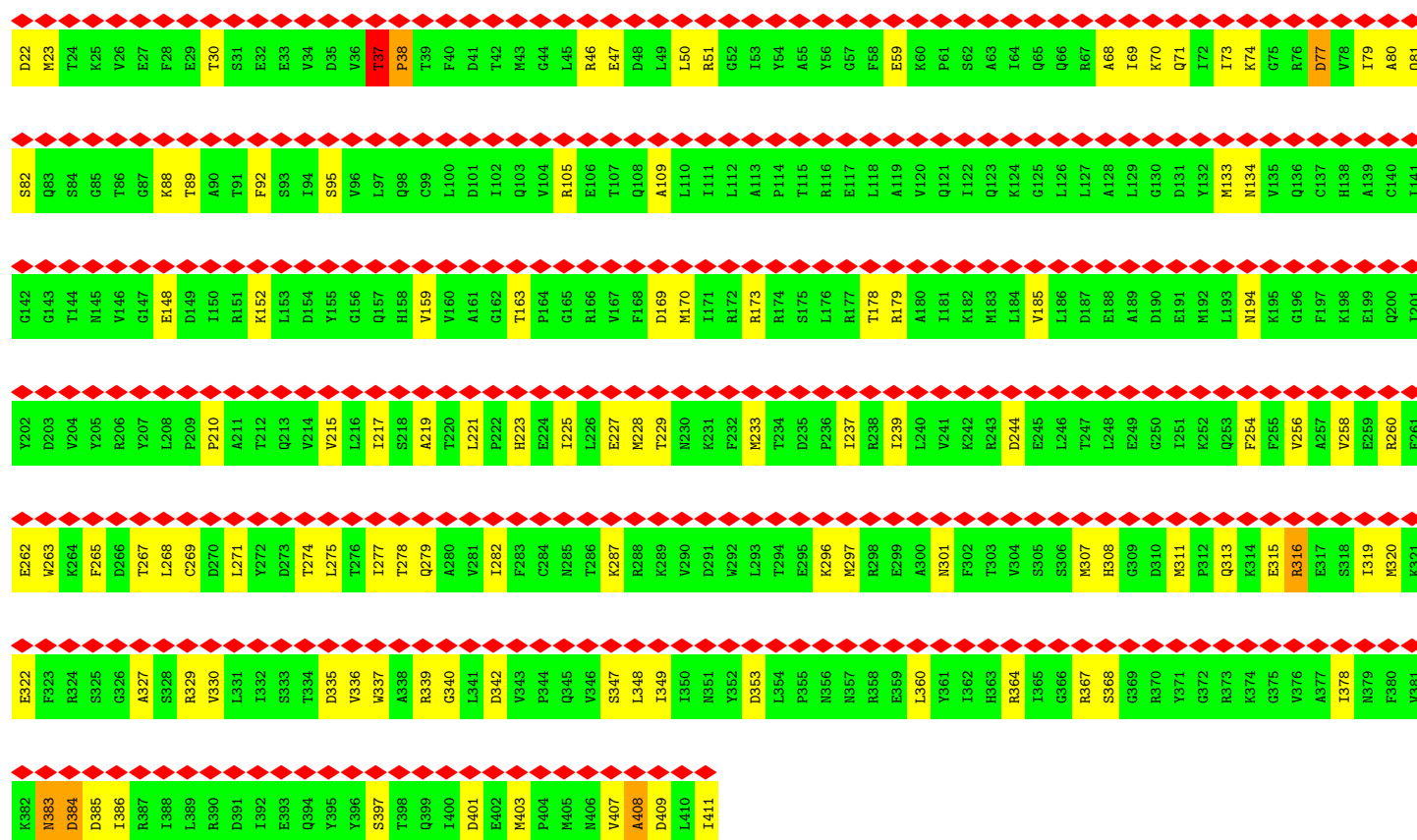
- Molecule 2: U5 snRNA



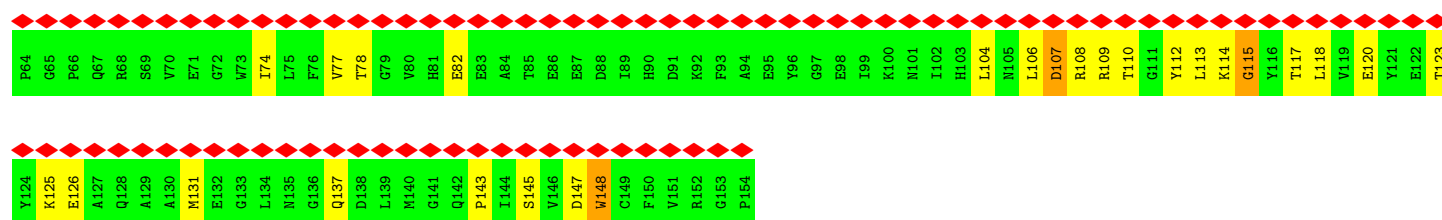
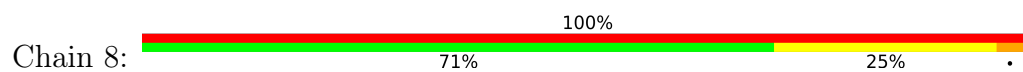
- Molecule 3: U6 snRNA



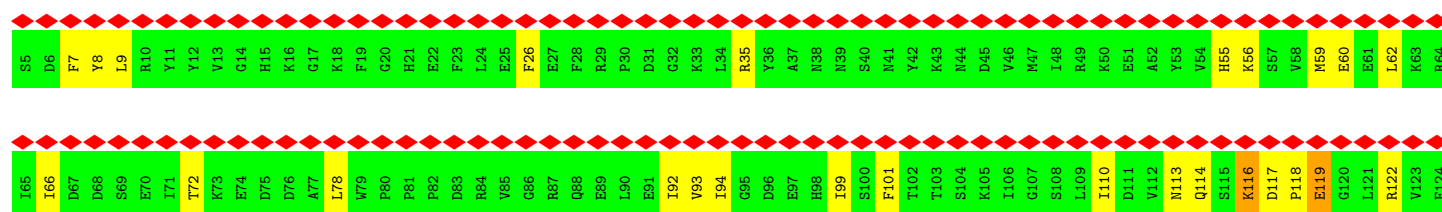
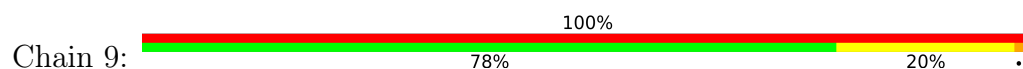
- Molecule 4: Eukaryotic initiation factor 4A-III, N-terminally processed

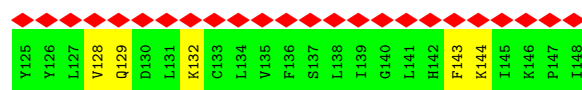


• Molecule 5: RNA-binding protein 8A

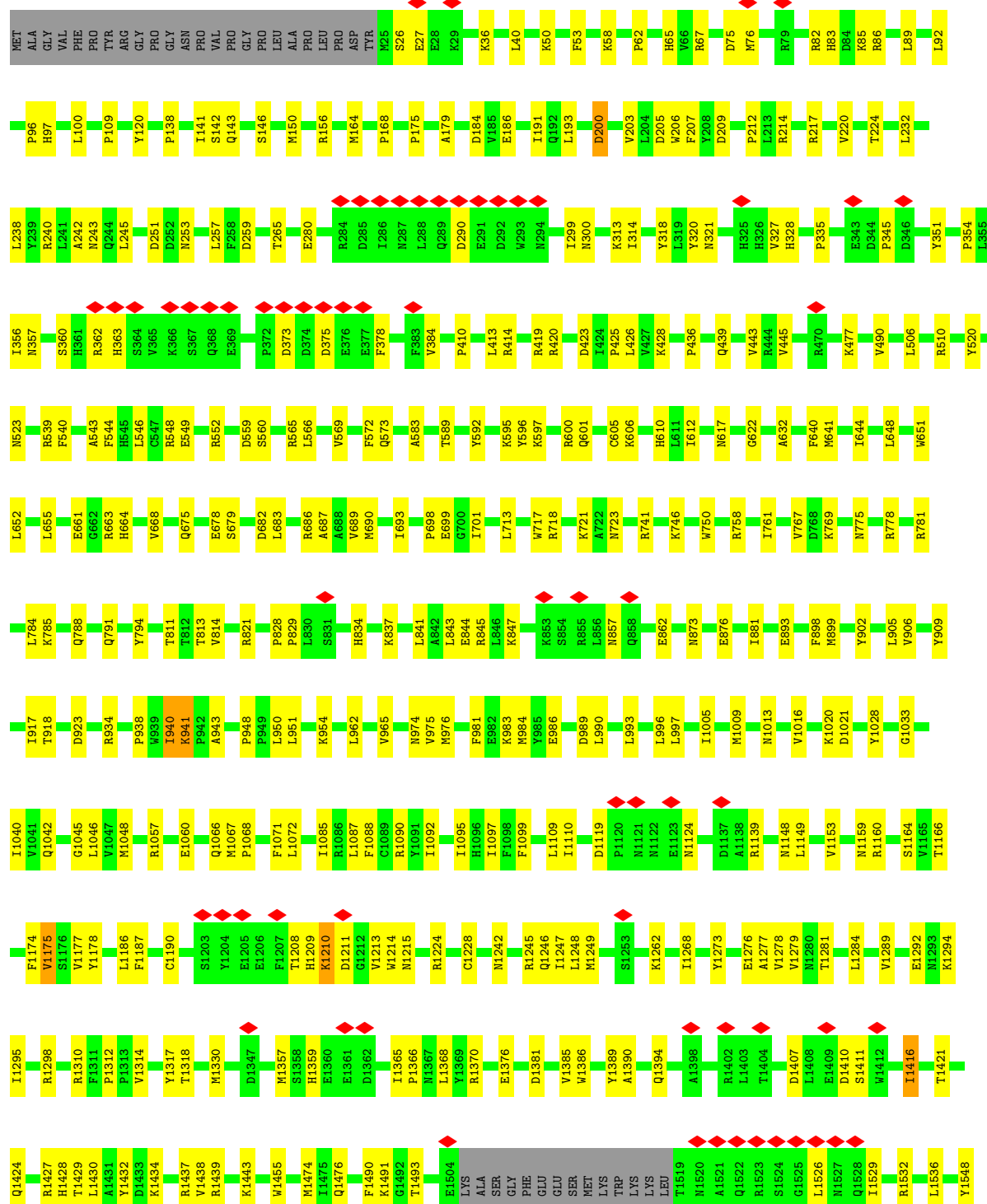


• Molecule 6: Protein mago nashi homolog 2





• Molecule 7: Pre-mRNA-processing-splicing factor 8



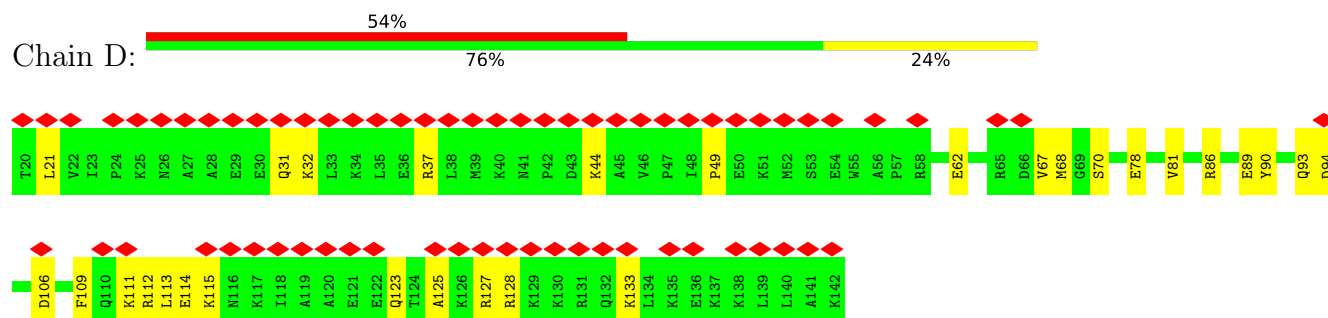
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L1184	E1185	L1186	S1187	V1188	H1189	L1129	R1130	L1070	K1071	L1072	E1073	G1074	F1075	A1076	L1077	M1078	A1079	D1080	M1081	V1082	Y1083	V1084	T1085	Q1086	S1087	A1088	G1089	R1090	L1091	M1092	R1093	A1094	I1095	F1096	E1097	I1098	V1099	L1100	N1101	R1102	G1103	W1104	A1105	R1166	L1107	L1108	D1109	K1110	T1111	L1112	L1113	L1114	C1115	K1116	M1117	I1118	D1119	K1120	M1121	W1122								
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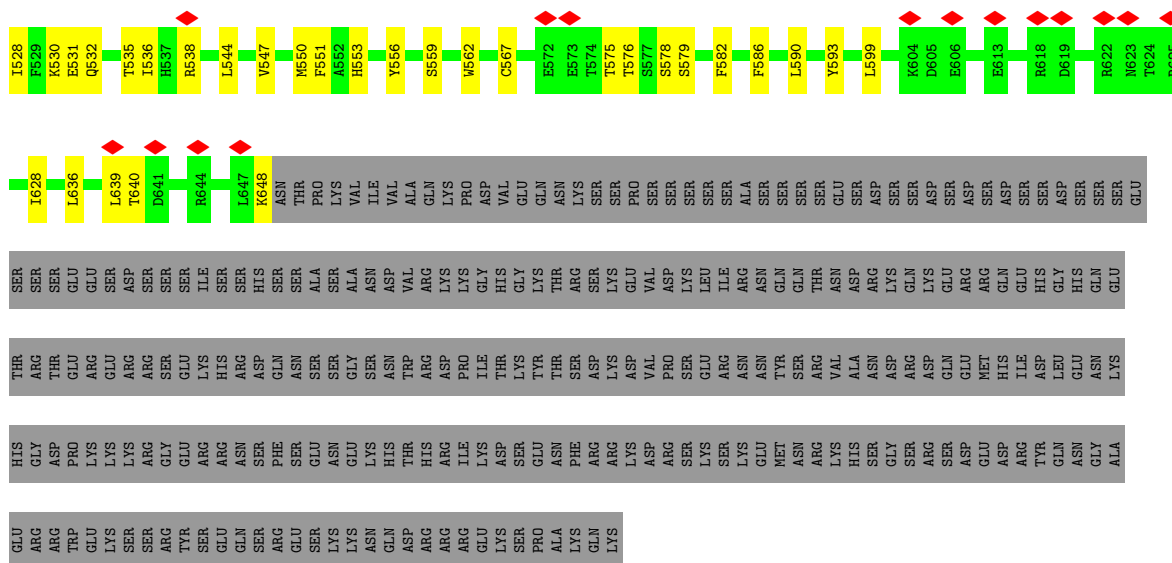
• Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component



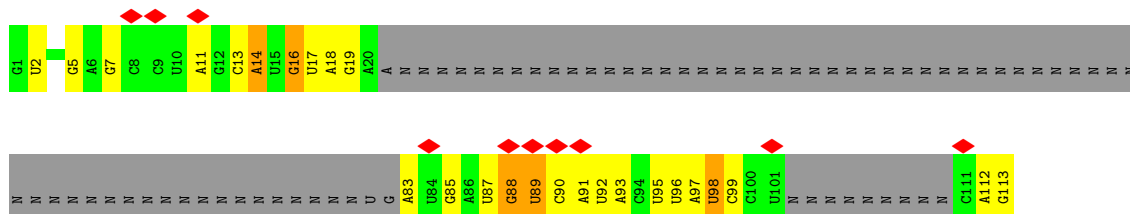
• Molecule 10: PRKR-interacting protein 1



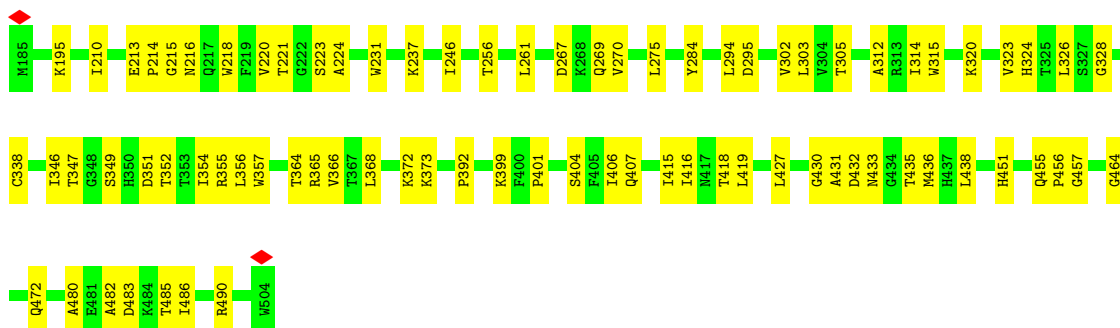
• Molecule 11: Ligated exons: MINX mRNA



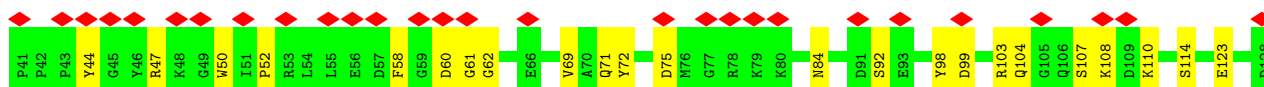
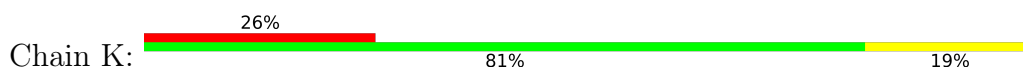
- Molecule 15: Intron lariat: MINX RNA

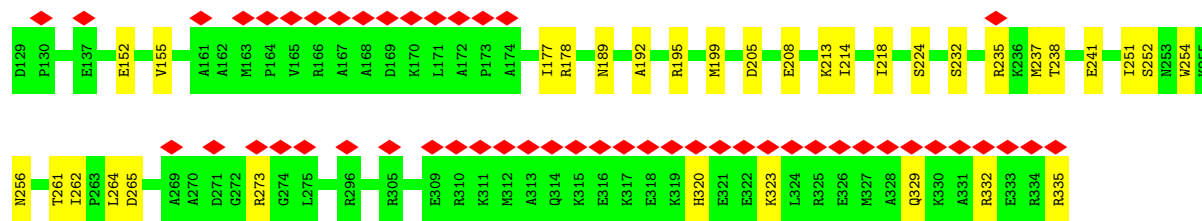


- Molecule 16: Pleiotropic regulator 1

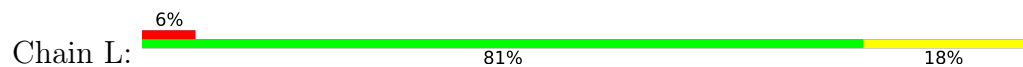


- Molecule 17: SNW domain-containing protein 1

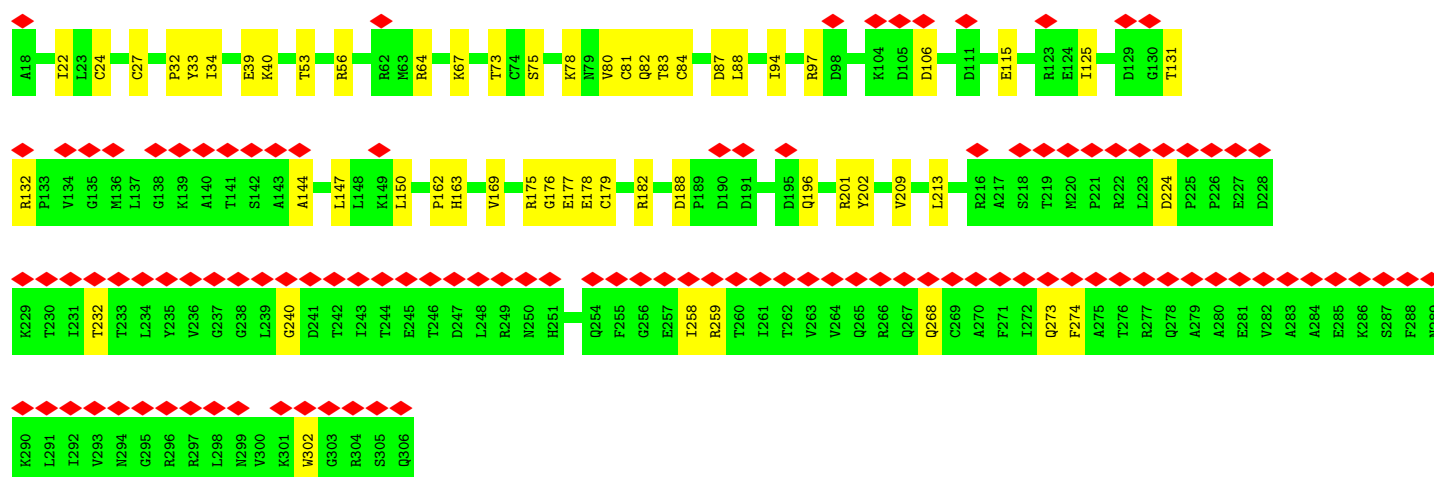
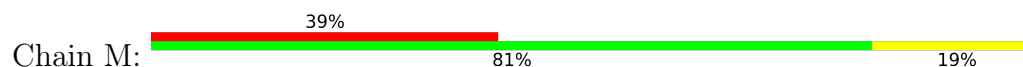




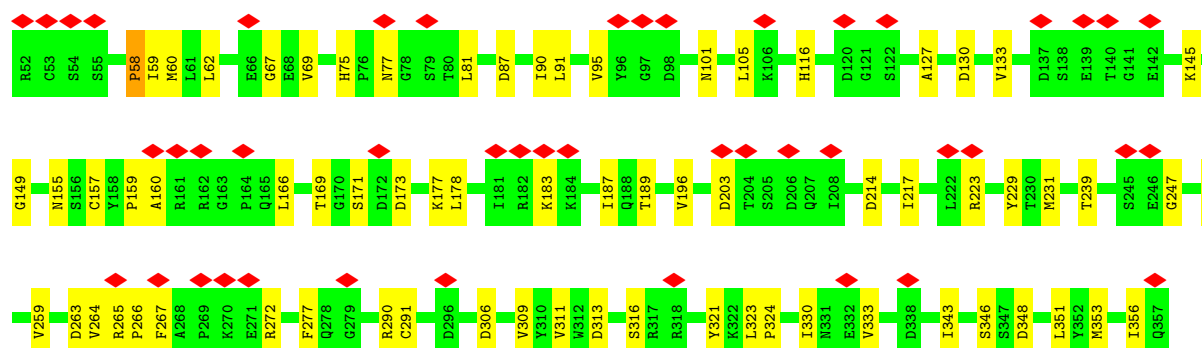
- Molecule 18: Protein BUD31 homolog



- Molecule 19: Pre-mRNA-splicing factor RBM22

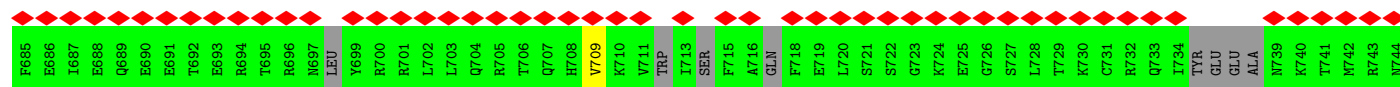


- Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein

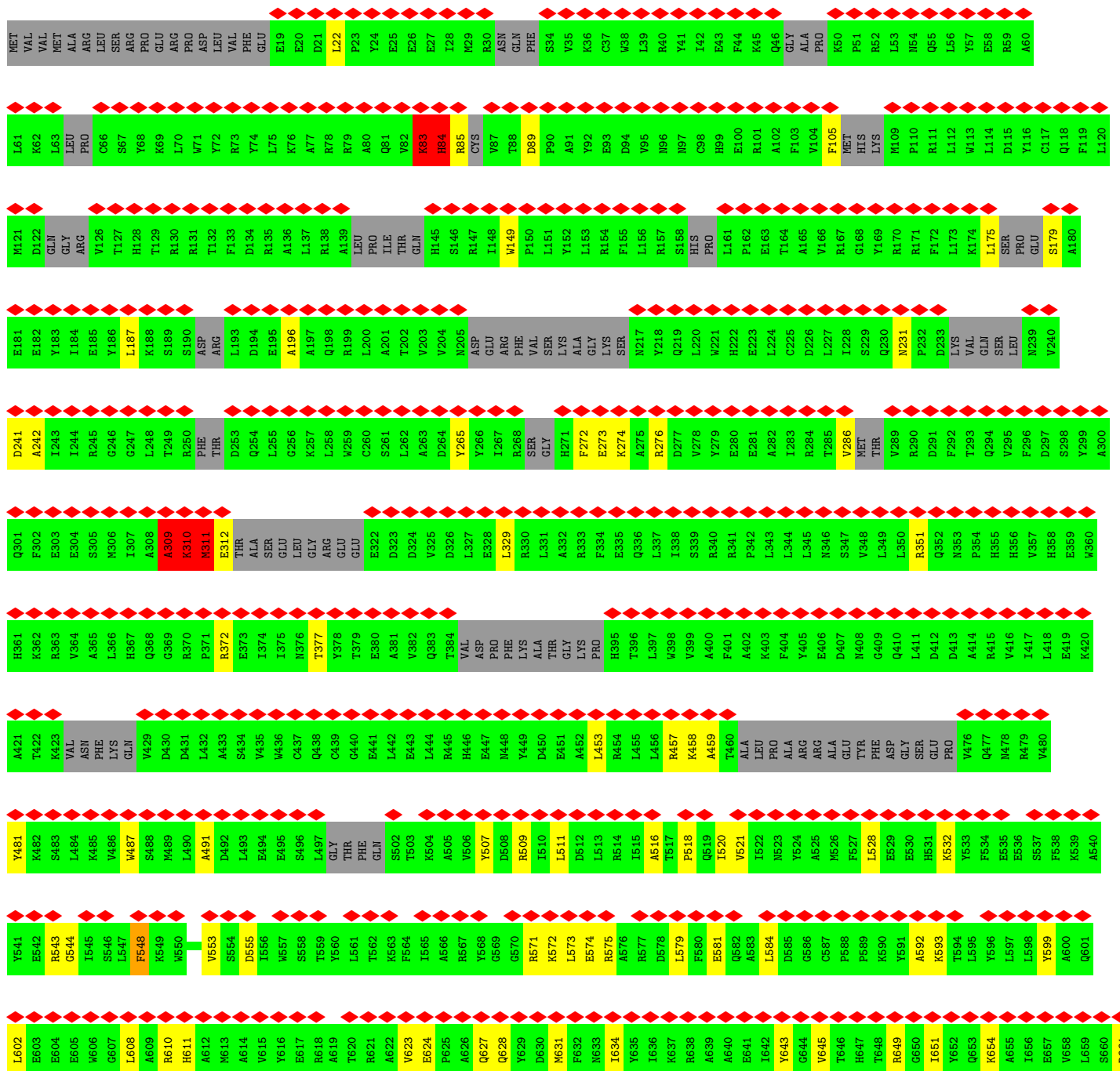
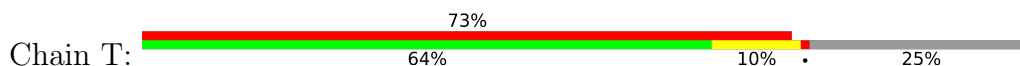


- Molecule 21: Cell division cycle 5-like protein

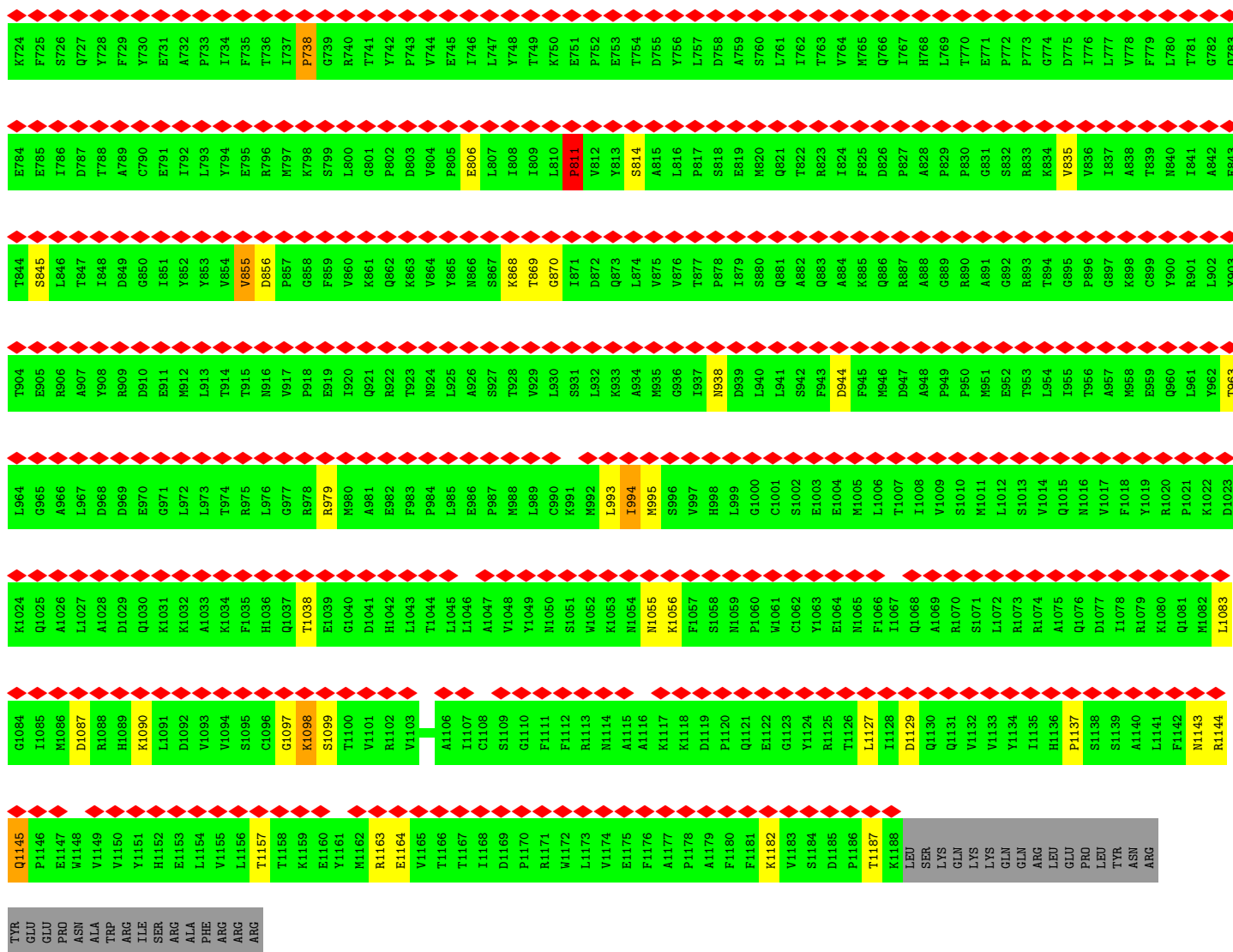




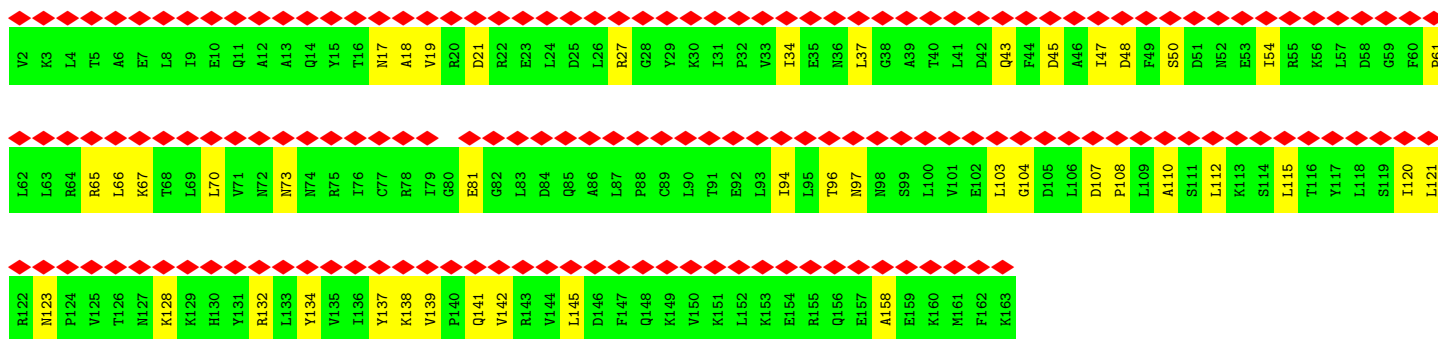
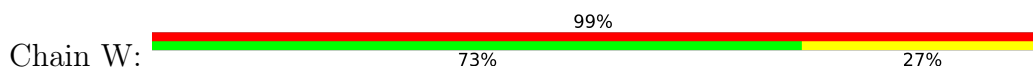
- Molecule 25: Pre-mRNA-splicing factor SYF1



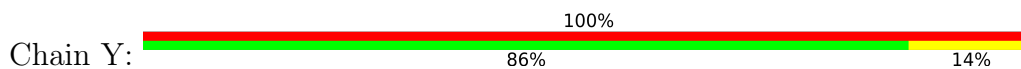
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P781	H782	F783	I784	P785	N786	R787	G788	F789	Y790	F791	Y792	N793	Q794	F795	K796	R797	N798	T799	I800	Q801	F802	T803	H804	T805	Q806	I807	E808	A809	I810	R811	A812	G813	M814	Q815	P816	G817	L818	T819	M820	V821	V822	G823	P824	P825	G826	T827	G828	K829	T830	D831	V832	A833	V834	Q835	I836	S837	N838	I840		
I721	E722	H723	L724	K725	A726	S727	F728	F729	G730	H731	N732	V733	K734	V735	T736	V737	F738	D739	P740	A741	L742	Q743	I744	F745	F746	R747	R748	I749	L869	T750	F751	P752	V753	ARG	SER	GLY	LYS	LYS	ARG	L879	M820	V821	V822	G823	P824	P825	G826	T827	G828	K829	T830	D831	V832	A833	V834	Q835	I836	S837	N838	I840
L601	D602	D603	K604	G605	R606	V607	I608	GLU	ASP	GLY	PRO	GLU	P614	R615	P616	N617	L618	R619	G620	E621	S622	C623	T624	F625	R626	V627	F628	L629	D630	P631	N632	Q633	Y634	Q635	Q636	M637	T639	N640	T641	I642	Q643	N644	G645	A646	E647	D648	V649	Y650	T652	F653	N654	I655	I656	M657	R658	Q659	K660			
P661	K662	E663	N664	N665	F666	K667	A668	V669	L670	E671	T672	I673	R674	N675	L676	M677	N678	T679	D680	C681	V682	G683	P684	D685	W686	L687	H688	D689	I690	I691	G692	G693	Y694	G695	D696	P697	S698	S699	A700	H701	I702	S703	K704	M705	P706	N707	Q708	I709	A710	T711	L712	D713	F714	N715	D716	T717	F718	L719	S720	
I541	N542	L543	N544	V545	R546	D547	I548	I549	K550	D551	E552	W553	E554	G555	L556	R557	K558	H559	D560	V561	C562	F563	L564	I565	T566	V567	R568	P569	T570	K571	P572	Y573	G574	T575	K576	F577	D578	R579	R580	R581	P582	F583	I584	E585	Q586	V587	L588	V590	Y591	V592	R593	G594	C595	I596	I597	Q598	G599	M600		

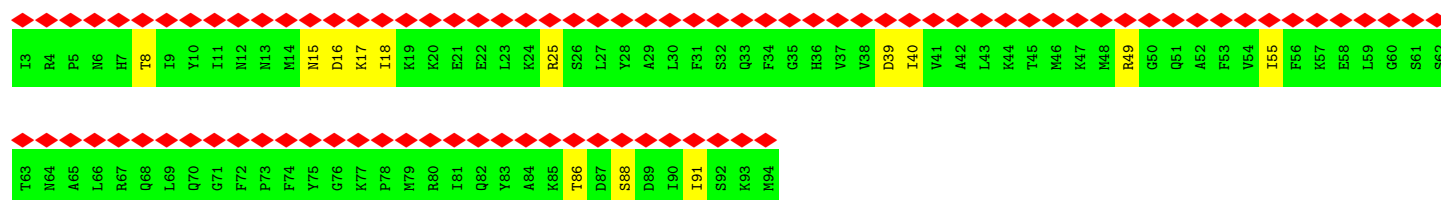


• Molecule 28: U2 small nuclear ribonucleoprotein A'

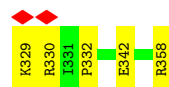
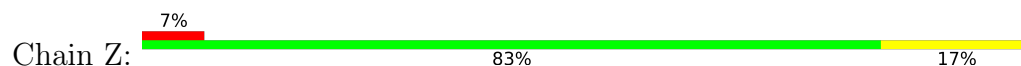


• Molecule 29: U2 small nuclear ribonucleoprotein B''

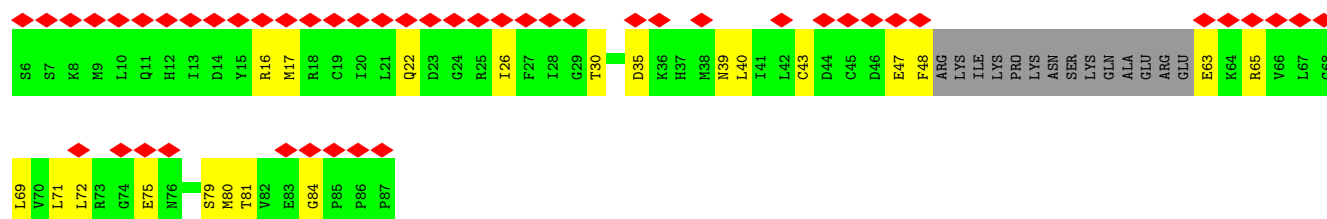




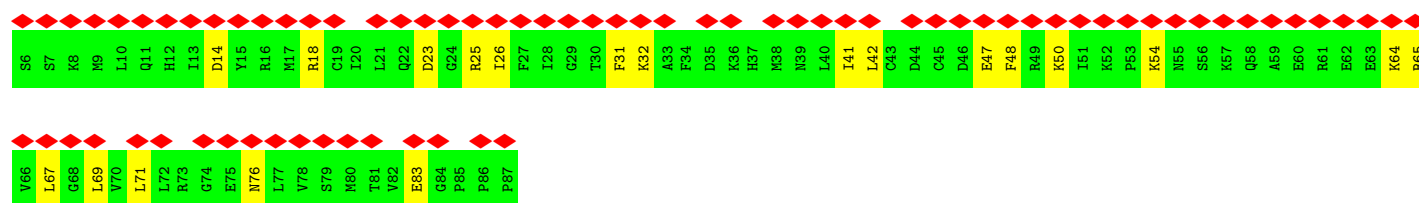
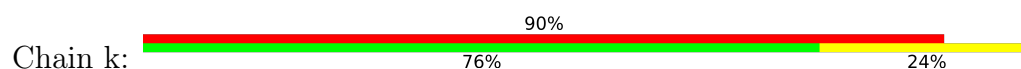
• Molecule 30: NF-kappa-B-activating protein



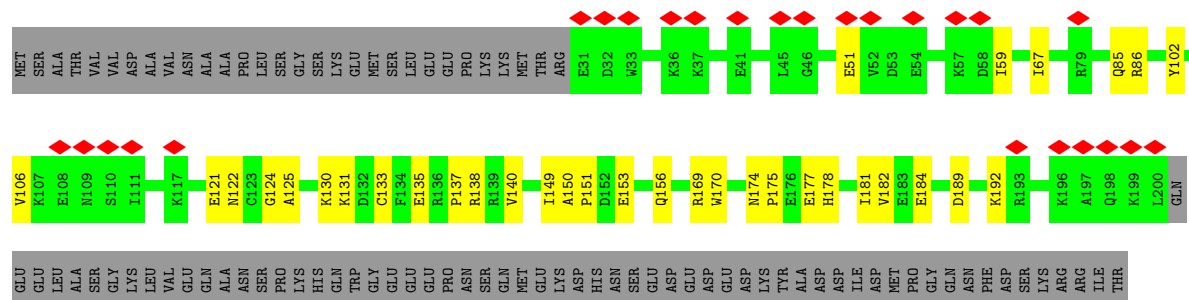
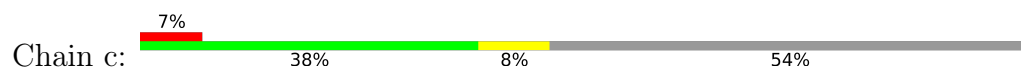
• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

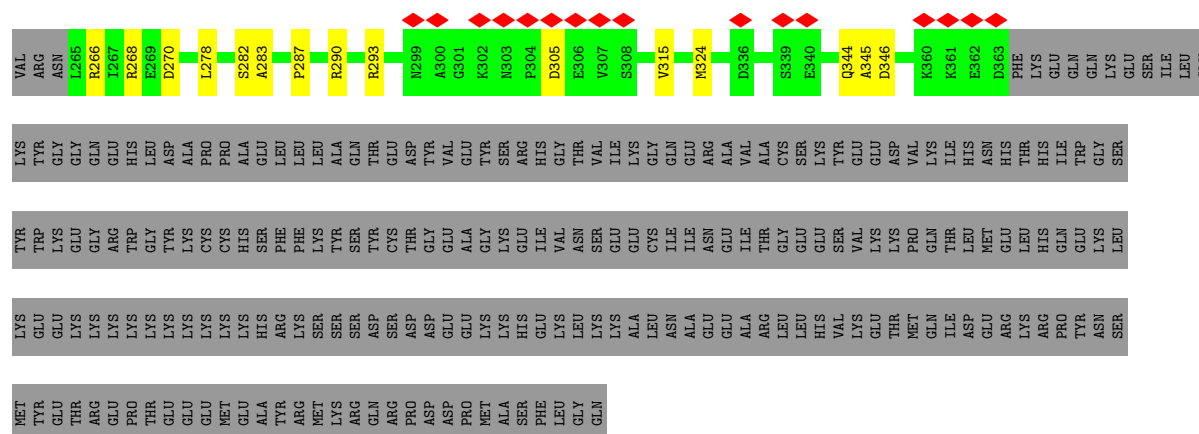


• Molecule 31: Small nuclear ribonucleoprotein-associated proteins B and B'

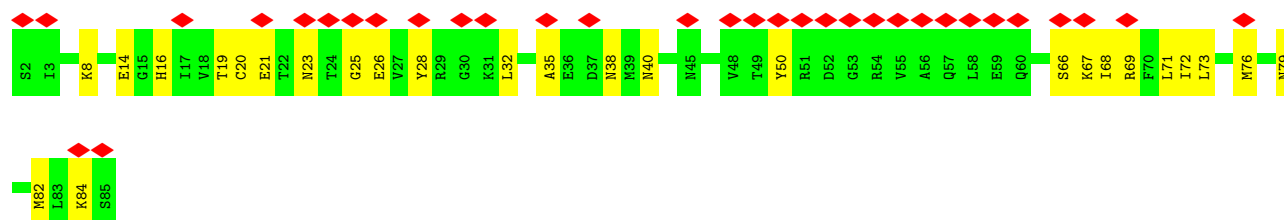
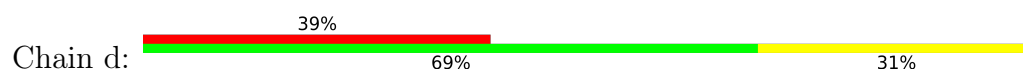


• Molecule 32: Pre-mRNA-splicing factor SLU7

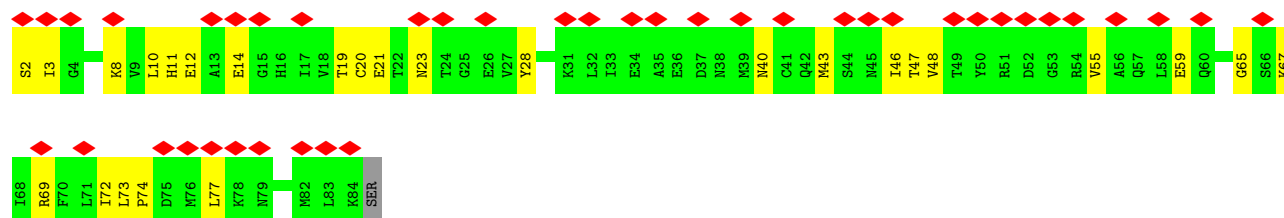




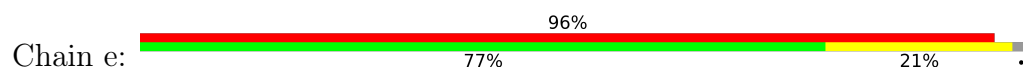
• Molecule 33: Small nuclear ribonucleoprotein Sm D3



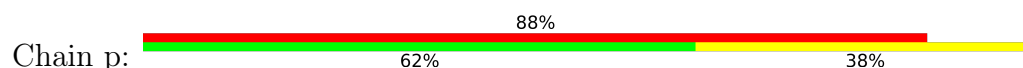
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

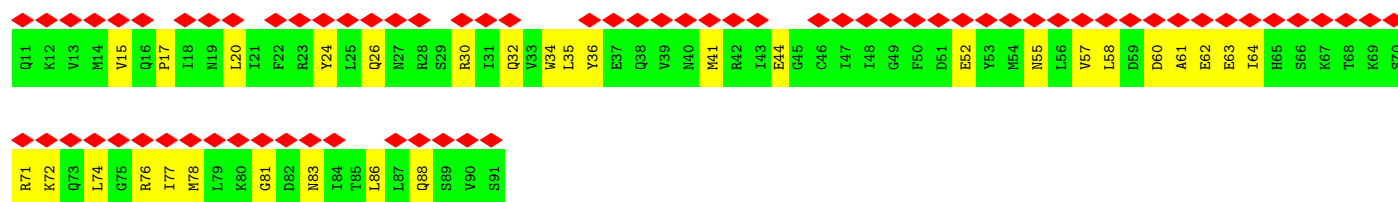


• Molecule 34: Small nuclear ribonucleoprotein E

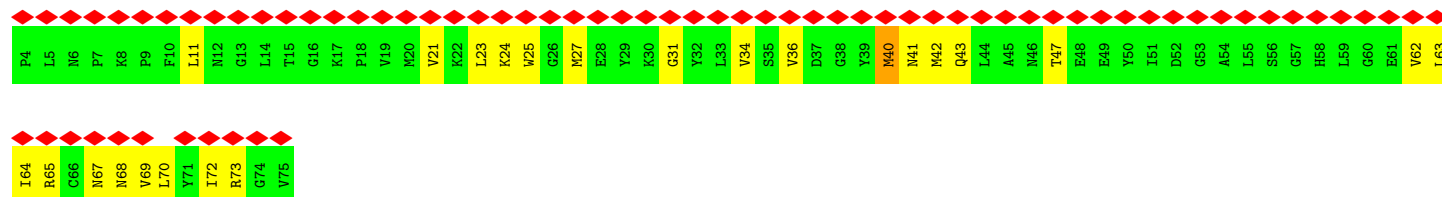


• Molecule 34: Small nuclear ribonucleoprotein E

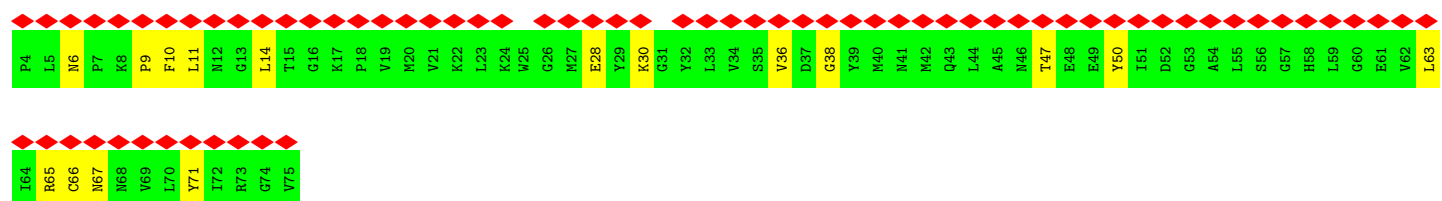
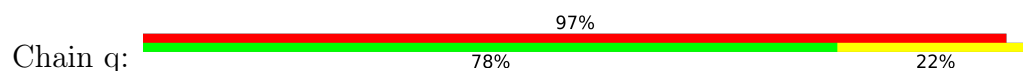




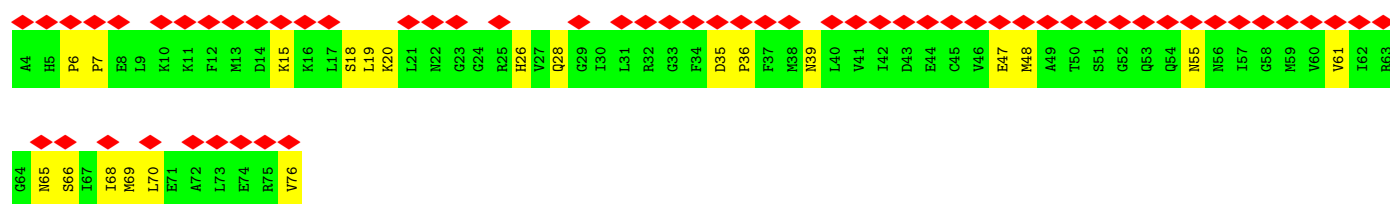
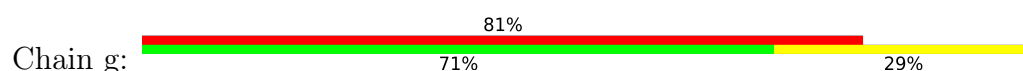
• Molecule 35: Small nuclear ribonucleoprotein F



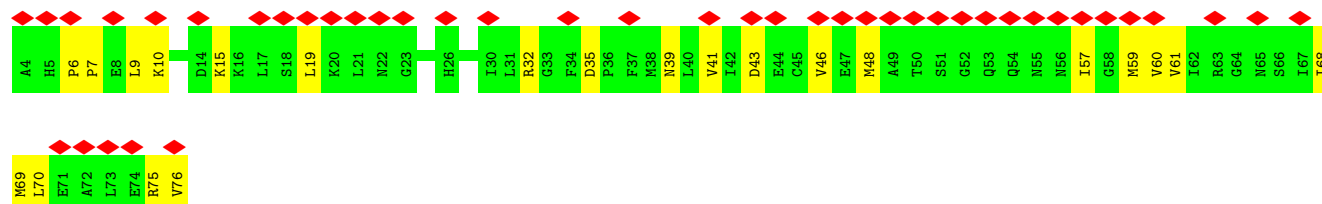
• Molecule 35: Small nuclear ribonucleoprotein F



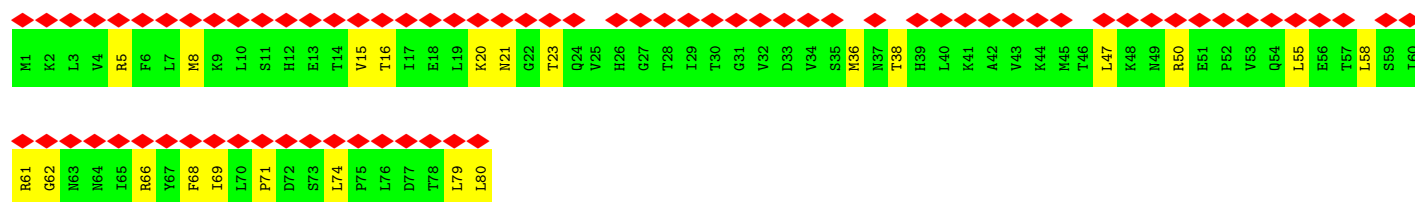
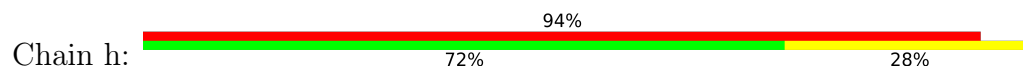
• Molecule 36: Small nuclear ribonucleoprotein G



• Molecule 36: Small nuclear ribonucleoprotein G



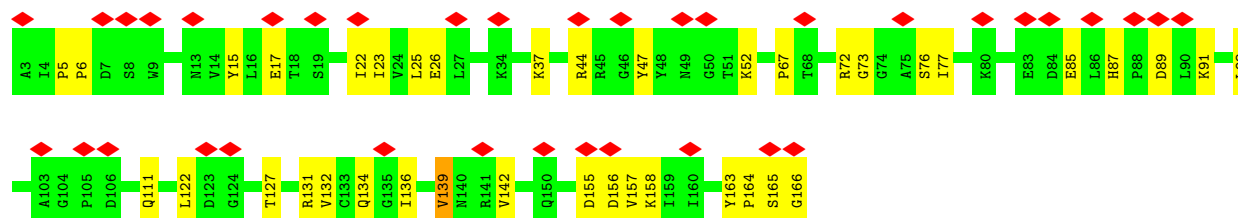
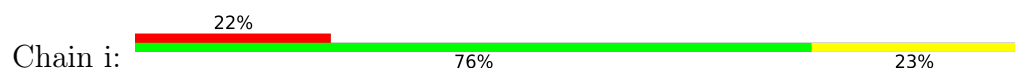
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



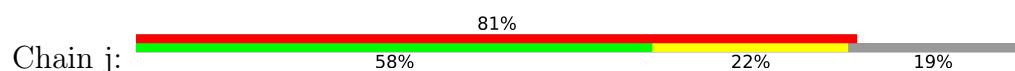
- Molecule 37: Small nuclear ribonucleoprotein Sm D1



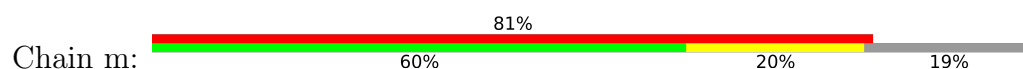
- Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1



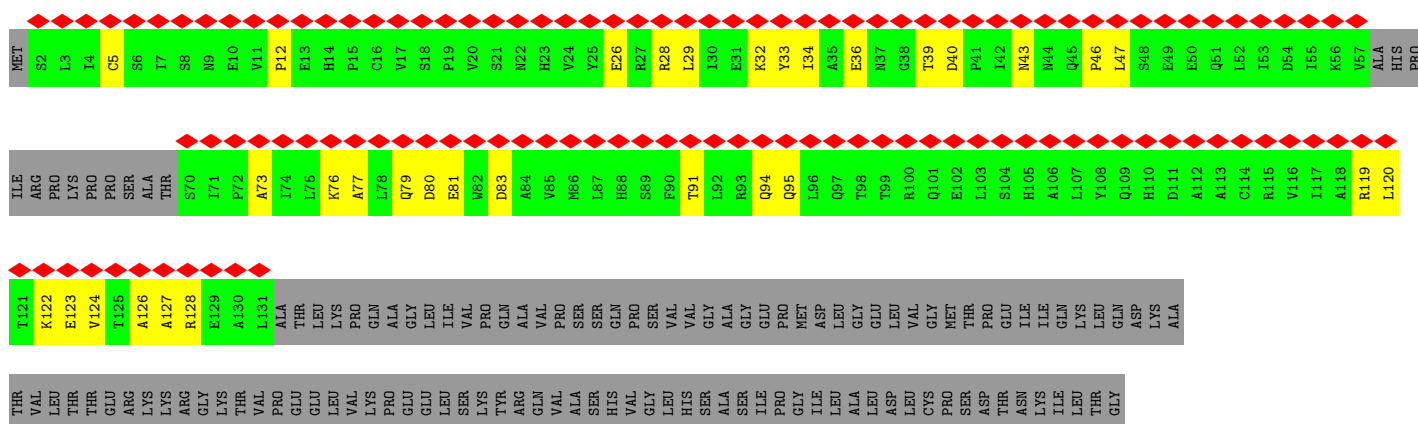
- Molecule 39: Small nuclear ribonucleoprotein Sm D2



- Molecule 39: Small nuclear ribonucleoprotein Sm D2

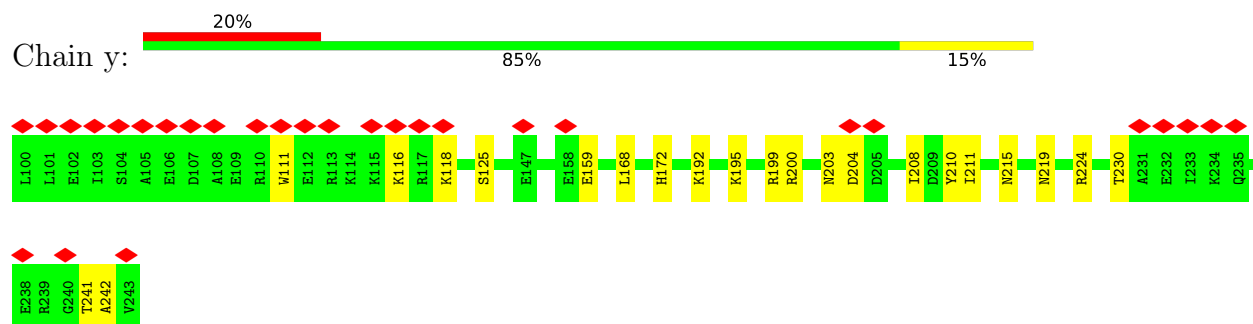




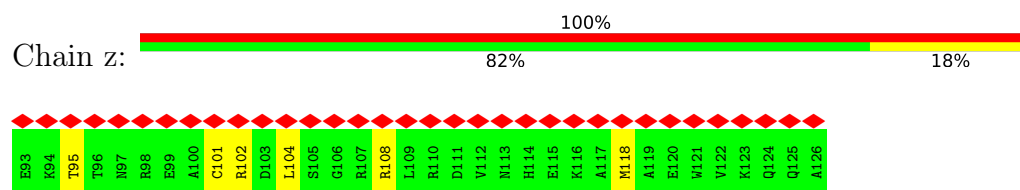


[illegible]

- Molecule 43: Pre-mRNA-splicing factor SYF2



- Molecule 44: Replication stress response regulator SDE2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GTP, K, MG, ZN, SEP, IHP

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	2	0.29	0/2827	0.47	0/4393
2	5	0.32	0/1760	0.50	0/2733
3	6	0.28	0/2323	0.44	0/3619
4	7	0.45	0/3179	1.00	14/4291 (0.3%)
5	8	0.40	0/748	0.98	4/1012 (0.4%)
6	9	0.40	0/1225	0.84	3/1648 (0.2%)
7	A	0.42	1/19172 (0.0%)	0.69	11/26014 (0.0%)
8	B	0.47	0/14140	0.92	27/19159 (0.1%)
9	C	0.33	0/7277	0.67	0/9887
10	D	0.31	0/1030	0.66	0/1371
11	E	0.34	0/329	0.52	0/510
12	F	0.30	1/1129 (0.1%)	0.55	0/1525
13	G	0.24	0/513	0.58	0/683
14	H	0.37	0/3779	0.68	0/5087
15	I	0.22	0/971	0.49	0/1504
16	J	0.42	0/2592	0.68	0/3535
17	K	0.31	0/2387	0.65	0/3205
18	L	0.34	0/1214	0.68	0/1627
19	M	0.30	0/2366	0.61	0/3193
20	N	0.25	0/2448	0.60	0/3316
21	O	0.29	0/3457	0.57	0/4627
22	P	0.28	0/902	0.63	1/1201 (0.1%)
23	R	0.39	0/196	0.49	0/265
24	S	0.40	0/4013	0.77	8/5432 (0.1%)
25	T	0.56	0/4031	1.35	21/5500 (0.4%)
26	U	0.57	71/11155 (0.6%)	0.70	3/15095 (0.0%)
27	V	0.81	0/3000	1.61	20/3777 (0.5%)
28	W	0.27	0/1299	0.64	0/1761
29	Y	0.33	0/759	0.50	0/1016
30	Z	0.25	0/232	0.60	0/307
31	b	0.29	0/553	0.59	0/739
31	k	0.44	0/674	0.59	0/899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.29	0/2268	0.61	0/3052
33	d	0.36	0/666	0.67	0/897
33	n	0.47	0/660	0.70	0/889
34	e	0.27	0/659	0.61	0/885
34	p	0.46	0/677	0.69	0/908
35	f	0.25	0/574	0.62	0/775
35	q	0.42	0/574	0.65	0/775
36	g	0.32	0/575	0.62	0/768
36	r	0.46	0/575	0.66	0/768
37	h	0.25	0/642	0.57	0/867
37	l	0.41	0/642	0.60	0/867
38	i	0.24	0/1304	0.57	0/1767
39	j	0.23	0/784	0.62	0/1053
39	m	0.39	0/784	0.65	0/1053
40	o	0.31	0/4265	0.66	0/5761
41	s	0.33	0/1423	0.65	0/1914
42	t	0.28	0/1004	0.56	0/1365
42	u	0.28	0/953	0.59	0/1295
42	v	0.31	0/1004	0.59	0/1365
42	w	0.26	0/953	0.57	0/1295
43	y	0.28	0/1241	0.63	0/1662
44	z	0.44	0/282	0.68	0/375
All	All	0.42	73/124189 (0.1%)	0.76	112/169287 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	4
8	B	0	1
9	C	0	2
17	K	0	1
18	L	0	2
25	T	0	5
27	V	0	15
35	f	0	1
41	s	0	3
All	All	0	34

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	867	MET	SD-CE	6.53	1.95	1.79
26	U	1093	MET	SD-CE	6.47	1.95	1.79
26	U	79	MET	SD-CE	6.41	1.95	1.79
26	U	1368	MET	SD-CE	6.41	1.95	1.79
26	U	176	MET	SD-CE	6.41	1.95	1.79
26	U	1214	MET	SD-CE	6.41	1.95	1.79
26	U	1037	MET	SD-CE	6.40	1.95	1.79
26	U	1115	MET	SD-CE	6.39	1.95	1.79
26	U	1294	MET	SD-CE	6.38	1.95	1.79
26	U	92	MET	SD-CE	6.34	1.95	1.79
26	U	65	MET	SD-CE	6.33	1.95	1.79
26	U	257	MET	SD-CE	6.31	1.95	1.79
26	U	492	MET	SD-CE	6.31	1.95	1.79
26	U	304	MET	SD-CE	6.30	1.95	1.79
12	F	714	PRO	C-N	6.29	1.39	1.33
26	U	1370	MET	SD-CE	6.29	1.95	1.79
26	U	424	MET	SD-CE	6.28	1.95	1.79
26	U	814	MET	SD-CE	6.27	1.95	1.79
26	U	244	MET	SD-CE	6.27	1.95	1.79
26	U	1061	MET	SD-CE	6.26	1.95	1.79
26	U	657	MET	SD-CE	6.24	1.95	1.79
26	U	1361	MET	SD-CE	6.22	1.95	1.79
26	U	207	MET	SD-CE	6.21	1.95	1.79
26	U	1107	MET	CG-SD	6.17	1.96	1.80
26	U	174	MET	SD-CE	6.17	1.95	1.79
26	U	1107	MET	SD-CE	6.16	1.95	1.79
26	U	97	MET	SD-CE	6.16	1.95	1.79
26	U	705	MET	SD-CE	6.15	1.95	1.79
26	U	638	MET	SD-CE	6.14	1.95	1.79
26	U	244	MET	CG-SD	6.14	1.96	1.80
26	U	79	MET	CG-SD	6.13	1.96	1.80
26	U	176	MET	CG-SD	6.13	1.96	1.80
26	U	1294	MET	CG-SD	6.12	1.96	1.80
26	U	600	MET	SD-CE	6.12	1.94	1.79
26	U	991	MET	CG-SD	6.11	1.96	1.80
26	U	1212	MET	SD-CE	6.09	1.94	1.79
26	U	1358	MET	CG-SD	6.08	1.96	1.80
26	U	424	MET	CG-SD	6.06	1.96	1.80
26	U	1358	MET	SD-CE	6.05	1.94	1.79
26	U	705	MET	CG-SD	6.03	1.95	1.80
26	U	941	MET	CG-SD	5.99	1.95	1.80
26	U	326	MET	SD-CE	5.97	1.94	1.79
26	U	257	MET	CG-SD	5.96	1.95	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	510	MET	CG-SD	5.96	1.95	1.80
26	U	510	MET	SD-CE	5.94	1.94	1.79
26	U	1368	MET	CG-SD	5.94	1.95	1.80
26	U	207	MET	CG-SD	5.93	1.95	1.80
26	U	1212	MET	CG-SD	5.91	1.95	1.80
26	U	638	MET	CG-SD	5.90	1.95	1.80
26	U	1214	MET	CG-SD	5.90	1.95	1.80
26	U	1370	MET	CG-SD	5.90	1.95	1.80
26	U	941	MET	SD-CE	5.89	1.94	1.79
26	U	600	MET	CG-SD	5.86	1.95	1.80
26	U	1361	MET	CG-SD	5.86	1.95	1.80
26	U	174	MET	CG-SD	5.85	1.95	1.80
26	U	677	MET	CG-SD	5.85	1.95	1.80
26	U	657	MET	CG-SD	5.83	1.95	1.80
26	U	92	MET	CG-SD	5.71	1.95	1.80
26	U	97	MET	CG-SD	5.68	1.95	1.80
26	U	991	MET	SD-CE	5.67	1.93	1.79
26	U	1037	MET	CG-SD	5.67	1.95	1.80
26	U	492	MET	CG-SD	5.66	1.95	1.80
26	U	677	MET	SD-CE	5.65	1.93	1.79
26	U	1093	MET	CG-SD	5.60	1.94	1.80
26	U	326	MET	CG-SD	5.60	1.94	1.80
26	U	1061	MET	CG-SD	5.59	1.94	1.80
26	U	65	MET	CG-SD	5.58	1.94	1.80
26	U	304	MET	CG-SD	5.57	1.94	1.80
26	U	1115	MET	CG-SD	5.50	1.94	1.80
26	U	814	MET	CG-SD	5.48	1.94	1.80
26	U	867	MET	CG-SD	5.43	1.94	1.80
26	U	820	MET	SD-CE	5.27	1.92	1.79
7	A	2105	ILE	CA-CB	-5.11	1.48	1.54

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	84	HIS	O-C-N	-12.04	109.67	122.07
25	T	83	LYS	O-C-N	-11.98	109.73	122.07
25	T	309	ALA	O-C-N	-11.96	109.76	122.07
25	T	311	MET	O-C-N	-11.95	109.76	122.07
25	T	310	LYS	O-C-N	-11.93	109.78	122.07
4	7	37	THR	CA-C-N	10.60	130.37	119.56
4	7	37	THR	C-N-CA	10.60	130.37	119.56
5	8	114	LYS	N-CA-C	-10.46	93.67	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	458	LYS	O-C-N	9.71	132.07	122.07
25	T	459	ALA	O-C-N	9.67	132.03	122.07
25	T	457	ARG	O-C-N	9.66	132.02	122.07
25	T	458	LYS	CA-C-O	-8.64	111.75	120.82
25	T	457	ARG	CA-C-O	-8.62	111.77	120.82
25	T	459	ALA	CA-C-O	-8.62	111.77	120.82
27	V	414	GLU	N-CA-C	8.35	120.38	111.28
26	U	1379	TYR	N-CA-C	7.64	122.69	112.30
8	B	1666	THR	N-CA-C	7.21	121.52	112.87
8	B	1044	VAL	CA-C-N	7.21	126.71	118.85
8	B	1044	VAL	C-N-CA	7.21	126.71	118.85
4	7	408	ALA	N-CA-C	7.20	118.77	111.07
24	S	522	PRO	N-CA-CB	7.16	110.03	103.08
4	7	77	ASP	N-CA-C	-7.10	99.77	110.28
8	B	533	VAL	N-CA-C	6.99	118.86	112.29
24	S	675	PRO	N-CA-CB	6.79	110.39	103.25
24	S	604	PRO	N-CA-CB	6.78	110.37	103.25
4	7	38	PRO	N-CA-C	6.56	122.37	113.84
24	S	637	PRO	N-CA-CB	6.52	110.43	103.52
24	S	523	PRO	N-CA-CB	6.49	110.40	103.52
27	V	1038	THR	N-CA-C	6.47	118.88	111.11
4	7	68	ALA	N-CA-C	6.29	119.43	111.69
27	V	994	ILE	O-C-N	-6.22	114.80	122.57
24	S	670	PRO	N-CA-CB	6.17	110.35	103.44
6	9	144	LYS	N-CA-C	6.11	118.60	109.25
8	B	1006	LYS	CA-C-N	6.09	126.26	119.32
8	B	1006	LYS	C-N-CA	6.09	126.26	119.32
4	7	339	ARG	N-CA-C	6.05	119.57	109.95
25	T	377	THR	CB-CA-C	-6.04	101.40	110.88
4	7	178	THR	N-CA-C	6.03	120.77	113.17
24	S	551	PRO	N-CA-CB	5.98	110.14	103.44
27	V	672	ILE	CA-C-N	5.98	127.54	122.28
27	V	672	ILE	C-N-CA	5.98	127.54	122.28
24	S	566	PRO	N-CA-CB	5.93	110.09	103.44
25	T	481	TYR	N-CA-C	5.86	118.61	111.82
7	A	2199	ILE	CB-CA-C	-5.82	104.39	112.02
4	7	336	VAL	N-CA-C	-5.73	104.02	112.04
8	B	1135	LEU	CA-C-N	5.72	125.66	119.76
8	B	1135	LEU	C-N-CA	5.72	125.66	119.76
27	V	811	PRO	CA-C-N	5.72	130.69	121.95
27	V	811	PRO	C-N-CA	5.72	130.69	121.95
8	B	782	PHE	N-CA-C	5.71	118.09	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	457	ARG	N-CA-C	5.70	117.17	111.07
7	A	2153	THR	N-CA-C	-5.69	101.75	109.95
27	V	663	ASP	O-C-N	-5.65	115.07	122.59
8	B	1291	LEU	CA-C-N	5.64	125.96	119.92
8	B	1291	LEU	C-N-CA	5.64	125.96	119.92
4	7	210	PRO	N-CA-C	5.64	121.37	113.53
6	9	116	LYS	N-CA-C	-5.60	100.55	109.96
27	V	1097	GLY	CA-C-N	5.58	132.20	121.54
27	V	1097	GLY	C-N-CA	5.58	132.20	121.54
8	B	1048	VAL	N-CA-C	-5.57	106.36	113.22
7	A	2225	LEU	N-CA-C	5.57	117.86	109.23
7	A	2241	ASN	N-CA-C	5.53	118.34	110.10
7	A	2203	ASN	N-CA-C	5.49	120.81	109.11
5	8	115	GLY	N-CA-C	5.48	126.16	113.18
27	V	738	PRO	N-CA-C	5.48	123.75	112.47
4	7	384	ASP	N-CA-C	5.46	117.67	111.11
27	V	869	THR	CA-C-N	5.43	132.06	121.41
27	V	869	THR	C-N-CA	5.43	132.06	121.41
8	B	1228	VAL	CB-CA-C	-5.42	104.94	112.04
7	A	2100	THR	N-CA-C	-5.38	106.71	113.28
8	B	1127	CYS	CA-C-N	5.33	125.65	119.47
8	B	1127	CYS	C-N-CA	5.33	125.65	119.47
8	B	1228	VAL	N-CA-C	5.31	116.68	110.62
8	B	811	SER	N-CA-C	5.30	115.13	108.45
8	B	749	GLY	N-CA-C	-5.29	108.39	114.69
8	B	2096	ALA	CA-C-N	5.28	125.48	120.31
8	B	2096	ALA	C-N-CA	5.28	125.48	120.31
27	V	979	ARG	CA-C-N	5.27	127.30	120.44
27	V	979	ARG	C-N-CA	5.27	127.30	120.44
7	A	375	ASP	CA-C-N	-5.25	114.69	122.56
7	A	375	ASP	C-N-CA	-5.25	114.69	122.56
8	B	1693	ARG	CA-C-N	5.25	125.05	119.28
8	B	1693	ARG	C-N-CA	5.25	125.05	119.28
4	7	367	ARG	N-CA-C	-5.23	106.16	112.54
25	T	487	TRP	N-CA-C	5.22	117.06	111.36
4	7	163	THR	N-CA-C	-5.20	103.63	110.39
8	B	488	LEU	N-CA-C	5.20	119.72	113.17
27	V	609	SER	CA-C-N	5.19	131.46	121.54
27	V	609	SER	C-N-CA	5.19	131.46	121.54
8	B	572	ASP	N-CA-C	-5.17	103.31	110.35
25	T	22	LEU	O-C-N	5.17	125.08	120.48
27	V	656	THR	CA-C-N	5.14	128.85	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	V	656	THR	C-N-CA	5.14	128.85	121.55
22	P	196	ASN	N-CA-C	5.13	118.23	110.64
5	8	107	ASP	N-CA-C	-5.11	102.08	109.59
25	T	231	ASN	O-C-N	5.10	125.02	120.48
27	V	814	SER	N-CA-C	5.09	118.27	111.75
4	7	342	ASP	N-CA-C	5.09	117.00	107.99
8	B	1875	VAL	CA-C-N	5.09	124.53	119.24
8	B	1875	VAL	C-N-CA	5.09	124.53	119.24
25	T	89	ASP	O-C-N	5.07	125.00	120.48
5	8	148	TRP	N-CA-C	-5.07	103.35	110.50
7	A	2310	ARG	CG-CD-NE	5.06	123.14	112.00
7	A	200	ASP	CA-C-N	5.06	127.26	120.58
7	A	200	ASP	C-N-CA	5.06	127.26	120.58
8	B	574	GLN	N-CA-C	5.06	117.91	111.69
25	T	149	TRP	O-C-N	5.06	124.98	120.48
6	9	143	PHE	N-CA-C	5.05	120.09	113.88
26	U	568	ARG	CA-C-N	5.01	125.01	119.90
26	U	568	ARG	C-N-CA	5.01	125.01	119.90
25	T	453	LEU	CA-C-N	5.01	126.99	120.28
25	T	453	LEU	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1210	LYS	Peptide
7	A	1416	ILE	Peptide
7	A	1635	TYR	Peptide
7	A	940	ILE	Peptide
8	B	430	LEU	Peptide
9	C	799	GLU	Peptide
9	C	93	ILE	Peptide
17	K	123	GLU	Peptide
18	L	127	GLU	Peptide
18	L	128	VAL	Peptide
25	T	309	ALA	Mainchain
25	T	310	LYS	Mainchain
25	T	311	MET	Mainchain
25	T	83	LYS	Mainchain
25	T	84	HIS	Mainchain
27	V	1098	LYS	Peptide
27	V	1127	LEU	Peptide

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Mol	Chain	Res	Type	Group
27	V	1163	ARG	Peptide
27	V	1187	THR	Peptide
27	V	515	ASP	Peptide
27	V	550	TYR	Peptide
27	V	563	GLU	Peptide
27	V	636	CYS	Peptide
27	V	662	THR	Peptide
27	V	811	PRO	Peptide
27	V	855	VAL	Peptide
27	V	868	LYS	Peptide
27	V	938	ASN	Peptide
27	V	963	THR	Peptide
27	V	993	LEU	Peptide
35	f	40	MET	Peptide
41	s	129	GLN	Peptide
41	s	77	GLN	Peptide
41	s	89	LEU	Peptide

5.2 Too-close contacts

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	2	2535	0	1281	48	0
2	5	1579	0	800	18	0
3	6	2075	0	1048	31	0
4	7	3130	0	3172	114	0
5	8	730	0	690	28	0
6	9	1196	0	1182	34	0
7	A	18655	0	18541	564	0
8	B	13846	0	13981	437	0
9	C	7116	0	7127	178	0
10	D	1013	0	1058	40	0
11	E	296	0	153	3	0
12	F	1084	0	1022	11	0
13	G	504	0	509	22	0
14	H	3713	0	3745	166	0
15	I	872	0	442	21	0
16	J	2523	0	2469	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	2360	0	2406	50	0
18	L	1188	0	1192	20	0
19	M	2318	0	2310	43	0
20	N	2394	0	2329	99	0
21	O	3416	0	3293	134	0
22	P	888	0	865	13	0
23	R	193	0	196	6	0
24	S	3965	0	3156	79	0
25	T	4003	0	2869	85	0
26	U	10885	0	10852	73	0
27	V	2995	0	991	102	0
28	W	1282	0	1305	26	0
29	Y	745	0	767	10	0
30	Z	230	0	229	3	0
31	b	545	0	557	16	0
31	k	664	0	690	20	0
32	c	2215	0	2165	39	0
33	d	658	0	675	32	0
33	n	652	0	670	36	0
34	e	651	0	671	12	0
34	p	669	0	692	26	0
35	f	562	0	574	22	0
35	q	562	0	574	12	0
36	g	568	0	590	15	0
36	r	568	0	590	33	0
37	h	634	0	680	14	0
37	l	634	0	680	16	0
38	i	1270	0	1244	27	0
39	j	774	0	802	20	0
39	m	774	0	802	17	0
40	o	4157	0	4060	140	0
41	s	1402	0	1379	39	0
42	t	988	0	994	27	0
42	u	938	0	938	25	0
42	v	988	0	994	27	0
42	w	938	0	938	20	0
43	y	1218	0	1194	21	0
44	z	280	0	276	24	0
45	6	5	0	0	0	0
45	7	1	0	0	0	0
45	C	1	0	0	0	0
46	6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	7	31	0	12	2	0
48	C	32	0	12	2	0
49	L	3	0	0	0	0
49	M	3	0	0	0	0
49	c	1	0	0	0	0
50	c	36	0	6	1	0
All	All	121152	0	113439	2491	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 11.

All (2491) 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)
7:A:1067:MET:HE3	27:V:413:LYS:CD	1.29	1.60
7:A:1067:MET:CE	27:V:413:LYS:HG2	1.27	1.59
27:V:393:ARG:HB3	27:V:1145:GLN:C	1.26	1.59
7:A:1067:MET:CE	27:V:413:LYS:CG	1.75	1.57
7:A:2333:LEU:CD2	8:B:545:ARG:CG	1.75	1.56
25:T:265:TYR:CB	25:T:274:LYS:CB	1.84	1.55
4:7:277:ILE:HG23	14:H:171:ASN:CG	1.33	1.53
7:A:2328:ALA:CB	8:B:788:GLY:HA2	1.35	1.53
20:N:267:PHE:CD1	41:s:195:ILE:HG23	1.43	1.53
7:A:357:ASN:HA	14:H:344:LYS:NZ	1.27	1.47
21:O:279:ILE:CD1	44:z:118:MET:HE1	1.42	1.46
4:7:277:ILE:HG23	14:H:171:ASN:ND2	1.30	1.45
24:S:480:TYR:CD2	24:S:502:GLU:CB	1.97	1.45
7:A:2333:LEU:HD23	8:B:545:ARG:CG	0.99	1.44
7:A:934:ARG:HH12	27:V:425:ILE:CG2	1.29	1.44
7:A:934:ARG:NH1	27:V:425:ILE:HG21	1.24	1.44
7:A:2328:ALA:HB3	8:B:788:GLY:CA	1.49	1.41
9:C:196:LYS:HZ2	33:d:14:GLU:CB	1.39	1.34
21:O:279:ILE:HD13	44:z:118:MET:CE	1.57	1.34
20:N:223:ARG:CZ	21:O:793:LEU:HD11	1.58	1.32
20:N:223:ARG:HE	21:O:793:LEU:CD2	1.39	1.32
24:S:512:GLU:CB	25:T:571:ARG:O	1.79	1.31
27:V:393:ARG:HB3	27:V:1145:GLN:O	1.19	1.29
7:A:2333:LEU:CD2	8:B:545:ARG:HG2	1.41	1.29
7:A:354:PRO:O	14:H:344:LYS:HD3	1.29	1.28
27:V:394:ILE:HA	27:V:1144:ARG:O	1.33	1.28
20:N:267:PHE:CD1	41:s:195:ILE:CG2	2.09	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:276:TYR:CE2	14:H:324:HIS:CE1	2.21	1.28
7:A:1067:MET:HE3	27:V:413:LYS:CG	1.43	1.27
7:A:2331:GLU:OE1	8:B:1082:VAL:CG1	1.82	1.27
14:H:320:ARG:NH1	14:H:340:PHE:CE1	2.02	1.27
27:V:393:ARG:HB3	27:V:1145:GLN:CA	1.58	1.27
17:K:335:ARG:NH1	27:V:1087:ASP:CA	2.00	1.25
10:D:106:ASP:OD1	36:r:75:ARG:CG	1.84	1.24
9:C:196:LYS:NZ	33:d:14:GLU:HB2	1.50	1.23
24:S:505:ALA:O	25:T:574:GLU:OE2	1.56	1.23
24:S:192:GLU:OE2	44:z:108:ARG:CZ	1.88	1.22
7:A:1067:MET:HE1	27:V:413:LYS:CG	1.47	1.21
21:O:279:ILE:CD1	44:z:118:MET:CE	2.11	1.21
7:A:2298:LEU:CD1	8:B:1265:GLN:OE1	1.88	1.20
20:N:267:PHE:CE1	41:s:195:ILE:HG23	1.77	1.20
27:V:393:ARG:CB	27:V:1145:GLN:CA	2.07	1.20
24:S:192:GLU:OE2	44:z:108:ARG:NH2	1.75	1.18
27:V:394:ILE:CA	27:V:1144:ARG:O	1.90	1.18
7:A:934:ARG:NH1	27:V:425:ILE:CG2	1.94	1.17
20:N:223:ARG:NE	21:O:793:LEU:HD21	1.59	1.16
7:A:2333:LEU:HA	8:B:545:ARG:NH1	1.57	1.16
4:7:277:ILE:CG2	14:H:171:ASN:ND2	2.08	1.16
7:A:360:SER:OG	14:H:337:GLU:OE1	1.64	1.16
7:A:354:PRO:O	14:H:344:LYS:CD	1.94	1.15
24:S:505:ALA:C	25:T:574:GLU:OE2	1.89	1.14
24:S:200:GLU:OE2	44:z:95:THR:HG23	1.46	1.14
24:S:512:GLU:CB	25:T:571:ARG:C	2.19	1.14
7:A:2298:LEU:HD11	8:B:1265:GLN:OE1	1.46	1.14
25:T:273:GLU:HA	26:U:357:ALA:HB2	1.16	1.14
4:7:277:ILE:CG2	14:H:171:ASN:CG	2.20	1.14
25:T:286:VAL:O	25:T:351:ARG:CB	1.96	1.14
7:A:2298:LEU:HD13	8:B:1265:GLN:CD	1.74	1.13
4:7:277:ILE:HG23	14:H:171:ASN:OD1	1.46	1.12
20:N:267:PHE:H	21:O:785:GLN:NE2	1.48	1.12
7:A:1067:MET:CE	27:V:413:LYS:CB	2.28	1.12
20:N:267:PHE:CB	21:O:785:GLN:HE21	1.62	1.11
27:V:393:ARG:CB	27:V:1145:GLN:O	1.97	1.11
7:A:2333:LEU:CD2	8:B:545:ARG:HG3	1.54	1.10
6:9:72:THR:HG21	6:9:94:ILE:HD11	1.29	1.10
20:N:223:ARG:NH2	21:O:793:LEU:HD11	1.65	1.10
27:V:393:ARG:CB	27:V:1145:GLN:C	2.22	1.10
7:A:2323:GLY:CA	8:B:1071:LYS:HE2	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:134:ASN:ND2	9:C:857:VAL:O	1.86	1.09
24:S:505:ALA:CA	25:T:574:GLU:OE2	1.98	1.09
20:N:267:PHE:CE1	41:s:195:ILE:CA	2.13	1.08
24:S:480:TYR:CE2	24:S:502:GLU:CB	2.36	1.08
10:D:106:ASP:OD1	36:r:75:ARG:CD	2.01	1.08
25:T:175:LEU:CB	25:T:179:SER:CB	2.33	1.07
7:A:354:PRO:HB3	14:H:344:LYS:HA	1.34	1.07
17:K:335:ARG:HH12	27:V:1087:ASP:CA	1.62	1.06
4:7:50:LEU:HD23	14:H:330:LYS:HE2	1.35	1.06
20:N:267:PHE:N	21:O:785:GLN:NE2	2.02	1.06
20:N:267:PHE:CE1	41:s:195:ILE:HA	1.67	1.06
7:A:357:ASN:CA	14:H:344:LYS:NZ	2.18	1.05
10:D:106:ASP:OD1	36:r:75:ARG:HG2	1.53	1.05
7:A:2333:LEU:HD22	8:B:545:ARG:HG2	1.11	1.05
24:S:505:ALA:O	25:T:574:GLU:CD	1.98	1.05
7:A:2333:LEU:CA	8:B:545:ARG:NH1	2.20	1.04
7:A:2298:LEU:HD22	8:B:1265:GLN:HE22	1.22	1.04
7:A:2298:LEU:CD1	8:B:1287:ARG:HH12	1.69	1.04
20:N:267:PHE:HB3	21:O:785:GLN:HE21	1.19	1.03
7:A:1067:MET:CE	27:V:413:LYS:CD	2.16	1.02
20:N:267:PHE:HE1	41:s:195:ILE:CA	1.60	1.02
9:C:196:LYS:HZ1	33:d:14:GLU:C	1.66	1.02
20:N:265:ARG:HB3	21:O:785:GLN:HE22	1.25	1.02
20:N:267:PHE:H	21:O:785:GLN:CD	1.66	1.02
4:7:277:ILE:HG23	14:H:171:ASN:HD21	1.22	1.02
14:H:320:ARG:NH1	14:H:340:PHE:CZ	2.28	1.02
20:N:267:PHE:HE1	41:s:195:ILE:HA	1.03	1.01
7:A:356:ILE:C	14:H:344:LYS:HE3	1.85	1.01
4:7:278:THR:HG23	4:7:279:GLN:H	1.26	1.01
24:S:192:GLU:OE2	44:z:108:ARG:NE	1.93	1.01
4:7:277:ILE:CG2	14:H:171:ASN:OD1	2.08	1.00
24:S:505:ALA:HA	25:T:574:GLU:OE2	1.60	1.00
7:A:354:PRO:O	14:H:344:LYS:CB	2.10	0.99
9:C:276:TYR:CE2	14:H:324:HIS:ND1	2.30	0.99
40:o:536:ASP:HB2	40:o:543:TYR:CE2	1.95	0.99
9:C:196:LYS:NZ	33:d:14:GLU:O	1.94	0.99
14:H:525:PHE:HA	14:H:528:ILE:HG22	1.42	0.99
7:A:1067:MET:HE3	27:V:413:LYS:HD2	1.01	0.99
7:A:357:ASN:HA	14:H:344:LYS:HZ2	1.25	0.99
7:A:354:PRO:CB	14:H:344:LYS:HA	1.92	0.98
9:C:196:LYS:NZ	33:d:14:GLU:C	2.21	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2331:GLU:OE1	8:B:1082:VAL:HG11	1.59	0.98
4:7:277:ILE:HG12	14:H:171:ASN:ND2	1.79	0.98
20:N:223:ARG:NE	21:O:793:LEU:CD2	2.19	0.98
19:M:27:CYS:HB3	19:M:84:CYS:SG	2.03	0.97
27:V:413:LYS:HG3	27:V:425:ILE:HD11	1.42	0.97
7:A:2333:LEU:C	8:B:545:ARG:NH1	2.23	0.97
24:S:480:TYR:CG	24:S:502:GLU:CB	2.46	0.97
7:A:2323:GLY:HA2	8:B:1071:LYS:HE2	1.42	0.97
25:T:329:LEU:O	26:U:353:LEU:O	1.83	0.97
25:T:273:GLU:CA	26:U:357:ALA:HB2	1.95	0.96
27:V:394:ILE:C	27:V:1144:ARG:O	2.08	0.96
10:D:106:ASP:OD1	36:r:75:ARG:HD2	1.64	0.96
7:A:1067:MET:HE1	27:V:413:LYS:CB	1.90	0.96
6:9:92:ILE:HG22	6:9:94:ILE:HG23	1.46	0.95
20:N:267:PHE:HD1	41:s:195:ILE:HG23	1.19	0.95
7:A:2298:LEU:HD12	8:B:1287:ARG:HH12	1.30	0.95
7:A:2331:GLU:OE1	8:B:1082:VAL:HG12	1.64	0.94
17:K:335:ARG:HH12	27:V:1087:ASP:N	1.63	0.94
7:A:2333:LEU:HD23	8:B:545:ARG:CB	1.97	0.94
7:A:1067:MET:CE	27:V:413:LYS:HB3	1.96	0.93
20:N:223:ARG:HE	21:O:793:LEU:HD21	0.78	0.93
7:A:357:ASN:N	14:H:344:LYS:HE3	1.84	0.93
20:N:223:ARG:CZ	21:O:793:LEU:CD1	2.47	0.93
20:N:267:PHE:CA	21:O:785:GLN:HE21	1.83	0.92
7:A:2333:LEU:CD2	8:B:545:ARG:CB	2.47	0.92
9:C:196:LYS:HZ2	33:d:14:GLU:HB2	0.76	0.91
7:A:1424:GLN:NE2	27:V:400:TRP:CZ2	2.39	0.91
21:O:275:LEU:HD23	44:z:118:MET:SD	2.10	0.91
24:S:512:GLU:CB	25:T:571:ARG:HB3	2.01	0.91
7:A:360:SER:OG	14:H:337:GLU:CD	2.13	0.91
7:A:821:ARG:HB2	27:V:426:LEU:HD11	1.53	0.91
24:S:200:GLU:OE2	44:z:95:THR:CG2	2.19	0.91
4:7:51:ARG:HG2	7:A:362:ARG:HH22	1.34	0.90
7:A:1066:GLN:CG	27:V:423:THR:O	2.18	0.90
7:A:354:PRO:O	14:H:344:LYS:HB2	1.71	0.90
7:A:357:ASN:CA	14:H:344:LYS:HZ1	1.83	0.90
9:C:196:LYS:HZ2	33:d:14:GLU:CA	1.84	0.90
14:H:320:ARG:HH12	14:H:340:PHE:HE1	0.91	0.89
20:N:267:PHE:CE1	41:s:195:ILE:CG2	2.17	0.89
21:O:275:LEU:CD2	44:z:118:MET:SD	2.60	0.89
4:7:277:ILE:HA	14:H:171:ASN:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:269:MET:HE1	36:r:10:LYS:HD3	1.53	0.89
25:T:329:LEU:HA	26:U:353:LEU:HG	1.54	0.89
40:o:269:MET:HE1	36:r:10:LYS:CE	2.03	0.88
7:A:1067:MET:HB3	27:V:413:LYS:HD2	1.55	0.88
7:A:2323:GLY:HA3	8:B:1071:LYS:HE2	1.55	0.88
9:C:276:TYR:HE2	14:H:324:HIS:CE1	1.88	0.88
7:A:1067:MET:CE	27:V:413:LYS:HD2	1.92	0.88
21:O:279:ILE:HD11	44:z:118:MET:CE	2.04	0.88
7:A:2333:LEU:HA	8:B:545:ARG:HH11	1.35	0.87
6:9:110:ILE:O	6:9:114:GLN:HG2	1.74	0.87
7:A:1068:PRO:O	27:V:413:LYS:HE2	1.75	0.87
20:N:265:ARG:HB3	21:O:785:GLN:NE2	1.80	0.87
7:A:1386:TRP:HB3	27:V:410:VAL:CG2	2.05	0.86
40:o:269:MET:HE1	36:r:10:LYS:CD	2.05	0.86
14:H:291:GLU:HG3	14:H:335:MET:SD	2.16	0.86
4:7:51:ARG:CG	7:A:362:ARG:HH22	1.90	0.85
4:7:278:THR:HG23	4:7:279:GLN:N	1.84	0.85
14:H:494:LEU:HD21	14:H:551:PHE:CE2	2.11	0.85
8:B:1538:ARG:NH1	8:B:1665:ASP:OD1	2.10	0.84
7:A:357:ASN:OD1	14:H:344:LYS:HE2	1.77	0.84
4:7:277:ILE:CG2	14:H:171:ASN:HD21	1.78	0.84
27:V:413:LYS:CG	27:V:425:ILE:HD11	2.06	0.84
24:S:192:GLU:CD	44:z:108:ARG:NH2	2.36	0.84
6:9:72:THR:CG2	6:9:94:ILE:HD11	2.08	0.83
7:A:2323:GLY:HA2	8:B:1071:LYS:CE	2.08	0.83
8:B:782:PHE:HB3	8:B:808:VAL:HB	1.59	0.83
7:A:2298:LEU:HD22	8:B:1265:GLN:NE2	1.94	0.83
21:O:279:ILE:CD1	44:z:118:MET:HE3	2.08	0.82
8:B:1218:SER:HB3	8:B:1240:LEU:HD21	1.61	0.82
27:V:394:ILE:C	27:V:1144:ARG:C	2.46	0.82
7:A:1067:MET:HE1	27:V:413:LYS:HG2	0.82	0.82
14:H:536:ILE:HG23	14:H:544:LEU:HD21	1.62	0.82
7:A:1434:LYS:NZ	27:V:403:LYS:HD3	1.95	0.82
7:A:2298:LEU:HD12	8:B:1287:ARG:NH1	1.94	0.82
8:B:425:ASN:ND2	8:B:886:GLN:O	2.13	0.81
10:D:106:ASP:OD1	36:r:75:ARG:CB	2.29	0.81
27:V:413:LYS:HB2	27:V:413:LYS:NZ	1.94	0.81
34:p:58:LEU:O	34:p:76:ARG:HA	1.80	0.81
7:A:1067:MET:SD	27:V:413:LYS:HG2	2.21	0.81
7:A:934:ARG:NH1	27:V:425:ILE:HG22	1.96	0.81
8:B:593:TRP:HD1	8:B:631:LEU:HD22	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:512:GLU:CB	25:T:571:ARG:CB	2.58	0.80
7:A:1386:TRP:HB3	27:V:410:VAL:HG21	1.62	0.80
7:A:2328:ALA:HB1	8:B:788:GLY:HA2	1.56	0.80
4:7:50:LEU:HD23	14:H:330:LYS:CE	2.09	0.80
7:A:354:PRO:CA	14:H:344:LYS:HA	2.11	0.80
4:7:383:ASN:CG	4:7:384:ASP:H	1.89	0.80
7:A:354:PRO:O	14:H:344:LYS:CG	2.30	0.80
14:H:152:LEU:HA	14:H:387:MET:HE1	1.62	0.80
4:7:79:ILE:HD11	4:7:229:THR:HG21	1.64	0.80
4:7:277:ILE:HG12	14:H:171:ASN:HD22	1.46	0.80
40:o:565:LYS:HG2	40:o:579:ASP:OD2	1.80	0.79
4:7:277:ILE:CG1	14:H:171:ASN:ND2	2.44	0.79
7:A:2327:SER:HB3	8:B:1078:MET:HE2	1.64	0.79
9:C:173:THR:O	9:C:177:ARG:HB3	1.82	0.79
17:K:335:ARG:HH12	27:V:1087:ASP:H	1.31	0.78
24:S:512:GLU:HA	25:T:571:ARG:HB3	1.65	0.78
25:T:241:ASP:C	26:U:528:GLY:CA	2.57	0.78
8:B:790:THR:HG21	8:B:793:ASP:HB2	1.64	0.78
25:T:105:PHE:O	26:U:934:TYR:CE2	2.37	0.78
9:C:276:TYR:HE2	14:H:324:HIS:ND1	1.80	0.78
20:N:267:PHE:HB3	21:O:785:GLN:NE2	1.96	0.78
7:A:2166:HIS:CD2	7:A:2272:MET:HE1	2.18	0.78
7:A:2333:LEU:C	8:B:545:ARG:HH12	1.91	0.77
8:B:539:ILE:HB	8:B:612:ILE:HG22	1.65	0.77
8:B:1380:THR:HG21	8:B:1385:LEU:HB3	1.64	0.77
5:8:108:ARG:HG3	6:9:129:GLN:HB3	1.64	0.77
27:V:393:ARG:CG	27:V:1145:GLN:O	2.33	0.77
40:o:565:LYS:CG	40:o:579:ASP:OD2	2.33	0.77
25:T:329:LEU:CB	26:U:353:LEU:HA	2.14	0.77
8:B:424:ALA:HB3	8:B:888:PRO:HG2	1.66	0.77
14:H:525:PHE:HA	14:H:528:ILE:CG2	2.15	0.76
40:o:269:MET:CE	36:r:10:LYS:HD3	2.16	0.76
7:A:2298:LEU:HD11	8:B:1287:ARG:HH12	1.47	0.76
7:A:2328:ALA:CB	8:B:788:GLY:CA	2.28	0.76
1:2:47:U:O2	10:D:21:LEU:HA	1.85	0.76
4:7:277:ILE:HA	14:H:171:ASN:CB	2.15	0.76
7:A:954:LYS:NZ	27:V:409:ASN:OD1	2.18	0.76
20:N:267:PHE:CA	21:O:785:GLN:NE2	2.48	0.76
14:H:264:ILE:HG13	14:H:274:CYS:SG	2.25	0.76
7:A:2298:LEU:CD2	8:B:1265:GLN:HE22	1.97	0.75
8:B:1205:THR:HG22	8:B:1249:GLU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:223:ARG:NH2	21:O:793:LEU:CD1	2.49	0.75
14:H:530:LYS:CD	14:H:567:CYS:HB3	2.17	0.75
20:N:266:PRO:HD2	21:O:785:GLN:HB3	1.68	0.75
7:A:1066:GLN:HG3	27:V:423:THR:O	1.86	0.75
33:n:11:HIS:HB3	40:o:259:GLN:HB3	1.69	0.75
7:A:2073:TRP:CD1	7:A:2074:ARG:HD2	2.22	0.75
4:7:278:THR:HG21	4:7:347:SER:HB2	1.69	0.75
16:J:216:ASN:HD21	16:J:472:GLN:H	1.35	0.75
25:T:272:PHE:CB	26:U:356:VAL:HB	2.16	0.75
4:7:50:LEU:CD2	14:H:330:LYS:HE2	2.13	0.74
17:K:335:ARG:HH11	27:V:1087:ASP:CA	1.99	0.74
24:S:512:GLU:CA	25:T:571:ARG:HB3	2.17	0.74
7:A:2328:ALA:HB3	8:B:788:GLY:HA2	0.76	0.74
7:A:2333:LEU:HA	8:B:545:ARG:CZ	2.17	0.74
33:n:48:VAL:O	33:n:55:VAL:HA	1.88	0.74
7:A:1068:PRO:HD2	27:V:425:ILE:HD12	1.68	0.73
6:9:99:ILE:HD12	6:9:101:PHE:CE1	2.24	0.73
7:A:2298:LEU:CD1	8:B:1265:GLN:CD	2.48	0.73
8:B:686:GLU:HB2	8:B:866:GLU:HG2	1.69	0.73
1:2:47:U:H5"	10:D:37:ARG:NH2	2.04	0.73
8:B:731:THR:HG22	8:B:784:ILE:HB	1.71	0.73
5:8:109:ARG:HG3	5:8:110:THR:N	2.03	0.73
7:A:354:PRO:HB3	14:H:344:LYS:CA	2.17	0.73
8:B:1739:GLU:HG3	8:B:1744:THR:HB	1.71	0.73
10:D:111:LYS:HA	10:D:114:GLU:HG2	1.70	0.73
20:N:266:PRO:CB	21:O:788:TYR:HD2	2.01	0.72
7:A:2300:ASN:ND2	8:B:1229:ASP:C	2.47	0.72
17:K:335:ARG:NH2	27:V:1083:LEU:O	2.22	0.72
7:A:356:ILE:C	14:H:344:LYS:CE	2.63	0.72
20:N:266:PRO:HD2	21:O:785:GLN:OE1	1.89	0.72
33:n:11:HIS:C	40:o:259:GLN:HB3	2.14	0.72
7:A:357:ASN:HA	14:H:344:LYS:HZ1	0.92	0.72
7:A:2300:ASN:HD21	8:B:1229:ASP:HA	1.52	0.72
14:H:330:LYS:O	14:H:333:GLN:HG3	1.89	0.72
25:T:329:LEU:CA	26:U:353:LEU:HA	2.20	0.72
8:B:1901:ARG:HH11	8:B:1961:LYS:HE2	1.54	0.72
25:T:575:ARG:O	25:T:579:LEU:HB2	1.89	0.72
4:7:275:LEU:HG	4:7:348:LEU:HD23	1.71	0.71
6:9:72:THR:HG21	6:9:94:ILE:CD1	2.16	0.71
7:A:1390:ALA:HB2	27:V:410:VAL:CG1	2.20	0.71
20:N:223:ARG:NE	21:O:793:LEU:HD11	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:241:ASP:C	26:U:528:GLY:N	2.48	0.71
20:N:267:PHE:CB	21:O:785:GLN:NE2	2.47	0.71
27:V:395:SER:N	27:V:1144:ARG:C	2.48	0.71
14:H:530:LYS:HD2	14:H:567:CYS:HB3	1.72	0.71
10:D:113:LEU:C	10:D:113:LEU:HD13	2.16	0.71
27:V:413:LYS:HB2	27:V:413:LYS:HZ2	1.55	0.71
6:9:119:GLU:OE1	6:9:119:GLU:HA	1.91	0.71
7:A:1067:MET:HB3	27:V:413:LYS:CD	2.20	0.71
26:U:1059:ILE:HG13	26:U:1088:LEU:HD11	1.72	0.71
7:A:1390:ALA:HB2	27:V:410:VAL:HG11	1.72	0.71
7:A:1571:ILE:HD13	13:G:112:LYS:HD2	1.73	0.71
7:A:2156:THR:OG1	7:A:2157:VAL:N	2.21	0.71
4:7:277:ILE:CB	14:H:171:ASN:ND2	2.53	0.70
8:B:1737:ASN:HB2	8:B:1796:LEU:HD21	1.73	0.70
10:D:106:ASP:OD1	36:r:75:ARG:HB3	1.91	0.70
25:T:273:GLU:CB	26:U:331:TYR:OH	2.38	0.70
7:A:2317:PHE:CZ	8:B:1141:LYS:HE3	2.26	0.70
14:H:494:LEU:HD21	14:H:551:PHE:HE2	1.53	0.70
4:7:275:LEU:O	4:7:275:LEU:HD23	1.90	0.70
25:T:241:ASP:CB	26:U:528:GLY:HA2	2.21	0.70
20:N:267:PHE:HA	21:O:788:TYR:CE2	2.27	0.70
4:7:69:ILE:O	4:7:73:ILE:HG12	1.91	0.70
7:A:1761:PRO:HD2	32:c:293:ARG:HH22	1.56	0.70
16:J:314:ILE:HD12	16:J:324:HIS:HB2	1.73	0.70
7:A:2328:ALA:HB3	8:B:788:GLY:HA3	1.65	0.70
7:A:2146:VAL:HG22	7:A:2272:MET:HB2	1.74	0.70
7:A:2324:GLU:HG2	7:A:2330:ARG:HH12	1.54	0.69
24:S:512:GLU:CB	25:T:571:ARG:CA	2.70	0.69
20:N:223:ARG:NE	21:O:793:LEU:CD1	2.55	0.69
7:A:357:ASN:HA	14:H:344:LYS:CE	2.20	0.69
8:B:2041:LEU:HB2	8:B:2088:ALA:HB3	1.74	0.69
1:2:51:A:C5	40:o:275:TYR:CD2	2.80	0.69
9:C:196:LYS:NZ	33:d:14:GLU:CB	2.22	0.69
1:2:46:U:N3	15:I:85:G:N2	2.40	0.69
7:A:1571:ILE:HD13	13:G:112:LYS:CD	2.23	0.69
18:L:118:ILE:HD12	18:L:132:ILE:HG23	1.74	0.69
7:A:1067:MET:HA	27:V:413:LYS:HD3	1.74	0.69
40:o:269:MET:SD	36:r:10:LYS:HE2	2.32	0.69
8:B:790:THR:O	8:B:794:ARG:NH1	2.25	0.68
33:n:11:HIS:O	40:o:259:GLN:CB	2.41	0.68
4:7:277:ILE:HA	14:H:171:ASN:CG	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:73:ILE:HD11	4:7:95:SER:HA	1.75	0.68
7:A:1394:GLN:NE2	27:V:415:GLU:OE2	2.27	0.68
7:A:2268:LEU:HD23	8:B:1261:PRO:HB2	1.74	0.68
8:B:1963:LEU:HD22	8:B:2007:VAL:HG13	1.76	0.68
25:T:241:ASP:C	26:U:528:GLY:HA2	2.19	0.68
8:B:1338:THR:O	8:B:1342:SER:OG	2.12	0.68
27:V:395:SER:N	27:V:1144:ARG:CA	2.57	0.68
41:s:73:LEU:HD23	41:s:76:ARG:HH12	1.59	0.68
8:B:637:ARG:NH1	8:B:918:ASN:OD1	2.27	0.68
7:A:2333:LEU:CD2	8:B:545:ARG:HB2	2.25	0.67
8:B:739:ARG:NH2	8:B:776:ASP:OD2	2.27	0.67
26:U:323:GLU:HA	26:U:326:MET:HE3	1.75	0.67
8:B:2043:ARG:HB3	8:B:2086:GLN:HA	1.76	0.67
9:C:276:TYR:CD2	14:H:324:HIS:CE1	2.81	0.67
7:A:1476:GLN:NE2	32:c:85:GLN:OE1	2.28	0.67
7:A:2333:LEU:HD21	8:B:545:ARG:HB2	1.76	0.67
9:C:300:LEU:HD13	9:C:306:ASN:HB3	1.77	0.67
7:A:357:ASN:N	14:H:344:LYS:CE	2.56	0.67
14:H:329:ASP:O	14:H:333:GLN:HG2	1.95	0.67
4:7:59:GLU:OE2	14:H:250:LYS:HE3	1.94	0.67
7:A:2306:HIS:CD2	7:A:2308:VAL:H	2.13	0.67
14:H:525:PHE:CA	14:H:528:ILE:HG22	2.23	0.67
8:B:1565:SER:HB3	8:B:1568:GLN:HB2	1.77	0.67
9:C:196:LYS:NZ	33:d:14:GLU:CA	2.52	0.67
20:N:266:PRO:HB2	21:O:788:TYR:HD2	1.60	0.67
6:9:92:ILE:CG2	6:9:94:ILE:HG23	2.21	0.67
7:A:2319:LEU:HD13	8:B:1069:GLN:O	1.95	0.66
4:7:335:ASP:OD1	4:7:364:ARG:HD2	1.95	0.66
7:A:67:ARG:HD3	7:A:179:ALA:HB2	1.78	0.66
10:D:109:PHE:HA	10:D:112:ARG:NH1	2.11	0.66
7:A:1068:PRO:CD	27:V:425:ILE:HD12	2.25	0.66
8:B:1433:ASP:OD1	8:B:1473:ARG:NH2	2.29	0.66
9:C:732:ILE:HG12	9:C:746:VAL:HG12	1.78	0.66
8:B:1130:ARG:NH1	8:B:1144:GLU:OE1	2.29	0.66
14:H:250:LYS:HD3	14:H:288:ASP:CG	2.21	0.66
7:A:1432:TYR:CE1	27:V:399:LYS:NZ	2.64	0.65
13:G:107:LYS:NZ	13:G:109:SER:OG	2.29	0.65
8:B:947:PRO:HG2	8:B:948:LEU:HD12	1.78	0.65
40:o:269:MET:HE1	36:r:10:LYS:NZ	2.10	0.65
7:A:934:ARG:HH12	27:V:425:ILE:HG21	0.50	0.65
7:A:1068:PRO:O	27:V:413:LYS:CE	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:88:SER:HG	29:Y:91:ILE:H	1.42	0.65
14:H:279:THR:O	14:H:283:GLU:HG3	1.96	0.65
25:T:241:ASP:CB	26:U:528:GLY:CA	2.74	0.65
7:A:1067:MET:HE3	27:V:413:LYS:CB	2.06	0.65
7:A:1771:LEU:HD22	7:A:1812:PRO:HG2	1.78	0.65
8:B:514:LEU:HA	8:B:517:MET:HE2	1.78	0.65
8:B:589:THR:H	8:B:592:LYS:HE2	1.62	0.65
8:B:1052:ILE:HG12	8:B:1053:GLU:H	1.60	0.65
8:B:1104:TRP:O	8:B:1108:THR:HG23	1.97	0.65
14:H:330:LYS:HA	14:H:333:GLN:CG	2.25	0.65
20:N:266:PRO:HG2	21:O:789:ALA:HB2	1.78	0.65
40:o:524:ILE:HG22	40:o:534:ILE:HG12	1.79	0.65
7:A:1421:THR:O	27:V:400:TRP:NE1	2.27	0.65
20:N:267:PHE:H	21:O:785:GLN:CG	2.08	0.65
7:A:2300:ASN:ND2	8:B:1229:ASP:O	2.30	0.65
27:V:394:ILE:CA	27:V:1144:ARG:C	2.69	0.65
21:O:279:ILE:HD11	44:z:118:MET:HE3	1.72	0.65
8:B:1456:VAL:HG11	8:B:1489:ALA:HB1	1.79	0.65
9:C:276:TYR:CZ	14:H:324:HIS:ND1	2.65	0.65
9:C:558:PRO:HG2	9:C:559:ILE:HG23	1.78	0.65
14:H:264:ILE:HD13	14:H:269:ALA:HB3	1.80	0.65
20:N:267:PHE:N	21:O:788:TYR:CD2	2.36	0.65
6:9:122:ARG:HG2	6:9:122:ARG:HH11	1.61	0.64
38:i:15:TYR:HB2	38:i:163:TYR:HB2	1.78	0.64
5:8:106:LEU:HD23	5:8:113:LEU:HD23	1.77	0.64
18:L:101:CYS:SG	18:L:102:CYS:N	2.69	0.64
7:A:899:MET:HE1	7:A:1246:GLN:HE22	1.61	0.64
24:S:200:GLU:OE2	44:z:95:THR:CB	2.44	0.64
33:n:11:HIS:O	40:o:259:GLN:HG2	1.97	0.64
5:8:125:LYS:HG3	5:8:126:GLU:N	2.12	0.64
7:A:1432:TYR:HE1	27:V:399:LYS:HZ3	1.45	0.64
8:B:1590:LEU:HD11	8:B:1597:LEU:HD11	1.78	0.64
8:B:447:VAL:HG22	8:B:687:GLN:HB2	1.80	0.64
25:T:329:LEU:HA	26:U:353:LEU:HA	1.80	0.64
7:A:1432:TYR:HE1	27:V:399:LYS:NZ	1.95	0.64
8:B:1765:THR:HG23	8:B:1781:LEU:HD13	1.79	0.64
22:P:23:LEU:HA	22:P:26:LEU:HD23	1.79	0.64
4:7:51:ARG:HD2	7:A:362:ARG:NH2	2.11	0.64
7:A:156:ARG:HD3	32:c:153:GLU:HG2	1.79	0.64
7:A:934:ARG:HH11	27:V:425:ILE:CG2	2.09	0.64
8:B:728:ARG:NH2	8:B:787:ALA:H	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:278:THR:CG2	4:7:279:GLN:N	2.57	0.63
5:8:78:THR:HG22	5:8:145:SER:HB2	1.80	0.63
8:B:1553:HIS:HB3	8:B:1701:ARG:HD2	1.79	0.63
9:C:137:HIS:HD2	9:C:238:ASN:H	1.46	0.63
17:K:62:GLY:HA3	38:i:131:ARG:HH11	1.63	0.63
25:T:187:LEU:CB	25:T:196:ALA:CB	2.76	0.63
3:6:21:U:O2'	40:o:130:ARG:NH2	2.31	0.63
40:o:552:VAL:HG13	40:o:571:TRP:HD1	1.62	0.63
9:C:853:ARG:HB3	9:C:879:ASP:HB3	1.80	0.63
8:B:1950:THR:OG1	8:B:2060:ARG:NH2	2.30	0.63
24:S:362:ALA:HA	24:S:365:ILE:HD12	1.81	0.63
35:q:28:GLU:HB2	35:q:50:TYR:O	1.99	0.63
7:A:941:LYS:HG3	7:A:951:LEU:HD22	1.81	0.63
7:A:357:ASN:CA	14:H:344:LYS:CE	2.77	0.63
7:A:2105:ILE:HD13	7:A:2266:ARG:HH22	1.64	0.63
33:d:19:THR:HB	33:d:72:ILE:HB	1.80	0.63
7:A:976:MET:O	7:A:1175:VAL:HA	1.98	0.63
8:B:1973:ARG:HD2	8:B:1997:LEU:HD11	1.80	0.63
7:A:209:ASP:HB2	7:A:212:PRO:HA	1.81	0.63
8:B:1563:VAL:HG12	8:B:1664:MET:HE2	1.79	0.63
8:B:1992:GLU:HA	8:B:1995:ALA:HB3	1.81	0.63
6:9:9:LEU:CD1	6:9:92:ILE:HG12	2.29	0.62
7:A:1066:GLN:HG2	27:V:423:THR:O	1.96	0.62
16:J:349:SER:OG	16:J:351:ASP:OD1	2.16	0.62
28:W:27:ARG:HG2	28:W:50:SER:HB3	1.81	0.62
41:s:74:ALA:HA	41:s:77:GLN:HB2	1.81	0.62
7:A:1641:ARG:HD2	32:c:175:PRO:HB2	1.80	0.62
7:A:2319:LEU:HG	7:A:2320:LEU:N	2.11	0.62
7:A:2331:GLU:OE2	8:B:1086:GLN:OE1	2.17	0.62
8:B:772:LEU:HB2	8:B:774:LEU:HG	1.81	0.62
14:H:330:LYS:HA	14:H:333:GLN:CD	2.24	0.62
40:o:272:GLU:OE2	36:r:6:PRO:CD	2.47	0.62
4:7:223:HIS:O	4:7:227:GLU:HG3	1.99	0.62
5:8:123:THR:HG1	5:8:126:GLU:HG3	1.62	0.62
9:C:664:GLU:HG2	9:C:779:LEU:HD12	1.81	0.62
38:i:52:LYS:HA	38:i:158:LYS:HA	1.81	0.62
31:k:26:ILE:HB	31:k:48:PHE:HB2	1.81	0.62
7:A:2074:ARG:HB2	8:B:1049:LYS:HE2	1.79	0.62
8:B:538:ILE:HB	8:B:585:ILE:HG12	1.79	0.62
20:N:267:PHE:CA	21:O:788:TYR:CE2	2.80	0.62
5:8:78:THR:CG2	5:8:145:SER:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:909:TYR:HB2	7:A:1033:GLY:HA3	1.82	0.62
20:N:266:PRO:CD	21:O:785:GLN:OE1	2.47	0.62
35:q:30:LYS:O	35:q:47:THR:HA	2.00	0.62
8:B:1936:LEU:HD22	8:B:1940:LEU:HD11	1.81	0.62
24:S:508:GLU:CB	25:T:573:LEU:CD2	2.77	0.62
7:A:2327:SER:HB3	8:B:1078:MET:CE	2.29	0.62
8:B:482:ASN:HB3	8:B:485:GLN:CD	2.24	0.62
1:2:101:U:O2'	37:l:61:ARG:NH1	2.33	0.62
4:7:275:LEU:CD2	4:7:330:VAL:HG22	2.30	0.62
19:M:78:LYS:O	19:M:97:ARG:NH2	2.33	0.62
21:O:189:ARG:NH2	24:S:213:LYS:O	2.33	0.61
24:S:200:GLU:CG	44:z:95:THR:OG1	2.48	0.61
1:2:2:U:H5''	43:y:116:LYS:HB2	1.81	0.61
1:2:46:U:N3	15:I:85:G:C2	2.66	0.61
10:D:68:MET:HA	12:F:757:ARG:HE	1.65	0.61
7:A:1571:ILE:CD1	13:G:112:LYS:CD	2.78	0.61
8:B:2067:VAL:HG22	8:B:2079:ILE:HG13	1.81	0.61
31:k:76:ASN:ND2	33:n:69:ARG:O	2.33	0.61
7:A:40:LEU:HD11	40:o:124:MET:HE1	1.82	0.61
20:N:62:LEU:HB2	20:N:351:LEU:HB2	1.82	0.61
43:y:159:GLU:HG2	43:y:168:LEU:HD11	1.81	0.61
7:A:821:ARG:CB	27:V:426:LEU:HD11	2.29	0.61
7:A:2073:TRP:CZ3	7:A:2310:ARG:HG2	2.36	0.61
27:V:401:GLU:O	27:V:405:MET:HG2	2.00	0.61
32:c:67:ILE:HG23	32:c:85:GLN:HE21	1.66	0.61
20:N:259:VAL:HB	20:N:277:PHE:HB2	1.81	0.61
32:c:51:GLU:HB2	32:c:59:ILE:HB	1.81	0.61
4:7:278:THR:HG21	4:7:347:SER:CB	2.29	0.61
8:B:704:MET:HG3	8:B:870:ILE:HG21	1.83	0.61
7:A:443:VAL:HG12	7:A:610:HIS:HB3	1.81	0.61
14:H:152:LEU:HA	14:H:387:MET:CE	2.30	0.61
14:H:532:GLN:OE1	14:H:547:VAL:HG11	2.01	0.61
40:o:565:LYS:HE3	40:o:579:ASP:OD2	1.99	0.61
7:A:2068:SER:HB2	7:A:2072:GLU:HB2	1.82	0.61
7:A:2106:LEU:HD12	7:A:2107:PRO:HD2	1.83	0.61
14:H:225:LYS:HG2	14:H:405:ILE:HG12	1.82	0.61
40:o:272:GLU:OE2	36:r:6:PRO:HD2	2.01	0.61
40:o:536:ASP:CB	40:o:543:TYR:CE2	2.79	0.61
4:7:148:GLU:OE1	4:7:148:GLU:HA	2.01	0.60
7:A:1424:GLN:NE2	27:V:400:TRP:HZ2	1.97	0.60
9:C:663:CYS:HB2	9:C:828:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:30:ARG:NH2	34:e:60:ASP:O	2.32	0.60
40:o:434:VAL:HG22	40:o:444:VAL:HG22	1.81	0.60
2:5:25:C:N4	9:C:162:ASP:OD2	2.34	0.60
4:7:277:ILE:HG22	14:H:171:ASN:OD1	1.98	0.60
7:A:1571:ILE:HD11	13:G:112:LYS:HD3	1.83	0.60
25:T:329:LEU:HA	26:U:353:LEU:CG	2.31	0.60
25:T:608:LEU:HB2	25:T:611:HIS:HB2	1.83	0.60
41:s:70:PHE:HA	41:s:73:LEU:HB2	1.83	0.60
4:7:278:THR:O	4:7:329:ARG:HD2	2.01	0.60
6:9:119:GLU:OE1	6:9:119:GLU:CA	2.49	0.60
7:A:362:ARG:NH1	14:H:334:TYR:HD1	1.99	0.60
7:A:1085:ILE:HD11	7:A:1160:ARG:HH12	1.66	0.60
8:B:844:LEU:HD11	8:B:849:ILE:HG23	1.83	0.60
8:B:905:ILE:HG22	8:B:981:VAL:HG22	1.82	0.60
19:M:64:ARG:HG3	19:M:162:PRO:HA	1.82	0.60
40:o:257:ILE:HD12	40:o:266:ARG:HE	1.67	0.60
34:p:30:ARG:NH2	34:p:60:ASP:O	2.35	0.60
8:B:451:LYS:HE2	8:B:451:LYS:H	1.66	0.60
9:C:476:CYS:SG	9:C:477:HIS:N	2.75	0.60
27:V:395:SER:OG	27:V:1143:ASN:O	2.16	0.60
2:5:45:C:H4'	7:A:596:TYR:HB3	1.83	0.60
4:7:51:ARG:CD	7:A:362:ARG:HH22	2.14	0.60
34:p:44:GLU:OE2	34:p:71:ARG:NH2	2.35	0.60
3:6:34:G:N2	15:I:13:C:O2	2.33	0.60
7:A:1124:ASN:ND2	7:A:1148:ASN:OD1	2.35	0.60
8:B:1777:SER:OG	8:B:1778:HIS:N	2.35	0.60
17:K:205:ASP:HB3	17:K:208:GLU:HB2	1.84	0.60
20:N:177:LYS:HG2	20:N:189:THR:HG22	1.82	0.60
17:K:320:HIS:HA	17:K:323:LYS:HB3	1.84	0.60
25:T:242:ALA:N	26:U:528:GLY:CA	2.61	0.60
7:A:641:MET:HA	7:A:644:ILE:HG22	1.84	0.60
7:A:2331:GLU:CD	8:B:1086:GLN:OE1	2.45	0.60
28:W:112:LEU:O	28:W:141:GLN:NE2	2.35	0.60
3:6:65:G:N7	7:A:663:ARG:NH2	2.44	0.59
7:A:1067:MET:CA	27:V:413:LYS:HD3	2.32	0.59
27:V:393:ARG:HB2	27:V:1145:GLN:CA	2.25	0.59
3:6:21:U:OP1	18:L:116:ASN:ND2	2.35	0.59
4:7:229:THR:HG23	4:7:233:MET:SD	2.41	0.59
8:B:764:THR:OG1	8:B:778:LEU:O	2.18	0.59
9:C:525:CYS:SG	9:C:557:GLN:NE2	2.75	0.59
25:T:187:LEU:CB	25:T:196:ALA:HB1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:423:MET:HE1	8:B:877:GLN:HG2	1.85	0.59
8:B:1135:LEU:HD22	8:B:1140:VAL:HG23	1.84	0.59
8:B:2124:VAL:O	8:B:2125:ASP:HB2	2.01	0.59
16:J:399:LYS:HB3	16:J:404:SER:HB2	1.83	0.59
17:K:189:ASN:HD21	17:K:195:ARG:HB3	1.68	0.59
33:n:67:LYS:HG3	36:r:68:ILE:HA	1.84	0.59
3:6:5:U:H3	3:6:15:A:H61	1.50	0.59
7:A:2268:LEU:HD21	8:B:1261:PRO:HG2	1.84	0.59
5:8:77:VAL:HB	5:8:117:THR:CG2	2.33	0.59
7:A:2333:LEU:HD23	8:B:545:ARG:HG3	0.60	0.59
8:B:1360:ALA:HB2	8:B:1490:LEU:HD11	1.85	0.59
2:5:91:U:O2'	37:h:61:ARG:NH1	2.36	0.59
7:A:200:ASP:OD1	7:A:240:ARG:NH2	2.35	0.59
7:A:549:GLU:OE1	7:A:552:ARG:NH1	2.35	0.59
7:A:1066:GLN:O	27:V:425:ILE:N	2.33	0.59
7:A:1214:TRP:HB2	7:A:1228:CYS:HB3	1.85	0.59
26:U:362:ARG:NH2	26:U:405:GLU:OE1	2.35	0.59
6:9:99:ILE:HD12	6:9:101:PHE:CZ	2.38	0.59
7:A:976:MET:HG2	7:A:1187:PHE:HB3	1.83	0.59
21:O:145:ASP:OD1	21:O:145:ASP:N	2.36	0.59
33:n:11:HIS:C	40:o:259:GLN:CB	2.75	0.59
7:A:881:ILE:HG23	7:A:918:THR:HG23	1.83	0.59
9:C:401:ILE:HD11	9:C:423:PHE:HB2	1.83	0.59
14:H:225:LYS:HE3	14:H:405:ILE:CG1	2.33	0.59
20:N:91:LEU:HD22	20:N:101:ASN:HD21	1.66	0.59
40:o:479:GLN:NE2	40:o:525:SER:OG	2.35	0.59
8:B:1661:VAL:HG23	8:B:1691:ALA:HB2	1.85	0.59
1:2:107:A:O2'	39:m:49:ASN:ND2	2.35	0.58
7:A:86:ARG:HH11	15:I:14:A:H5'	1.68	0.58
7:A:318:TYR:O	9:C:645:ARG:NH1	2.36	0.58
9:C:148:CYS:SG	9:C:417:ARG:NH2	2.76	0.58
33:d:26:GLU:HG2	33:d:50:TYR:HA	1.84	0.58
37:h:16:THR:HB	37:h:69:ILE:HB	1.85	0.58
2:5:93:U:O2'	35:f:65:ARG:NH2	2.36	0.58
7:A:357:ASN:OD1	14:H:344:LYS:CE	2.50	0.58
8:B:728:ARG:HH21	8:B:787:ALA:H	1.51	0.58
8:B:1570:ARG:NH2	8:B:1608:THR:HG21	2.18	0.58
20:N:223:ARG:HE	21:O:793:LEU:HD22	1.56	0.58
7:A:552:ARG:NH1	7:A:589:THR:O	2.36	0.58
12:F:682:TYR:HB3	12:F:685:LEU:HD11	1.85	0.58
17:K:238:THR:HG23	17:K:241:GLU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:887:LEU:HD23	8:B:888:PRO:HD2	1.85	0.58
8:B:1040:LEU:HD11	8:B:1072:LEU:HD22	1.85	0.58
26:U:867:MET:HE1	26:U:889:GLU:HB3	1.86	0.58
35:q:10:PHE:O	35:q:14:LEU:HB2	2.04	0.58
7:A:1609:VAL:O	32:c:268:ARG:NH2	2.36	0.58
7:A:1768:TYR:OH	32:c:344:GLN:NE2	2.36	0.58
20:N:266:PRO:CB	21:O:788:TYR:CD2	2.83	0.58
36:g:18:SER:OG	36:g:26:HIS:NE2	2.36	0.58
36:g:28:GLN:NE2	36:g:48:MET:SD	2.75	0.58
33:n:11:HIS:O	40:o:259:GLN:HB3	2.03	0.58
3:6:10:U:O2'	3:6:12:G:N7	2.37	0.58
6:9:8:TYR:HB3	6:9:93:VAL:HB	1.83	0.58
7:A:2073:TRP:CD1	7:A:2074:ARG:N	2.71	0.58
7:A:2298:LEU:CD1	8:B:1287:ARG:NH1	2.51	0.58
7:A:2298:LEU:HD13	8:B:1265:GLN:NE2	2.18	0.58
7:A:2300:ASN:HD21	8:B:1229:ASP:CA	2.16	0.58
9:C:103:THR:HA	9:C:171:LEU:HA	1.84	0.58
9:C:846:VAL:HG22	9:C:887:LEU:HD11	1.85	0.58
40:o:103:GLN:NE2	40:o:111:LEU:O	2.37	0.58
7:A:357:ASN:CA	14:H:344:LYS:HZ2	1.97	0.58
7:A:1581:LEU:HD22	7:A:1746:ARG:HH11	1.68	0.58
7:A:1214:TRP:NE1	7:A:1276:GLU:OE1	2.36	0.58
7:A:1434:LYS:NZ	27:V:403:LYS:CD	2.67	0.58
7:A:2095:ASP:OD2	7:A:2258:ARG:NE	2.36	0.58
8:B:1307:LEU:H	8:B:1333:THR:HG21	1.69	0.58
9:C:779:LEU:O	9:C:938:ARG:NH1	2.35	0.58
20:N:267:PHE:CA	21:O:788:TYR:CD2	2.85	0.58
28:W:47:ILE:HG12	28:W:66:LEU:HD21	1.84	0.58
2:5:88:A:H61	35:f:40:MET:HG3	1.68	0.58
7:A:1430:LEU:HB3	27:V:400:TRP:CZ3	2.39	0.58
21:O:279:ILE:HD13	44:z:118:MET:HE1	0.64	0.58
42:w:5:CYS:HB2	42:w:12:PRO:HG3	1.86	0.58
1:2:175:G:OP2	10:D:133:LYS:NZ	2.37	0.58
7:A:490:VAL:HG21	7:A:565:ARG:HG3	1.86	0.58
40:o:333:LYS:H	40:o:353:ASP:HB3	1.69	0.58
8:B:724:PHE:CG	8:B:852:MET:HE2	2.39	0.57
14:H:225:LYS:HE3	14:H:405:ILE:HG12	1.86	0.57
16:J:210:ILE:HG13	16:J:480:ALA:HB2	1.85	0.57
24:S:188:GLN:O	44:z:101:CYS:HB3	2.04	0.57
39:j:70:VAL:HG21	39:j:99:MET:HG2	1.84	0.57
1:2:45:C:C5	1:2:46:U:C4	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:186:GLU:O	13:G:72:ARG:NH2	2.37	0.57
7:A:837:LYS:HG2	7:A:1429:THR:HG22	1.86	0.57
7:A:2300:ASN:ND2	8:B:1229:ASP:HA	2.19	0.57
7:A:2326:TYR:HE1	8:B:1071:LYS:HZ3	1.52	0.57
16:J:294:LEU:HD12	16:J:303:LEU:HD11	1.85	0.57
31:b:79:SER:HB2	37:h:58:LEU:HD11	1.87	0.57
8:B:681:ARG:HH21	8:B:854:GLY:HA2	1.69	0.57
8:B:1122:MET:HE3	8:B:1126:MET:HB2	1.86	0.57
7:A:2310:ARG:NH1	7:A:2314:PHE:HE1	2.02	0.57
9:C:618:THR:HB	9:C:630:LEU:HB2	1.85	0.57
14:H:590:LEU:HD22	14:H:599:LEU:HD13	1.86	0.57
17:K:103:ARG:NH1	17:K:110:LYS:O	2.37	0.57
19:M:56:ARG:HG2	19:M:67:LYS:HB3	1.85	0.57
35:f:31:GLY:HA3	35:f:47:THR:HG22	1.87	0.57
33:n:11:HIS:HB3	40:o:259:GLN:O	2.03	0.57
40:o:432:ARG:NH2	40:o:446:GLU:OE2	2.37	0.57
3:6:20:A:O2'	18:L:120:ARG:NH2	2.37	0.57
3:6:64:U:OP2	7:A:663:ARG:NH1	2.32	0.57
4:7:46:ARG:HD3	4:7:133:MET:HE3	1.85	0.57
7:A:2268:LEU:CD2	8:B:1261:PRO:HB2	2.35	0.57
8:B:1120:LYS:HG2	8:B:1131:GLN:HG2	1.86	0.57
20:N:95:VAL:HG13	20:N:353:MET:HE1	1.85	0.57
7:A:335:PRO:HG3	9:C:139:HIS:HB3	1.86	0.57
7:A:354:PRO:O	14:H:344:LYS:CA	2.52	0.57
7:A:678:GLU:OE2	7:A:778:ARG:NH2	2.38	0.57
7:A:962:LEU:HB3	7:A:965:VAL:HB	1.87	0.57
7:A:2298:LEU:HD13	8:B:1265:GLN:OE1	1.63	0.57
17:K:98:TYR:OH	24:S:331:GLN:NE2	2.38	0.57
19:M:162:PRO:HG2	19:M:182:ARG:HG3	1.87	0.57
33:n:11:HIS:O	40:o:259:GLN:CG	2.53	0.57
40:o:304:LEU:HD11	40:o:567:ILE:HG21	1.86	0.57
40:o:422:ASN:N	40:o:436:THR:O	2.38	0.57
7:A:1777:ILE:HG12	7:A:1860:GLN:HB2	1.85	0.57
7:A:2331:GLU:OE1	8:B:1086:GLN:OE1	2.23	0.57
8:B:545:ARG:O	8:B:549:GLN:HG2	2.03	0.57
8:B:1586:ARG:HG2	8:B:1587:GLN:HG3	1.86	0.57
37:l:22:GLY:HA3	37:l:48:LYS:HD2	1.87	0.57
9:C:276:TYR:OH	14:H:324:HIS:CG	2.58	0.57
33:d:28:TYR:OH	36:g:20:LYS:NZ	2.37	0.57
42:u:75:LEU:HG	42:u:79:GLN:HE21	1.70	0.57
42:w:39:THR:HA	42:w:46:PRO:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:280:GLU:OE2	23:R:11:ARG:NH1	2.38	0.57
7:A:606:LYS:NZ	7:A:1548:TYR:O	2.35	0.57
8:B:690:VAL:HG21	8:B:707:ILE:HD13	1.87	0.57
19:M:131:THR:O	40:o:108:ARG:NH2	2.38	0.57
21:O:743:GLU:OE2	42:t:93:ARG:NH2	2.32	0.57
39:m:107:ILE:HG22	39:m:108:VAL:HG23	1.87	0.57
42:t:70:SER:N	42:u:10:GLU:OE1	2.38	0.57
42:t:125:THR:HA	42:t:128:ARG:HD2	1.85	0.57
31:b:26:ILE:HB	31:b:48:PHE:HB2	1.87	0.57
5:8:109:ARG:HG3	5:8:110:THR:HG23	1.86	0.56
8:B:828:ILE:HD12	8:B:869:LEU:HD12	1.87	0.56
21:O:766:ARG:NH2	41:s:14:ASP:O	2.38	0.56
41:s:22:GLY:O	41:s:29:ARG:NH2	2.38	0.56
8:B:1861:ARG:HD2	8:B:1864:GLU:OE2	2.05	0.56
21:O:147:ASP:OD1	21:O:147:ASP:N	2.34	0.56
6:9:117:ASP:N	6:9:118:PRO:HD3	2.21	0.56
7:A:1389:TYR:CD2	27:V:405:MET:SD	2.98	0.56
8:B:1777:SER:HB3	8:B:1780:HIS:ND1	2.21	0.56
9:C:177:ARG:NH2	9:C:638:ASP:OD2	2.37	0.56
14:H:287:ASP:HB3	14:H:331:ARG:CZ	2.35	0.56
14:H:316:PHE:CE2	14:H:343:ARG:HD3	2.40	0.56
14:H:374:ASP:HB2	14:H:376:TYR:CZ	2.41	0.56
14:H:474:HIS:HD2	23:R:23:LEU:H	1.52	0.56
20:N:267:PHE:CD1	41:s:195:ILE:HG21	2.29	0.56
24:S:286:GLU:HB2	24:S:295:ALA:HB2	1.88	0.56
35:f:34:VAL:HB	35:f:43:GLN:HB3	1.86	0.56
8:B:1670:ASN:ND2	8:B:1673:ILE:HG12	2.20	0.56
17:K:261:THR:HG23	21:O:24:MET:HB3	1.86	0.56
21:O:282:THR:HA	43:y:203:ASN:HD22	1.69	0.56
28:W:45:ASP:OD2	31:k:64:LYS:NZ	2.37	0.56
4:7:268:LEU:HD11	4:7:282:ILE:HD13	1.87	0.56
4:7:315:GLU:O	4:7:319:ILE:HG12	2.05	0.56
7:A:873:ASN:ND2	7:A:876:GLU:OE1	2.38	0.56
7:A:1618:LYS:NZ	7:A:1628:ASP:OD2	2.35	0.56
8:B:2014:TYR:OH	8:B:2114:MET:O	2.22	0.56
9:C:475:MET:HA	9:C:565:ILE:O	2.04	0.56
10:D:111:LYS:CA	10:D:114:GLU:HG2	2.36	0.56
14:H:494:LEU:HD13	14:H:550:MET:SD	2.46	0.56
20:N:81:LEU:HD21	20:N:343:ILE:HD12	1.88	0.56
28:W:43:GLN:NE2	31:k:83:GLU:O	2.39	0.56
40:o:126:GLU:HA	40:o:129:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1790:ILE:HG22	7:A:1800:THR:HG22	1.87	0.56
7:A:2300:ASN:HD21	8:B:1229:ASP:C	2.13	0.56
9:C:350:ASN:O	9:C:354:ARG:N	2.39	0.56
9:C:687:MET:HG2	9:C:791:ILE:HD13	1.88	0.56
25:T:734:TYR:HB3	25:T:739:ASN:HD22	1.70	0.56
40:o:436:THR:HG21	40:o:464:MET:HB2	1.86	0.56
7:A:2153:THR:HG22	7:A:2154:HIS:H	1.70	0.56
7:A:2320:LEU:HD23	7:A:2322:GLU:H	1.71	0.56
18:L:51:ARG:O	18:L:54:HIS:HB3	2.06	0.56
20:N:266:PRO:CG	21:O:789:ALA:HB2	2.35	0.56
26:U:204:ASP:HA	26:U:207:MET:HE2	1.87	0.56
38:i:26:GLU:OE1	38:i:131:ARG:NH2	2.38	0.56
40:o:435:SER:HB3	40:o:445:TRP:HE1	1.71	0.56
1:2:12:G:N7	43:y:200:ARG:NH2	2.53	0.56
1:2:46:U:H3	15:I:85:G:N2	2.02	0.56
1:2:46:U:OP2	1:2:46:U:H6	1.88	0.56
4:7:275:LEU:HD23	4:7:275:LEU:C	2.31	0.56
7:A:1215:ASN:HB3	7:A:1224:ARG:HD3	1.88	0.56
7:A:2073:TRP:HD1	7:A:2074:ARG:N	2.04	0.56
8:B:1223:ILE:HG22	8:B:1270:VAL:HG22	1.87	0.56
20:N:183:LYS:HG3	20:N:187:ILE:HD11	1.87	0.56
26:U:310:GLY:O	26:U:414:ARG:NH2	2.37	0.56
39:j:47:ARG:HA	39:j:107:ILE:HD11	1.88	0.56
33:n:19:THR:HB	33:n:72:ILE:HB	1.86	0.56
7:A:354:PRO:C	14:H:344:LYS:HD3	2.21	0.56
20:N:267:PHE:HB2	21:O:785:GLN:CG	2.36	0.56
21:O:785:GLN:HA	21:O:788:TYR:HB3	1.87	0.56
40:o:269:MET:CE	36:r:10:LYS:CE	2.81	0.56
4:7:59:GLU:OE2	14:H:250:LYS:CE	2.54	0.56
20:N:267:PHE:HA	21:O:788:TYR:CD2	2.41	0.56
28:W:132:ARG:HG3	28:W:145:LEU:HD23	1.88	0.56
31:k:47:GLU:HG2	31:k:65:ARG:HB2	1.88	0.56
37:l:67:TYR:OH	39:m:94:ARG:NH2	2.39	0.56
42:t:74:ILE:HG12	42:u:78:LEU:HD22	1.87	0.56
4:7:77:ASP:HB3	4:7:233:MET:HE2	1.86	0.55
20:N:346:SER:OG	20:N:348:ASP:OD1	2.24	0.55
7:A:546:LEU:HD11	7:A:595:LYS:HB2	1.88	0.55
7:A:1592:ASP:OD1	32:c:266:ARG:NH2	2.39	0.55
10:D:106:ASP:CG	36:r:75:ARG:HD2	2.30	0.55
17:K:218:ILE:O	22:P:16:ARG:NH1	2.34	0.55
17:K:237:MET:O	43:y:125:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:87:TYR:O	41:s:113:GLN:NE2	2.39	0.55
1:2:37:U:OP1	40:o:454:LYS:NZ	2.39	0.55
7:A:143:GLN:NE2	7:A:207:PHE:O	2.32	0.55
7:A:378:PHE:O	9:C:342:ARG:NH2	2.39	0.55
7:A:1042:GLN:HA	7:A:1090:ARG:HH12	1.71	0.55
7:A:1779:PHE:O	7:A:1809:ILE:HA	2.06	0.55
8:B:1985:ILE:O	8:B:1993:ARG:NH1	2.39	0.55
10:D:31:GLN:NE2	36:r:35:ASP:OD2	2.39	0.55
13:G:80:LYS:HA	13:G:88:ARG:HH22	1.72	0.55
21:O:270:LYS:HG3	21:O:278:ALA:HB2	1.86	0.55
21:O:782:LYS:O	21:O:786:HIS:N	2.39	0.55
7:A:923:ASP:OD2	7:A:1439:ARG:NH1	2.38	0.55
7:A:940:ILE:HD11	7:A:1046:LEU:HB2	1.89	0.55
7:A:1042:GLN:OE1	7:A:1090:ARG:NH1	2.39	0.55
7:A:1389:TYR:HD2	27:V:405:MET:SD	2.30	0.55
8:B:871:THR:OG1	8:B:872:SER:N	2.39	0.55
28:W:121:LEU:O	28:W:123:ASN:ND2	2.38	0.55
7:A:205:ASP:OD1	7:A:205:ASP:N	2.37	0.55
8:B:727:SER:HB3	8:B:730:GLU:HB3	1.88	0.55
8:B:927:ILE:HB	8:B:931:ARG:HH21	1.71	0.55
8:B:1564:PRO:O	8:B:1648:ARG:NH2	2.39	0.55
9:C:485:ASP:N	9:C:485:ASP:OD1	2.38	0.55
14:H:576:THR:H	14:H:579:SER:HB3	1.72	0.55
17:K:104:GLN:NE2	21:O:222:LEU:O	2.38	0.55
42:v:31:GLU:HG2	42:v:49:GLU:HG2	1.89	0.55
2:5:67:A:H5"	18:L:90:ALA:HB1	1.89	0.55
4:7:89:THR:HB	47:7:702:ATP:O1A	2.06	0.55
7:A:265:THR:HG23	7:A:327:VAL:HG13	1.87	0.55
17:K:44:TYR:HA	17:K:47:ARG:HD2	1.88	0.55
18:L:133:GLU:OE2	18:L:140:ARG:NE	2.38	0.55
26:U:571:LYS:HD2	26:U:586:GLN:O	2.07	0.55
40:o:565:LYS:CE	40:o:579:ASP:OD2	2.55	0.55
41:s:110:SER:HA	41:s:113:GLN:HB2	1.88	0.55
42:t:108:TYR:HA	42:t:111:ASP:HB2	1.89	0.55
12:F:739:GLN:NE2	12:F:746:GLN:OE1	2.40	0.55
21:O:713:MET:HA	21:O:716:LYS:HD2	1.88	0.55
7:A:362:ARG:HG3	14:H:337:GLU:OE2	2.06	0.55
7:A:1072:LEU:HD13	7:A:1087:LEU:HD13	1.87	0.55
8:B:793:ASP:HA	8:B:796:LEU:HB2	1.89	0.55
14:H:218:LEU:HD23	14:H:218:LEU:C	2.31	0.55
20:N:265:ARG:H	20:N:272:ARG:HH12	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:67:LYS:HG3	36:g:68:ILE:HA	1.87	0.55
7:A:360:SER:HG	14:H:337:GLU:CD	2.03	0.55
7:A:539:ARG:NH1	11:E:-3:A:O2'	2.40	0.55
7:A:682:ASP:OD2	7:A:746:LYS:NZ	2.38	0.55
20:N:263:ASP:OD1	20:N:263:ASP:N	2.39	0.55
4:7:287:LYS:HG2	4:7:308:HIS:HB2	1.89	0.55
8:B:1877:HIS:HB2	8:B:1896:GLN:NE2	2.21	0.55
16:J:270:VAL:HB	16:J:284:TYR:HB2	1.89	0.55
20:N:324:PRO:HG3	40:o:88:MET:HE1	1.89	0.55
21:O:60:LYS:HB2	43:y:241:THR:HG22	1.89	0.55
37:l:19:LEU:HD21	37:l:60:ILE:HD13	1.88	0.55
36:r:19:LEU:HD13	36:r:70:LEU:HB3	1.88	0.55
7:A:164:MET:HE1	7:A:560:SER:HA	1.89	0.54
7:A:523:ASN:OD1	7:A:552:ARG:NH2	2.40	0.54
8:B:1048:VAL:O	8:B:1050:GLU:N	2.40	0.54
8:B:1982:VAL:HG12	8:B:1986:MET:HE3	1.88	0.54
8:B:1989:GLU:HG2	8:B:1991:GLU:H	1.70	0.54
25:T:740:PHE:O	25:T:744:GLN:NE2	2.40	0.54
1:2:51:A:C6	40:o:275:TYR:CD2	2.95	0.54
7:A:1164:SER:HA	9:C:59:LEU:HD11	1.87	0.54
7:A:2117:ILE:O	7:A:2304:PHE:HB2	2.07	0.54
20:N:311:VAL:HB	20:N:321:TYR:HB2	1.88	0.54
35:f:62:VAL:HA	39:j:110:LEU:HA	1.89	0.54
37:h:36:MET:SD	39:j:102:ARG:NH2	2.80	0.54
34:p:64:ILE:HG12	34:p:71:ARG:HG2	1.90	0.54
4:7:275:LEU:HD21	4:7:330:VAL:HG22	1.90	0.54
5:8:123:THR:OG1	5:8:126:GLU:HG3	2.07	0.54
7:A:1366:PRO:HA	14:H:465:SER:HA	1.89	0.54
8:B:602:GLU:HG2	8:B:606:THR:HG23	1.88	0.54
8:B:752:LEU:O	8:B:807:GLN:NE2	2.40	0.54
8:B:1005:LEU:HD11	8:B:1095:ILE:HG23	1.90	0.54
9:C:174:GLU:HG2	9:C:181:ILE:HG12	1.88	0.54
15:I:18:A:O2'	19:M:83:THR:O	2.24	0.54
20:N:309:VAL:HB	20:N:323:LEU:HB2	1.88	0.54
31:b:69:LEU:HD23	33:d:73:LEU:HB2	1.88	0.54
32:c:189:ASP:HA	32:c:192:LYS:HB2	1.88	0.54
37:h:20:LYS:HD3	37:h:66:ARG:HG3	1.89	0.54
4:7:105:ARG:NH2	9:C:855:GLY:C	2.65	0.54
7:A:290:ASP:HB3	7:A:1139:ARG:HH12	1.73	0.54
7:A:2073:TRP:HD1	7:A:2074:ARG:HD2	1.68	0.54
8:B:1093:ARG:HD2	8:B:1115:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:169:VAL:HA	40:o:216:LEU:HD13	1.88	0.54
20:N:239:THR:O	20:N:290:ARG:NH1	2.40	0.54
28:W:137:TYR:HB2	28:W:158:ALA:HB1	1.90	0.54
6:9:55:HIS:CE1	6:9:56:LYS:HG2	2.43	0.54
7:A:698:PRO:HD2	7:A:701:ILE:HG13	1.90	0.54
7:A:1245:ARG:O	7:A:1249:MET:HB2	2.07	0.54
7:A:2333:LEU:O	8:B:545:ARG:NH1	2.41	0.54
8:B:1448:ILE:HD11	8:B:1474:MET:HE2	1.90	0.54
16:J:312:ALA:HB3	16:J:326:LEU:HB2	1.88	0.54
16:J:365:ARG:HH22	16:J:401:PRO:HB2	1.73	0.54
19:M:24:CYS:SG	19:M:81:CYS:HB2	2.47	0.54
24:S:334:GLU:OE2	24:S:368:ARG:NH1	2.41	0.54
26:U:913:LYS:HD2	26:U:917:LYS:HE2	1.90	0.54
27:V:402:ILE:O	27:V:406:ILE:HD12	2.07	0.54
7:A:141:ILE:HD12	7:A:410:PRO:HG3	1.88	0.54
8:B:1134:LYS:HE2	8:B:1177:TYR:CE1	2.43	0.54
8:B:1985:ILE:HG22	8:B:1988:MET:HE3	1.89	0.54
9:C:854:ARG:NH1	9:C:879:ASP:OD2	2.41	0.54
31:b:47:GLU:OE1	31:b:65:ARG:NH1	2.41	0.54
38:i:25:LEU:HD23	38:i:98:LEU:HD21	1.89	0.54
4:7:307:MET:HE1	4:7:320:MET:HG2	1.90	0.54
20:N:223:ARG:CZ	21:O:793:LEU:HD21	2.34	0.54
39:j:45:ASN:HB2	39:j:108:VAL:HG12	1.90	0.54
37:l:68:PHE:HB2	39:m:100:PHE:HB3	1.90	0.54
7:A:2129:TYR:HB3	7:A:2172:MET:HE3	1.89	0.54
24:S:438:TYR:O	24:S:442:ARG:HB2	2.08	0.54
26:U:1027:LEU:HA	26:U:1031:GLU:HB3	1.90	0.54
1:2:168:A:C8	33:n:47:THR:HG21	2.43	0.54
4:7:51:ARG:HD2	7:A:362:ARG:HH22	1.73	0.54
4:7:313:GLN:HA	4:7:316:ARG:HG3	1.90	0.54
6:9:99:ILE:HD12	6:9:101:PHE:HE1	1.70	0.54
8:B:991:TYR:O	8:B:1090:ARG:HD2	2.07	0.54
8:B:2069:GLY:HA2	8:B:2077:ILE:HB	1.89	0.54
37:h:74:LEU:O	39:j:98:LYS:NZ	2.41	0.54
1:2:15:U:OP1	43:y:224:ARG:NH2	2.41	0.54
7:A:2067:PHE:CE2	7:A:2069:SER:HA	2.43	0.54
7:A:2095:ASP:OD1	7:A:2095:ASP:N	2.41	0.54
7:A:2310:ARG:HH12	7:A:2314:PHE:HE1	1.56	0.54
21:O:15:GLU:HG2	21:O:151:MET:HE1	1.91	0.54
25:T:624:GLU:O	25:T:628:GLN:N	2.41	0.54
39:j:70:VAL:HB	39:j:96:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:n:3:ILE:HG21	40:o:262:GLY:HA2	1.88	0.54
40:o:400:ILE:HB	40:o:414:TYR:HB2	1.90	0.54
42:t:70:SER:O	42:t:74:ILE:N	2.38	0.54
21:O:33:ARG:O	21:O:158:ARG:NH2	2.40	0.53
24:S:508:GLU:CB	25:T:573:LEU:HD21	2.37	0.53
25:T:592:ALA:HB3	25:T:623:VAL:HG12	1.90	0.53
17:K:107:SER:OG	17:K:108:LYS:N	2.41	0.53
25:T:309:ALA:O	25:T:310:LYS:C	2.51	0.53
40:o:442:LEU:HB2	40:o:456:ILE:HB	1.91	0.53
34:p:78:MET:HE2	35:q:11:LEU:HD11	1.90	0.53
42:w:26:GLU:HB2	42:w:29:LEU:HB2	1.90	0.53
14:H:291:GLU:OE1	14:H:331:ARG:NH2	2.41	0.53
20:N:266:PRO:HG2	21:O:785:GLN:O	2.08	0.53
33:d:20:CYS:SG	33:d:21:GLU:N	2.81	0.53
38:i:156:ASP:OD1	38:i:156:ASP:N	2.40	0.53
40:o:390:LEU:HD22	40:o:402:GLN:HE21	1.72	0.53
40:o:552:VAL:HG13	40:o:571:TRP:CD1	2.43	0.53
1:2:166:G:OP2	1:2:166:G:N2	2.36	0.53
2:5:89:U:H1'	36:g:65:ASN:HB3	1.91	0.53
7:A:1009:MET:O	7:A:1013:ASN:ND2	2.41	0.53
7:A:1042:GLN:HE22	7:A:1092:ILE:HA	1.73	0.53
7:A:1808:PHE:HE2	7:A:1893:PHE:HB3	1.73	0.53
8:B:791:ARG:HH21	8:B:794:ARG:HH12	1.55	0.53
8:B:1375:ARG:CZ	8:B:1420:GLY:HA2	2.39	0.53
21:O:243:ARG:HA	24:S:213:LYS:HA	1.90	0.53
40:o:274:CYS:O	40:o:522:TYR:HE2	1.91	0.53
7:A:1021:ASP:OD1	7:A:1021:ASP:N	2.40	0.53
8:B:425:ASN:ND2	8:B:888:PRO:HD3	2.23	0.53
8:B:785:HIS:CE1	8:B:815:LEU:HD23	2.43	0.53
8:B:1099:VAL:HG13	8:B:1108:THR:HG22	1.91	0.53
8:B:1443:LYS:H	8:B:1443:LYS:HD3	1.73	0.53
9:C:764:ASP:HA	9:C:767:VAL:HG22	1.89	0.53
21:O:250:GLU:OE2	21:O:258:ARG:NH2	2.41	0.53
7:A:1430:LEU:CB	27:V:400:TRP:CZ3	2.91	0.53
7:A:2333:LEU:C	8:B:545:ARG:HH11	2.15	0.53
25:T:272:PHE:CB	26:U:356:VAL:H	2.21	0.53
4:7:307:MET:HA	4:7:311:MET:SD	2.49	0.53
5:8:125:LYS:CG	5:8:126:GLU:N	2.72	0.53
10:D:111:LYS:HA	10:D:114:GLU:CG	2.39	0.53
16:J:221:THR:HG21	16:J:486:ILE:HG12	1.91	0.53
17:K:61:GLY:HA3	38:i:136:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:178:ARG:HB2	40:o:118:ALA:HB2	1.91	0.53
19:M:106:ASP:OD1	19:M:106:ASP:N	2.42	0.53
25:T:84:HIS:O	25:T:85:ARG:C	2.51	0.53
25:T:105:PHE:C	26:U:934:TYR:CE2	2.87	0.53
32:c:282:SER:OG	32:c:283:ALA:N	2.42	0.53
36:g:15:LYS:HG3	36:g:76:VAL:HG12	1.89	0.53
7:A:1607:GLU:HG2	7:A:1608:THR:HG23	1.91	0.53
7:A:1780:VAL:HG22	7:A:1809:ILE:HG12	1.90	0.53
17:K:177:ILE:HG22	40:o:117:PRO:HA	1.91	0.53
20:N:231:MET:HE1	20:N:264:VAL:HG22	1.91	0.53
25:T:310:LYS:O	25:T:311:MET:C	2.51	0.53
35:f:42:MET:HB2	35:f:64:ILE:HD11	1.89	0.53
37:l:61:ARG:NH2	37:l:63:ASN:OD1	2.42	0.53
1:2:51:A:N6	40:o:564:SER:HB2	2.24	0.53
7:A:156:ARG:NH1	32:c:153:GLU:OE2	2.42	0.53
7:A:721:LYS:HB3	7:A:781:ARG:HD3	1.90	0.53
7:A:2073:TRP:CH2	7:A:2310:ARG:HG2	2.44	0.53
20:N:160:ALA:HB3	20:N:166:LEU:H	1.74	0.53
25:T:311:MET:O	25:T:312:GLU:C	2.51	0.53
31:k:69:LEU:O	33:n:73:LEU:N	2.40	0.53
40:o:258:PRO:HD2	40:o:265:LEU:HD12	1.91	0.53
42:v:27:ARG:NH2	42:v:31:GLU:OE2	2.42	0.53
7:A:89:LEU:O	7:A:92:LEU:HB3	2.09	0.53
7:A:214:ARG:HA	7:A:220:VAL:HG21	1.91	0.53
7:A:1676:ILE:HD13	7:A:1706:ASP:HB2	1.91	0.53
8:B:606:THR:HA	8:B:609:VAL:HG22	1.90	0.53
8:B:930:LEU:HD23	8:B:949:LEU:HD23	1.91	0.53
8:B:1380:THR:HG22	8:B:1382:MET:H	1.74	0.53
19:M:87:ASP:OD1	19:M:88:LEU:N	2.41	0.53
36:r:35:ASP:OD2	36:r:39:ASN:ND2	2.42	0.53
42:u:21:SER:O	42:u:23:HIS:ND1	2.41	0.53
4:7:383:ASN:O	4:7:386:ILE:HG22	2.09	0.52
6:9:94:ILE:O	6:9:94:ILE:HG13	2.09	0.52
7:A:1312:PRO:HG2	7:A:1314:VAL:HG12	1.91	0.52
8:B:1134:LYS:HE2	8:B:1177:TYR:HE1	1.74	0.52
9:C:162:ASP:OD1	9:C:162:ASP:N	2.42	0.52
9:C:850:LEU:HB3	9:C:855:GLY:HA3	1.91	0.52
16:J:215:GLY:O	22:P:57:ARG:NH2	2.43	0.52
7:A:2133:PRO:HD2	7:A:2139:VAL:HG13	1.92	0.52
8:B:1842:VAL:O	8:B:1846:ILE:HG12	2.08	0.52
9:C:95:LYS:O	22:P:48:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:100:LYS:NZ	9:C:650:GLU:OE2	2.39	0.52
17:K:265:ASP:OD1	17:K:265:ASP:N	2.41	0.52
21:O:746:HIS:O	21:O:750:ARG:NH1	2.43	0.52
33:n:74:PRO:HG2	33:n:77:LEU:HD13	1.91	0.52
4:7:30:THR:HG23	4:7:239:ILE:HA	1.89	0.52
7:A:698:PRO:HB2	17:K:237:MET:HE1	1.90	0.52
7:A:1370:ARG:NH2	14:H:504:GLU:OE1	2.42	0.52
9:C:208:HIS:HB3	9:C:211:PHE:HD2	1.74	0.52
21:O:178:GLU:OE2	21:O:181:ARG:NH1	2.41	0.52
25:T:241:ASP:CB	26:U:528:GLY:HA3	2.40	0.52
37:h:5:ARG:HG3	37:h:8:MET:HE2	1.91	0.52
40:o:210:GLU:HA	40:o:213:GLN:HB2	1.90	0.52
4:7:46:ARG:NH1	4:7:133:MET:HE3	2.24	0.52
7:A:109:PRO:HB2	7:A:191:ILE:HD12	1.91	0.52
7:A:243:ASN:O	32:c:131:LYS:NZ	2.41	0.52
8:B:2026:LYS:NZ	8:B:2027:ASP:OD2	2.43	0.52
10:D:113:LEU:HD13	10:D:113:LEU:O	2.08	0.52
14:H:234:LEU:HB3	14:H:370:LEU:HD12	1.92	0.52
20:N:127:ALA:HB2	20:N:157:CYS:HB3	1.91	0.52
21:O:176:LEU:HD22	40:o:440:LYS:HD3	1.90	0.52
26:U:673:ILE:HG22	26:U:677:MET:HE2	1.90	0.52
28:W:96:THR:HG23	28:W:121:LEU:HB2	1.91	0.52
37:l:74:LEU:O	39:m:98:LYS:NZ	2.41	0.52
7:A:419:ARG:NH2	7:A:423:ASP:O	2.42	0.52
7:A:1694:ILE:HG12	13:G:88:ARG:HB3	1.91	0.52
8:B:2105:THR:HG23	8:B:2121:LYS:HG3	1.90	0.52
16:J:352:THR:OG1	24:S:274:ARG:NH1	2.43	0.52
18:L:51:ARG:NH2	40:o:192:PHE:O	2.43	0.52
20:N:67:GLY:N	20:N:87:ASP:OD1	2.43	0.52
21:O:214:ILE:HG12	24:S:260:ARG:HG2	1.92	0.52
31:k:25:ARG:NH2	33:n:21:GLU:OE2	2.41	0.52
34:p:62:GLU:OE2	34:p:71:ARG:NH2	2.39	0.52
42:u:70:SER:O	42:u:74:ILE:N	2.36	0.52
42:w:119:ARG:NH2	42:w:123:GLU:OE2	2.42	0.52
7:A:26:SER:OG	7:A:27:GLU:N	2.42	0.52
7:A:36:LYS:NZ	40:o:163:GLN:O	2.43	0.52
7:A:76:MET:O	7:A:85:LYS:NZ	2.42	0.52
9:C:224:GLY:HA3	9:C:438:ILE:HD12	1.90	0.52
19:M:258:ILE:HA	19:M:274:PHE:HA	1.90	0.52
37:l:72:ASP:OD1	39:m:97:SER:OG	2.27	0.52
40:o:505:HIS:HB2	40:o:527:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:r:15:LYS:HE2	36:r:76:VAL:HA	1.91	0.52
3:6:20:A:N3	18:L:143:SER:OG	2.43	0.52
3:6:46:G:OP1	21:O:169:ARG:NH1	2.38	0.52
4:7:71:GLN:HG3	4:7:237:ILE:HG21	1.92	0.52
5:8:82:GLU:CG	5:8:112:TYR:HB3	2.40	0.52
8:B:1028:THR:O	8:B:1058:LYS:NZ	2.31	0.52
8:B:1228:VAL:CG1	8:B:1264:PRO:HD2	2.40	0.52
8:B:1732:MET:HE3	8:B:1788:LEU:HD21	1.92	0.52
9:C:853:ARG:NH1	9:C:879:ASP:O	2.41	0.52
13:G:54:GLY:O	32:c:174:ASN:ND2	2.40	0.52
19:M:97:ARG:HA	19:M:147:LEU:HD11	1.91	0.52
5:8:104:LEU:HD22	5:8:113:LEU:HD13	1.91	0.52
7:A:1786:TYR:HE1	7:A:1802:PRO:HB3	1.75	0.52
7:A:2090:ILE:HA	7:A:2223:CYS:O	2.10	0.52
7:A:2323:GLY:HA2	8:B:1071:LYS:NZ	2.25	0.52
9:C:137:HIS:O	9:C:142:LYS:NZ	2.43	0.52
9:C:531:TRP:HB2	9:C:551:LEU:HB2	1.92	0.52
10:D:109:PHE:CE1	33:n:59:GLU:HB2	2.44	0.52
10:D:123:GLN:O	10:D:127:ARG:NH1	2.42	0.52
16:J:419:LEU:HD22	16:J:427:LEU:HD11	1.92	0.52
19:M:144:ALA:HB3	19:M:147:LEU:HB2	1.91	0.52
21:O:276:PRO:HA	21:O:279:ILE:HG12	1.92	0.52
25:T:83:LYS:O	25:T:84:HIS:C	2.51	0.52
35:f:21:VAL:HG11	35:f:64:ILE:HD13	1.92	0.52
37:h:38:THR:HG21	37:h:68:PHE:HZ	1.75	0.52
4:7:59:GLU:OE1	14:H:291:GLU:OE2	2.28	0.52
7:A:981:PHE:O	7:A:1166:THR:OG1	2.28	0.52
7:A:1860:GLN:HG2	7:A:1883:VAL:HB	1.91	0.52
7:A:2306:HIS:HD2	7:A:2308:VAL:H	1.54	0.52
7:A:2327:SER:CB	8:B:1078:MET:HE2	2.37	0.52
8:B:1538:ARG:HG3	8:B:1542:MET:HE3	1.91	0.52
13:G:91:ASP:OD1	13:G:94:ARG:NH2	2.41	0.52
16:J:347:THR:HG22	16:J:357:TRP:HE1	1.74	0.52
18:L:64:PHE:HZ	18:L:72:ARG:HD2	1.73	0.52
24:S:457:ILE:HA	24:S:460:LYS:HG2	1.92	0.52
28:W:21:ASP:HB3	28:W:45:ASP:HB2	1.92	0.52
28:W:48:ASP:HA	28:W:70:LEU:HB2	1.91	0.52
31:k:23:ASP:OD2	33:n:69:ARG:NH1	2.43	0.52
7:A:300:ASN:O	9:C:939:ARG:NH1	2.42	0.52
7:A:1617:ARG:HD2	13:G:99:LEU:HD22	1.91	0.52
7:A:1930:TYR:HB2	32:c:324:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:532:GLN:OE1	14:H:547:VAL:CG1	2.58	0.52
16:J:373:LYS:HD2	16:J:392:PRO:HB2	1.92	0.52
17:K:261:THR:H	43:y:215:ASN:HD21	1.58	0.52
39:j:19:ARG:O	39:j:23:GLU:N	2.41	0.52
40:o:190:ASP:OD1	40:o:190:ASP:N	2.42	0.52
7:A:1211:ASP:HB3	7:A:1276:GLU:HG2	1.91	0.51
7:A:1686:ASP:OD1	32:c:169:ARG:NH1	2.43	0.51
14:H:517:LEU:HD21	23:R:24:SER:HA	1.91	0.51
20:N:266:PRO:HB2	21:O:788:TYR:CD2	2.42	0.51
40:o:274:CYS:O	40:o:522:TYR:CE2	2.63	0.51
40:o:572:ASP:OD1	40:o:572:ASP:N	2.43	0.51
4:7:225:ILE:HD13	4:7:228:MET:HE3	1.93	0.51
7:A:75:ASP:OD1	7:A:75:ASP:N	2.43	0.51
7:A:761:ILE:HD12	7:A:775:ASN:HD22	1.75	0.51
7:A:2268:LEU:CD2	8:B:1261:PRO:HG2	2.39	0.51
9:C:140:HIS:CD2	9:C:230:ASP:HB2	2.45	0.51
16:J:392:PRO:HG3	16:J:415:ILE:HA	1.93	0.51
17:K:47:ARG:HA	17:K:50:TRP:HE1	1.75	0.51
21:O:192:ARG:NH2	24:S:218:GLU:OE1	2.43	0.51
26:U:225:LEU:HG	26:U:253:PHE:HE1	1.75	0.51
40:o:284:TRP:HE1	40:o:322:ARG:HB3	1.76	0.51
40:o:384:ASP:O	40:o:388:GLN:NE2	2.44	0.51
7:A:138:PRO:HB2	7:A:238:LEU:HD13	1.93	0.51
7:A:1536:LEU:HG	7:A:1572:SER:HB3	1.93	0.51
8:B:1182:PRO:HA	8:B:1208:PHE:CG	2.45	0.51
20:N:203:ASP:HB3	20:N:247:GLY:HA3	1.91	0.51
4:7:307:MET:HE1	4:7:320:MET:SD	2.51	0.51
8:B:1891:THR:O	8:B:1895:LEU:HB2	2.11	0.51
9:C:130:ARG:NH2	9:C:435:VAL:O	2.42	0.51
10:D:44:LYS:O	34:p:26:GLN:NE2	2.43	0.51
10:D:89:GLU:O	10:D:93:GLN:N	2.40	0.51
16:J:355:ARG:HH11	16:J:364:THR:HG21	1.75	0.51
21:O:715:LYS:HA	21:O:718:LYS:HB2	1.92	0.51
7:A:1067:MET:HE2	27:V:413:LYS:HB3	1.89	0.51
7:A:1571:ILE:CD1	13:G:112:LYS:HD3	2.40	0.51
7:A:1984:LYS:HG3	32:c:345:ALA:HB1	1.93	0.51
9:C:186:VAL:HA	9:C:534:VAL:HA	1.91	0.51
21:O:714:GLU:OE2	41:s:120:ARG:NH1	2.44	0.51
21:O:798:LEU:HD13	41:s:209:ILE:HB	1.93	0.51
38:i:25:LEU:HG	38:i:132:VAL:HG12	1.93	0.51
42:t:43:ASN:O	42:t:45:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:175:G:H2'	1:2:176:G:H8	1.75	0.51
3:6:2:U:O2	18:L:95:GLN:NE2	2.44	0.51
4:7:80:ALA:HB3	4:7:217:ILE:HD13	1.91	0.51
4:7:256:VAL:CG2	4:7:403:MET:HE2	2.41	0.51
4:7:277:ILE:CA	14:H:171:ASN:CG	2.84	0.51
6:9:128:VAL:HG12	6:9:132:LYS:HE2	1.93	0.51
7:A:948:PRO:HD2	7:A:1455:TRP:HB2	1.92	0.51
7:A:1005:ILE:HG22	7:A:1009:MET:HE2	1.93	0.51
7:A:2327:SER:CB	8:B:1078:MET:CE	2.88	0.51
8:B:1519:ARG:NH1	8:B:1521:VAL:O	2.44	0.51
8:B:1979:VAL:HG11	8:B:1985:ILE:HG23	1.92	0.51
10:D:90:TYR:O	10:D:94:ASP:N	2.42	0.51
14:H:494:LEU:CD2	14:H:551:PHE:CZ	2.94	0.51
20:N:267:PHE:HB2	21:O:785:GLN:HG2	1.93	0.51
24:S:417:VAL:HB	24:S:454:ASN:HD22	1.75	0.51
4:7:383:ASN:CG	4:7:384:ASP:N	2.58	0.51
7:A:1067:MET:SD	27:V:413:LYS:CD	2.99	0.51
7:A:1434:LYS:HZ3	27:V:403:LYS:HD3	1.72	0.51
8:B:512:VAL:HA	8:B:515:MET:HE2	1.93	0.51
8:B:792:VAL:HG12	8:B:796:LEU:HD13	1.92	0.51
8:B:1127:CYS:SG	8:B:1129:LEU:HB2	2.51	0.51
9:C:471:ASP:N	9:C:471:ASP:OD1	2.44	0.51
14:H:628:ILE:HA	14:H:640:THR:HG21	1.93	0.51
16:J:195:LYS:HZ3	16:J:490:ARG:HH21	1.58	0.51
29:Y:39:ASP:HB3	29:Y:55:ILE:HD12	1.93	0.51
4:7:383:ASN:OD1	4:7:384:ASP:N	2.38	0.51
5:8:74:ILE:HD13	5:8:120:GLU:HG3	1.93	0.51
7:A:1946:ASN:HD22	7:A:1986:LEU:HD11	1.75	0.51
8:B:424:ALA:HB1	8:B:935:LEU:HD11	1.93	0.51
8:B:544:MET:HG3	8:B:817:TRP:CE2	2.45	0.51
8:B:1601:LEU:HD23	8:B:1604:LEU:HD12	1.91	0.51
9:C:676:ALA:HB2	9:C:815:VAL:HB	1.92	0.51
32:c:125:ALA:HB2	32:c:150:ALA:HB3	1.93	0.51
33:n:2:SER:OG	33:n:3:ILE:N	2.43	0.51
7:A:265:THR:OG1	7:A:328:HIS:O	2.29	0.51
10:D:106:ASP:CG	36:r:75:ARG:CD	2.80	0.51
13:G:107:LYS:O	13:G:110:TRP:HB3	2.11	0.51
7:A:2073:TRP:HH2	7:A:2310:ARG:NH1	2.09	0.50
8:B:530:THR:C	8:B:531:ILE:HG13	2.36	0.50
8:B:1135:LEU:HD23	8:B:1136:PRO:HD2	1.92	0.50
9:C:700:ILE:O	9:C:740:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:200:GLU:OE2	44:z:95:THR:OG1	2.29	0.50
28:W:81:GLU:HA	28:W:108:PRO:HB3	1.93	0.50
39:j:57:LYS:HB2	39:j:66:VAL:HG23	1.93	0.50
33:n:40:ASN:HD22	33:n:65:GLY:H	1.57	0.50
42:t:108:TYR:O	42:t:112:ALA:N	2.43	0.50
7:A:1732:LYS:HG2	32:c:278:LEU:HA	1.93	0.50
8:B:1351:PRO:O	8:B:1354:SER:OG	2.29	0.50
8:B:1418:LEU:O	8:B:1421:LYS:HG2	2.11	0.50
8:B:1982:VAL:O	8:B:1986:MET:HG2	2.11	0.50
9:C:644:LEU:O	9:C:649:SER:OG	2.29	0.50
16:J:356:LEU:HB2	16:J:366:VAL:HB	1.93	0.50
34:e:30:ARG:HH12	34:e:60:ASP:HB2	1.76	0.50
36:g:19:LEU:HD13	36:g:70:LEU:HB3	1.93	0.50
36:g:35:ASP:OD1	36:g:39:ASN:N	2.41	0.50
41:s:19:PHE:O	41:s:21:GLN:NE2	2.44	0.50
42:v:20:VAL:HG12	42:v:43:ASN:HD22	1.76	0.50
3:6:33:G:H1	15:I:13:C:H42	1.59	0.50
4:7:185:VAL:HG22	4:7:215:VAL:HB	1.94	0.50
4:7:322:GLU:HG3	4:7:327:ALA:HB3	1.94	0.50
8:B:406:ARG:HG2	8:B:954:LEU:HG	1.93	0.50
8:B:1271:VAL:HG12	8:B:1279:GLU:HB2	1.92	0.50
8:B:1636:PHE:CE1	8:B:1644:VAL:HG22	2.45	0.50
8:B:1890:LYS:NZ	8:B:1894:LEU:HD11	2.26	0.50
8:B:2064:TRP:CZ3	8:B:2110:SER:HB2	2.46	0.50
20:N:267:PHE:H	21:O:785:GLN:HG2	1.76	0.50
25:T:692:SER:HA	25:T:695:CYS:HB3	1.93	0.50
26:U:204:ASP:O	26:U:212:ARG:NH1	2.45	0.50
4:7:59:GLU:OE2	14:H:250:LYS:NZ	2.43	0.50
7:A:76:MET:HB3	7:A:85:LYS:HG2	1.94	0.50
7:A:597:LYS:O	7:A:600:ARG:HB3	2.11	0.50
33:d:79:ASN:HA	33:d:84:LYS:HE2	1.92	0.50
39:m:62:HIS:O	35:q:65:ARG:NH1	2.45	0.50
40:o:157:GLU:O	40:o:161:LYS:HB2	2.12	0.50
42:u:41:PRO:O	42:w:94:GLN:NE2	2.44	0.50
7:A:690:MET:HA	7:A:693:ILE:HG12	1.94	0.50
8:B:423:MET:HE1	8:B:877:GLN:CG	2.40	0.50
9:C:86:THR:HG21	16:J:237:LYS:HE3	1.93	0.50
16:J:210:ILE:HG12	16:J:221:THR:HG22	1.93	0.50
21:O:59:LYS:O	21:O:91:ARG:NH1	2.44	0.50
25:T:265:TYR:CA	25:T:274:LYS:CB	2.80	0.50
40:o:286:GLY:HA3	40:o:316:TRP:HH2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:80:ASP:HA	42:t:83:ASP:HB2	1.93	0.50
3:6:24:A:N3	3:6:26:U:O2'	2.37	0.50
7:A:954:LYS:CE	27:V:409:ASN:OD1	2.59	0.50
7:A:983:LYS:HB3	7:A:986:GLU:HB2	1.93	0.50
8:B:1309:VAL:HA	8:B:1328:PHE:HE2	1.77	0.50
8:B:1872:ALA:HB2	8:B:1893:LEU:HD13	1.93	0.50
9:C:210:ASN:HB3	9:C:636:TYR:HB2	1.92	0.50
42:w:119:ARG:HA	42:w:122:LYS:HD2	1.92	0.50
2:5:12:U:H5'	7:A:224:THR:HG23	1.94	0.50
7:A:569:VAL:HG13	7:A:573:GLN:HB2	1.93	0.50
7:A:1776:ILE:HB	7:A:1858:PRO:HA	1.93	0.50
8:B:1081:MET:O	8:B:1085:THR:HG23	2.11	0.50
9:C:811:THR:HA	9:C:814:ARG:HG2	1.94	0.50
9:C:880:SER:O	9:C:880:SER:OG	2.28	0.50
14:H:166:ILE:O	14:H:170:ILE:HG12	2.11	0.50
14:H:294:ILE:HG22	14:H:298:LYS:HE3	1.94	0.50
40:o:301:GLY:O	40:o:559:HIS:NE2	2.39	0.50
2:5:22:U:OP1	9:C:160:ARG:NH1	2.45	0.50
7:A:1314:VAL:O	7:A:1318:THR:OG1	2.29	0.50
8:B:1100:LEU:HA	8:B:1108:THR:HG21	1.94	0.50
8:B:1534:HIS:CE1	8:B:1536:GLN:HB2	2.47	0.50
19:M:224:ASP:O	19:M:302:TRP:NE1	2.45	0.50
33:d:32:LEU:HD11	33:d:35:ALA:HB2	1.94	0.50
36:g:15:LYS:HE2	36:g:76:VAL:HA	1.94	0.50
40:o:428:ASP:OD2	40:o:431:ARG:NH1	2.40	0.50
42:u:19:PRO:HG3	42:u:51:GLN:HB3	1.92	0.50
7:A:299:ILE:HD12	9:C:920:PRO:HB2	1.94	0.50
7:A:1900:GLU:HG2	10:D:86:ARG:HG3	1.94	0.50
7:A:2073:TRP:CH2	7:A:2310:ARG:NH1	2.80	0.50
8:B:420:SER:HA	8:B:621:HIS:CD2	2.47	0.50
8:B:833:VAL:CG1	8:B:844:LEU:HB3	2.42	0.50
19:M:176:GLY:HA2	40:o:206:ALA:HB2	1.94	0.50
24:S:480:TYR:CE2	24:S:502:GLU:CA	2.95	0.50
32:c:122:ASN:ND2	32:c:133:CYS:SG	2.71	0.50
35:f:25:TRP:NE1	35:f:68:ASN:OD1	2.44	0.50
7:A:1045:GLY:HA2	7:A:1048:MET:HE2	1.92	0.49
8:B:1496:ASN:HD22	8:B:1763:ARG:NH1	2.09	0.49
8:B:1764:MET:HE1	8:B:1784:HIS:CD2	2.47	0.49
8:B:1890:LYS:HZ2	8:B:1894:LEU:HD11	1.77	0.49
21:O:750:ARG:HA	21:O:753:GLU:HB2	1.94	0.49
25:T:272:PHE:CB	26:U:356:VAL:CB	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:35:ASP:OD2	31:b:39:ASN:ND2	2.45	0.49
34:e:77:ILE:HG22	35:f:73:ARG:HB3	1.94	0.49
35:f:67:ASN:OD1	35:f:68:ASN:ND2	2.44	0.49
33:n:11:HIS:CB	40:o:259:GLN:O	2.60	0.49
41:s:77:GLN:O	41:s:79:ILE:N	2.45	0.49
42:u:43:ASN:O	42:u:45:GLN:NE2	2.45	0.49
2:5:24:G:OP1	2:5:58:U:O2'	2.29	0.49
7:A:83:HIS:NE2	15:I:16:G:N7	2.57	0.49
7:A:1782:ASP:OD2	7:A:1865:ARG:NH2	2.46	0.49
9:C:151:GLU:O	9:C:158:ARG:NH1	2.44	0.49
13:G:111:THR:O	13:G:112:LYS:OXT	2.30	0.49
14:H:636:LEU:HB3	14:H:639:LEU:HD13	1.93	0.49
20:N:69:VAL:HG11	20:N:351:LEU:HD21	1.94	0.49
25:T:511:LEU:HD12	25:T:543:ARG:HD2	1.92	0.49
38:i:72:ARG:HD2	40:o:74:PRO:HG3	1.94	0.49
40:o:404:ASP:HB3	40:o:407:SER:HB3	1.95	0.49
6:9:7:PHE:CE1	6:9:94:ILE:HG22	2.46	0.49
7:A:2303:GLU:CD	7:A:2303:GLU:H	2.19	0.49
9:C:829:GLU:HB2	9:C:907:VAL:HG13	1.94	0.49
10:D:111:LYS:HA	10:D:114:GLU:OE2	2.12	0.49
14:H:582:PHE:O	14:H:586:PHE:HB2	2.12	0.49
20:N:166:LEU:HD23	20:N:178:LEU:HD11	1.94	0.49
24:S:211:GLN:HB2	40:o:483:ASN:HD21	1.76	0.49
25:T:491:ALA:HB1	25:T:507:TYR:CE2	2.47	0.49
26:U:19:ASN:HB3	26:U:22:PHE:HB3	1.94	0.49
32:c:102:TYR:HB3	32:c:156:GLN:HE21	1.77	0.49
33:n:23:ASN:N	33:n:67:LYS:O	2.46	0.49
40:o:358:LEU:HD23	40:o:367:ILE:HB	1.94	0.49
42:v:85:VAL:HG13	42:v:86:MET:HE2	1.94	0.49
5:8:108:ARG:HG3	6:9:129:GLN:CB	2.36	0.49
7:A:601:GLN:HG2	7:A:640:PHE:HB2	1.92	0.49
7:A:1434:LYS:O	7:A:1439:ARG:NH2	2.42	0.49
7:A:1904:ASP:HB3	7:A:1908:LYS:HE2	1.93	0.49
7:A:2147:MET:O	7:A:2274:PRO:HD3	2.10	0.49
8:B:772:LEU:HD23	8:B:789:MET:HB2	1.94	0.49
9:C:250:ARG:NH2	9:C:450:GLU:OE2	2.45	0.49
28:W:17:ASN:HD21	28:W:21:ASP:HB2	1.77	0.49
32:c:135:GLU:OE1	32:c:138:ARG:NH1	2.46	0.49
42:v:123:GLU:O	42:v:127:ALA:N	2.44	0.49
1:2:47:U:O2'	1:2:48:A:H5'	2.12	0.49
7:A:1873:GLU:O	32:c:290:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1956:PRO:HD2	7:A:1960:THR:HG21	1.94	0.49
8:B:787:ALA:HA	8:B:794:ARG:HD3	1.94	0.49
8:B:1747:ASN:HB2	8:B:1809:ASP:HA	1.95	0.49
31:k:18:ARG:HG3	31:k:26:ILE:HG23	1.94	0.49
40:o:270:PRO:HB3	40:o:518:PRO:HB3	1.94	0.49
1:2:39:U:O4	40:o:493:ARG:NH1	2.46	0.49
5:8:125:LYS:HZ3	5:8:126:GLU:CG	2.25	0.49
6:9:9:LEU:HD22	6:9:66:ILE:HD11	1.93	0.49
7:A:1808:PHE:HB2	7:A:1817:LEU:HD11	1.95	0.49
7:A:2073:TRP:CD1	7:A:2073:TRP:C	2.91	0.49
7:A:2149:PRO:O	7:A:2160:PRO:HD3	2.13	0.49
8:B:1478:SER:HA	8:B:1481:ILE:HG22	1.93	0.49
8:B:1512:PHE:HB3	8:B:1514:PHE:CE2	2.48	0.49
9:C:256:CYS:SG	9:C:310:SER:OG	2.65	0.49
9:C:564:THR:HG21	9:C:576:ILE:HA	1.95	0.49
10:D:113:LEU:C	10:D:113:LEU:CD1	2.86	0.49
10:D:123:GLN:HB3	10:D:127:ARG:HH12	1.77	0.49
18:L:51:ARG:HH21	40:o:193:LEU:HD23	1.77	0.49
26:U:830:THR:HG22	26:U:865:LYS:HD2	1.94	0.49
31:b:71:LEU:HB2	33:d:73:LEU:HD11	1.93	0.49
34:e:62:GLU:OE1	34:e:71:ARG:NH1	2.40	0.49
7:A:245:LEU:HD13	7:A:426:LEU:HB3	1.93	0.49
7:A:425:PRO:HB2	7:A:428:LYS:HB2	1.95	0.49
7:A:652:LEU:HD23	7:A:655:LEU:HD23	1.94	0.49
7:A:857:ASN:N	7:A:857:ASN:OD1	2.46	0.49
7:A:1292:GLU:OE2	7:A:1317:TYR:OH	2.27	0.49
8:B:1566:ARG:O	8:B:1569:THR:HG22	2.13	0.49
27:V:394:ILE:C	27:V:1144:ARG:CA	2.85	0.49
28:W:107:ASP:OD1	28:W:134:TYR:OH	2.26	0.49
33:n:12:GLU:HA	40:o:259:GLN:HB2	1.93	0.49
41:s:177:LYS:O	41:s:181:MET:N	2.40	0.49
7:A:1210:LYS:HE2	14:H:468:ASP:HA	1.94	0.49
9:C:529:ARG:H	9:C:553:GLU:HB3	1.77	0.49
14:H:294:ILE:HD13	14:H:335:MET:C	2.37	0.49
14:H:494:LEU:HD21	14:H:551:PHE:CZ	2.46	0.49
20:N:214:ASP:OD1	20:N:214:ASP:N	2.46	0.49
20:N:251:LEU:HD23	20:N:291:CYS:HB3	1.95	0.49
24:S:196:ARG:HA	43:y:208:ILE:HD11	1.94	0.49
27:V:397:PRO:O	27:V:400:TRP:HB3	2.13	0.49
41:s:71:GLU:OE1	42:v:93:ARG:NH2	2.46	0.49
42:t:3:LEU:HD11	42:u:15:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:51:A:N7	40:o:275:TYR:CG	2.81	0.49
8:B:1559:VAL:HG22	8:B:1660:LEU:HB3	1.95	0.49
8:B:1982:VAL:HG13	8:B:1985:ILE:HD11	1.95	0.49
9:C:196:LYS:CE	33:d:14:GLU:HB2	2.37	0.49
9:C:342:ARG:HE	9:C:356:PHE:HB2	1.77	0.49
9:C:641:MET:HE2	9:C:655:VAL:HG22	1.95	0.49
9:C:856:HIS:ND1	9:C:856:HIS:O	2.46	0.49
10:D:109:PHE:CZ	33:n:59:GLU:HB2	2.48	0.49
14:H:152:LEU:HA	14:H:387:MET:SD	2.53	0.49
16:J:455:GLN:HG2	16:J:456:PRO:HD2	1.95	0.49
21:O:16:ASP:OD2	21:O:49:ARG:NH2	2.42	0.49
25:T:593:LYS:HE2	25:T:631:MET:HG3	1.95	0.49
34:e:48:ILE:HD11	34:e:59:ASP:HB2	1.94	0.49
33:n:23:ASN:OD1	33:n:69:ARG:NH2	2.42	0.49
7:A:723:ASN:OD1	7:A:785:LYS:NZ	2.38	0.49
8:B:725:VAL:HG12	8:B:727:SER:H	1.77	0.49
8:B:1329:ASN:O	8:B:1333:THR:HG23	2.12	0.49
28:W:115:LEU:HD22	28:W:142:VAL:HG22	1.95	0.49
35:f:11:LEU:HD13	35:f:36:VAL:HG11	1.95	0.49
38:i:23:ILE:HD13	38:i:139:VAL:HG12	1.95	0.49
40:o:208:PRO:HG2	40:o:213:GLN:HG2	1.95	0.49
40:o:386:ASP:OD2	40:o:387:LYS:NZ	2.46	0.49
34:p:32:GLN:N	34:p:88:GLN:O	2.44	0.49
35:q:11:LEU:HD13	35:q:36:VAL:HG11	1.93	0.49
4:7:70:LYS:O	4:7:74:LYS:HG3	2.13	0.48
5:8:125:LYS:HZ3	5:8:126:GLU:HG3	1.78	0.48
7:A:1555:LEU:HD22	7:A:1560:ILE:HD12	1.95	0.48
9:C:115:GLU:OE2	33:d:84:LYS:HG3	2.13	0.48
9:C:277:LYS:NZ	9:C:864:PRO:O	2.39	0.48
9:C:463:GLU:HA	9:C:466:SER:HB2	1.94	0.48
12:F:694:TYR:HA	12:F:709:ARG:O	2.13	0.48
14:H:294:ILE:HD13	14:H:335:MET:O	2.13	0.48
16:J:436:MET:HE3	16:J:438:LEU:HD11	1.94	0.48
17:K:265:ASP:HB2	43:y:230:THR:HB	1.95	0.48
19:M:75:SER:OG	19:M:80:VAL:O	2.31	0.48
40:o:484:GLN:HG2	40:o:503:LYS:HB3	1.95	0.48
40:o:565:LYS:HA	40:o:578:TRP:O	2.11	0.48
42:t:103:LEU:O	42:t:107:LEU:N	2.38	0.48
3:6:56:A:OP1	7:A:675:GLN:NE2	2.45	0.48
4:7:89:THR:HA	4:7:92:PHE:CE2	2.48	0.48
7:A:1119:ASP:OD1	7:A:1119:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:143:THR:OG1	48:C:1500:GTP:O2B	2.30	0.48
20:N:90:ILE:HB	20:N:105:LEU:HB2	1.95	0.48
24:S:296:ARG:HH22	43:y:172:HIS:CD2	2.31	0.48
28:W:73:ASN:HA	28:W:97:ASN:HB3	1.96	0.48
30:Z:329:LYS:HE3	30:Z:342:GLU:HG3	1.93	0.48
42:u:15:PRO:HG2	42:u:55:ILE:HB	1.95	0.48
1:2:48:A:C5	40:o:273:LYS:HE3	2.48	0.48
1:2:103:U:O2'	35:q:65:ARG:NH2	2.38	0.48
7:A:718:ARG:NH1	17:K:252:SER:OG	2.46	0.48
7:A:1559:GLY:HA3	7:A:1622:MET:HE3	1.95	0.48
8:B:1356:LYS:O	8:B:1359:CYS:HB2	2.13	0.48
9:C:609:LYS:HD2	9:C:648:TYR:HB3	1.96	0.48
17:K:192:ALA:O	40:o:142:SER:OG	2.27	0.48
38:i:87:HIS:ND1	38:i:89:ASP:OD1	2.46	0.48
31:k:14:ASP:OD2	31:k:32:LYS:NZ	2.44	0.48
40:o:233:LYS:NZ	40:o:355:TYR:OH	2.45	0.48
4:7:244:ASP:HB2	4:7:397:SER:HB2	1.95	0.48
7:A:1268:ILE:HG22	7:A:1368:LEU:HD21	1.95	0.48
7:A:1639:VAL:HG13	7:A:1717:ASN:HB3	1.95	0.48
7:A:2097:ILE:HD12	7:A:2099:GLU:HB2	1.94	0.48
9:C:375:GLU:HG2	9:C:379:LYS:HE3	1.94	0.48
9:C:496:VAL:O	9:C:547:GLY:N	2.41	0.48
28:W:34:ILE:HD11	28:W:54:ILE:HD13	1.95	0.48
6:9:99:ILE:CD1	6:9:101:PHE:HE1	2.27	0.48
7:A:841:LEU:HA	7:A:844:GLU:HG2	1.95	0.48
8:B:441:GLY:O	8:B:693:THR:N	2.36	0.48
8:B:1139:VAL:O	8:B:1143:ILE:HG23	2.14	0.48
8:B:1560:ILE:HG13	8:B:1658:ALA:HB2	1.96	0.48
20:N:133:VAL:HG21	20:N:169:THR:HG21	1.96	0.48
20:N:330:ILE:HG12	20:N:346:SER:HB3	1.96	0.48
7:A:1640:SER:OG	7:A:1641:ARG:N	2.46	0.48
7:A:1768:TYR:O	7:A:1771:LEU:HB2	2.13	0.48
8:B:837:GLU:HG2	8:B:1083:TYR:CZ	2.48	0.48
8:B:1616:GLY:HA2	8:B:1641:ILE:HG22	1.95	0.48
9:C:383:GLN:OE1	9:C:391:SER:OG	2.31	0.48
16:J:220:VAL:HG11	16:J:261:LEU:HD11	1.96	0.48
21:O:37:LEU:HD13	21:O:158:ARG:HD3	1.94	0.48
21:O:755:LEU:HD11	42:t:108:TYR:HB3	1.95	0.48
41:s:19:PHE:N	41:s:171:GLN:OE1	2.46	0.48
42:w:77:ALA:O	42:w:81:GLU:N	2.42	0.48
8:B:1066:PHE:CG	8:B:1085:THR:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:151:SER:O	14:H:155:GLN:HG3	2.13	0.48
25:T:661:ASP:HA	25:T:664:ALA:HB3	1.95	0.48
35:f:36:VAL:HG22	35:f:42:MET:HG2	1.96	0.48
33:n:40:ASN:ND2	33:n:65:GLY:H	2.11	0.48
35:q:66:CYS:SG	35:q:67:ASN:N	2.86	0.48
7:A:251:ASP:HB3	7:A:253:ASN:H	1.79	0.48
7:A:843:LEU:O	7:A:847:LYS:HB2	2.13	0.48
7:A:1067:MET:CB	27:V:413:LYS:CD	2.89	0.48
7:A:1386:TRP:HB3	27:V:410:VAL:HG23	1.91	0.48
7:A:1800:THR:HG21	15:I:98:U:H5'	1.96	0.48
8:B:493:LEU:HD11	8:B:515:MET:HB3	1.96	0.48
8:B:1476:TYR:O	8:B:1479:SER:HB3	2.13	0.48
14:H:330:LYS:C	14:H:333:GLN:HG3	2.38	0.48
26:U:790:TYR:OH	26:U:976:ASN:ND2	2.47	0.48
39:j:44:ILE:HG12	39:j:109:VAL:HG22	1.96	0.48
42:v:90:PHE:HD1	42:v:93:ARG:HH11	1.62	0.48
7:A:902:TYR:HB2	7:A:1242:ASN:HB3	1.96	0.48
7:A:2121:ARG:HA	7:A:2121:ARG:HD2	1.55	0.48
8:B:495:THR:HG22	8:B:497:GLU:H	1.77	0.48
8:B:1265:GLN:O	8:B:1265:GLN:HG2	2.13	0.48
9:C:121:ASP:HB3	33:d:76:MET:HB2	1.95	0.48
9:C:168:THR:HG22	9:C:184:THR:HB	1.96	0.48
9:C:276:TYR:CZ	14:H:324:HIS:CG	3.01	0.48
12:F:742:ASN:HB2	12:F:744:ILE:HD12	1.94	0.48
14:H:369:MET:HE3	14:H:369:MET:O	2.13	0.48
19:M:22:ILE:HD13	40:o:111:LEU:HD23	1.95	0.48
26:U:1355:ILE:HG21	26:U:1361:MET:HB2	1.96	0.48
36:g:7:PRO:HD3	36:g:36:PRO:HA	1.96	0.48
3:6:40:U:H2'	3:6:41:A:H8	1.79	0.48
8:B:496:ASP:CG	8:B:519:ARG:HH11	2.22	0.48
8:B:1839:LYS:O	8:B:1841:LYS:HE3	2.13	0.48
9:C:829:GLU:OE2	9:C:854:ARG:NH2	2.46	0.48
17:K:199:MET:HE3	17:K:199:MET:HB3	1.73	0.48
20:N:171:SER:OG	20:N:173:ASP:OD1	2.32	0.48
24:S:317:THR:O	24:S:321:GLU:N	2.47	0.48
40:o:121:ASN:HB3	40:o:124:MET:HG2	1.95	0.48
42:u:107:LEU:O	42:u:111:ASP:N	2.43	0.48
4:7:307:MET:HE2	4:7:319:ILE:CG2	2.44	0.47
5:8:77:VAL:HB	5:8:117:THR:HG22	1.95	0.47
7:A:146:SER:HB2	7:A:193:LEU:HD22	1.96	0.47
7:A:862:GLU:HG3	21:O:6:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:994:THR:HG22	8:B:1023:GLU:OE1	2.14	0.47
8:B:1359:CYS:HA	8:B:1362:PHE:CD2	2.49	0.47
8:B:1408:LEU:HD22	8:B:1425:ILE:HG22	1.95	0.47
8:B:2076:LEU:HD21	8:B:2079:ILE:HB	1.96	0.47
9:C:226:VAL:HA	9:C:254:THR:O	2.14	0.47
14:H:260:VAL:O	14:H:264:ILE:HG12	2.13	0.47
17:K:99:ASP:OD1	17:K:114:SER:OG	2.31	0.47
19:M:196:GLN:HE22	19:M:209:VAL:HG23	1.79	0.47
21:O:211:ASN:ND2	24:S:221:ASN:O	2.47	0.47
21:O:517:ASP:CB	25:T:532:LYS:NZ	2.77	0.47
38:i:6:PRO:O	38:i:37:LYS:NZ	2.47	0.47
40:o:158:GLU:HA	40:o:161:LYS:HB3	1.95	0.47
6:9:113:ASN:HA	6:9:118:PRO:HB3	1.95	0.47
7:A:583:ALA:HA	7:A:605:CYS:HB3	1.95	0.47
7:A:2252:LEU:HD23	7:A:2253:PRO:HD2	1.96	0.47
8:B:500:LEU:HD23	8:B:662:ALA:HA	1.95	0.47
8:B:1962:GLN:HE22	8:B:2014:TYR:HE1	1.61	0.47
16:J:354:ILE:HB	16:J:368:LEU:HB2	1.95	0.47
40:o:506:MET:HE2	40:o:506:MET:HB2	1.76	0.47
4:7:349:ILE:HG12	4:7:368:SER:HB3	1.95	0.47
7:A:2326:TYR:HE1	8:B:1071:LYS:NZ	2.11	0.47
8:B:969:LEU:HD12	8:B:985:GLY:HA2	1.96	0.47
8:B:972:TYR:HB2	8:B:979:PHE:HD1	1.79	0.47
9:C:304:LEU:O	9:C:437:HIS:NE2	2.39	0.47
9:C:731:SER:HB2	9:C:747:ASP:HB3	1.96	0.47
20:N:116:HIS:HB3	20:N:159:PRO:HD3	1.96	0.47
39:j:65:MET:HE1	39:j:109:VAL:HG21	1.96	0.47
39:m:29:LEU:HD23	39:m:32:LEU:HD12	1.95	0.47
34:p:63:GLU:O	34:p:71:ARG:HA	2.14	0.47
42:t:75:LEU:HD13	42:w:79:GLN:HG3	1.96	0.47
42:u:71:ILE:HA	42:u:74:ILE:HB	1.96	0.47
43:y:211:ILE:H	43:y:215:ASN:HD22	1.62	0.47
5:8:107:ASP:OD1	5:8:109:ARG:HG2	2.14	0.47
7:A:1066:GLN:CB	27:V:423:THR:O	2.62	0.47
7:A:1090:ARG:NH2	7:A:1092:ILE:O	2.47	0.47
7:A:1942:ALA:HB1	7:A:1986:LEU:HD23	1.96	0.47
14:H:352:ILE:HG22	14:H:353:ILE:HG13	1.95	0.47
18:L:107:GLN:OE1	18:L:109:ARG:NH1	2.43	0.47
19:M:150:LEU:HD13	19:M:213:LEU:HD23	1.95	0.47
21:O:192:ARG:NH2	21:O:197:GLU:OE2	2.46	0.47
32:c:124:GLY:HA3	32:c:149:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:79:GLN:HE21	42:v:28:ARG:HD2	1.79	0.47
2:5:11:U:O2'	7:A:217:ARG:NH2	2.47	0.47
7:A:679:SER:O	7:A:683:LEU:N	2.48	0.47
7:A:975:VAL:HB	7:A:1099:PHE:HB2	1.97	0.47
8:B:618:HIS:CD2	8:B:847:LEU:HD22	2.49	0.47
8:B:1408:LEU:HD23	8:B:1427:SER:HB2	1.95	0.47
9:C:222:SER:O	9:C:448:LYS:NZ	2.39	0.47
10:D:114:GLU:HG3	10:D:115:LYS:N	2.29	0.47
17:K:60:ASP:HB3	38:i:134:GLN:HA	1.97	0.47
20:N:223:ARG:NE	21:O:793:LEU:HD22	2.18	0.47
26:U:1237:ILE:O	26:U:1241:ILE:HG12	2.14	0.47
40:o:307:CYS:HB3	40:o:335:VAL:HG13	1.95	0.47
1:2:97:G:OP2	39:m:61:ARG:NH1	2.43	0.47
5:8:125:LYS:NZ	5:8:126:GLU:HG3	2.29	0.47
7:A:313:LYS:O	7:A:321:ASN:ND2	2.48	0.47
7:A:320:TYR:OH	9:C:881:PHE:O	2.26	0.47
7:A:699:GLU:HG2	16:J:372:LYS:HD3	1.96	0.47
7:A:769:LYS:HD3	7:A:1249:MET:HG2	1.97	0.47
7:A:2148:VAL:O	7:A:2150:GLN:HG2	2.14	0.47
8:B:1264:PRO:HB2	8:B:1265:GLN:OE1	2.15	0.47
8:B:1375:ARG:HG2	8:B:1448:ILE:HG22	1.97	0.47
8:B:1713:PHE:N	8:B:1713:PHE:CD1	2.82	0.47
9:C:82:GLN:HB2	16:J:231:TRP:HZ3	1.79	0.47
20:N:306:ASP:HA	40:o:143:LEU:HD22	1.96	0.47
35:f:63:LEU:N	39:j:109:VAL:O	2.43	0.47
1:2:18:U:N3	17:K:256:ASN:OD1	2.42	0.47
1:2:22:U:OP1	7:A:717:TRP:NE1	2.43	0.47
3:6:27:A:OP1	19:M:175:ARG:NH2	2.35	0.47
5:8:77:VAL:HB	5:8:117:THR:HG23	1.95	0.47
6:9:26:PHE:HA	6:9:35:ARG:O	2.14	0.47
7:A:184:ASP:OD1	7:A:184:ASP:N	2.36	0.47
7:A:257:LEU:HD22	7:A:314:ILE:HG22	1.95	0.47
7:A:881:ILE:HD11	7:A:917:ILE:HG22	1.97	0.47
7:A:893:GLU:HG2	7:A:1016:VAL:HB	1.96	0.47
7:A:954:LYS:HE3	27:V:409:ASN:OD1	2.14	0.47
7:A:1428:HIS:HB2	27:V:396:ASP:HB3	1.96	0.47
7:A:1552:GLN:HG2	7:A:1561:PHE:HB3	1.96	0.47
8:B:538:ILE:HG12	8:B:611:LEU:HB3	1.96	0.47
8:B:720:GLN:HG2	8:B:807:GLN:HA	1.96	0.47
9:C:101:LYS:NZ	9:C:103:THR:O	2.42	0.47
17:K:69:VAL:O	17:K:71:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:144:MET:HG3	21:O:149:LEU:HG	1.97	0.47
28:W:134:TYR:O	28:W:138:LYS:HB2	2.15	0.47
38:i:17:GLU:HB3	38:i:22:ILE:HG12	1.97	0.47
38:i:73:GLY:O	38:i:111:GLN:NE2	2.43	0.47
39:j:60:ASP:N	39:j:60:ASP:OD1	2.48	0.47
39:m:30:SER:O	39:m:34:GLN:N	2.45	0.47
40:o:218:GLU:HG2	40:o:222:LYS:HE3	1.96	0.47
41:s:189:VAL:HG21	42:v:131:LEU:HB3	1.96	0.47
1:2:20:G:OP1	7:A:686:ARG:NH2	2.48	0.47
4:7:225:ILE:HA	4:7:228:MET:HE3	1.96	0.47
7:A:362:ARG:HD2	14:H:337:GLU:OE1	2.13	0.47
7:A:664:HIS:HE1	17:K:214:ILE:HG22	1.80	0.47
8:B:729:LYS:HD2	8:B:729:LYS:HA	1.72	0.47
19:M:188:ASP:OD1	19:M:188:ASP:N	2.43	0.47
24:S:250:GLN:NE2	24:S:253:GLU:OE2	2.48	0.47
31:b:71:LEU:HB3	33:d:71:LEU:HB2	1.96	0.47
7:A:50:LYS:HB3	7:A:53:PHE:HB2	1.96	0.47
7:A:1595:GLN:NE2	32:c:270:ASP:O	2.48	0.47
7:A:1832:ARG:NH2	15:I:2:U:OP1	2.47	0.47
8:B:1024:PHE:HB3	8:B:1027:ILE:HD12	1.96	0.47
8:B:1113:ASN:O	8:B:1117:MET:HG3	2.14	0.47
8:B:2104:TYR:HB2	8:B:2122:PHE:CZ	2.50	0.47
9:C:128:LEU:HD12	33:d:16:HIS:CE1	2.50	0.47
16:J:305:THR:OG1	16:J:315:TRP:NE1	2.44	0.47
19:M:33:TYR:OH	40:o:139:LEU:O	2.32	0.47
19:M:94:ILE:HD12	19:M:202:TYR:HA	1.96	0.47
20:N:263:ASP:O	20:N:272:ARG:NH1	2.44	0.47
40:o:239:THR:HG21	40:o:364:GLY:HA3	1.97	0.47
40:o:536:ASP:HB2	40:o:543:TYR:CD2	2.45	0.47
34:p:36:TYR:N	34:p:83:ASN:O	2.45	0.47
42:t:128:ARG:O	42:t:132:ALA:N	2.48	0.47
6:9:7:PHE:HE1	6:9:94:ILE:HG22	1.80	0.47
7:A:1630:LEU:HD11	7:A:1696:PRO:HG3	1.97	0.47
8:B:420:SER:HB3	8:B:622:ASP:HA	1.97	0.47
8:B:772:LEU:H	8:B:772:LEU:HD12	1.79	0.47
8:B:1725:GLU:OE1	8:B:1763:ARG:NE	2.46	0.47
8:B:2109:MET:HG3	8:B:2117:ASP:CG	2.39	0.47
14:H:530:LYS:HD2	14:H:567:CYS:CB	2.43	0.47
36:g:47:GLU:OE2	36:g:55:ASN:ND2	2.43	0.47
34:p:44:GLU:O	34:p:61:ALA:HA	2.15	0.47
1:2:46:U:C2	15:I:85:G:N2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:9:LEU:HD12	6:9:92:ILE:HG12	1.95	0.46
7:A:356:ILE:O	14:H:344:LYS:CE	2.62	0.46
7:A:1687:TYR:O	7:A:1693:SER:OG	2.30	0.46
7:A:2335:ALA:HA	8:B:570:THR:O	2.15	0.46
8:B:1324:LYS:NZ	8:B:1400:ARG:HH12	2.14	0.46
8:B:1395:GLU:HA	8:B:1399:ASP:HB2	1.98	0.46
9:C:619:THR:HA	9:C:628:VAL:O	2.15	0.46
9:C:774:THR:HG22	9:C:784:ILE:HD12	1.97	0.46
21:O:517:ASP:CB	25:T:532:LYS:HZ1	2.28	0.46
22:P:68:ARG:HD3	22:P:72:ARG:HH11	1.80	0.46
42:t:15:PRO:HB2	42:t:55:ILE:HD12	1.97	0.46
42:v:97:GLN:O	42:v:101:GLN:NE2	2.48	0.46
42:w:80:ASP:HA	42:w:83:ASP:HB2	1.96	0.46
1:2:51:A:H62	40:o:275:TYR:HB2	1.80	0.46
6:9:56:LYS:O	6:9:60:GLU:HG2	2.15	0.46
7:A:362:ARG:CD	14:H:337:GLU:OE1	2.64	0.46
7:A:687:ALA:HA	7:A:690:MET:HG2	1.97	0.46
7:A:965:VAL:O	7:A:974:ASN:ND2	2.45	0.46
8:B:506:GLY:O	8:B:682:PRO:HG3	2.15	0.46
8:B:969:LEU:CD1	8:B:985:GLY:HA2	2.45	0.46
16:J:328:GLY:O	16:J:355:ARG:NH2	2.49	0.46
16:J:435:THR:HG23	16:J:451:HIS:HD2	1.80	0.46
20:N:267:PHE:N	21:O:785:GLN:HG2	2.31	0.46
21:O:19:LEU:HD23	21:O:54:LEU:HD22	1.98	0.46
26:U:509:ARG:HG3	26:U:549:ILE:HD12	1.97	0.46
39:j:87:SER:OG	39:j:88:LYS:N	2.47	0.46
40:o:441:SER:HA	40:o:456:ILE:O	2.16	0.46
42:u:4:ILE:HA	42:u:12:PRO:HD3	1.97	0.46
1:2:161:U:O2	1:2:163:G:N2	2.49	0.46
4:7:269:CYS:SG	4:7:297:MET:HE1	2.56	0.46
5:8:82:GLU:HG3	5:8:112:TYR:HB3	1.96	0.46
5:8:109:ARG:CG	5:8:110:THR:N	2.77	0.46
6:9:122:ARG:HG2	6:9:122:ARG:NH1	2.30	0.46
7:A:142:SER:HA	7:A:242:ALA:HB2	1.96	0.46
7:A:938:PRO:HB2	7:A:1071:PHE:HA	1.97	0.46
7:A:1248:LEU:HD21	7:A:1295:ILE:HD13	1.98	0.46
8:B:828:ILE:HD13	8:B:849:ILE:HG22	1.96	0.46
14:H:531:GLU:OE1	14:H:531:GLU:HA	2.16	0.46
17:K:52:PRO:HG2	17:K:71:GLN:HG2	1.97	0.46
41:s:164:ASN:O	41:s:168:LYS:N	2.39	0.46
1:2:165:A:N6	29:Y:86:THR:OG1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:750:TRP:HH2	7:A:781:ARG:HB3	1.81	0.46
7:A:2268:LEU:CD2	8:B:1261:PRO:CB	2.94	0.46
8:B:1320:LEU:HA	8:B:1400:ARG:NH1	2.30	0.46
9:C:295:ASP:N	9:C:295:ASP:OD1	2.48	0.46
14:H:228:GLN:HG2	14:H:229:ILE:N	2.29	0.46
28:W:110:ALA:HA	28:W:139:VAL:HG13	1.97	0.46
4:7:105:ARG:HH22	9:C:855:GLY:C	2.22	0.46
7:A:2121:ARG:O	7:A:2154:HIS:HA	2.16	0.46
8:B:1948:MET:HE3	8:B:1955:SER:N	2.31	0.46
9:C:137:HIS:HA	9:C:238:ASN:HB3	1.98	0.46
13:G:80:LYS:NZ	32:c:184:GLU:OE2	2.41	0.46
14:H:234:LEU:HD21	14:H:263:LEU:HD13	1.96	0.46
29:Y:16:ASP:OD1	29:Y:16:ASP:N	2.46	0.46
34:e:61:ALA:O	34:e:74:LEU:N	2.46	0.46
39:j:48:ASN:OD1	39:j:48:ASN:N	2.41	0.46
34:p:17:PRO:HG2	36:r:39:ASN:HB2	1.96	0.46
42:t:12:PRO:HB3	42:t:26:GLU:HA	1.97	0.46
42:u:39:THR:OG1	42:u:40:ASP:N	2.48	0.46
42:w:34:ILE:HD11	42:w:47:LEU:HD23	1.98	0.46
7:A:1330:MET:HB2	7:A:1330:MET:HE3	1.84	0.46
8:B:591:GLU:H	8:B:591:GLU:HG2	1.42	0.46
8:B:967:ASN:ND2	8:B:995:ASN:O	2.48	0.46
14:H:544:LEU:HD11	14:H:578:SER:HB2	1.96	0.46
26:U:362:ARG:HH22	26:U:405:GLU:CD	2.24	0.46
41:s:165:TRP:HA	41:s:168:LYS:HB2	1.98	0.46
42:v:108:TYR:O	42:v:112:ALA:N	2.41	0.46
7:A:351:TYR:HA	9:C:270:PRO:HG3	1.97	0.46
8:B:531:ILE:HD12	8:B:531:ILE:O	2.16	0.46
24:S:505:ALA:CB	25:T:574:GLU:OE2	2.63	0.46
26:U:1284:LEU:HD23	26:U:1310:PHE:CE1	2.51	0.46
31:b:48:PHE:HA	31:b:63:GLU:HA	1.98	0.46
34:e:78:MET:HE2	35:f:11:LEU:HD11	1.98	0.46
42:t:5:CYS:HB2	42:t:12:PRO:HG3	1.96	0.46
42:w:33:TYR:HA	42:w:36:GLU:HB2	1.96	0.46
42:w:91:THR:O	42:w:95:GLN:NE2	2.49	0.46
7:A:2117:ILE:H	7:A:2117:ILE:HG12	1.64	0.46
8:B:593:TRP:CD1	8:B:631:LEU:HD22	2.37	0.46
8:B:1329:ASN:HB2	8:B:1330:PRO:HD2	1.98	0.46
9:C:270:PRO:HD2	9:C:273:ASP:HB2	1.98	0.46
9:C:561:LYS:H	9:C:561:LYS:HG3	1.48	0.46
9:C:603:MET:O	9:C:607:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:246:ILE:HG13	16:J:269:GLN:HE22	1.80	0.46
20:N:217:ILE:HB	20:N:231:MET:HB2	1.98	0.46
21:O:28:LYS:HE3	21:O:28:LYS:HB2	1.68	0.46
26:U:790:TYR:HB3	26:U:792:TYR:CE2	2.51	0.46
34:p:63:GLU:HG3	34:p:74:LEU:HD11	1.98	0.46
41:s:195:ILE:O	41:s:198:THR:OG1	2.26	0.46
3:6:40:U:H3	15:I:7:G:H22	1.63	0.46
5:8:131:MET:HE1	5:8:148:TRP:CD1	2.51	0.46
7:A:997:LEU:HD13	7:A:1009:MET:HE3	1.98	0.46
7:A:1208:THR:HG21	14:H:553:HIS:HE1	1.79	0.46
8:B:1328:PHE:HB2	8:B:1333:THR:HG22	1.97	0.46
21:O:30:GLN:HB3	21:O:33:ARG:HB3	1.98	0.46
35:f:23:LEU:HD12	35:f:27:MET:HB2	1.98	0.46
38:i:5:PRO:HD2	38:i:37:LYS:HE3	1.97	0.46
38:i:155:ASP:OD1	38:i:155:ASP:N	2.46	0.46
42:u:108:TYR:HA	42:u:111:ASP:HB2	1.98	0.46
42:w:123:GLU:HA	42:w:126:ALA:HB3	1.97	0.46
7:A:445:VAL:HG21	11:E:-9:C:H2'	1.98	0.46
8:B:669:PRO:HA	8:B:673:LEU:HB2	1.97	0.46
8:B:1018:PHE:O	8:B:1021:SER:OG	2.32	0.46
8:B:1760:LEU:O	8:B:1764:MET:HG3	2.15	0.46
19:M:24:CYS:HB2	19:M:27:CYS:SG	2.56	0.46
21:O:218:LYS:NZ	24:S:270:ASP:OD1	2.49	0.46
29:Y:15:ASN:HD22	29:Y:18:ILE:HG23	1.81	0.46
32:c:102:TYR:HD1	32:c:156:GLN:HB3	1.81	0.46
33:d:19:THR:O	33:d:72:ILE:N	2.43	0.46
31:k:47:GLU:OE2	31:k:65:ARG:NH1	2.49	0.46
42:w:124:VAL:HG12	42:w:128:ARG:HH21	1.81	0.46
1:2:100:U:O2	33:n:40:ASN:ND2	2.49	0.45
7:A:1682:ALA:O	7:A:1686:ASP:HB2	2.16	0.45
7:A:2169:LEU:HD21	7:A:2272:MET:HG3	1.99	0.45
7:A:2310:ARG:HH11	7:A:2310:ARG:CG	2.28	0.45
8:B:728:ARG:NH2	8:B:786:HIS:HB2	2.31	0.45
9:C:311:SER:HB3	9:C:316:ILE:HB	1.98	0.45
9:C:678:THR:HG23	9:C:680:ASN:H	1.82	0.45
16:J:416:ILE:HA	16:J:431:ALA:HA	1.98	0.45
17:K:235:ARG:NH1	17:K:241:GLU:OE1	2.41	0.45
24:S:196:ARG:NH2	43:y:204:ASP:O	2.49	0.45
24:S:454:ASN:HA	24:S:457:ILE:HG12	1.96	0.45
25:T:599:TYR:HA	25:T:602:LEU:HG	1.99	0.45
26:U:444:TYR:CZ	26:U:446:GLY:HA2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:W:65:ARG:O	28:W:67:LYS:NZ	2.49	0.45
36:g:35:ASP:OD2	36:g:39:ASN:ND2	2.49	0.45
42:w:123:GLU:O	42:w:127:ALA:N	2.50	0.45
1:2:151:C:H2'	1:2:152:G:C8	2.51	0.45
4:7:179:ARG:HH22	9:C:906:ILE:HG13	1.80	0.45
4:7:265:PHE:CZ	4:7:296:LYS:HG2	2.51	0.45
7:A:566:LEU:O	13:G:72:ARG:NH1	2.49	0.45
7:A:2333:LEU:CG	8:B:545:ARG:HG3	2.38	0.45
8:B:598:ARG:HA	8:B:907:LEU:HD21	1.98	0.45
8:B:881:SER:HA	8:B:886:GLN:HB2	1.99	0.45
9:C:105:MET:HE3	9:C:105:MET:HB3	1.83	0.45
14:H:234:LEU:CD2	14:H:263:LEU:HD13	2.46	0.45
14:H:515:CYS:HB2	14:H:559:SER:HB3	1.98	0.45
24:S:202:GLU:HB3	24:S:205:LEU:HB3	1.99	0.45
24:S:250:GLN:HA	24:S:253:GLU:HG2	1.98	0.45
34:p:88:GLN:HG3	36:r:57:ILE:HB	1.99	0.45
42:v:20:VAL:HG11	42:v:45:GLN:HB2	1.98	0.45
1:2:51:A:N6	40:o:275:TYR:HB2	2.31	0.45
4:7:277:ILE:CB	14:H:171:ASN:CG	2.88	0.45
7:A:2320:LEU:HD21	7:A:2322:GLU:CD	2.41	0.45
8:B:418:GLN:HE22	8:B:842:THR:HG22	1.81	0.45
8:B:1127:CYS:HA	8:B:1128:PRO:HD3	1.83	0.45
8:B:1542:MET:C	8:B:1545:PRO:HD2	2.42	0.45
15:I:19:G:OP2	19:M:64:ARG:NH1	2.43	0.45
16:J:267:ASP:HB3	16:J:269:GLN:HG2	1.97	0.45
17:K:261:THR:H	43:y:215:ASN:ND2	2.14	0.45
19:M:40:LYS:HA	19:M:53:THR:HG23	1.99	0.45
21:O:263:ASP:OD2	43:y:199:ARG:NH2	2.36	0.45
25:T:329:LEU:CB	26:U:352:ALA:O	2.64	0.45
25:T:516:ALA:HA	25:T:520:ILE:HD11	1.98	0.45
26:U:748:ARG:NH1	26:U:780:GLU:OE1	2.43	0.45
26:U:987:TYR:CZ	26:U:991:MET:HE3	2.51	0.45
35:f:24:LYS:HA	35:f:70:LEU:HD12	1.97	0.45
42:t:75:LEU:O	42:t:79:GLN:N	2.45	0.45
4:7:148:GLU:OE2	4:7:152:LYS:HE2	2.17	0.45
7:A:741:ARG:HH22	16:J:464:GLY:HA3	1.81	0.45
7:A:2074:ARG:O	7:A:2078:ILE:HD13	2.17	0.45
7:A:2279:TRP:CD1	7:A:2279:TRP:H	2.35	0.45
8:B:846:ALA:O	8:B:849:ILE:HG13	2.17	0.45
9:C:224:GLY:HA3	9:C:438:ILE:HG23	1.99	0.45
9:C:276:TYR:HH	14:H:324:HIS:CG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:796:GLU:HA	21:O:799:LYS:HB2	1.97	0.45
25:T:555:ASP:N	25:T:555:ASP:OD1	2.46	0.45
38:i:142:VAL:HG22	38:i:157:VAL:HG11	1.99	0.45
37:l:25:VAL:HG22	37:l:45:MET:HG3	1.99	0.45
36:r:69:MET:HE3	36:r:69:MET:HB3	1.74	0.45
42:w:28:ARG:O	42:w:32:LYS:NZ	2.47	0.45
7:A:941:LYS:HD2	7:A:941:LYS:HA	1.50	0.45
7:A:1491:LYS:O	7:A:1710:ASN:ND2	2.49	0.45
7:A:2196:HIS:HB3	7:A:2230:LEU:HD11	1.98	0.45
8:B:1314:ASN:OD1	8:B:1317:PHE:N	2.47	0.45
8:B:1532:ILE:HG21	8:B:1537:THR:HB	1.97	0.45
9:C:241:ARG:HD2	9:C:900:VAL:HG11	1.97	0.45
16:J:214:PRO:HG3	16:J:256:THR:HG22	1.98	0.45
21:O:170:LYS:HA	21:O:170:LYS:HD3	1.81	0.45
24:S:184:PRO:HB2	44:z:104:LEU:HD21	1.99	0.45
28:W:104:GLY:O	28:W:107:ASP:HB2	2.16	0.45
31:b:30:THR:N	31:b:43:CYS:O	2.48	0.45
2:5:53:U:O2'	22:P:36:PRO:O	2.33	0.45
7:A:794:TYR:OH	7:A:989:ASP:OD1	2.29	0.45
7:A:943:ALA:O	7:A:1437:ARG:NE	2.39	0.45
7:A:1670:ASP:N	7:A:1670:ASP:OD1	2.47	0.45
8:B:419:GLY:C	8:B:421:HIS:H	2.25	0.45
8:B:728:ARG:HH21	8:B:787:ALA:N	2.13	0.45
8:B:1228:VAL:HG11	8:B:1264:PRO:HD2	1.97	0.45
8:B:1349:GLY:HA2	8:B:1491:SER:O	2.16	0.45
9:C:150:ILE:O	9:C:154:HIS:N	2.39	0.45
14:H:399:LYS:O	14:H:403:LYS:HG3	2.17	0.45
14:H:517:LEU:HD11	23:R:24:SER:HB2	1.99	0.45
17:K:251:ILE:HG21	17:K:262:ILE:HG21	1.98	0.45
19:M:22:ILE:H	19:M:82:GLN:HE21	1.65	0.45
28:W:18:ALA:HB1	29:Y:40:ILE:HG12	1.97	0.45
42:v:40:ASP:N	42:v:45:GLN:O	2.47	0.45
4:7:82:SER:O	4:7:219:ALA:HA	2.17	0.45
4:7:275:LEU:CD2	4:7:330:VAL:CG2	2.94	0.45
7:A:1009:MET:HB3	7:A:1040:ILE:HD11	1.99	0.45
8:B:421:HIS:NE2	8:B:875:GLU:OE1	2.50	0.45
8:B:665:LEU:HB2	8:B:667:VAL:HG23	1.99	0.45
8:B:833:VAL:HG11	8:B:844:LEU:HB3	1.98	0.45
8:B:1439:TRP:CD2	8:B:1477:ILE:HD13	2.52	0.45
8:B:1775:GLY:HA3	8:B:1780:HIS:CD2	2.51	0.45
9:C:560:VAL:HG12	9:C:561:LYS:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:491:ALA:HB1	25:T:507:TYR:HE2	1.80	0.45
25:T:624:GLU:HB3	25:T:627:GLN:HB2	1.97	0.45
37:h:21:ASN:ND2	37:h:23:THR:OG1	2.50	0.45
1:2:51:A:H61	40:o:564:SER:HB2	1.82	0.45
7:A:65:HIS:ND1	7:A:120:TYR:OH	2.45	0.45
7:A:240:ARG:HG2	32:c:137:PRO:HB2	1.99	0.45
7:A:1095:ILE:HD12	7:A:1097:ILE:HD11	1.97	0.45
7:A:1900:GLU:OE1	7:A:1951:LYS:NZ	2.45	0.45
7:A:2333:LEU:CA	8:B:545:ARG:HH11	2.04	0.45
8:B:826:VAL:O	8:B:868:ILE:HD12	2.16	0.45
12:F:686:ILE:HG12	12:F:715:PRO:HB3	1.99	0.45
16:J:464:GLY:O	16:J:482:ALA:N	2.50	0.45
26:U:1021:LEU:HD22	26:U:1021:LEU:HA	1.84	0.45
43:y:192:LYS:HA	43:y:195:LYS:HE2	1.99	0.45
7:A:150:MET:HE3	7:A:572:PHE:HZ	1.82	0.45
7:A:834:HIS:HA	7:A:837:LYS:HE3	1.99	0.45
7:A:975:VAL:HG22	7:A:1177:VAL:HG22	1.99	0.45
7:A:1434:LYS:HZ3	27:V:403:LYS:CD	2.29	0.45
7:A:2237:TRP:HZ2	7:A:2248:PRO:HB2	1.81	0.45
7:A:2326:TYR:CE1	8:B:1071:LYS:NZ	2.80	0.45
8:B:791:ARG:HH21	8:B:794:ARG:NH1	2.13	0.45
8:B:1028:THR:OG1	8:B:1029:VAL:N	2.49	0.45
8:B:1128:PRO:HG2	8:B:1150:PHE:CD2	2.52	0.45
8:B:1732:MET:HE3	8:B:1788:LEU:CD2	2.47	0.45
14:H:294:ILE:HD12	14:H:335:MET:HB3	1.98	0.45
15:I:19:G:H21	19:M:196:GLN:HG3	1.81	0.45
21:O:216:PHE:HB2	24:S:267:ARG:HD2	1.99	0.45
21:O:721:LEU:O	21:O:725:GLN:N	2.39	0.45
28:W:37:LEU:HD23	28:W:61:PRO:HD2	1.99	0.45
28:W:70:LEU:HA	28:W:94:ILE:HB	1.98	0.45
29:Y:8:THR:HG22	29:Y:55:ILE:HG23	1.98	0.45
33:d:38:ASN:OD1	33:d:40:ASN:ND2	2.50	0.45
42:u:120:LEU:HD22	42:w:120:LEU:HB3	1.99	0.45
7:A:1526:LEU:HA	7:A:1529:ILE:HD12	1.98	0.45
7:A:2070:LYS:HD3	7:A:2070:LYS:HA	1.67	0.45
7:A:2315:LEU:HA	7:A:2315:LEU:HD13	1.83	0.45
8:B:822:PRO:HG2	8:B:859:PRO:HD3	1.99	0.45
9:C:276:TYR:OH	14:H:324:HIS:HB3	2.17	0.45
16:J:457:GLY:O	22:P:212:ASN:HB3	2.17	0.45
17:K:152:GLU:HA	17:K:155:VAL:HG22	1.99	0.45
17:K:195:ARG:HH11	19:M:34:ILE:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:749:LEU:O	21:O:753:GLU:N	2.45	0.45
32:c:346:ASP:OD1	32:c:346:ASP:N	2.50	0.45
34:e:36:TYR:N	34:e:83:ASN:O	2.47	0.45
39:m:43:LEU:HD23	39:m:110:LEU:HD21	1.98	0.45
1:2:151:C:H2'	1:2:152:G:H8	1.82	0.44
3:6:14:C:H2'	3:6:15:A:H8	1.82	0.44
6:9:7:PHE:HE2	6:9:62:LEU:HD23	1.82	0.44
7:A:203:VAL:HG13	7:A:206:TRP:CH2	2.52	0.44
8:B:612:ILE:HD11	8:B:648:LEU:HG	1.98	0.44
8:B:1969:GLU:H	8:B:1969:GLU:HG3	1.58	0.44
9:C:343:LEU:HD13	9:C:373:ILE:HD11	1.99	0.44
24:S:266:GLU:OE2	24:S:301:ARG:NH1	2.50	0.44
37:h:15:VAL:HG12	37:h:71:PRO:HD3	1.99	0.44
37:h:79:LEU:HD12	37:h:80:LEU:HG	1.98	0.44
40:o:188:ASN:OD1	40:o:188:ASN:N	2.48	0.44
42:u:6:SER:N	42:u:24:VAL:O	2.47	0.44
42:v:96:LEU:HD23	42:v:96:LEU:HA	1.84	0.44
3:6:19:C:H1'	18:L:95:GLN:HG3	1.99	0.44
4:7:267:THR:O	4:7:271:LEU:HD13	2.17	0.44
7:A:1427:ARG:HB2	27:V:400:TRP:CG	2.51	0.44
7:A:1560:ILE:HG21	7:A:1573:LEU:HD13	1.99	0.44
7:A:2073:TRP:CZ3	7:A:2313:HIS:CE1	3.05	0.44
7:A:2222:SER:OG	7:A:2223:CYS:N	2.50	0.44
8:B:535:ASP:OD1	8:B:535:ASP:N	2.50	0.44
8:B:1733:HIS:CD2	8:B:1792:THR:HG23	2.52	0.44
9:C:103:THR:HG22	9:C:171:LEU:HB3	2.00	0.44
9:C:441:PRO:O	9:C:445:ALA:HB2	2.18	0.44
9:C:481:MET:HB3	9:C:481:MET:HE3	1.73	0.44
9:C:850:LEU:HD23	9:C:875:ILE:HD12	1.99	0.44
13:G:79:LYS:O	13:G:88:ARG:NH2	2.50	0.44
20:N:149:GLY:O	20:N:177:LYS:NZ	2.43	0.44
33:d:25:GLY:HA2	33:d:69:ARG:HH12	1.83	0.44
39:m:30:SER:O	39:m:33:THR:HB	2.18	0.44
5:8:123:THR:OG1	5:8:126:GLU:CG	2.66	0.44
7:A:2284:MET:HE1	7:A:2311:PRO:HG3	1.99	0.44
8:B:692:ILE:HG22	8:B:694:GLU:H	1.83	0.44
8:B:1534:HIS:HE1	8:B:1536:GLN:HB2	1.81	0.44
8:B:1889:VAL:O	8:B:1893:LEU:HG	2.17	0.44
8:B:2027:ASP:OD1	8:B:2027:ASP:N	2.49	0.44
9:C:92:PRO:O	9:C:95:LYS:NZ	2.49	0.44
9:C:762:VAL:HG11	9:C:803:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:155:ASN:O	20:N:290:ARG:NH2	2.51	0.44
21:O:142:ILE:HB	24:S:181:ASN:HB3	2.00	0.44
31:k:67:LEU:HB3	33:n:72:ILE:HG12	2.00	0.44
33:n:14:GLU:HG2	40:o:259:GLN:HG2	1.99	0.44
40:o:228:LYS:HD2	40:o:228:LYS:HA	1.83	0.44
40:o:443:ARG:NH1	40:o:452:ASP:OD2	2.46	0.44
36:r:32:ARG:HB3	36:r:41:VAL:HG12	1.98	0.44
41:s:197:ARG:NH2	42:t:137:GLN:OE1	2.50	0.44
2:5:12:U:OP1	7:A:224:THR:OG1	2.31	0.44
7:A:62:PRO:HG3	18:L:53:HIS:CG	2.53	0.44
7:A:259:ASP:OD1	7:A:259:ASP:N	2.49	0.44
14:H:294:ILE:CD1	14:H:335:MET:HB3	2.47	0.44
14:H:476:LEU:HD13	14:H:489:LEU:HD11	2.00	0.44
21:O:59:LYS:HA	43:y:242:ALA:H	1.82	0.44
25:T:548:PHE:HD1	25:T:553:VAL:HG22	1.82	0.44
37:l:46:THR:O	37:l:46:THR:OG1	2.35	0.44
42:t:91:THR:O	42:t:95:GLN:NE2	2.51	0.44
42:u:125:THR:O	42:u:129:GLU:N	2.51	0.44
42:v:34:ILE:HD12	42:v:49:GLU:HG3	1.99	0.44
4:7:81:GLN:HB2	4:7:221:LEU:HD12	1.99	0.44
4:7:88:LYS:NZ	47:7:702:ATP:O1G	2.50	0.44
4:7:134:ASN:HB3	9:C:858:THR:O	2.16	0.44
4:7:274:THR:HG21	4:7:409:ASP:OD1	2.17	0.44
7:A:168:PRO:HG2	7:A:559:ASP:HB3	1.98	0.44
7:A:1411:SER:O	7:A:1411:SER:OG	2.28	0.44
7:A:1737:ASN:HB3	7:A:1740:LEU:HB2	1.99	0.44
8:B:439:ARG:HA	8:B:439:ARG:HD2	1.87	0.44
21:O:780:ARG:HH11	42:v:135:LYS:HZ2	1.65	0.44
22:P:213:ASP:OD2	22:P:216:ARG:NH1	2.45	0.44
24:S:286:GLU:HB3	24:S:291:GLN:HB2	2.00	0.44
26:U:894:ARG:HE	26:U:1024:SER:HB2	1.82	0.44
36:g:69:MET:HE3	36:g:69:MET:HB3	1.94	0.44
34:p:63:GLU:OE2	35:q:71:TYR:OH	2.33	0.44
7:A:1209:HIS:HB3	7:A:1213:VAL:HG21	1.98	0.44
7:A:1949:ARG:NH1	10:D:62:GLU:O	2.51	0.44
8:B:544:MET:HG3	8:B:817:TRP:CD2	2.53	0.44
8:B:828:ILE:HD11	8:B:853:LEU:HD13	2.00	0.44
8:B:1735:HIS:O	8:B:1739:GLU:HB2	2.17	0.44
9:C:833:PHE:HB2	9:C:902:HIS:HB2	2.00	0.44
15:I:88:G:N7	15:I:89:U:N3	2.65	0.44
21:O:755:LEU:HD23	21:O:755:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:41:ILE:HD11	31:k:71:LEU:HD12	2.00	0.44
34:p:55:ASN:OD1	34:p:81:GLY:N	2.42	0.44
3:6:64:U:O2'	7:A:539:ARG:O	2.28	0.44
4:7:47:GLU:HG3	14:H:330:LYS:NZ	2.33	0.44
6:9:72:THR:CG2	6:9:94:ILE:CD1	2.89	0.44
7:A:592:TYR:OH	7:A:1551:PHE:N	2.51	0.44
8:B:1475:ARG:NH1	8:B:1505:GLY:HA3	2.32	0.44
9:C:115:GLU:CD	33:d:84:LYS:HG3	2.43	0.44
21:O:25:LYS:HD2	21:O:159:LEU:HA	2.00	0.44
21:O:779:GLU:HA	21:O:782:LYS:HD2	1.98	0.44
22:P:40:LYS:HB2	22:P:40:LYS:HE3	1.77	0.44
31:b:81:THR:HG21	37:h:55:LEU:HD13	1.98	0.44
38:i:26:GLU:N	38:i:131:ARG:O	2.49	0.44
42:t:74:ILE:HG23	42:u:78:LEU:HD13	2.00	0.44
42:u:115:ARG:O	42:u:119:ARG:N	2.50	0.44
42:w:32:LYS:O	42:w:36:GLU:N	2.50	0.44
4:7:307:MET:HA	4:7:311:MET:CE	2.47	0.44
7:A:360:SER:CB	14:H:337:GLU:CD	2.91	0.44
7:A:384:VAL:HG22	9:C:331:PHE:HB3	2.00	0.44
7:A:741:ARG:NH1	16:J:432:ASP:O	2.44	0.44
7:A:828:PRO:HA	7:A:829:PRO:HD3	1.89	0.44
7:A:1088:PHE:HD1	7:A:1097:ILE:HG23	1.83	0.44
8:B:1083:TYR:O	8:B:1087:SER:OG	2.35	0.44
9:C:809:ILE:HG13	9:C:810:PRO:HD3	2.00	0.44
9:C:812:ALA:HA	9:C:815:VAL:HG12	2.00	0.44
13:G:58:ARG:HD2	13:G:62:GLN:HB3	1.99	0.44
13:G:58:ARG:NH2	32:c:177:GLU:OE1	2.49	0.44
16:J:270:VAL:HG21	16:J:305:THR:HG21	1.99	0.44
17:K:84:ASN:ND2	21:O:228:SER:OG	2.51	0.44
26:U:987:TYR:CE2	26:U:991:MET:HE3	2.53	0.44
31:k:31:PHE:HA	31:k:42:LEU:HD23	1.99	0.44
39:m:74:TRP:NE1	39:m:76:GLU:OE2	2.42	0.44
41:s:81:LEU:HD12	42:u:73:ALA:HB2	1.99	0.44
42:t:85:VAL:HG21	42:v:86:MET:HE1	2.00	0.44
4:7:23:MET:O	4:7:227:GLU:HG2	2.18	0.44
4:7:265:PHE:CE1	4:7:297:MET:HE3	2.53	0.44
7:A:791:GLN:OE1	7:A:1028:TYR:N	2.41	0.44
7:A:1759:THR:HG21	30:Z:358:ARG:HH22	1.82	0.44
7:A:2125:ALA:O	7:A:2150:GLN:NE2	2.50	0.44
7:A:2300:ASN:ND2	8:B:1229:ASP:CA	2.78	0.44
8:B:411:LEU:O	8:B:415:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:412:GLU:O	8:B:415:VAL:HG22	2.17	0.44
8:B:1416:LEU:O	8:B:1419:LEU:HD23	2.18	0.44
16:J:483:ASP:OD1	16:J:485:THR:OG1	2.35	0.44
3:6:84:A:H1'	24:S:277:THR:HG21	1.99	0.43
7:A:1901:LYS:HE2	7:A:1917:PHE:HE2	1.83	0.43
7:A:2280:ASN:HB3	7:A:2309:HIS:CD2	2.53	0.43
8:B:1346:VAL:HG23	8:B:1488:VAL:HG13	2.01	0.43
8:B:1457:HIS:CE1	8:B:1492:SER:HB3	2.53	0.43
9:C:502:HIS:HB2	9:C:505:GLN:HB2	2.00	0.43
16:J:346:ILE:HD12	16:J:356:LEU:HG	2.00	0.43
37:h:62:GLY:O	39:j:102:ARG:NH2	2.51	0.43
41:s:207:TYR:HA	41:s:210:LYS:HB2	2.00	0.43
1:2:45:C:H2'	1:2:46:U:O4'	2.18	0.43
4:7:148:GLU:OE1	4:7:148:GLU:CA	2.65	0.43
4:7:260:ARG:HG2	4:7:262:GLU:H	1.83	0.43
7:A:1109:LEU:HD13	7:A:1153:VAL:HG22	2.00	0.43
8:B:721:VAL:HA	8:B:825:THR:O	2.18	0.43
8:B:1324:LYS:HZ1	8:B:1400:ARG:HH12	1.65	0.43
9:C:474:LEU:HB3	9:C:567:GLU:HG3	1.99	0.43
9:C:770:PHE:HA	9:C:816:VAL:HG21	2.00	0.43
10:D:70:SER:OG	12:F:758:ARG:O	2.36	0.43
12:F:709:ARG:NH2	12:F:718:ASP:OD2	2.51	0.43
18:L:121:VAL:HG21	18:L:126:LEU:HD13	1.98	0.43
23:R:24:SER:O	23:R:24:SER:OG	2.31	0.43
24:S:400:GLU:HA	24:S:403:VAL:HG12	2.01	0.43
25:T:509:ARG:HA	25:T:509:ARG:HD3	1.79	0.43
34:p:57:VAL:HA	34:p:77:ILE:O	2.18	0.43
1:2:26:A:OP1	7:A:1020:LYS:NZ	2.50	0.43
1:2:45:C:C5	1:2:46:U:C5	3.06	0.43
4:7:22:ASP:C	4:7:22:ASP:OD1	2.61	0.43
6:9:92:ILE:CG2	6:9:94:ILE:CG2	2.95	0.43
7:A:898:PHE:HD2	7:A:905:LEU:HB3	1.82	0.43
7:A:1784:ASN:HD22	7:A:1897:LEU:HD12	1.83	0.43
8:B:837:GLU:HG2	8:B:1083:TYR:CE1	2.54	0.43
9:C:756:LYS:HA	9:C:759:LEU:HB3	2.00	0.43
10:D:32:LYS:HD3	34:p:52:GLU:HG2	1.99	0.43
12:F:643:PRO:HD2	12:F:719:ILE:HD11	1.99	0.43
21:O:646:GLY:O	21:O:650:GLY:N	2.52	0.43
21:O:699:ASN:O	21:O:703:MET:N	2.50	0.43
24:S:220:LEU:HG	24:S:224:LYS:HE3	2.00	0.43
30:Z:330:ARG:HH11	30:Z:332:PRO:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:40:LEU:HD12	31:b:72:LEU:HD23	1.98	0.43
35:f:62:VAL:HG23	39:j:110:LEU:HB3	2.00	0.43
38:i:85:GLU:HB2	38:i:127:THR:HG23	2.00	0.43
42:t:117:ILE:HD12	42:v:120:LEU:HD12	2.00	0.43
4:7:254:PHE:HA	4:7:401:ASP:O	2.18	0.43
4:7:403:MET:HG3	4:7:411:ILE:HD12	2.00	0.43
7:A:506:LEU:O	7:A:510:ARG:HB2	2.17	0.43
7:A:543:ALA:HB2	7:A:651:TRP:HB3	2.01	0.43
7:A:813:THR:HG21	7:A:996:LEU:HD22	2.00	0.43
7:A:2067:PHE:HB2	7:A:2072:GLU:HG2	2.00	0.43
8:B:592:LYS:HA	8:B:595:ILE:HD11	2.00	0.43
8:B:791:ARG:HE	8:B:794:ARG:HH22	1.64	0.43
8:B:1566:ARG:HG3	8:B:1622:GLU:HG2	2.00	0.43
9:C:388:VAL:HA	9:C:392:LEU:HB2	2.00	0.43
9:C:587:VAL:HG12	9:C:588:ILE:HD13	2.00	0.43
10:D:111:LYS:HG2	10:D:114:GLU:OE2	2.19	0.43
24:S:385:PHE:HA	24:S:388:LYS:HE2	2.01	0.43
42:u:5:CYS:HB2	42:u:12:PRO:HG3	1.99	0.43
7:A:96:PRO:HG3	7:A:648:LEU:HB3	2.00	0.43
7:A:1277:ALA:O	7:A:1281:THR:OG1	2.27	0.43
7:A:1717:ASN:HD21	32:c:178:HIS:CE1	2.36	0.43
7:A:1813:ARG:HA	7:A:1929:SER:HB2	2.00	0.43
8:B:1139:VAL:HA	8:B:1167:MET:HE1	1.99	0.43
8:B:1191:GLN:HE21	8:B:1199:LYS:HE2	1.82	0.43
8:B:1728:LEU:O	8:B:1732:MET:HE2	2.18	0.43
8:B:1855:TYR:CE1	8:B:1915:ILE:HG23	2.54	0.43
9:C:173:THR:O	9:C:177:ARG:CB	2.60	0.43
10:D:49:PRO:HD2	34:p:15:VAL:HG22	2.00	0.43
16:J:406:ILE:HG22	16:J:407:GLN:HB2	1.99	0.43
17:K:58:PHE:HZ	17:K:71:GLN:HB3	1.83	0.43
20:N:75:HIS:ND1	20:N:77:ASN:OD1	2.52	0.43
24:S:192:GLU:CD	44:z:108:ARG:HH21	2.16	0.43
25:T:518:PRO:HA	25:T:521:VAL:HG12	2.00	0.43
25:T:734:TYR:HB3	25:T:739:ASN:ND2	2.34	0.43
40:o:103:GLN:HG2	40:o:108:ARG:HD3	2.01	0.43
40:o:265:LEU:HB3	40:o:300:SER:HB2	2.01	0.43
40:o:326:ARG:NH2	40:o:362:GLU:O	2.51	0.43
42:v:5:CYS:HB2	42:v:12:PRO:HG3	2.00	0.43
43:y:204:ASP:OD1	43:y:204:ASP:N	2.52	0.43
7:A:82:ARG:NH2	15:I:16:G:N7	2.66	0.43
7:A:811:THR:HA	7:A:814:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2072:GLU:O	7:A:2076:ARG:HG3	2.19	0.43
7:A:2074:ARG:H	7:A:2074:ARG:HG2	1.63	0.43
8:B:462:LEU:HD11	8:B:466:LYS:HB2	2.01	0.43
8:B:821:LEU:HA	8:B:822:PRO:HD3	1.82	0.43
8:B:890:GLU:OE1	8:B:936:TYR:OH	2.31	0.43
8:B:1475:ARG:HH12	8:B:1505:GLY:HA3	1.82	0.43
9:C:126:SER:O	9:C:126:SER:OG	2.35	0.43
9:C:711:ARG:O	9:C:730:ARG:NH2	2.52	0.43
14:H:231:GLU:O	14:H:235:LYS:HG3	2.19	0.43
14:H:463:ILE:HG23	14:H:506:PHE:HE2	1.84	0.43
14:H:474:HIS:CD2	23:R:23:LEU:H	2.33	0.43
21:O:10:VAL:HG11	21:O:138:ARG:HD3	2.01	0.43
21:O:214:ILE:HB	21:O:217:GLU:HB3	2.01	0.43
24:S:357:LYS:HD2	24:S:357:LYS:HA	1.83	0.43
24:S:464:ASP:HB3	24:S:467:GLY:H	1.83	0.43
27:V:662:THR:C	27:V:663:ASP:O	2.61	0.43
32:c:106:VAL:HB	32:c:151:PRO:HB2	2.00	0.43
34:e:40:ASN:OD1	34:e:40:ASN:N	2.49	0.43
34:e:85:THR:HG23	36:g:66:SER:HB3	1.99	0.43
35:f:21:VAL:HB	35:f:72:ILE:HD13	2.00	0.43
40:o:527:ASP:OD1	40:o:531:LYS:N	2.51	0.43
40:o:565:LYS:HD3	40:o:577:LEU:HD21	2.01	0.43
42:w:73:ALA:HA	42:w:76:LYS:HB2	2.01	0.43
7:A:1247:ILE:HG12	7:A:1262:LYS:HB3	2.00	0.43
7:A:1555:LEU:HD13	7:A:1560:ILE:HB	1.99	0.43
8:B:464:VAL:HG21	8:B:478:PHE:O	2.18	0.43
8:B:726:HIS:CG	8:B:833:VAL:HG12	2.54	0.43
8:B:1359:CYS:HA	8:B:1362:PHE:HD2	1.82	0.43
8:B:1455:GLU:HG3	8:B:1457:HIS:CE1	2.53	0.43
9:C:352:LYS:HA	9:C:352:LYS:HD2	1.80	0.43
16:J:320:LYS:HE3	16:J:320:LYS:HB2	1.91	0.43
40:o:127:GLN:O	40:o:131:THR:OG1	2.31	0.43
41:s:175:GLY:HA2	41:s:178:LEU:HB2	2.00	0.43
43:y:111:TRP:CD1	43:y:111:TRP:H	2.35	0.43
1:2:15:U:H5'	1:2:16:U:H2'	2.01	0.43
7:A:610:HIS:NE2	50:c:601:IHP:O21	2.43	0.43
7:A:1021:ASP:OD2	17:K:254:TRP:NE1	2.44	0.43
7:A:1067:MET:SD	27:V:425:ILE:HG13	2.58	0.43
7:A:1681:ARG:NH2	32:c:170:TRP:O	2.46	0.43
7:A:1764:SER:H	7:A:1767:ASN:HB2	1.84	0.43
8:B:1094:ALA:O	8:B:1098:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1313:ARG:HD2	8:B:1313:ARG:HA	1.68	0.43
8:B:1340:TYR:O	8:B:1366:ARG:HD2	2.18	0.43
8:B:1836:LEU:HB3	8:B:1930:LEU:HD21	2.01	0.43
9:C:141:GLY:O	9:C:258:ASN:ND2	2.51	0.43
9:C:614:TYR:OH	9:C:643:ASP:OD2	2.34	0.43
17:K:72:TYR:HB3	17:K:75:ASP:HA	2.01	0.43
20:N:173:ASP:OD1	20:N:173:ASP:N	2.50	0.43
24:S:472:ILE:HD13	25:T:575:ARG:HA	2.01	0.43
25:T:511:LEU:HD11	25:T:521:VAL:HG23	2.01	0.43
25:T:673:ASP:OD1	25:T:677:LYS:HE3	2.19	0.43
26:U:163:ARG:O	26:U:167:GLN:HG2	2.19	0.43
33:n:8:LYS:HG2	40:o:260:ASP:O	2.19	0.43
40:o:180:LYS:HA	40:o:199:TYR:HA	2.01	0.43
34:p:20:LEU:HD22	36:r:61:VAL:HG23	2.01	0.43
42:v:14:HIS:HD2	42:v:28:ARG:HH22	1.67	0.43
7:A:689:VAL:HG21	7:A:713:LEU:HD22	2.01	0.43
7:A:1174:PHE:HE2	7:A:1186:LEU:HB2	1.84	0.43
7:A:2310:ARG:HH11	7:A:2310:ARG:HB3	1.83	0.43
8:B:639:ILE:HD11	8:B:646:VAL:HB	2.01	0.43
8:B:646:VAL:HG12	8:B:647:ARG:O	2.19	0.43
16:J:295:ASP:OD2	16:J:338:CYS:N	2.50	0.43
24:S:242:ILE:HG13	24:S:275:ASN:HD22	1.84	0.43
29:Y:16:ASP:HB2	29:Y:49:ARG:HH21	1.83	0.43
4:7:307:MET:HE2	4:7:319:ILE:HG22	2.01	0.43
7:A:414:ARG:NH1	9:C:410:LEU:O	2.50	0.43
7:A:1892:PRO:HD3	7:A:1941:ARG:HH21	1.83	0.43
8:B:1385:LEU:O	8:B:1389:VAL:HG23	2.19	0.43
9:C:863:ILE:HA	9:C:864:PRO:HD3	1.91	0.43
14:H:182:ILE:O	14:H:186:LEU:HG	2.18	0.43
14:H:387:MET:HA	14:H:387:MET:HE3	2.01	0.43
22:P:195:LYS:HA	22:P:195:LYS:HD3	1.86	0.43
24:S:190:THR:CG2	44:z:102:ARG:HG3	2.49	0.43
31:k:71:LEU:HD13	33:n:10:LEU:HB2	2.01	0.43
40:o:297:PHE:HB2	40:o:303:LEU:HB2	2.00	0.43
34:p:20:LEU:HD11	36:r:59:MET:HG2	2.01	0.43
36:r:7:PRO:HB2	36:r:9:LEU:HG	2.01	0.43
3:6:14:C:H2'	3:6:15:A:C8	2.54	0.42
4:7:307:MET:HE1	4:7:320:MET:CG	2.49	0.42
5:8:137:GLN:O	5:8:143:PRO:HA	2.19	0.42
7:A:58:LYS:NZ	7:A:477:LYS:O	2.49	0.42
7:A:976:MET:HE2	7:A:976:MET:HB2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1428:HIS:CB	27:V:396:ASP:HB3	2.48	0.42
8:B:509:LYS:HE2	8:B:509:LYS:HB2	1.66	0.42
8:B:1713:PHE:N	8:B:1713:PHE:HD1	2.17	0.42
9:C:313:GLN:HB2	48:C:1500:GTP:C6	2.54	0.42
19:M:259:ARG:N	19:M:273:GLN:O	2.49	0.42
21:O:781:GLU:HA	21:O:784:LEU:HB2	2.00	0.42
26:U:1208:VAL:HG13	26:U:1241:ILE:HD13	2.00	0.42
28:W:103:LEU:HD23	28:W:128:LYS:HE3	2.01	0.42
33:d:68:ILE:HG21	33:d:71:LEU:HD22	2.00	0.42
37:l:7:LEU:HD12	37:l:10:LEU:HD12	2.01	0.42
40:o:173:LYS:NZ	40:o:175:THR:O	2.52	0.42
34:p:88:GLN:HA	36:r:60:VAL:HG12	2.00	0.42
1:2:45:C:C6	1:2:46:U:C5	3.07	0.42
2:5:44:A:O2'	11:E:-5:G:N2	2.49	0.42
4:7:51:ARG:HG2	7:A:362:ARG:NH2	2.17	0.42
6:9:7:PHE:HD2	6:9:59:MET:HE3	1.84	0.42
7:A:1381:ASP:O	7:A:1385:VAL:HB	2.19	0.42
7:A:1890:GLN:O	10:D:70:SER:OG	2.32	0.42
7:A:2302:LYS:HD2	7:A:2306:HIS:CE1	2.54	0.42
8:B:598:ARG:HD3	8:B:989:SER:OG	2.19	0.42
8:B:1234:LEU:HD12	8:B:1234:LEU:HA	1.85	0.42
8:B:1388:GLN:HG3	8:B:1655:ASN:OD1	2.19	0.42
8:B:1918:LYS:H	8:B:1918:LYS:HG2	1.72	0.42
8:B:1945:LEU:O	8:B:1949:VAL:HG23	2.18	0.42
8:B:2032:GLY:HA2	8:B:2095:VAL:HG23	2.00	0.42
14:H:304:LEU:HA	14:H:304:LEU:HD23	1.76	0.42
20:N:145:LYS:HE2	20:N:145:LYS:HB2	1.89	0.42
25:T:581:GLU:HA	25:T:584:LEU:HD12	2.01	0.42
25:T:649:ARG:HG2	25:T:674:MET:HE1	2.00	0.42
37:l:17:ILE:HD12	37:l:40:LEU:HD11	2.00	0.42
40:o:536:ASP:HB2	40:o:543:TYR:CZ	2.51	0.42
4:7:50:LEU:HD23	14:H:330:LYS:NZ	2.33	0.42
4:7:73:ILE:CD1	4:7:95:SER:HA	2.46	0.42
7:A:362:ARG:HD2	14:H:337:GLU:CD	2.45	0.42
7:A:661:GLU:HA	17:K:213:LYS:HA	2.01	0.42
7:A:1159:ASN:ND2	22:P:197:CYS:O	2.52	0.42
7:A:2073:TRP:CH2	7:A:2313:HIS:CG	3.06	0.42
8:B:566:VAL:HG23	8:B:585:ILE:O	2.20	0.42
8:B:655:LEU:HD21	8:B:882:LEU:HD23	2.02	0.42
8:B:1368:LEU:HD11	8:B:1403:LYS:HG3	2.00	0.42
8:B:1986:MET:HE1	8:B:2011:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:183:SER:OG	9:C:480:LYS:NZ	2.49	0.42
9:C:654:LYS:HE3	9:C:654:LYS:HB2	1.75	0.42
9:C:843:VAL:O	9:C:846:VAL:HB	2.19	0.42
16:J:223:SER:OG	16:J:224:ALA:N	2.51	0.42
17:K:273:ARG:NH2	21:O:55:ASP:OD2	2.52	0.42
17:K:329:GLN:HA	17:K:332:ARG:HB2	2.02	0.42
18:L:28:LYS:HD2	40:o:189:ILE:HG22	2.00	0.42
18:L:131:ILE:HD11	19:M:177:GLU:HB3	2.01	0.42
25:T:651:ILE:HD12	25:T:654:LYS:HE2	2.00	0.42
26:U:61:ILE:O	26:U:65:MET:HG3	2.19	0.42
27:V:405:MET:HB3	27:V:411:LEU:HG	2.00	0.42
31:k:71:LEU:HB2	33:n:73:LEU:HD11	2.01	0.42
37:l:74:LEU:HD23	37:l:74:LEU:HA	1.91	0.42
39:m:75:THR:HG22	39:m:89:PRO:HB2	2.01	0.42
8:B:752:LEU:HB3	8:B:807:GLN:HE21	1.85	0.42
8:B:1647:SER:HB3	8:B:1650:LEU:HD13	2.02	0.42
8:B:1860:ILE:HG13	8:B:1885:ASN:O	2.19	0.42
9:C:276:TYR:OH	14:H:324:HIS:ND1	2.52	0.42
12:F:741:ALA:HA	24:S:182:LYS:HB2	2.01	0.42
14:H:284:ARG:HG3	14:H:284:ARG:O	2.19	0.42
24:S:319:MET:HE2	24:S:319:MET:HB3	1.81	0.42
26:U:735:VAL:HG11	26:U:743:GLN:HG2	2.02	0.42
31:b:16:ARG:HB3	31:b:84:GLY:HA3	2.02	0.42
40:o:209:SER:O	40:o:213:GLN:N	2.46	0.42
40:o:520:MET:HE3	40:o:520:MET:HB3	1.84	0.42
42:u:40:ASP:N	42:u:45:GLN:O	2.51	0.42
42:v:79:GLN:O	42:v:83:ASP:N	2.39	0.42
4:7:271:LEU:HD11	4:7:408:ALA:HB1	2.00	0.42
7:A:436:PRO:HG2	7:A:439:GLN:HG3	2.00	0.42
7:A:1490:PHE:O	7:A:1493:THR:OG1	2.37	0.42
7:A:1532:ARG:NH2	7:A:1575:GLN:OE1	2.52	0.42
7:A:1827:TRP:O	7:A:1830:GLN:NE2	2.41	0.42
7:A:1838:LYS:HB3	7:A:1871:PRO:HG2	2.00	0.42
7:A:2310:ARG:HG2	7:A:2310:ARG:HH11	1.85	0.42
8:B:423:MET:HB2	8:B:878:TYR:HD1	1.85	0.42
8:B:618:HIS:CE1	8:B:653:ALA:H	2.38	0.42
8:B:704:MET:HE2	8:B:870:ILE:HG22	2.00	0.42
8:B:739:ARG:HD3	8:B:780:TYR:CE2	2.55	0.42
8:B:753:ARG:NE	8:B:756:SER:O	2.52	0.42
8:B:862:ASP:OD1	8:B:863:THR:N	2.52	0.42
8:B:924:TYR:O	8:B:927:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1542:MET:O	8:B:1546:VAL:HG23	2.19	0.42
8:B:1953:MET:HE2	8:B:1953:MET:HB3	1.84	0.42
8:B:1996:LEU:HD12	8:B:1997:LEU:HD23	2.00	0.42
8:B:2051:VAL:HG13	8:B:2113:TYR:CZ	2.54	0.42
14:H:535:THR:HG23	14:H:538:ARG:HD3	2.01	0.42
17:K:92:SER:HB2	38:i:155:ASP:HB2	2.00	0.42
21:O:764:PRO:HA	21:O:767:LEU:HB2	2.01	0.42
25:T:273:GLU:C	26:U:357:ALA:HB2	2.44	0.42
31:b:35:ASP:OD1	31:b:35:ASP:N	2.53	0.42
1:2:98:A:N6	35:q:38:GLY:O	2.49	0.42
7:A:58:LYS:HE2	7:A:58:LYS:HB3	1.85	0.42
7:A:612:ILE:HD11	7:A:632:ALA:HB3	2.01	0.42
7:A:761:ILE:O	7:A:1245:ARG:NH2	2.41	0.42
7:A:2112:LYS:HB3	7:A:2112:LYS:HE2	1.67	0.42
7:A:2332:ASP:C	7:A:2334:TYR:H	2.28	0.42
8:B:462:LEU:HD21	8:B:467:LEU:HB3	2.01	0.42
8:B:1062:LEU:HD12	8:B:1062:LEU:HA	1.87	0.42
8:B:1244:LYS:HE2	8:B:1245:TYR:CE2	2.54	0.42
8:B:1583:ASP:C	8:B:1585:GLN:H	2.26	0.42
8:B:1825:ASN:OD1	8:B:1826:TYR:N	2.52	0.42
12:F:710:PHE:HE1	12:F:747:LEU:HD13	1.84	0.42
14:H:322:ILE:O	14:H:326:SER:HB2	2.19	0.42
14:H:494:LEU:HD23	14:H:528:ILE:HG13	2.02	0.42
16:J:433:ASN:OD1	16:J:435:THR:OG1	2.36	0.42
33:d:8:LYS:HB3	33:d:82:MET:SD	2.60	0.42
35:f:41:ASN:HD22	35:f:65:ARG:HA	1.85	0.42
33:n:46:ILE:HA	33:n:46:ILE:HD13	1.84	0.42
3:6:25:C:N4	19:M:39:GLU:OE2	2.51	0.42
5:8:131:MET:HE2	5:8:147:ASP:C	2.44	0.42
7:A:345:PRO:HG3	32:c:140:VAL:HG22	2.01	0.42
7:A:845:ARG:HA	7:A:845:ARG:HD3	1.83	0.42
7:A:981:PHE:HB3	7:A:984:MET:HB2	2.02	0.42
7:A:1443:LYS:HA	7:A:1443:LYS:HD3	1.83	0.42
7:A:1571:ILE:HG12	13:G:112:LYS:HE3	2.01	0.42
8:B:623:ASP:O	8:B:626:PRO:HD2	2.19	0.42
8:B:991:TYR:CE2	8:B:1097:GLU:HG3	2.54	0.42
9:C:276:TYR:OH	14:H:324:HIS:CB	2.67	0.42
19:M:240:GLY:H	19:M:268:GLN:HB2	1.84	0.42
21:O:780:ARG:O	21:O:784:LEU:N	2.43	0.42
26:U:1358:MET:HB3	26:U:1359:PRO:HD3	2.02	0.42
32:c:305:ASP:OD1	32:c:305:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:464:MET:HE1	40:o:486:LEU:HD12	2.01	0.42
41:s:125:GLU:O	41:s:128:SER:OG	2.37	0.42
7:A:758:ARG:HA	7:A:758:ARG:HD2	1.72	0.42
7:A:1110:ILE:HD11	7:A:1149:LEU:HB2	2.00	0.42
7:A:1248:LEU:HD11	7:A:1294:LYS:HB3	2.02	0.42
7:A:1407:ASP:N	7:A:1407:ASP:OD1	2.44	0.42
8:B:791:ARG:HE	8:B:794:ARG:HH12	1.68	0.42
8:B:1680:PRO:O	8:B:1683:ASP:HB2	2.19	0.42
10:D:125:ALA:HA	10:D:128:ARG:HB2	2.00	0.42
19:M:73:THR:HG23	19:M:125:ILE:HD12	2.01	0.42
20:N:130:ASP:N	20:N:130:ASP:OD1	2.49	0.42
20:N:229:TYR:HE1	20:N:231:MET:HE3	1.85	0.42
21:O:775:GLN:HA	21:O:778:GLN:HB2	2.00	0.42
24:S:358:GLU:HB3	24:S:361:ARG:HB3	2.00	0.42
24:S:431:ARG:HA	24:S:434:VAL:HG12	2.02	0.42
38:i:76:SER:OG	38:i:77:ILE:N	2.53	0.42
33:n:20:CYS:HB2	33:n:43:MET:HE1	2.00	0.42
40:o:255:LEU:HD21	40:o:362:GLU:HB3	2.02	0.42
42:v:120:LEU:HD23	42:v:120:LEU:HA	1.93	0.42
7:A:384:VAL:HG21	9:C:334:ILE:HD11	2.02	0.42
7:A:950:LEU:HD22	7:A:1416:ILE:HG21	2.02	0.42
7:A:1214:TRP:CD1	7:A:1376:GLU:HB3	2.55	0.42
7:A:1390:ALA:HB2	27:V:410:VAL:HG13	2.00	0.42
7:A:2272:MET:HE3	7:A:2296:LEU:HB3	2.01	0.42
9:C:320:LEU:HD21	9:C:344:TRP:HB2	2.01	0.42
14:H:330:LYS:HA	14:H:333:GLN:OE1	2.20	0.42
24:S:200:GLU:HG2	44:z:95:THR:OG1	2.18	0.42
25:T:276:ARG:H	26:U:357:ALA:HB3	1.81	0.42
27:V:411:LEU:HD23	27:V:411:LEU:HA	1.90	0.42
38:i:91:LYS:HA	38:i:91:LYS:HD3	1.93	0.42
33:n:28:TYR:HB3	33:n:46:ILE:HD12	2.02	0.42
2:5:90:U:H5''	33:d:66:SER:HB3	2.02	0.42
7:A:1683:LYS:HD3	7:A:1683:LYS:HA	1.76	0.42
7:A:1945:VAL:HA	10:D:67:VAL:HG11	2.01	0.42
7:A:2120:LEU:HD12	7:A:2120:LEU:N	2.35	0.42
8:B:1077:LEU:H	8:B:1077:LEU:HD12	1.85	0.42
8:B:1380:THR:HG21	8:B:1385:LEU:HD22	2.01	0.42
8:B:1883:LYS:HA	8:B:1883:LYS:HD3	1.87	0.42
9:C:519:GLU:O	9:C:522:SER:OG	2.35	0.42
9:C:699:ASP:OD2	9:C:722:TYR:OH	2.38	0.42
13:G:83:LYS:HE3	13:G:83:LYS:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:320:ARG:NH1	14:H:340:PHE:HE1	1.76	0.42
16:J:213:GLU:HG3	16:J:218:TRP:CZ2	2.55	0.42
19:M:259:ARG:HD2	19:M:273:GLN:HB3	2.01	0.42
20:N:266:PRO:N	21:O:785:GLN:OE1	2.53	0.42
21:O:49:ARG:HA	21:O:133:GLU:HB3	2.02	0.42
24:S:505:ALA:O	25:T:574:GLU:OE1	2.31	0.42
26:U:565:ILE:HB	26:U:655:ILE:HB	2.02	0.42
40:o:269:MET:CE	36:r:10:LYS:HE2	2.48	0.42
40:o:400:ILE:HG12	40:o:421:VAL:HG11	2.01	0.42
1:2:150:U:H2'	1:2:151:C:C6	2.55	0.41
3:6:40:U:H2'	3:6:41:A:C8	2.54	0.41
8:B:481:LEU:HD23	8:B:486:SER:HA	2.02	0.41
8:B:1148:PHE:CE2	8:B:1152:ARG:HB3	2.54	0.41
8:B:1590:LEU:HD22	8:B:1614:LEU:O	2.20	0.41
8:B:1936:LEU:HA	8:B:1936:LEU:HD23	1.79	0.41
9:C:769:GLY:HA3	9:C:812:ALA:HB3	2.01	0.41
15:I:18:A:H2	19:M:201:ARG:HD3	1.84	0.41
16:J:418:THR:HG1	16:J:430:GLY:H	1.68	0.41
21:O:633:GLN:O	21:O:637:VAL:N	2.50	0.41
21:O:741:GLN:HA	21:O:744:GLN:HB2	2.02	0.41
21:O:795:LYS:NZ	41:s:205:GLU:OE1	2.53	0.41
24:S:262:ARG:NH2	24:S:291:GLN:OE1	2.53	0.41
25:T:717:GLU:HA	25:T:720:ILE:HB	2.02	0.41
26:U:21:GLU:CD	26:U:21:GLU:H	2.28	0.41
35:f:23:LEU:HD22	35:f:68:ASN:HB3	2.01	0.41
42:w:40:ASP:OD2	42:w:43:ASN:N	2.47	0.41
3:6:29:A:N6	15:I:16:G:O2'	2.47	0.41
3:6:46:G:H2'	3:6:47:A:C8	2.56	0.41
7:A:1057:ARG:NH1	7:A:1060:GLU:OE1	2.53	0.41
8:B:1010:SER:OG	8:B:1013:GLU:OE2	2.33	0.41
9:C:166:CYS:O	9:C:168:THR:N	2.50	0.41
9:C:255:VAL:HG21	9:C:285:VAL:HG11	2.00	0.41
9:C:277:LYS:HD2	9:C:865:GLY:HA3	2.02	0.41
9:C:755:ASP:HB3	9:C:758:LEU:HB3	2.01	0.41
16:J:261:LEU:HB2	16:J:275:LEU:HD11	2.02	0.41
19:M:32:PRO:HG3	40:o:153:ILE:HD11	2.02	0.41
19:M:132:ARG:HG3	40:o:104:MET:HE1	2.02	0.41
25:T:272:PHE:O	26:U:357:ALA:HB3	2.20	0.41
26:U:208:ASP:OD1	26:U:210:GLU:HG2	2.20	0.41
26:U:826:GLY:HA3	26:U:1138:ARG:HG2	2.02	0.41
26:U:961:VAL:HG12	26:U:987:TYR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:134:LEU:HD13	42:v:134:LEU:HD21	2.01	0.41
4:7:265:PHE:CE1	4:7:297:MET:CE	3.03	0.41
7:A:974:ASN:HB2	7:A:1178:TYR:HB3	2.01	0.41
7:A:1536:LEU:HD23	7:A:1536:LEU:HA	1.81	0.41
7:A:2111:LEU:HD21	7:A:2225:LEU:HD21	2.02	0.41
8:B:580:ILE:HB	8:B:605:TYR:OH	2.20	0.41
9:C:135:CYS:O	9:C:227:LEU:HA	2.20	0.41
9:C:350:ASN:HB3	9:C:353:THR:HB	2.02	0.41
21:O:256:GLU:O	21:O:260:ARG:HB2	2.19	0.41
21:O:720:LEU:HD23	21:O:720:LEU:HA	1.92	0.41
24:S:429:PHE:HD1	24:S:458:PHE:HE1	1.67	0.41
39:j:46:CYS:HB3	39:j:50:LYS:HB2	2.02	0.41
40:o:513:GLN:HB3	40:o:555:GLY:HA2	2.02	0.41
41:s:68:ASN:HA	41:s:71:GLU:CD	2.46	0.41
43:y:210:TYR:HB3	43:y:219:ASN:HD22	1.85	0.41
44:z:118:MET:HE2	44:z:118:MET:HB2	1.96	0.41
8:B:488:LEU:HD21	8:B:501:LEU:HD23	2.02	0.41
8:B:760:GLU:HB3	8:B:763:ARG:HB2	2.01	0.41
8:B:1033:GLU:HB3	8:B:1077:LEU:HD11	2.01	0.41
8:B:1481:ILE:C	8:B:1483:ARG:H	2.28	0.41
8:B:1814:ASN:O	8:B:1818:ILE:HG13	2.20	0.41
8:B:2109:MET:HG3	8:B:2117:ASP:OD1	2.20	0.41
10:D:109:PHE:HA	10:D:112:ARG:HH11	1.85	0.41
13:G:107:LYS:O	13:G:110:TRP:CB	2.69	0.41
17:K:264:LEU:HD13	21:O:50:TRP:HH2	1.85	0.41
21:O:8:GLY:N	21:O:40:ARG:O	2.53	0.41
21:O:703:MET:O	41:s:117:GLN:NE2	2.50	0.41
33:d:23:ASN:N	33:d:67:LYS:O	2.53	0.41
37:h:47:LEU:HB2	37:h:50:ARG:HB2	2.01	0.41
38:i:122:LEU:HD21	40:o:95:PRO:HB3	2.02	0.41
40:o:463:SER:HB3	40:o:481:MET:HE2	2.02	0.41
42:t:130:ALA:O	42:t:133:THR:OG1	2.35	0.41
42:v:48:SER:N	42:v:51:GLN:OE1	2.44	0.41
4:7:353:ASP:O	4:7:364:ARG:NH2	2.53	0.41
7:A:420:ARG:NH2	7:A:423:ASP:OD1	2.53	0.41
7:A:1190:CYS:O	7:A:1273:TYR:OH	2.31	0.41
7:A:1698:PRO:HB2	32:c:182:VAL:HG22	2.03	0.41
7:A:2073:TRP:CZ3	7:A:2313:HIS:CG	3.09	0.41
7:A:2216:CYS:HA	7:A:2225:LEU:HB3	2.01	0.41
8:B:991:TYR:HE2	8:B:1097:GLU:HG3	1.86	0.41
8:B:1576:ILE:O	8:B:1580:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:836:VAL:HB	9:C:871:ILE:HB	2.02	0.41
14:H:387:MET:CE	14:H:387:MET:HA	2.50	0.41
14:H:466:SER:HB2	14:H:471:GLU:HB3	2.01	0.41
26:U:173:PRO:HG3	26:U:200:ILE:HD13	2.01	0.41
40:o:284:TRP:NE1	40:o:322:ARG:HB3	2.35	0.41
1:2:45:C:N4	15:I:85:G:H1	2.19	0.41
7:A:164:MET:HE2	7:A:164:MET:HB3	1.90	0.41
7:A:1068:PRO:HD3	27:V:425:ILE:HD12	2.02	0.41
7:A:1736:ALA:HA	32:c:287:PRO:HG3	2.03	0.41
8:B:598:ARG:CZ	8:B:992:TYR:CE1	3.03	0.41
8:B:709:TYR:O	8:B:712:ILE:HG22	2.20	0.41
8:B:1351:PRO:HG3	8:B:1516:PRO:HA	2.01	0.41
9:C:589:LYS:HG3	9:C:628:VAL:HG13	2.01	0.41
14:H:155:GLN:CD	14:H:387:MET:HE2	2.45	0.41
25:T:521:VAL:HG21	25:T:544:GLY:HA3	2.02	0.41
25:T:631:MET:HA	25:T:634:ILE:HB	2.03	0.41
29:Y:15:ASN:HD21	29:Y:17:LYS:HB2	1.85	0.41
35:f:42:MET:HE1	35:f:69:VAL:HG21	2.03	0.41
42:u:97:GLN:O	42:u:101:GLN:N	2.50	0.41
2:5:56:C:H5''	7:A:97:HIS:HE1	1.85	0.41
2:5:56:C:H4'	7:A:100:LEU:HD21	2.02	0.41
5:8:131:MET:HE1	5:8:148:TRP:CG	2.56	0.41
7:A:356:ILE:O	14:H:344:LYS:NZ	2.49	0.41
7:A:373:ASP:OD1	7:A:373:ASP:N	2.51	0.41
7:A:690:MET:HE3	7:A:690:MET:HB2	1.86	0.41
7:A:899:MET:HB3	7:A:906:VAL:HB	2.03	0.41
7:A:1877:LEU:HA	7:A:1877:LEU:HD23	1.83	0.41
7:A:2120:LEU:HD12	7:A:2120:LEU:H	1.86	0.41
8:B:577:LYS:O	8:B:581:SER:N	2.54	0.41
8:B:2114:MET:HE3	8:B:2114:MET:HB3	1.86	0.41
9:C:586:SER:OG	9:C:616:SER:O	2.28	0.41
9:C:664:GLU:HB3	9:C:820:PHE:CZ	2.56	0.41
9:C:828:MET:HE3	9:C:904:TRP:HB2	2.02	0.41
16:J:261:LEU:HD13	16:J:275:LEU:HD21	2.02	0.41
19:M:175:ARG:HB2	19:M:179:CYS:HB2	2.02	0.41
21:O:710:ALA:HA	21:O:713:MET:HB2	2.02	0.41
22:P:187:ARG:HA	22:P:187:ARG:HD3	1.92	0.41
24:S:480:TYR:CE2	24:S:502:GLU:HA	2.56	0.41
26:U:61:ILE:HD11	26:U:103:ARG:NE	2.35	0.41
40:o:434:VAL:HG21	40:o:476:LEU:HD11	2.02	0.41
40:o:439:ASP:OD2	40:o:441:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:199:ILE:HD13	41:s:202:LEU:HD12	2.01	0.41
4:7:378:ILE:HD13	4:7:403:MET:HE1	2.02	0.41
7:A:76:MET:HG3	7:A:506:LEU:HD11	2.03	0.41
7:A:1067:MET:CB	27:V:413:LYS:HD3	2.51	0.41
7:A:1248:LEU:O	7:A:1298:ARG:NH2	2.53	0.41
8:B:406:ARG:H	8:B:406:ARG:HD2	1.86	0.41
8:B:434:SER:HB3	8:B:447:VAL:HG12	2.03	0.41
8:B:617:ILE:HG22	8:B:652:SER:HB3	2.03	0.41
16:J:399:LYS:HB2	16:J:406:ILE:HD11	2.03	0.41
18:L:70:ILE:HG23	18:L:74:LEU:HB3	2.03	0.41
20:N:58:PRO:O	20:N:60:MET:N	2.45	0.41
21:O:696:LEU:HD23	21:O:696:LEU:HA	1.97	0.41
28:W:19:VAL:HG21	29:Y:25:ARG:HG2	2.02	0.41
32:c:86:ARG:HA	32:c:86:ARG:HD3	1.83	0.41
31:k:26:ILE:O	31:k:47:GLU:HA	2.20	0.41
37:l:9:LYS:HB3	37:l:9:LYS:HE3	1.85	0.41
40:o:398:LYS:HD3	40:o:419:GLY:H	1.85	0.41
1:2:175:G:H2'	1:2:176:G:C8	2.54	0.41
3:6:36:A:N6	15:I:11:A:OP2	2.54	0.41
4:7:109:ALA:HB3	4:7:159:VAL:HG22	2.02	0.41
4:7:169:ASP:OD1	4:7:170:MET:HE2	2.20	0.41
4:7:173:ARG:HH21	4:7:173:ARG:CB	2.33	0.41
6:9:78:LEU:HB3	6:9:116:LYS:HB2	2.02	0.41
7:A:232:LEU:HD21	9:C:412:ILE:HD11	2.03	0.41
7:A:544:PHE:O	7:A:548:ARG:HB2	2.20	0.41
7:A:617:ASN:HB3	7:A:622:GLY:O	2.21	0.41
7:A:990:LEU:HA	7:A:993:LEU:HB3	2.02	0.41
7:A:1410:ASP:OD1	7:A:1410:ASP:N	2.53	0.41
7:A:1784:ASN:HB3	7:A:1787:ARG:HD3	2.03	0.41
7:A:2259:VAL:HG22	7:A:2260:GLN:H	1.86	0.41
8:B:564:ILE:HG13	8:B:584:GLN:HG3	2.02	0.41
8:B:681:ARG:NH2	8:B:854:GLY:HA2	2.33	0.41
8:B:1312:LEU:H	8:B:1312:LEU:HD12	1.85	0.41
8:B:1858:ILE:HA	8:B:1859:PRO:HD3	1.80	0.41
8:B:2038:LEU:HD13	8:B:2091:LYS:HB3	2.03	0.41
9:C:532:ILE:HG23	9:C:539:ILE:HB	2.02	0.41
14:H:215:TYR:O	14:H:219:VAL:HG23	2.21	0.41
14:H:494:LEU:HD23	14:H:528:ILE:CG1	2.51	0.41
14:H:648:LYS:HA	14:H:648:LYS:HD3	1.87	0.41
19:M:232:THR:OG1	19:M:274:PHE:O	2.30	0.41
20:N:155:ASN:ND2	20:N:196:VAL:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:313:ASP:HB3	20:N:316:SER:HB3	2.03	0.41
24:S:232:GLU:OE2	24:S:267:ARG:NH1	2.40	0.41
24:S:262:ARG:HG3	24:S:285:MET:HE1	2.03	0.41
24:S:421:LYS:HA	24:S:424:GLU:HG2	2.03	0.41
26:U:1088:LEU:HD12	26:U:1088:LEU:HA	1.93	0.41
26:U:1138:ARG:NE	26:U:1267:GLN:OE1	2.48	0.41
31:b:22:GLN:NE2	31:b:75:GLU:O	2.54	0.41
34:e:32:GLN:HA	34:e:44:GLU:HA	2.03	0.41
35:f:47:THR:HG21	35:f:62:VAL:HG12	2.01	0.41
34:p:34:TRP:CE2	34:p:86:LEU:HD22	2.55	0.41
41:s:21:GLN:OE1	41:s:179:ARG:NH2	2.39	0.41
41:s:83:SER:OG	42:v:79:GLN:NE2	2.44	0.41
4:7:258:VAL:HB	4:7:263:TRP:HB2	2.02	0.41
7:A:357:ASN:ND2	9:C:866:SER:O	2.54	0.41
7:A:1279:VAL:HA	14:H:467:LEU:HD21	2.03	0.41
7:A:1389:TYR:CE2	27:V:405:MET:SD	3.14	0.41
7:A:2090:ILE:HD13	7:A:2090:ILE:H	1.86	0.41
8:B:752:LEU:HB3	8:B:807:GLN:NE2	2.36	0.41
8:B:1368:LEU:HD13	8:B:1368:LEU:HA	1.87	0.41
8:B:1779:ARG:HD3	8:B:1779:ARG:H	1.86	0.41
8:B:1796:LEU:HD12	8:B:1796:LEU:HA	1.70	0.41
9:C:119:LEU:HD11	9:C:187:THR:HG22	2.03	0.41
25:T:610:ARG:HE	25:T:643:TYR:HE2	1.69	0.41
26:U:109:TRP:CD2	26:U:162:ILE:HD11	2.56	0.41
33:d:21:GLU:OE2	33:d:69:ARG:NH1	2.45	0.41
36:g:6:PRO:HA	36:g:36:PRO:HA	2.02	0.41
31:k:50:LYS:HA	31:k:50:LYS:HD2	1.89	0.41
39:m:104:ASP:OD1	39:m:104:ASP:N	2.54	0.41
39:m:109:VAL:HB	35:q:63:LEU:HB3	2.03	0.41
40:o:88:MET:HE3	40:o:88:MET:HB2	1.88	0.41
40:o:422:ASN:H	40:o:437:SER:HA	1.85	0.41
35:q:6:ASN:HB2	35:q:9:PRO:HD2	2.02	0.41
42:u:82:TRP:NE1	42:v:71:ILE:HG21	2.36	0.41
2:5:91:U:H3'	2:5:92:U:H3'	2.02	0.40
3:6:22:A:H2'	40:o:130:ARG:HH11	1.86	0.40
7:A:2090:ILE:HD13	7:A:2090:ILE:N	2.37	0.40
7:A:2117:ILE:HG21	7:A:2301:PRO:HB2	2.02	0.40
7:A:2272:MET:HE3	7:A:2272:MET:HB3	1.74	0.40
8:B:1023:GLU:H	8:B:1023:GLU:HG2	1.65	0.40
8:B:1186:LEU:HD13	8:B:1282:LEU:HB2	2.02	0.40
8:B:1481:ILE:O	8:B:1481:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2036:VAL:HG22	8:B:2093:ASP:HB3	2.02	0.40
8:B:2072:LYS:HD2	8:B:2072:LYS:HA	1.87	0.40
9:C:710:ASN:OD1	9:C:713:LYS:N	2.46	0.40
10:D:78:GLU:HA	10:D:81:VAL:HG22	2.03	0.40
14:H:562:TRP:HH2	14:H:590:LEU:HD21	1.86	0.40
38:i:165:SER:OG	38:i:166:GLY:N	2.52	0.40
37:l:37:ASN:OD1	37:l:62:GLY:N	2.54	0.40
40:o:449:ILE:HG22	40:o:451:VAL:H	1.85	0.40
40:o:538:LYS:HE2	40:o:538:LYS:HB2	1.87	0.40
34:p:35:LEU:HD12	34:p:41:MET:HB3	2.02	0.40
36:r:48:MET:HE2	36:r:48:MET:HB3	1.93	0.40
43:y:118:LYS:HD3	43:y:118:LYS:HA	1.76	0.40
7:A:363:HIS:HD2	9:C:283:ASP:HB3	1.87	0.40
7:A:540:PHE:HB3	7:A:544:PHE:HB3	2.04	0.40
7:A:1365:ILE:HG23	7:A:1474:MET:HE1	2.02	0.40
8:B:436:ARG:HG3	8:B:445:VAL:HG22	2.03	0.40
8:B:612:ILE:O	8:B:612:ILE:HD12	2.21	0.40
8:B:654:THR:OG1	8:B:885:GLN:HG2	2.21	0.40
8:B:887:LEU:HA	8:B:888:PRO:HD3	1.92	0.40
8:B:1979:VAL:HG13	8:B:1984:ASP:HB2	2.02	0.40
8:B:1987:GLU:OE2	8:B:1988:MET:HG2	2.22	0.40
15:I:18:A:OP2	19:M:163:HIS:NE2	2.46	0.40
20:N:127:ALA:HA	20:N:133:VAL:HG22	2.03	0.40
20:N:321:TYR:CZ	20:N:356:ILE:HG13	2.56	0.40
20:N:348:ASP:HA	40:o:119:HIS:CG	2.56	0.40
21:O:238:ASP:O	21:O:242:LEU:N	2.53	0.40
25:T:572:LYS:HD3	25:T:575:ARG:HD3	2.03	0.40
34:e:64:ILE:HG12	34:e:71:ARG:HG2	2.03	0.40
39:j:51:LYS:HE2	39:j:51:LYS:HB2	1.94	0.40
40:o:398:LYS:HD2	40:o:418:LEU:HA	2.04	0.40
34:p:72:LYS:HE3	34:p:74:LEU:HD21	2.03	0.40
42:v:26:GLU:HB2	42:v:29:LEU:HD12	2.01	0.40
3:6:57:U:H2'	3:6:58:G:C8	2.57	0.40
4:7:268:LEU:HD11	4:7:282:ILE:CD1	2.50	0.40
7:A:1310:ARG:HH22	7:A:1563:HIS:C	2.29	0.40
8:B:597:THR:HG23	8:B:602:GLU:CD	2.46	0.40
8:B:703:ILE:O	8:B:707:ILE:HG13	2.21	0.40
8:B:777:LEU:HB3	8:B:782:PHE:O	2.21	0.40
9:C:560:VAL:HG12	9:C:561:LYS:H	1.85	0.40
14:H:344:LYS:HZ3	14:H:344:LYS:HG2	1.54	0.40
14:H:556:TYR:CG	14:H:593:TYR:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:696:LEU:O	21:O:700:ARG:N	2.54	0.40
26:U:789:PRO:O	26:U:791:PRO:HD3	2.21	0.40
31:b:16:ARG:HA	31:b:30:THR:HA	2.04	0.40
32:c:121:GLU:HG2	32:c:130:LYS:HD3	2.03	0.40
39:m:67:LEU:HB2	39:m:99:MET:HG2	2.02	0.40
42:t:71:ILE:HA	42:t:74:ILE:HB	2.03	0.40
1:2:182:U:OP2	31:k:54:LYS:NZ	2.38	0.40
4:7:37:THR:HA	4:7:38:PRO:HD2	1.88	0.40
7:A:175:PRO:HD3	7:A:520:TYR:CD1	2.56	0.40
7:A:784:LEU:O	7:A:788:GLN:HB2	2.21	0.40
8:B:538:ILE:O	8:B:585:ILE:HA	2.21	0.40
8:B:933:PRO:HG3	8:B:943:LEU:HD22	2.02	0.40
8:B:1494:LEU:HD12	8:B:1494:LEU:HA	1.79	0.40
9:C:603:MET:HB2	9:C:651:ILE:HD11	2.04	0.40
18:L:94:LYS:HD3	18:L:94:LYS:HA	1.80	0.40
19:M:175:ARG:HB3	19:M:178:GLU:HG3	2.03	0.40
26:U:902:LEU:O	26:U:906:ILE:HG12	2.21	0.40
26:U:1248:ASN:HA	26:U:1249:PRO:HD3	1.90	0.40
31:b:17:MET:HE2	31:b:80:MET:HE2	2.04	0.40
38:i:44:ARG:HG3	38:i:164:PRO:HG3	2.03	0.40
31:k:23:ASP:OD1	31:k:23:ASP:N	2.55	0.40
37:l:14:THR:HA	37:l:28:THR:HA	2.02	0.40
34:p:24:TYR:OH	36:r:59:MET:O	2.40	0.40
3:6:49:G:OP1	21:O:33:ARG:NH1	2.55	0.40
3:6:82:A:OP1	21:O:252:ARG:NH2	2.50	0.40
7:A:1278:VAL:HG22	7:A:1284:LEU:HD23	2.04	0.40
7:A:1289:VAL:HG13	7:A:1357:MET:HG3	2.03	0.40
7:A:2117:ILE:HG22	7:A:2303:GLU:HA	2.03	0.40
8:B:436:ARG:HH11	8:B:445:VAL:HG21	1.86	0.40
8:B:882:LEU:HD23	8:B:882:LEU:HA	1.79	0.40
8:B:928:ARG:HB3	8:B:936:TYR:CE1	2.57	0.40
8:B:1188:VAL:CG2	8:B:1200:VAL:HG13	2.51	0.40
8:B:1588:ARG:HG3	8:B:1589:PHE:CD1	2.57	0.40
8:B:1890:LYS:NZ	8:B:1908:LEU:HD22	2.37	0.40
9:C:617:LEU:HD12	9:C:617:LEU:HA	1.83	0.40
9:C:830:PRO:HG2	9:C:877:ALA:HB3	2.03	0.40
21:O:706:GLU:HA	21:O:709:ARG:HB2	2.03	0.40
22:P:54:VAL:HB	22:P:59:PHE:HZ	1.86	0.40
26:U:49:ILE:O	26:U:53:GLU:HB2	2.21	0.40
26:U:696:ASP:HA	26:U:697:PRO:HD2	1.97	0.40
38:i:47:TYR:CZ	38:i:67:PRO:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:29:LEU:HD23	39:j:32:LEU:HD12	2.03	0.40
40:o:72:LEU:HD21	40:o:81:TYR:HE1	1.87	0.40
40:o:534:ILE:HB	40:o:544:SER:HB3	2.03	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	
4	7	388/390 (100%)	376 (97%)	9 (2%)	3 (1%)	16	45
5	8	89/91 (98%)	87 (98%)	1 (1%)	1 (1%)	11	39
6	9	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
7	A	2244/2335 (96%)	2105 (94%)	139 (6%)	0	100	100
8	B	1720/1722 (100%)	1633 (95%)	84 (5%)	3 (0%)	43	71
9	C	897/899 (100%)	828 (92%)	67 (8%)	2 (0%)	43	71
10	D	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
12	F	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
13	G	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
14	H	455/908 (50%)	440 (97%)	15 (3%)	0	100	100
16	J	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
17	K	291/295 (99%)	271 (93%)	20 (7%)	0	100	100
18	L	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
19	M	287/289 (99%)	271 (94%)	16 (6%)	0	100	100
20	N	304/306 (99%)	283 (93%)	19 (6%)	2 (1%)	18	49
21	O	429/802 (54%)	416 (97%)	12 (3%)	1 (0%)	43	71
22	P	100/229 (44%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	R	24/26 (92%)	17 (71%)	7 (29%)	0	100	100
24	S	531/848 (63%)	500 (94%)	28 (5%)	3 (1%)	21	52
25	T	597/855 (70%)	584 (98%)	12 (2%)	1 (0%)	43	71
26	U	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
27	V	709/1220 (58%)	617 (87%)	60 (8%)	32 (4%)	2	13
28	W	160/162 (99%)	147 (92%)	13 (8%)	0	100	100
29	Y	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
30	Z	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
31	b	64/82 (78%)	62 (97%)	2 (3%)	0	100	100
31	k	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
32	c	265/586 (45%)	248 (94%)	17 (6%)	0	100	100
33	d	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
33	n	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	e	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
34	p	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
35	f	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
35	q	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
36	g	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
36	r	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
37	h	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
37	l	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
38	i	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
39	j	91/118 (77%)	87 (96%)	4 (4%)	0	100	100
39	m	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
40	o	511/513 (100%)	465 (91%)	45 (9%)	1 (0%)	43	71
41	s	161/225 (72%)	148 (92%)	13 (8%)	0	100	100
42	t	121/504 (24%)	118 (98%)	3 (2%)	0	100	100
42	u	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
42	v	121/504 (24%)	119 (98%)	2 (2%)	0	100	100
42	w	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
43	y	142/144 (99%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	z	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
All	All	14378/18759 (77%)	13605 (95%)	724 (5%)	49 (0%)	37	65

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	383	ASN
8	B	957	VAL
8	B	1584	ILE
20	N	59	ILE
27	V	531	MET
27	V	610	ARG
27	V	855	VAL
27	V	944	ASP
27	V	995	MET
27	V	1090	LYS
27	V	1098	LYS
27	V	1099	SER
27	V	1129	ASP
27	V	1145	GLN
27	V	1164	GLU
4	7	340	GLY
4	7	385	ASP
5	8	115	GLY
9	C	94	ILE
24	S	709	VAL
27	V	517	GLU
27	V	845	SER
27	V	870	GLY
27	V	1182	LYS
27	V	524	ASN
27	V	550	TYR
27	V	806	GLU
27	V	994	ILE
27	V	1056	LYS
20	N	58	PRO
24	S	604	PRO
27	V	590	THR
27	V	663	ASP
27	V	722	ALA
27	V	835	VAL
27	V	1055	ASN

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Mol	Chain	Res	Type
40	o	248	ASP
9	C	680	ASN
24	S	341	PRO
27	V	811	PRO
27	V	1157	THR
25	T	372	ARG
27	V	523	ALA
27	V	856	ASP
21	O	215	PRO
27	V	738	PRO
27	V	521	ILE
27	V	1137	PRO
8	B	585	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7	345/345 (100%)	338 (98%)	7 (2%)	48	68
5	8	76/76 (100%)	75 (99%)	1 (1%)	61	74
6	9	132/132 (100%)	131 (99%)	1 (1%)	73	79
7	A	2033/2108 (96%)	1989 (98%)	44 (2%)	45	66
8	B	1541/1541 (100%)	1346 (87%)	195 (13%)	4	18
9	C	799/799 (100%)	794 (99%)	5 (1%)	78	81
10	D	106/106 (100%)	106 (100%)	0	100	100
12	F	110/110 (100%)	110 (100%)	0	100	100
13	G	54/55 (98%)	54 (100%)	0	100	100
14	H	410/838 (49%)	404 (98%)	6 (2%)	57	72
16	J	276/276 (100%)	274 (99%)	2 (1%)	76	80
17	K	246/247 (100%)	246 (100%)	0	100	100
18	L	130/130 (100%)	129 (99%)	1 (1%)	73	79
19	M	254/254 (100%)	253 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	N	263/263 (100%)	262 (100%)	1 (0%)	84	84
21	O	322/709 (45%)	320 (99%)	2 (1%)	78	81
22	P	94/203 (46%)	94 (100%)	0	100	100
23	R	21/21 (100%)	21 (100%)	0	100	100
24	S	275/751 (37%)	275 (100%)	0	100	100
25	T	213/749 (28%)	209 (98%)	4 (2%)	50	68
26	U	1202/1336 (90%)	1196 (100%)	6 (0%)	81	83
27	V	31/1085 (3%)	29 (94%)	2 (6%)	15	43
28	W	139/147 (95%)	138 (99%)	1 (1%)	76	80
29	Y	81/82 (99%)	81 (100%)	0	100	100
30	Z	25/25 (100%)	25 (100%)	0	100	100
31	b	62/75 (83%)	62 (100%)	0	100	100
31	k	75/75 (100%)	75 (100%)	0	100	100
32	c	236/520 (45%)	234 (99%)	2 (1%)	73	79
33	d	74/74 (100%)	74 (100%)	0	100	100
33	n	73/74 (99%)	73 (100%)	0	100	100
34	e	74/76 (97%)	74 (100%)	0	100	100
34	p	76/76 (100%)	76 (100%)	0	100	100
35	f	61/61 (100%)	61 (100%)	0	100	100
35	q	61/61 (100%)	61 (100%)	0	100	100
36	g	63/63 (100%)	62 (98%)	1 (2%)	55	72
36	r	63/63 (100%)	61 (97%)	2 (3%)	34	60
37	h	75/75 (100%)	75 (100%)	0	100	100
37	l	75/75 (100%)	75 (100%)	0	100	100
38	i	133/133 (100%)	132 (99%)	1 (1%)	73	79
39	j	91/110 (83%)	91 (100%)	0	100	100
39	m	91/110 (83%)	91 (100%)	0	100	100
40	o	451/451 (100%)	448 (99%)	3 (1%)	76	80
41	s	152/196 (78%)	152 (100%)	0	100	100
42	t	111/435 (26%)	111 (100%)	0	100	100
42	u	106/435 (24%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	v	111/435 (26%)	111 (100%)	0	100	100
42	w	106/435 (24%)	106 (100%)	0	100	100
43	y	129/129 (100%)	129 (100%)	0	100	100
44	z	29/29 (100%)	29 (100%)	0	100	100
All	All	11756/16654 (71%)	11468 (98%)	288 (2%)	42	65

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	7	37	THR
4	7	194	ASN
4	7	301	ASN
4	7	316	ARG
4	7	337	TRP
4	7	360	LEU
4	7	407	VAL
5	8	118	LEU
6	9	119	GLU
7	A	413	LEU
7	A	668	VAL
7	A	767	VAL
7	A	941	LYS
7	A	1175	VAL
7	A	1359	HIS
7	A	1438	VAL
7	A	1868	MET
7	A	2011	ILE
7	A	2073	TRP
7	A	2074	ARG
7	A	2078	ILE
7	A	2085	LEU
7	A	2087	THR
7	A	2090	ILE
7	A	2103	THR
7	A	2108	LYS
7	A	2117	ILE
7	A	2139	VAL
7	A	2143	ARG
7	A	2156	THR
7	A	2157	VAL
7	A	2159	LEU

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Mol	Chain	Res	Type
7	A	2171	GLU
7	A	2193	VAL
7	A	2194	THR
7	A	2219	THR
7	A	2223	CYS
7	A	2226	THR
7	A	2233	SER
7	A	2242	THR
7	A	2254	SER
7	A	2258	ARG
7	A	2259	VAL
7	A	2261	MET
7	A	2268	LEU
7	A	2273	VAL
7	A	2284	MET
7	A	2293	LYS
7	A	2298	LEU
7	A	2303	GLU
7	A	2310	ARG
7	A	2312	SER
7	A	2319	LEU
8	B	406	ARG
8	B	409	LEU
8	B	410	ASP
8	B	412	GLU
8	B	414	LEU
8	B	420	SER
8	B	430	LEU
8	B	436	ARG
8	B	446	HIS
8	B	447	VAL
8	B	450	LEU
8	B	451	LYS
8	B	464	VAL
8	B	467	LEU
8	B	488	LEU
8	B	495	THR
8	B	500	LEU
8	B	501	LEU
8	B	505	THR
8	B	525	ILE
8	B	533	VAL

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Mol	Chain	Res	Type
8	B	547	LEU
8	B	550	GLU
8	B	566	VAL
8	B	572	ASP
8	B	576	CYS
8	B	578	GLU
8	B	580	ILE
8	B	584	GLN
8	B	591	GLU
8	B	592	LYS
8	B	595	ILE
8	B	602	GLU
8	B	612	ILE
8	B	614	LEU
8	B	643	GLN
8	B	673	LEU
8	B	683	VAL
8	B	690	VAL
8	B	693	THR
8	B	712	ILE
8	B	728	ARG
8	B	739	ARG
8	B	743	LEU
8	B	750	LEU
8	B	759	THR
8	B	773	GLU
8	B	782	PHE
8	B	791	ARG
8	B	806	ILE
8	B	807	GLN
8	B	809	LEU
8	B	810	VAL
8	B	820	ASN
8	B	833	VAL
8	B	847	LEU
8	B	849	ILE
8	B	850	LEU
8	B	852	MET
8	B	855	ARG
8	B	868	ILE
8	B	869	LEU
8	B	877	GLN

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Mol	Chain	Res	Type
8	B	885	GLN
8	B	887	LEU
8	B	894	VAL
8	B	897	LEU
8	B	900	MET
8	B	901	LEU
8	B	906	VAL
8	B	910	VAL
8	B	920	LEU
8	B	934	THR
8	B	941	ASP
8	B	942	ASP
8	B	957	VAL
8	B	972	TYR
8	B	975	LYS
8	B	981	VAL
8	B	992	TYR
8	B	1004	LEU
8	B	1016	ARG
8	B	1020	LEU
8	B	1028	THR
8	B	1037	LEU
8	B	1051	SER
8	B	1062	LEU
8	B	1063	LEU
8	B	1087	SER
8	B	1091	LEU
8	B	1100	LEU
8	B	1101	ASN
8	B	1108	THR
8	B	1125	SER
8	B	1135	LEU
8	B	1143	ILE
8	B	1153	LEU
8	B	1158	HIS
8	B	1165	ILE
8	B	1166	ARG
8	B	1186	LEU
8	B	1187	SER
8	B	1204	ILE
8	B	1224	LEU
8	B	1225	VAL

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Mol	Chain	Res	Type
8	B	1228	VAL
8	B	1232	VAL
8	B	1234	LEU
8	B	1240	LEU
8	B	1241	LEU
8	B	1242	LYS
8	B	1262	LEU
8	B	1287	ARG
8	B	1301	LEU
8	B	1312	LEU
8	B	1320	LEU
8	B	1337	ASN
8	B	1368	LEU
8	B	1375	ARG
8	B	1385	LEU
8	B	1399	ASP
8	B	1406	VAL
8	B	1408	LEU
8	B	1413	SER
8	B	1419	LEU
8	B	1421	LYS
8	B	1425	ILE
8	B	1430	GLU
8	B	1436	SER
8	B	1441	GLN
8	B	1442	ARG
8	B	1443	LYS
8	B	1453	VAL
8	B	1455	GLU
8	B	1456	VAL
8	B	1474	MET
8	B	1477	ILE
8	B	1480	GLN
8	B	1481	ILE
8	B	1482	GLU
8	B	1492	SER
8	B	1528	GLN
8	B	1567	LYS
8	B	1580	CYS
8	B	1629	ARG
8	B	1655	ASN
8	B	1707	GLN

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Mol	Chain	Res	Type
8	B	1713	PHE
8	B	1728	LEU
8	B	1734	ASP
8	B	1742	THR
8	B	1747	ASN
8	B	1752	VAL
8	B	1756	THR
8	B	1762	ARG
8	B	1779	ARG
8	B	1781	LEU
8	B	1788	LEU
8	B	1817	MET
8	B	1829	ILE
8	B	1831	LEU
8	B	1834	MET
8	B	1840	THR
8	B	1842	VAL
8	B	1849	ILE
8	B	1854	GLU
8	B	1865	ASP
8	B	1912	THR
8	B	1936	LEU
8	B	1956	LYS
8	B	1957	ASP
8	B	1970	HIS
8	B	1988	MET
8	B	1996	LEU
8	B	1999	LEU
8	B	2000	THR
8	B	2017	ILE
8	B	2026	LYS
8	B	2027	ASP
8	B	2029	ILE
8	B	2031	SER
8	B	2047	VAL
8	B	2055	LEU
8	B	2070	ASP
8	B	2076	LEU
8	B	2077	ILE
8	B	2082	LEU
8	B	2084	LEU
8	B	2092	LEU

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Mol	Chain	Res	Type
8	B	2095	VAL
8	B	2105	THR
8	B	2109	MET
8	B	2114	MET
8	B	2121	LYS
8	B	2125	ASP
9	C	168	THR
9	C	189	VAL
9	C	215	VAL
9	C	801	LEU
9	C	824	THR
14	H	333	GLN
14	H	344	LYS
14	H	387	MET
14	H	461	LEU
14	H	494	LEU
14	H	575	THR
16	J	302	VAL
16	J	323	VAL
18	L	131	ILE
19	M	115	GLU
20	N	333	VAL
21	O	147	ASP
21	O	208	VAL
25	T	528	LEU
25	T	548	PHE
25	T	645	VAL
25	T	724	LEU
26	U	51	GLU
26	U	84	GLU
26	U	881	HIS
26	U	960	ASP
26	U	986	SER
26	U	1021	LEU
27	V	413	LYS
27	V	414	GLU
28	W	120	ILE
32	c	181	ILE
32	c	315	VAL
36	g	61	VAL
38	i	139	VAL
40	o	335	VAL

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Mol	Chain	Res	Type
40	o	436	THR
40	o	552	VAL
36	r	43	ASP
36	r	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
4	7	136	GLN
4	7	301	ASN
4	7	394	GLN
7	A	160	HIS
7	A	270	ASN
7	A	495	GLN
7	A	664	HIS
7	A	755	HIS
7	A	775	ASN
7	A	792	HIS
7	A	793	ASN
7	A	815	HIS
7	A	834	HIS
7	A	994	ASN
7	A	1014	ASN
7	A	1026	ASN
7	A	1066	GLN
7	A	1096	HIS
7	A	1121	ASN
7	A	1129	ASN
7	A	1159	ASN
7	A	1169	GLN
7	A	1188	ASN
7	A	1209	HIS
7	A	1246	GLN
7	A	1280	ASN
7	A	1304	ASN
7	A	1337	GLN
7	A	1363	GLN
7	A	1394	GLN
7	A	1468	ASN
7	A	1476	GLN
7	A	1487	HIS
7	A	1520	ASN

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Mol	Chain	Res	Type
7	A	1563	HIS
7	A	1586	HIS
7	A	1599	GLN
7	A	1610	GLN
7	A	1717	ASN
7	A	1946	ASN
7	A	1947	ASN
7	A	2089	HIS
7	A	2123	GLN
7	A	2155	GLN
7	A	2291	ASN
7	A	2300	ASN
7	A	2306	HIS
8	B	425	ASN
8	B	482	ASN
8	B	726	HIS
8	B	785	HIS
8	B	873	HIS
8	B	877	GLN
8	B	1113	ASN
8	B	1189	HIS
8	B	1322	GLN
8	B	1337	ASN
8	B	1423	ASN
8	B	1528	GLN
8	B	1568	GLN
8	B	1814	ASN
8	B	1862	HIS
8	B	1898	HIS
8	B	2012	ASN
8	B	2058	GLN
9	C	60	HIS
9	C	125	ASN
9	C	137	HIS
9	C	175	GLN
9	C	350	ASN
9	C	411	ASN
9	C	451	HIS
9	C	477	HIS
9	C	557	GLN
9	C	596	ASN
9	C	743	ASN

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Mol	Chain	Res	Type
9	C	903	HIS
9	C	905	GLN
10	D	116	ASN
12	F	656	ASN
14	H	171	ASN
14	H	474	HIS
14	H	499	GLN
14	H	542	ASN
14	H	600	ASN
14	H	623	ASN
16	J	216	ASN
16	J	269	GLN
16	J	417	ASN
16	J	446	ASN
16	J	451	HIS
16	J	500	HIS
17	K	84	ASN
17	K	133	GLN
17	K	194	GLN
18	L	116	ASN
19	M	82	GLN
19	M	289	ASN
20	N	101	ASN
20	N	165	GLN
21	O	95	GLN
21	O	161	ASN
21	O	175	GLN
21	O	186	GLN
21	O	245	GLN
22	P	56	ASN
23	R	20	GLN
24	S	221	ASN
24	S	250	GLN
24	S	293	ASN
24	S	331	GLN
24	S	454	ASN
25	T	601	GLN
25	T	705	GLN
25	T	739	ASN
25	T	744	GLN
26	U	71	GLN
26	U	152	HIS

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Mol	Chain	Res	Type
26	U	165	GLN
26	U	355	ASN
26	U	393	ASN
26	U	469	ASN
26	U	542	ASN
26	U	544	ASN
26	U	632	ASN
26	U	1007	GLN
26	U	1082	GLN
26	U	1255	ASN
26	U	1311	GLN
27	V	404	GLN
28	W	43	GLN
28	W	72	ASN
29	Y	15	ASN
29	Y	68	GLN
31	b	76	ASN
32	c	85	GLN
32	c	92	GLN
32	c	154	HIS
32	c	156	GLN
32	c	171	ASN
32	c	178	HIS
32	c	328	GLN
32	c	344	GLN
35	f	41	ASN
36	g	56	ASN
37	h	21	ASN
37	h	64	ASN
38	i	10	GLN
38	i	140	ASN
38	i	148	ASN
39	j	39	ASN
39	j	91	ASN
31	k	76	ASN
37	l	64	ASN
39	m	25	ASN
39	m	49	ASN
33	n	16	HIS
33	n	40	ASN
33	n	45	ASN
40	o	80	GLN

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Mol	Chain	Res	Type
40	o	128	GLN
40	o	145	ASN
40	o	147	GLN
40	o	250	GLN
40	o	402	GLN
40	o	412	GLN
40	o	462	HIS
40	o	479	GLN
40	o	513	GLN
40	o	533	ASN
34	p	88	GLN
35	q	68	ASN
36	r	26	HIS
36	r	55	ASN
36	r	56	ASN
41	s	164	ASN
41	s	192	ASN
42	t	9	ASN
42	t	22	ASN
42	t	79	GLN
42	t	94	GLN
42	u	22	ASN
42	u	45	GLN
42	u	79	GLN
42	v	14	HIS
42	v	22	ASN
42	v	43	ASN
42	v	94	GLN
42	v	101	GLN
42	w	22	ASN
42	w	44	ASN
43	y	131	GLN
43	y	156	HIS
43	y	165	ASN
43	y	169	HIS
43	y	172	HIS
43	y	215	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	117/189 (61%)	30 (25%)	5 (4%)
11	E	14/14 (100%)	5 (35%)	1 (7%)
15	I	39/113 (34%)	19 (48%)	2 (5%)
2	5	73/116 (62%)	24 (32%)	2 (2%)
3	6	96/106 (90%)	37 (38%)	5 (5%)
All	All	339/538 (63%)	115 (33%)	15 (4%)

All (115) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	U
1	2	17	U
1	2	19	G
1	2	20	G
1	2	24	A
1	2	25	G
1	2	29	A
1	2	30	A
1	2	32	U
1	2	40	C
1	2	41	U
1	2	46	U
1	2	47	U
1	2	51	A
1	2	53	U
1	2	54	U
1	2	96	A
1	2	97	G
1	2	99	U
1	2	100	U
1	2	101	U
1	2	102	U
1	2	103	U
1	2	104	G
1	2	105	G
1	2	106	A
1	2	109	U
1	2	157	G
1	2	171	U
1	2	178	A
2	5	10	U

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Mol	Chain	Res	Type
2	5	11	U
2	5	20	G
2	5	21	A
2	5	34	U
2	5	35	U
2	5	36	C
2	5	38	C
2	5	39	C
2	5	42	U
2	5	45	C
2	5	47	A
2	5	52	U
2	5	53	U
2	5	57	G
2	5	69	A
2	5	86	C
2	5	89	U
2	5	91	U
2	5	92	U
2	5	93	U
2	5	94	U
2	5	95	G
2	5	96	A
3	6	6	C
3	6	7	G
3	6	8	C
3	6	9	U
3	6	11	C
3	6	12	G
3	6	26	U
3	6	28	A
3	6	29	A
3	6	33	G
3	6	34	G
3	6	35	A
3	6	37	C
3	6	38	G
3	6	41	A
3	6	44	G
3	6	45	A
3	6	46	G
3	6	48	A

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Mol	Chain	Res	Type
3	6	49	G
3	6	51	U
3	6	54	G
3	6	56	A
3	6	58	G
3	6	59	G
3	6	60	C
3	6	61	C
3	6	62	C
3	6	67	G
3	6	68	C
3	6	74	U
3	6	79	C
3	6	81	C
3	6	84	A
3	6	85	U
3	6	87	C
3	6	88	G
11	E	-11	G
11	E	-7	C
11	E	-6	C
11	E	1	C
11	E	2	U
15	I	5	G
15	I	14	A
15	I	16	G
15	I	17	U
15	I	83	A
15	I	87	U
15	I	88	G
15	I	89	U
15	I	90	C
15	I	91	A
15	I	92	U
15	I	93	A
15	I	95	U
15	I	96	U
15	I	97	A
15	I	98	U
15	I	99	C
15	I	112	A
15	I	113	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	39	U
1	2	46	U
1	2	95	A
1	2	102	U
1	2	105	G
2	5	92	U
2	5	95	G
3	6	5	U
3	6	33	G
3	6	37	C
3	6	50	A
3	6	58	G
11	E	-12	G
15	I	90	C
15	I	95	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
17	SEP	K	232	17	8,9,10	1.63	1 (12%)	7,12,14	1.17	1 (14%)
17	SEP	K	224	17	8,9,10	1.60	1 (12%)	7,12,14	0.88	0

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
17	SEP	K	232	17	-	3/6/8/10	-
17	SEP	K	224	17	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	232	SEP	P-O1P	3.53	1.61	1.50
17	K	224	SEP	P-O1P	3.49	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	232	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	232	SEP	CB-OG-P-O2P
17	K	232	SEP	CB-OG-P-O3P
17	K	232	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z > 2$
50	IHP	c	601	-	36,36,36	0.75	0	60,60,60	1.01	3 (5%)
47	ATP	7	702	45	32,33,33	1.22	4 (12%)	48,52,52	1.84	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	GTP	C	1500	45	33,34,34	0.94	0	50,54,54	1.59	9 (18%)

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
50	IHP	c	601	-	-	6/30/54/54	0/1/1/1
47	ATP	7	702	45	-	0/22/38/38	0/3/3/3
48	GTP	C	1500	45	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	7	702	ATP	C4-N9	-3.20	1.31	1.37
47	7	702	ATP	PB-O3B	2.75	1.62	1.59
47	7	702	ATP	C5-N7	-2.12	1.35	1.39
47	7	702	ATP	PA-O3A	2.01	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	7	702	ATP	C5-C4-N3	-6.38	117.93	126.72
48	C	1500	GTP	C5-C4-N3	-4.88	120.63	128.39
48	C	1500	GTP	C2-N3-C4	4.56	120.16	112.30
47	7	702	ATP	N3-C2-N1	-4.16	122.29	128.58
47	7	702	ATP	N3-C4-N9	4.08	134.10	127.17
47	7	702	ATP	C4-C5-N7	-4.04	105.97	110.58
47	7	702	ATP	C2-N3-C4	3.64	120.71	111.83
47	7	702	ATP	N9-C8-N7	-3.15	109.46	113.94
48	C	1500	GTP	N9-C4-N3	3.12	132.19	125.95
47	7	702	ATP	C5-N7-C8	3.09	108.31	103.45
50	c	601	IHP	C5-C4-C3	3.05	117.13	110.43
48	C	1500	GTP	C2-N1-C6	-3.03	119.62	125.11
50	c	601	IHP	C6-C1-C2	-2.95	103.96	110.43
48	C	1500	GTP	N9-C8-N7	-2.73	108.34	113.40
48	C	1500	GTP	C5-C6-N1	2.68	120.07	113.25
48	C	1500	GTP	O6-C6-C5	-2.58	119.72	126.53
48	C	1500	GTP	C8-N7-C5	2.49	108.69	104.26
47	7	702	ATP	C4-N9-C8	2.43	108.29	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	c	601	IHP	C4-C3-C2	2.05	114.92	110.43
48	C	1500	GTP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	C	1500	GTP	C5'-O5'-PA-O3A
48	C	1500	GTP	C5'-O5'-PA-O1A
48	C	1500	GTP	C5'-O5'-PA-O2A
48	C	1500	GTP	C3'-C4'-C5'-O5'
48	C	1500	GTP	O4'-C4'-C5'-O5'
50	c	601	IHP	C5-O15-P5-O25
50	c	601	IHP	C1-O11-P1-O31
50	c	601	IHP	C2-O12-P2-O42
50	c	601	IHP	C6-O16-P6-O46
50	c	601	IHP	C1-O11-P1-O41
50	c	601	IHP	C6-O16-P6-O26

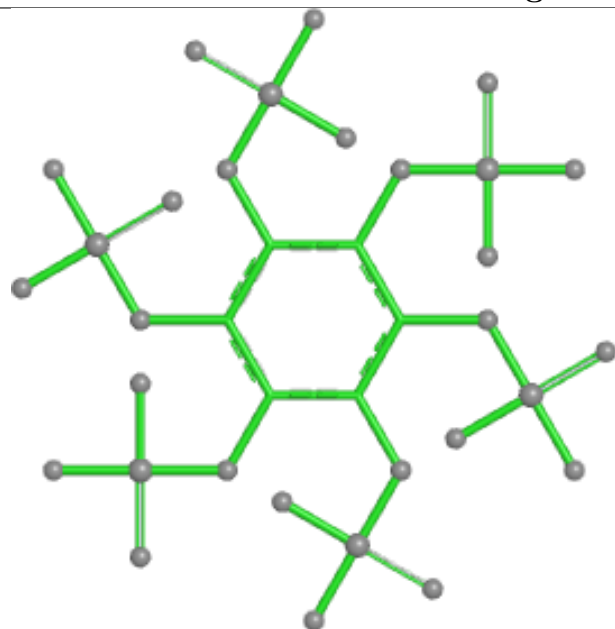
There are no ring outliers.

3 monomers are involved in 5 short contacts:

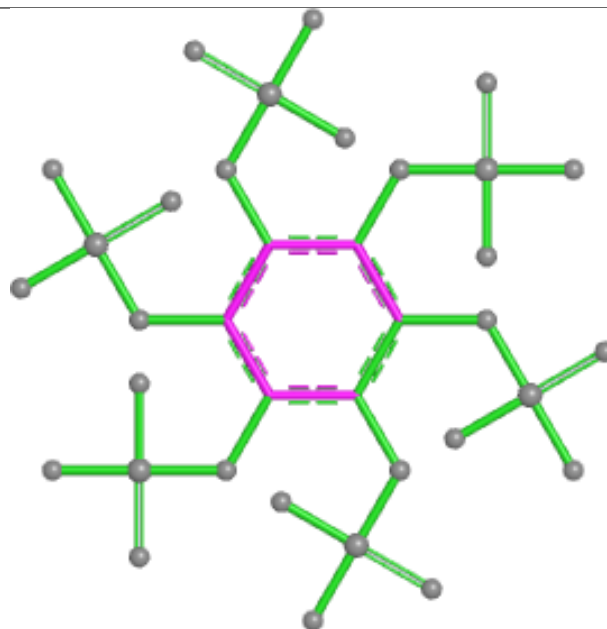
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	c	601	IHP	1	0
47	7	702	ATP	2	0
48	C	1500	GTP	2	0

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 than 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.

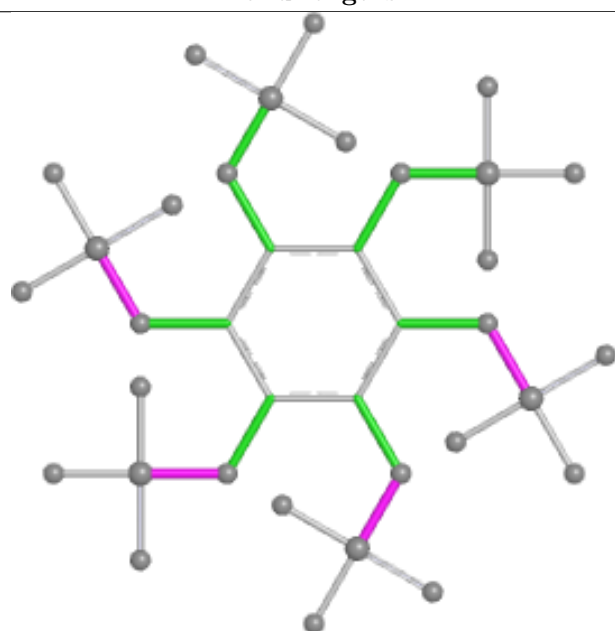
Ligand IHP c 601



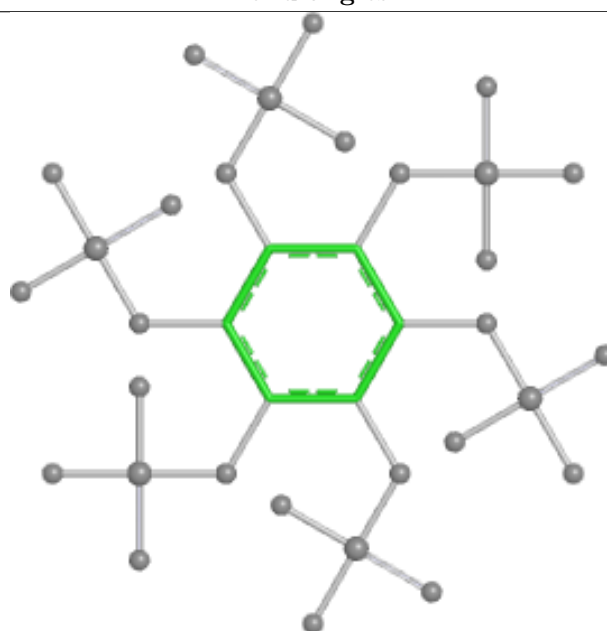
Bond lengths



Bond angles

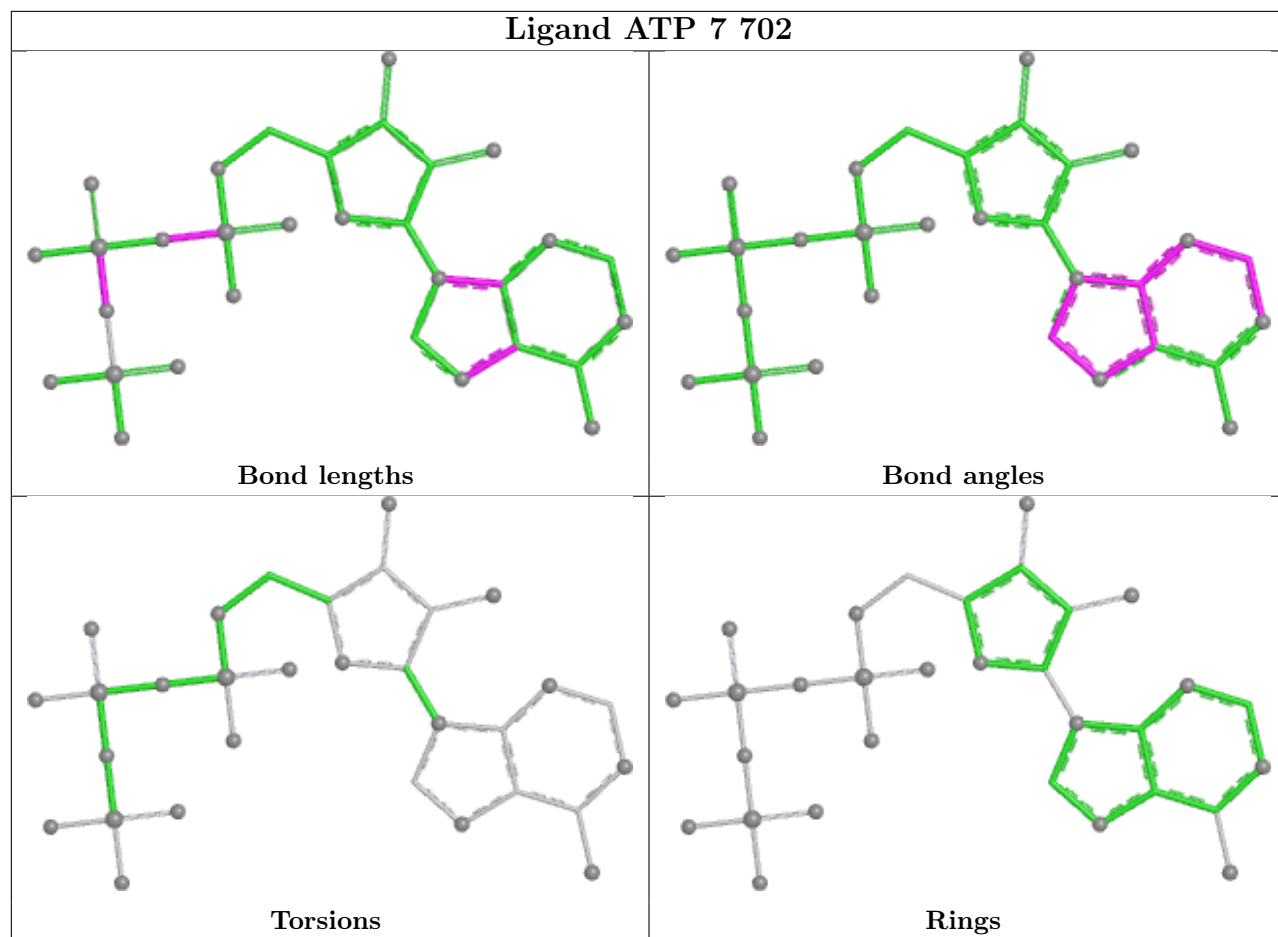


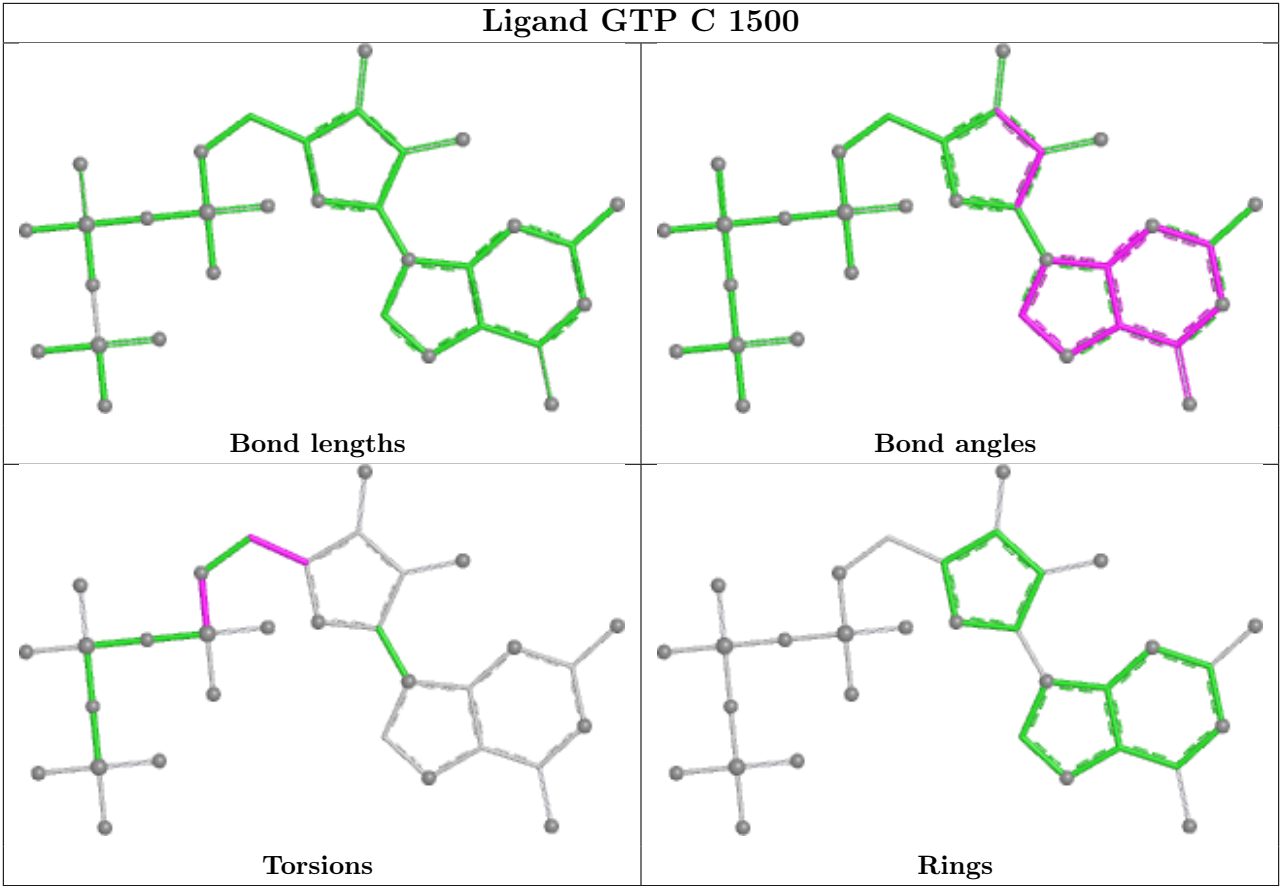
Torsions



Rings

Ligand ATP 7 702





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	83:A	O3'	84:U	P	83.48

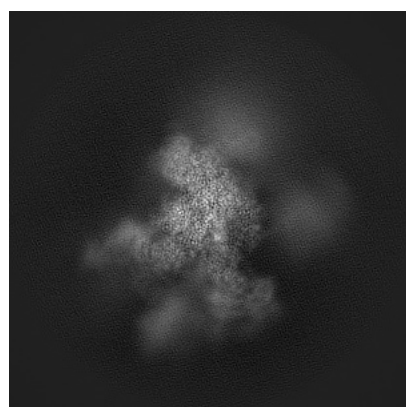
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

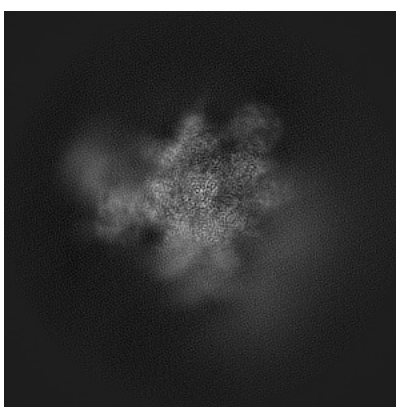
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

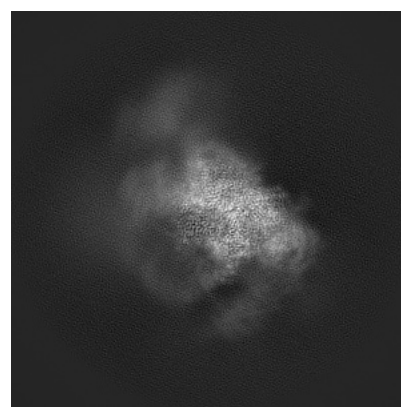
6.1.1 Primary map



X



Y

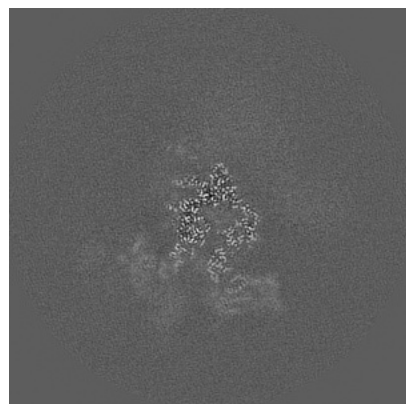


Z

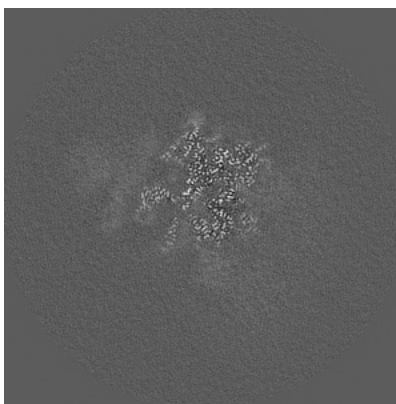
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

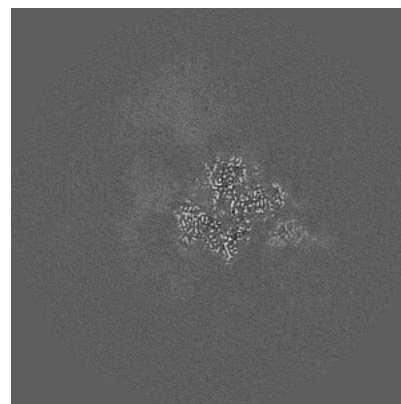
6.2.1 Primary map



X Index: 205



Y Index: 205

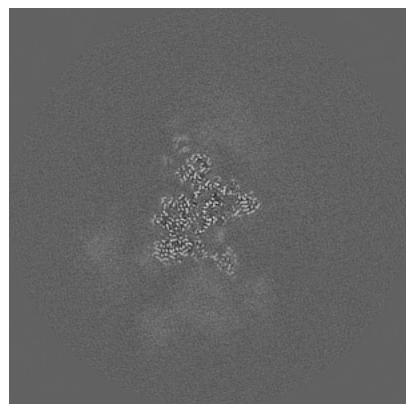


Z Index: 205

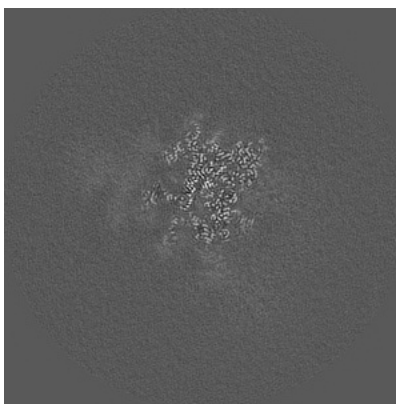
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

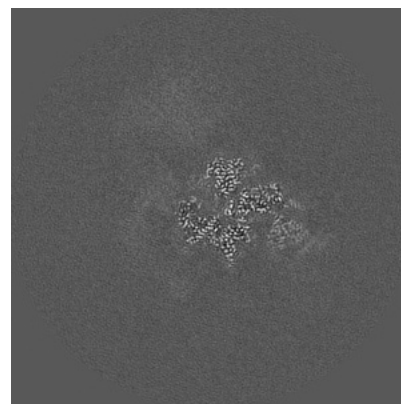
6.3.1 Primary map



X Index: 231



Y Index: 203

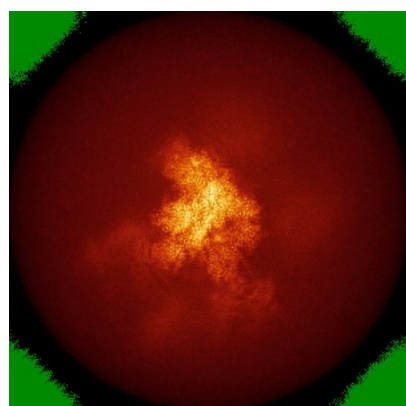


Z Index: 202

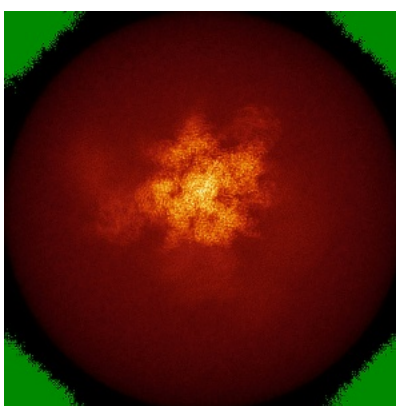
The images above show the largest variance slices of the map in three orthogonal directions.

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

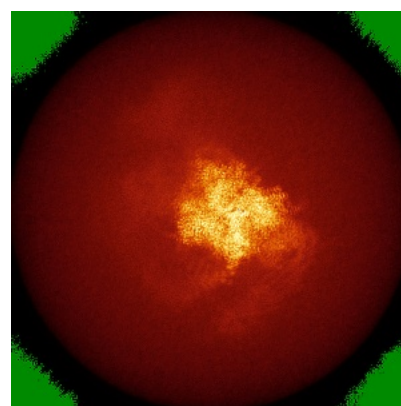
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

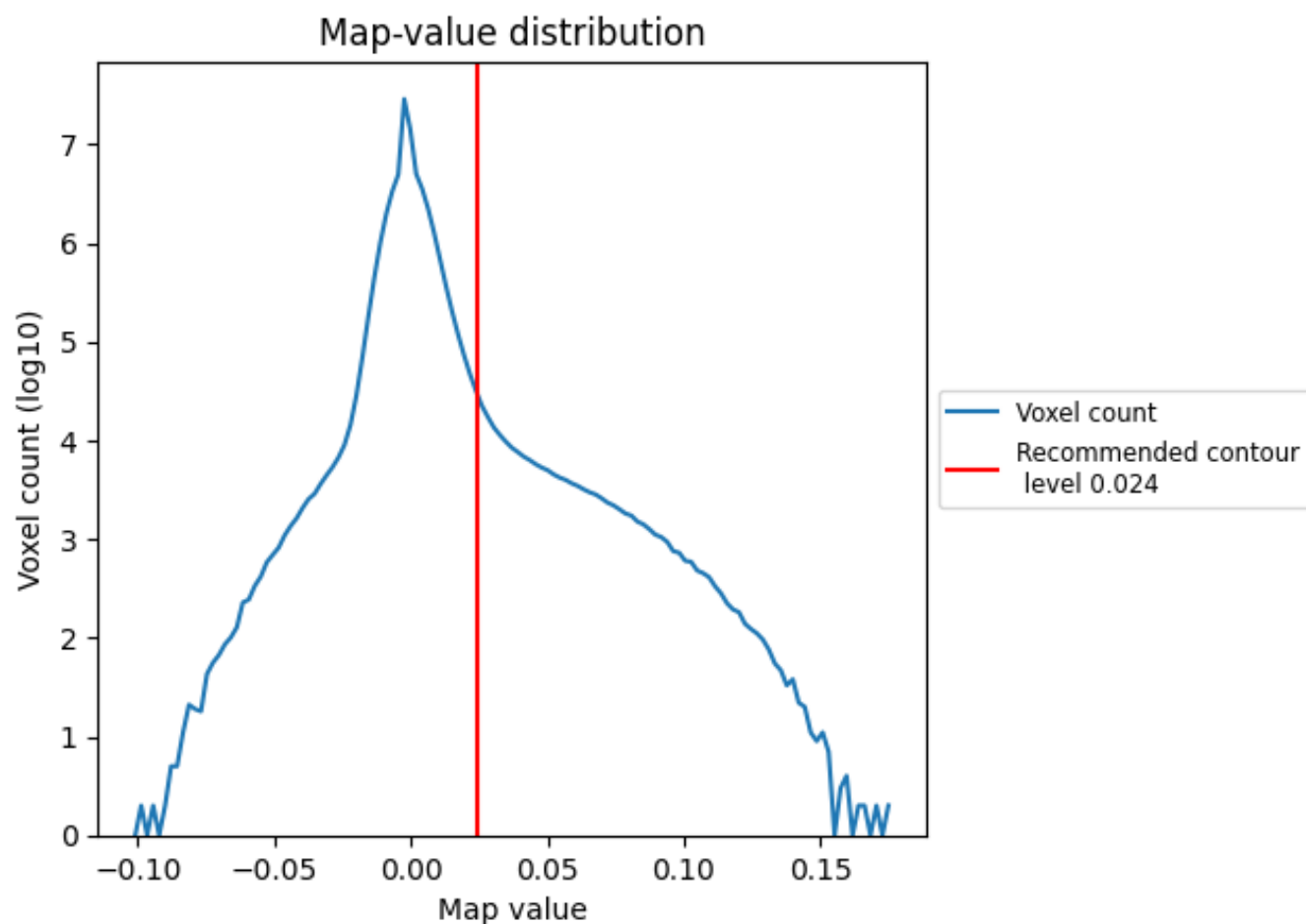
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

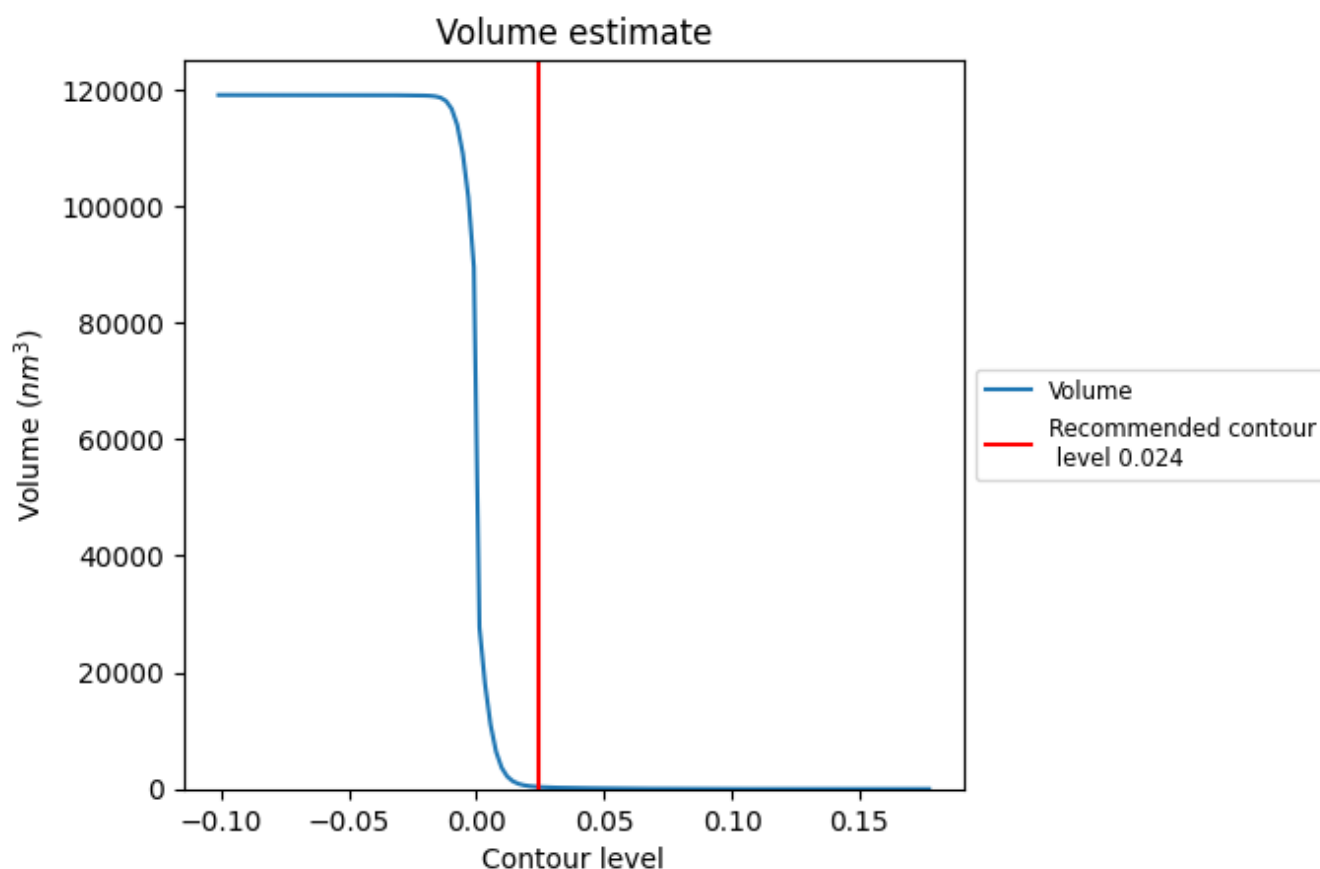
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

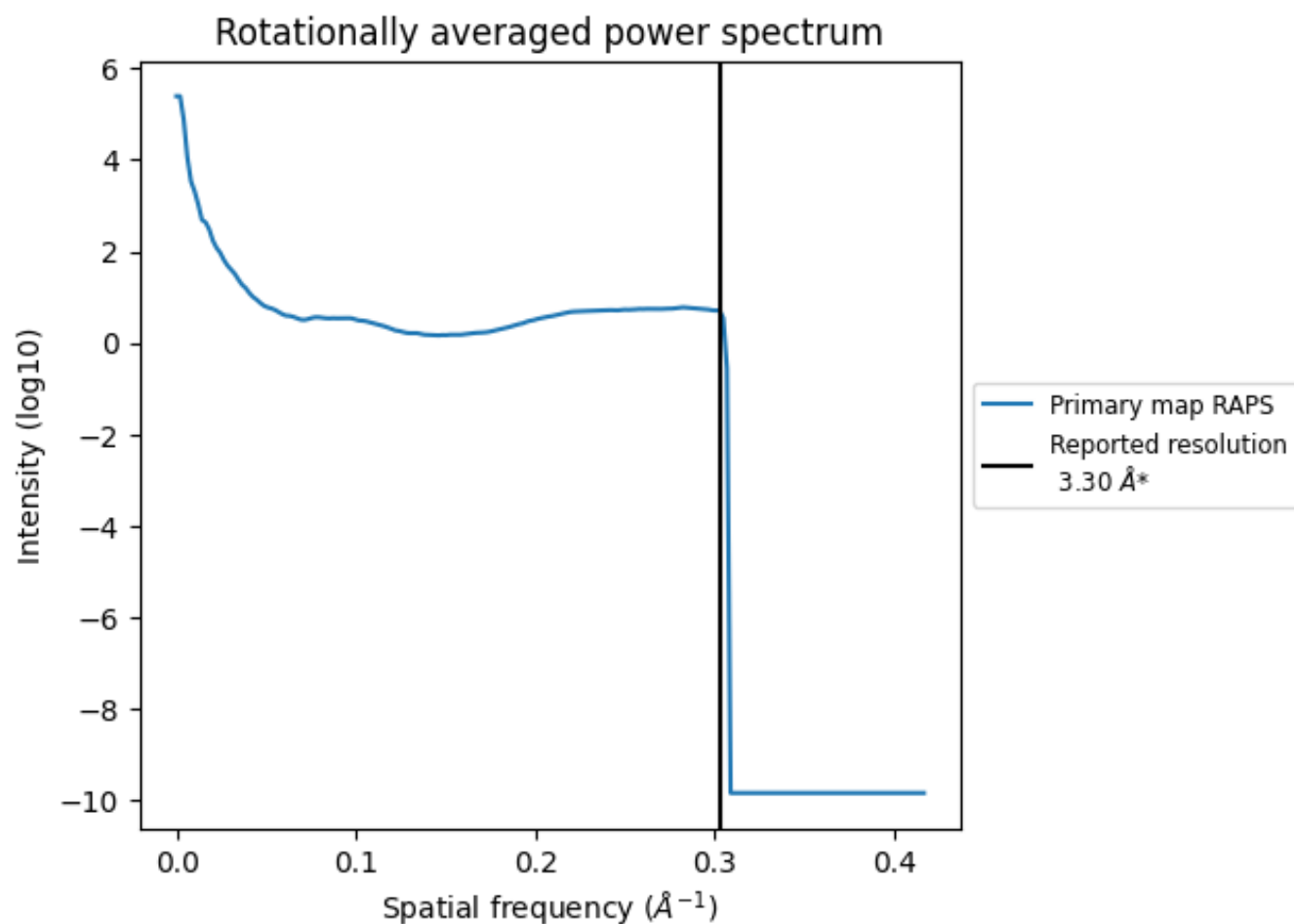
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

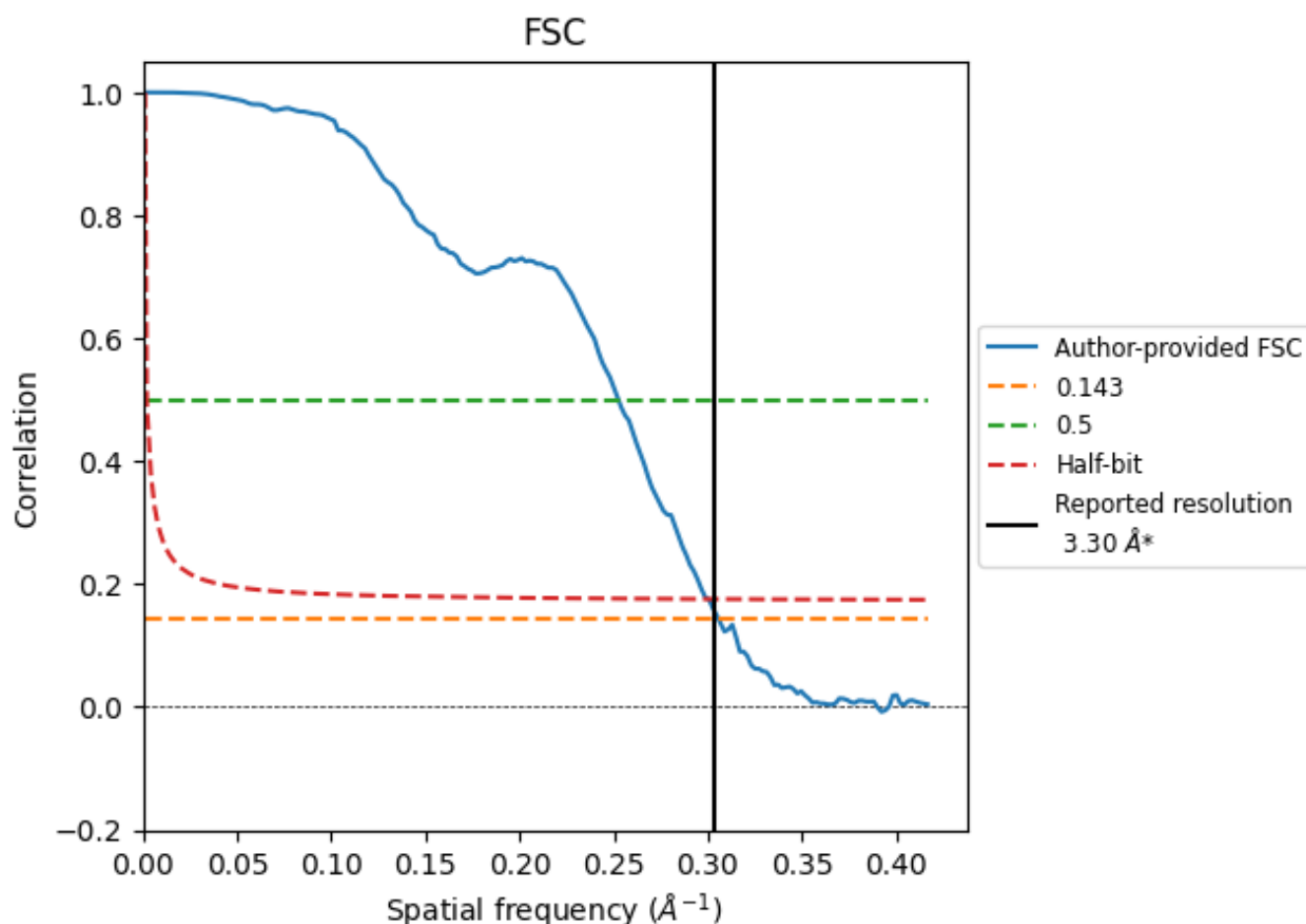


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

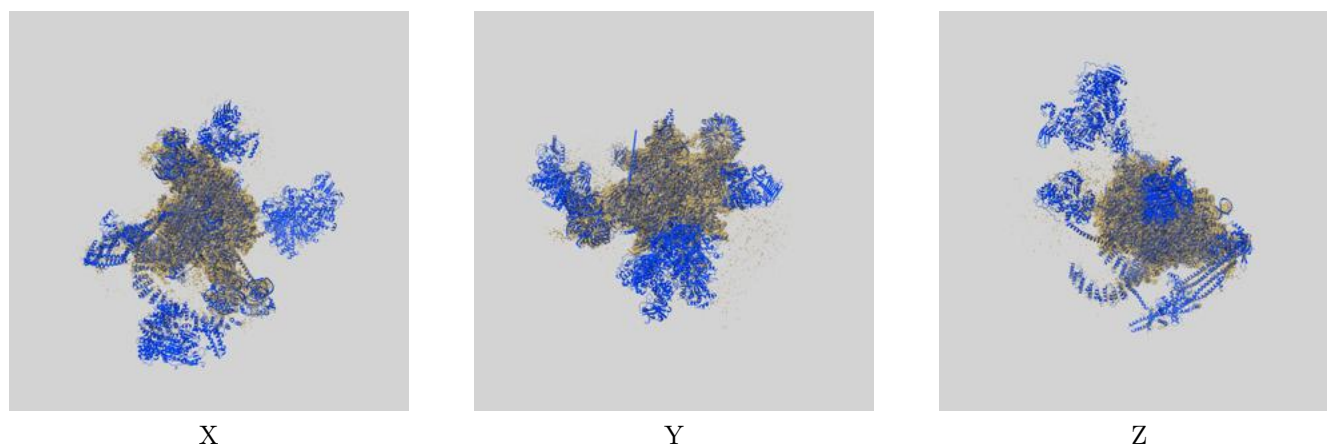
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

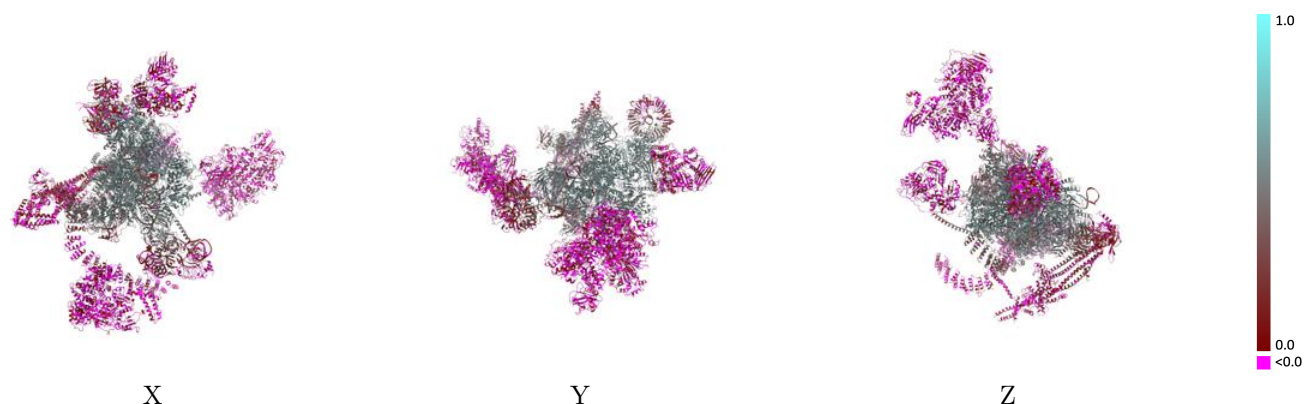
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 6QDV. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



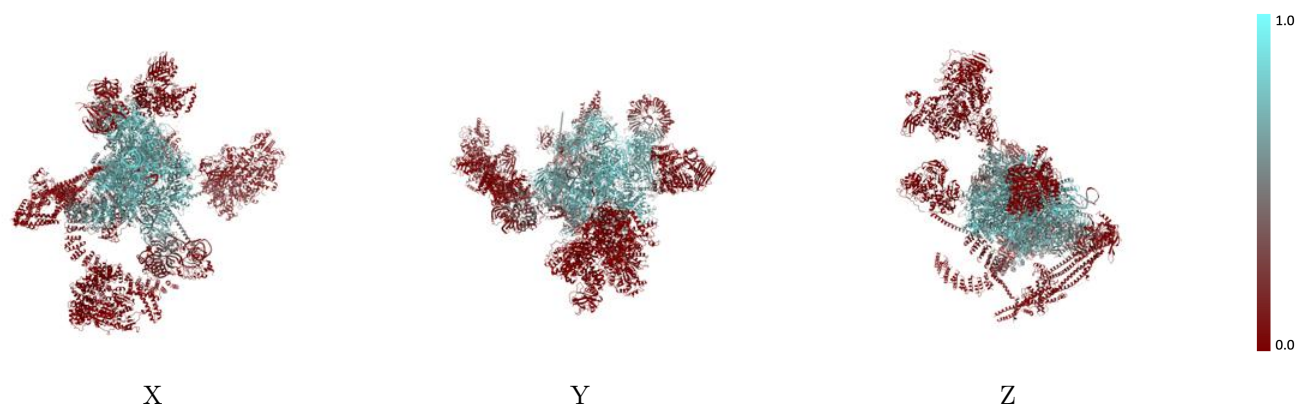
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



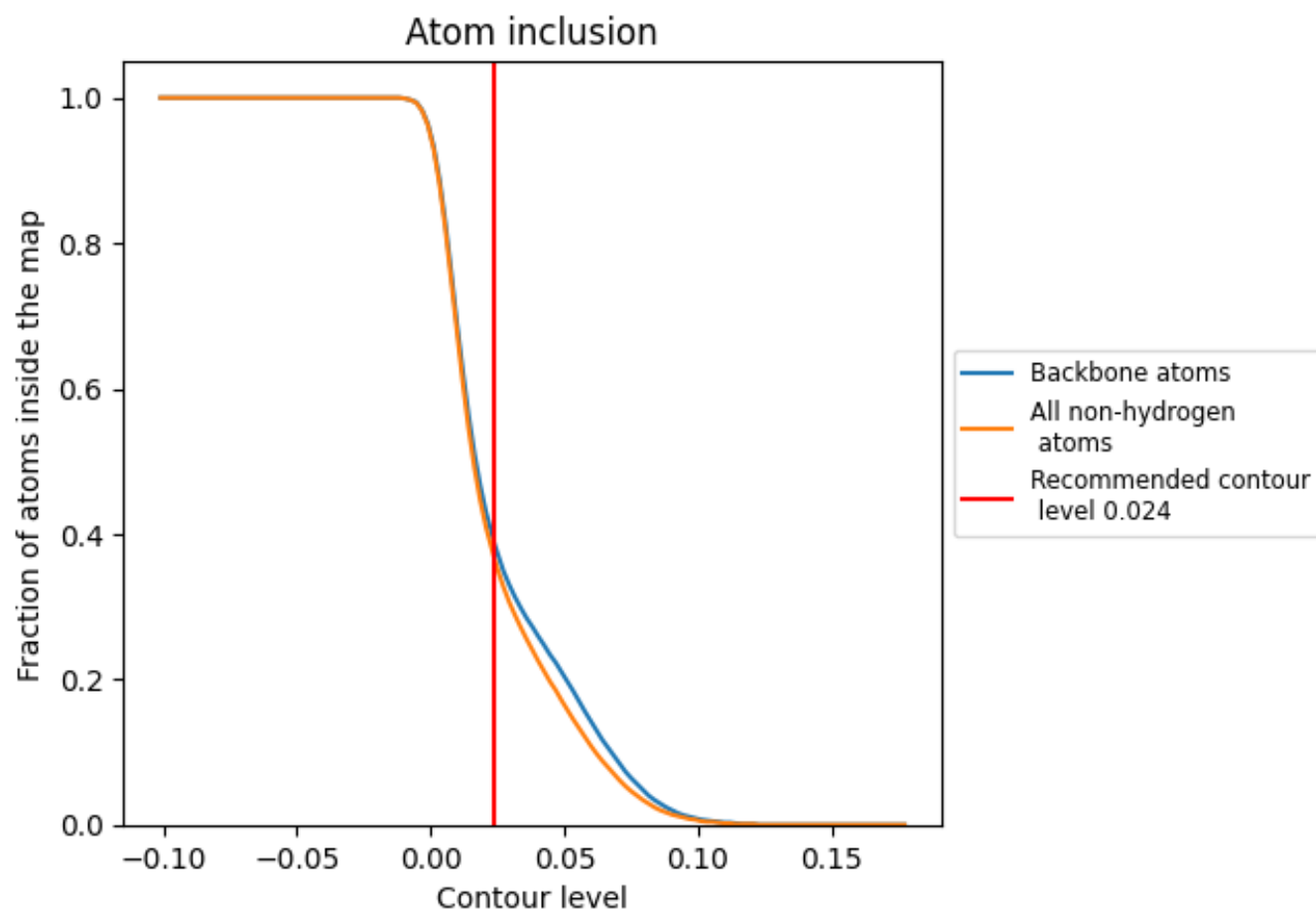
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3640	 0.2780
2	 0.4150	 0.2640
5	 0.7510	 0.4540
6	 0.7380	 0.4570
7	 0.0050	 0.0600
8	 0.0000	 -0.0230
9	 0.0000	 0.0230
A	 0.6840	 0.4780
B	 0.0010	 0.0020
C	 0.6850	 0.5010
D	 0.4080	 0.3490
E	 0.8410	 0.5300
F	 0.6280	 0.4670
G	 0.5770	 0.5060
H	 0.3250	 0.2530
I	 0.6040	 0.3950
J	 0.8350	 0.5600
K	 0.5780	 0.4700
L	 0.7400	 0.5240
M	 0.5150	 0.4410
N	 0.6240	 0.4720
O	 0.4300	 0.3550
P	 0.6530	 0.5150
R	 0.8340	 0.5500
S	 0.4420	 0.3340
T	 0.0660	 0.1560
U	 0.0010	 -0.0010
V	 0.0730	 0.0630
W	 0.0210	 0.0440
Y	 0.0480	 0.0930
Z	 0.6520	 0.5040
b	 0.2810	 0.2660
c	 0.6520	 0.4960
d	 0.4340	 0.3790
e	 0.0740	 0.1380



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Chain	Atom inclusion	Q-score
f	 0.0420	 0.1010
g	 0.2160	 0.2880
h	 0.1070	 0.1720
i	 0.5730	 0.4500
j	 0.0500	 0.0950
k	 0.2060	 0.2370
l	 0.1230	 0.1500
m	 0.0610	 0.0830
n	 0.3690	 0.3190
o	 0.6620	 0.4960
p	 0.2240	 0.2290
q	 0.1140	 0.1190
r	 0.3480	 0.3330
s	 0.0730	 0.1200
t	 0.0260	 0.0690
u	 0.0160	 0.0240
v	 0.0240	 0.1160
w	 0.0100	 0.0760
y	 0.6400	 0.4900
z	 0.0110	 0.1960