



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:49 AM UTC

PDB ID : 7DVQ / pdb_00007dvq
EMDB ID : EMD-30875
Title : Cryo-EM Structure of the Activated Human Minor Spliceosome (minor Bact Complex)
Authors : Bai, R.; Wan, R.; Wang, L.; Xu, K.; Zhang, Q.; Lei, J.; Shi, Y.
Deposited on : 2021-01-14
Resolution : 2.89 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:

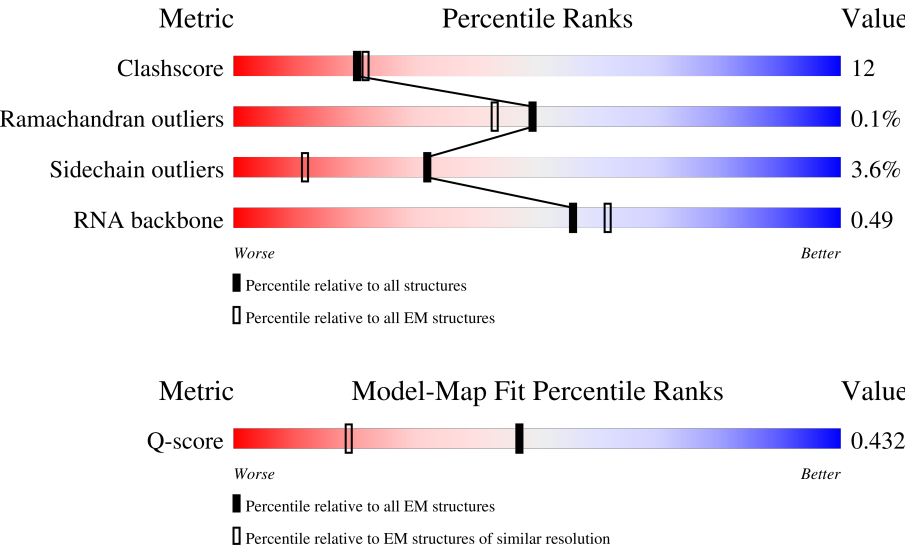
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.89 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	12148 (2.39 - 3.39)

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	A	2335	11% 77% 17% • 5%
2	B	117	24% 40% 30% 7% 23%
3	C	972	• 74% 18% • 7%

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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	a	126	
6	h	126	
7	b	240	
7	i	240	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	124	
14	G	142	
15	H	150	
16	v	230	
17	1	1304	
18	2	895	
19	3	1217	
20	4	424	
21	5	125	

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Mol	Chain	Length	Quality of chain
22	6	110	
23	7	86	
24	L	802	
25	J	848	
26	P	229	
27	R	536	
28	T	514	
29	X	396	
30	Y	322	
31	Z	619	
32	9	520	
33	z	472	
34	x	1041	
35	y	476	
36	M	343	
37	U	2752	
38	V	908	
39	8	904	
40	0	101	
41	I	367	
42	K	198	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 99906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2223	Total	C	N	O	S	0	0
			18354	11832	3206	3236	80		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	90	Total	C	N	O	P	0	0
			1898	850	320	638	90		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	902	Total	C	N	O	S	0	0
			7125	4560	1185	1345	35		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1803	Total	C	N	O	S	0	0
			9215	5522	1841	1851	1		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	299	Total	C	N	O	S	0	0
			2337	1470	409	445	13		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	a	81	Total	C	N	O	0	0
			399	237	81	81		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	h	80	Total	C	N	O	0	0
			392	233	79	80		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	82	Total	C	N	O	0	0
			405	241	82	82		
7	i	86	Total	C	N	O	0	0
			422	250	86	86		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	c	82	Total	C	N	O	0	0
			406	242	82	82		
8	j	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	d	97	Total	C	N	O	0	0
			480	286	97	97		
9	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	f	74	Total	C	N	O	0	0
			361	213	74	74		
10	m	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	79	Total	C	N	O	0	0
			391	233	79	79		
11	l	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	g	74	Total	C	N	O	0	0
			363	215	74	74		
12	n	68	Total	C	N	O	0	0
			334	198	68	68		

- Molecule 13 is a RNA chain called U6atac snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	60	Total	C	N	O	P	0	0
			1294	577	242	415	60		

- Molecule 14 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	63	Total	C	N	O	P	0	0
			1303	585	197	458	63		

- Molecule 15 is a RNA chain called U12 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	63	Total	C	N	O	P	0	0
			1350	604	247	436	63		

- Molecule 16 is a protein called Sodium channel modifier 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	v	119	Total	C	N	O	S	0	0
			963	601	179	178	5		

- Molecule 17 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	1	986	Total	C	N	O	P	S	0	0
			7879	5035	1361	1435	1	47		

- Molecule 18 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	216	Total	C	N	O	S	0	0
			1674	1067	296	305	6		

- Molecule 19 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	1193	Total	C	N	O	P	S	
			9352	5932	1590	1784	1	45	
								0	0

- Molecule 20 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	4	78	Total	C	N	O		
			383	227	78	78		
							0	0

- Molecule 21 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	109	Total	C	N	O	S		
			906	582	157	163	4		
								0	0

- Molecule 22 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	105	Total	C	N	O	S		
			811	502	145	151	13		
								0	0

- Molecule 23 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7	81	Total	C	N	O	S		
			669	422	117	124	6		
								0	0

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	101	Total	C	N	O	S		
			843	540	152	147	4		
								0	0

- Molecule 25 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	522	Total	C	N	O	S		
			3457	2153	654	645	5		
								0	0

- Molecule 26 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	44	Total	C	N	O	S	0	0
			384	243	71	68	2		

- Molecule 27 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	241	Total	C	N	O	S	0	0
			1923	1191	347	374	11		

- Molecule 28 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 29 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	156	Total	C	N	O	S	0	0
			1271	815	227	227	2		

- Molecule 30 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	140	Total	C	N	O	S	0	0
			1095	692	192	206	5		

- Molecule 31 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	140	Total	C	N	O	S	0	0
			1129	703	214	207	5		

- Molecule 32 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	409	Total	C	N	O	S	0	0
			2691	1672	487	525	7		

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	177	Total	C	N	O	S	0	0
			1400	883	245	267	5		

- Molecule 34 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	x	599	Total	C	N	O	S	0	0
			3007	1794	607	605	1		

- Molecule 35 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	y	13	Total	C	N	O	0	0
			105	66	22	17		

- Molecule 36 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	191	Total	C	N	O	S	0	0
			1572	983	282	295	12		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 38 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	468	Total	C	N	O	S	0	0
			3008	1873	548	574	13		

- Molecule 39 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	126	Total	C	N	O	S	0	0
			1011	652	168	185	6		

- Molecule 40 is a protein called Cysteine-rich PDZ-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	0	100	Total	C	N	O	S	0	0
			770	475	142	144	9		

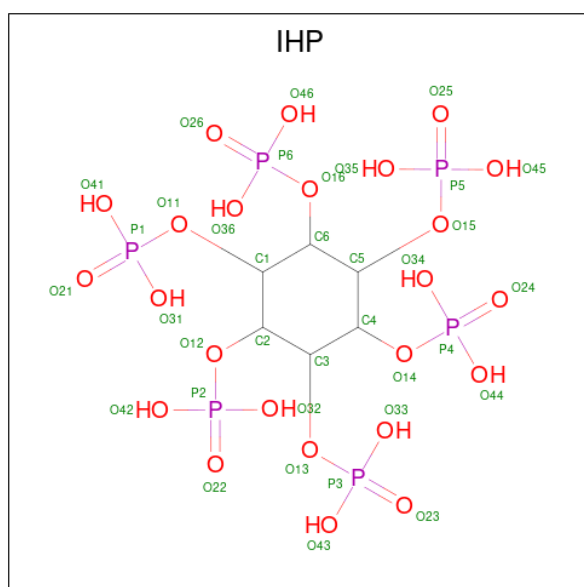
- Molecule 41 is a protein called RNA-binding protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	128	Total	C	N	O	S	0	0
			1062	683	184	190	5		

- Molecule 42 is a protein called Armadillo repeat-containing protein 7.

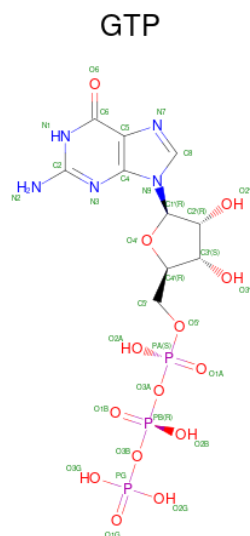
Mol	Chain	Residues	Atoms					AltConf	Trace
42	K	188	Total	C	N	O	S	0	0
			1314	824	229	256	5		

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
43	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

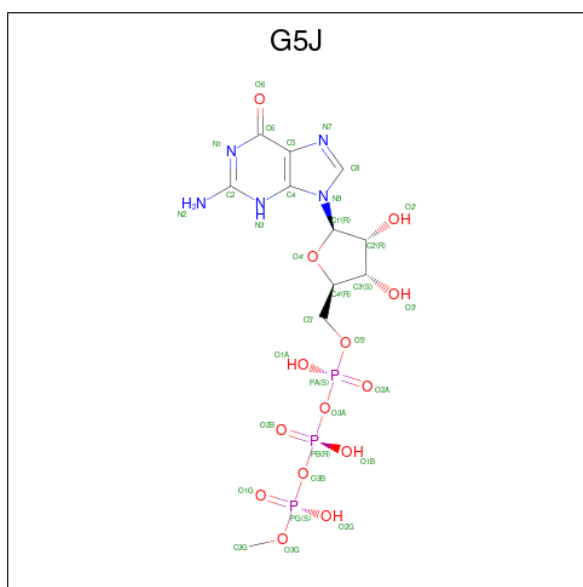
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
45	C	1	Total Mg 1 1	0
45	F	4	Total Mg 4 4	0

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	F	2	Total 2	K 2	0

- Molecule 47 is 5'-O-[(S)-hydroxy{[(R)-hydroxy{[(S)-hydroxy(methoxy)phosphoryl]oxy}phosphoryl]oxy}phosphoryl]guanosine (CCD ID: G5J) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
47	F	1	Total 33	C 11	N 5	O 14	P 3	0

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
48	v	1	Total Zn 1 1	0
48	6	3	Total Zn 3 3	0
48	M	1	Total Zn 1 1	0
48	0	2	Total Zn 2 2	0

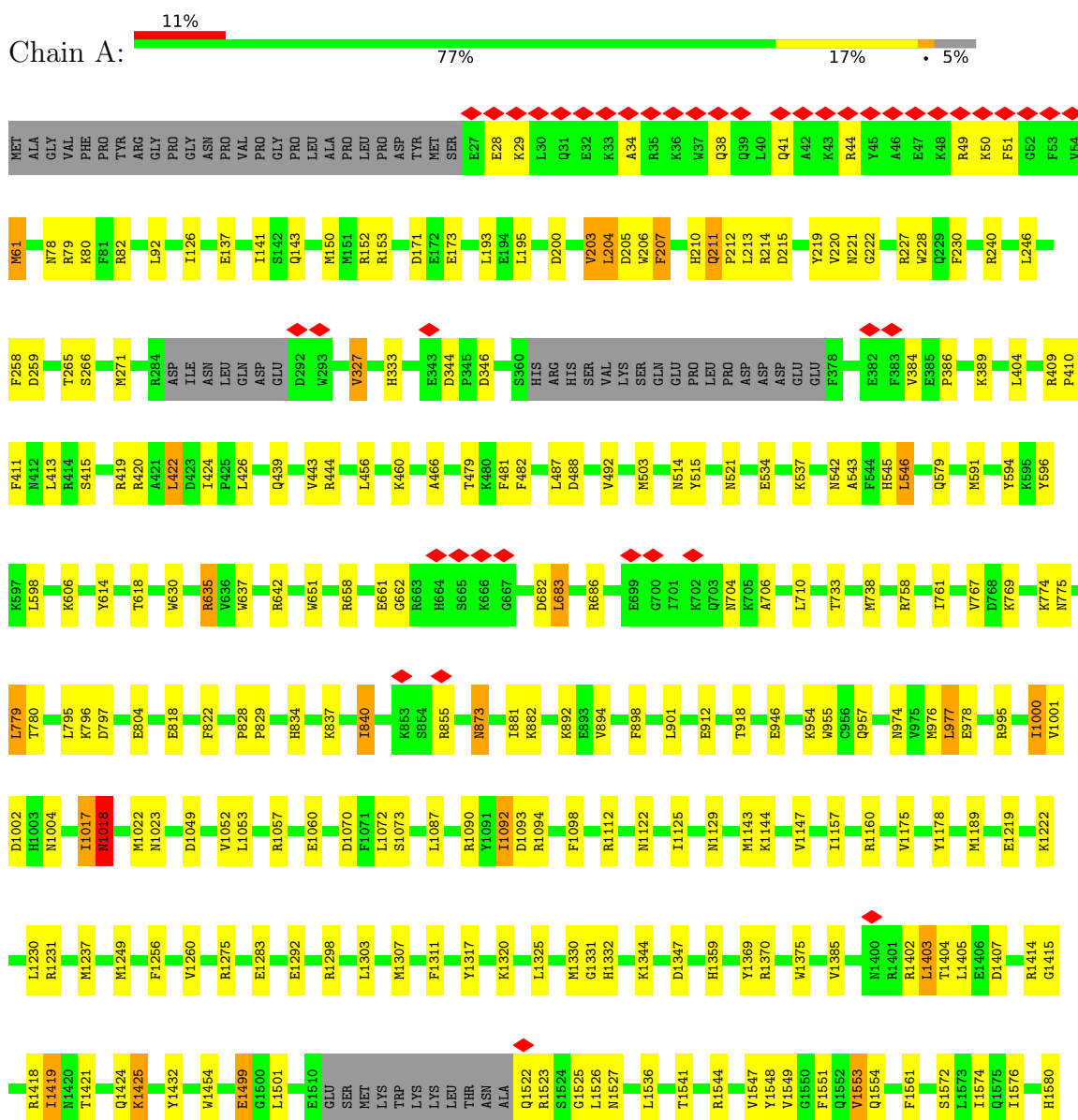
- Molecule 49 is water.

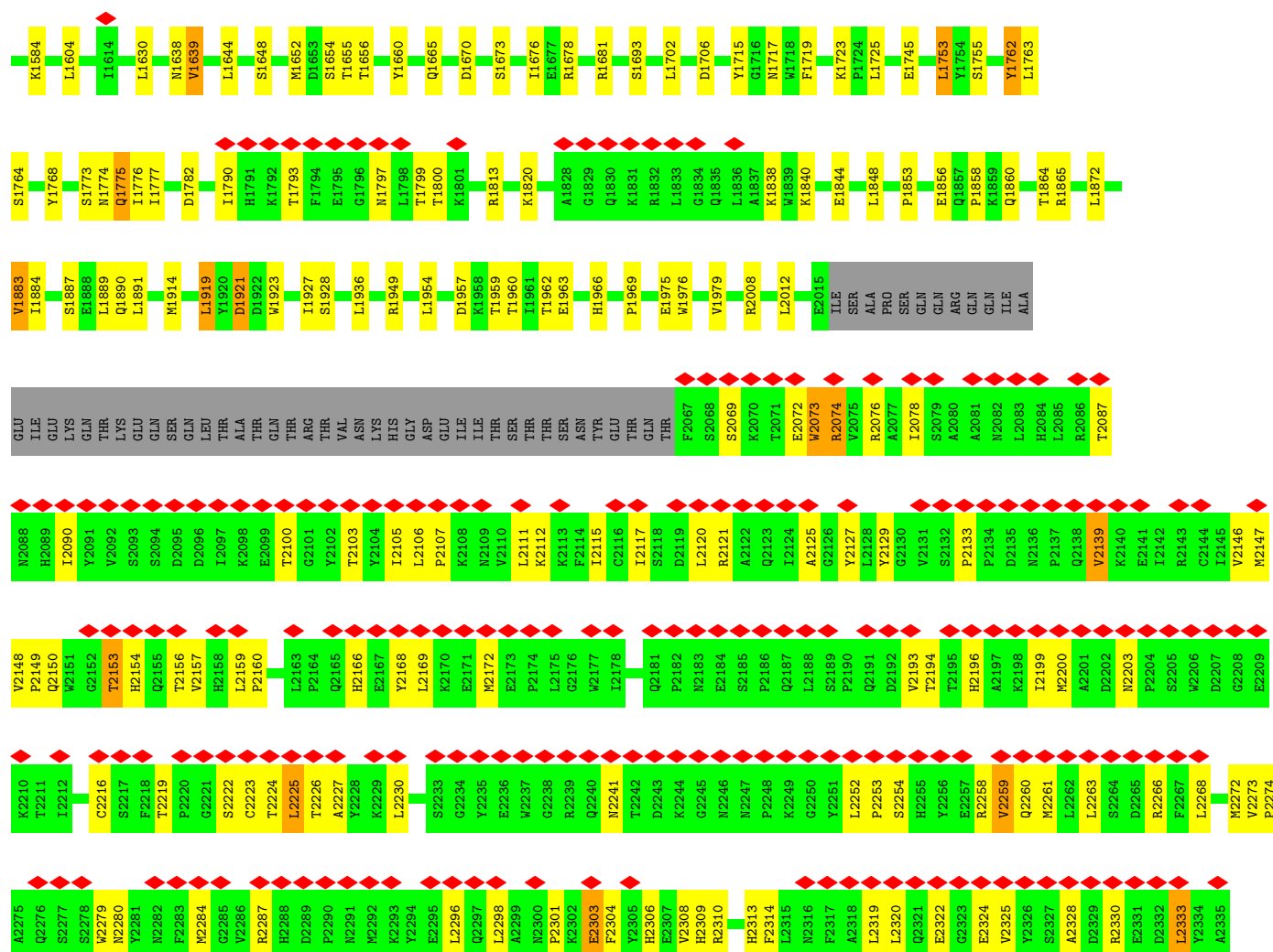
Mol	Chain	Residues	Atoms	AltConf
49	C	3	Total O 3 3	0

3 Residue-property plots

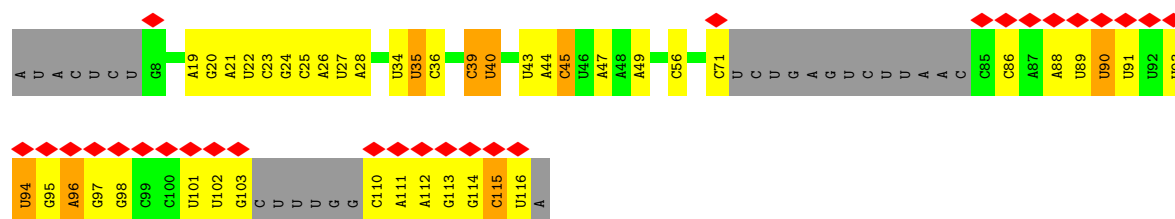
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Pre-mRNA-processing-splicing factor 8

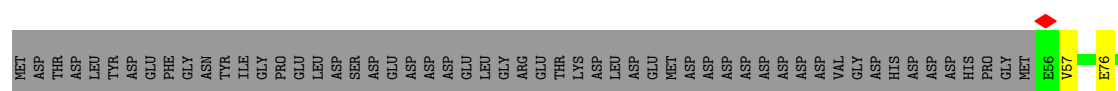
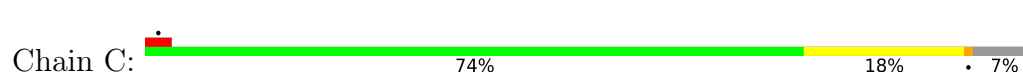




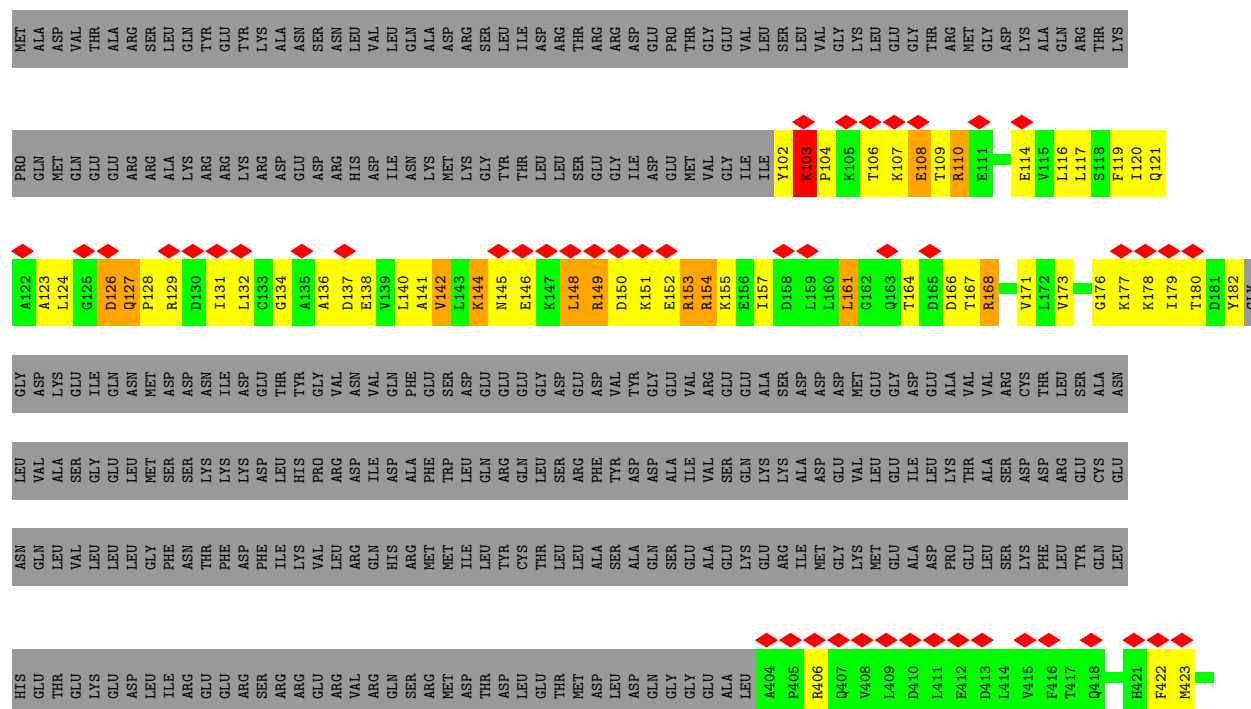
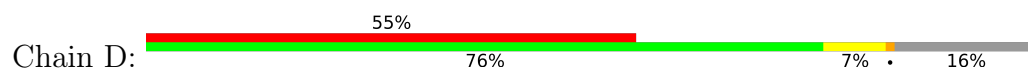
• Molecule 2: U5 snRNA



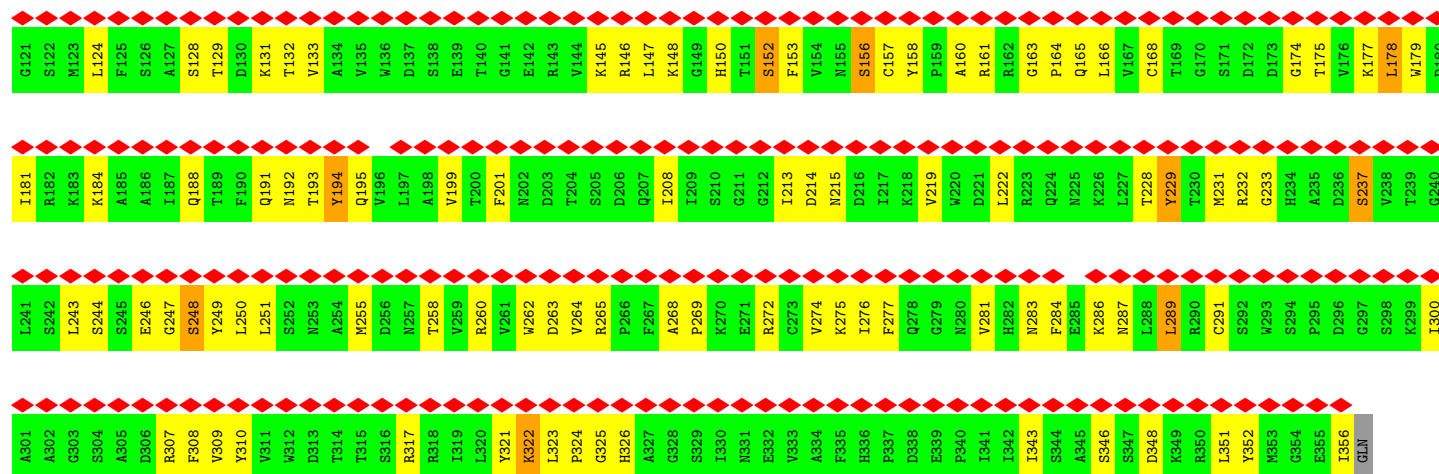
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component



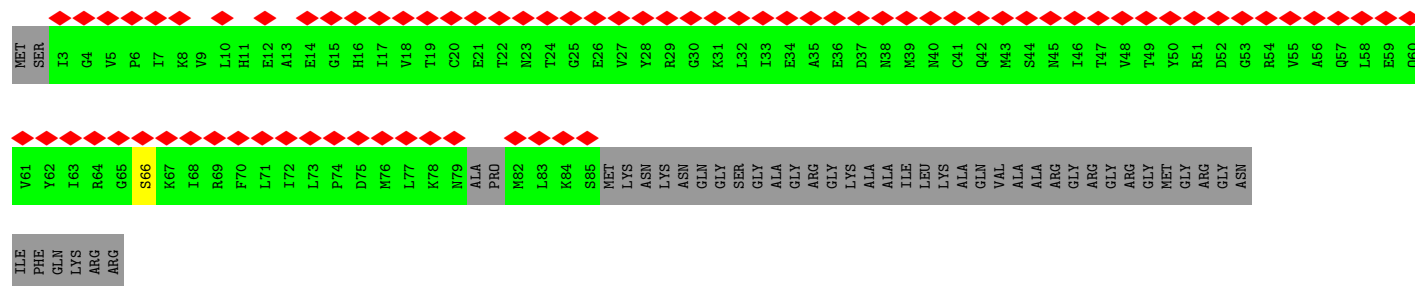
- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase



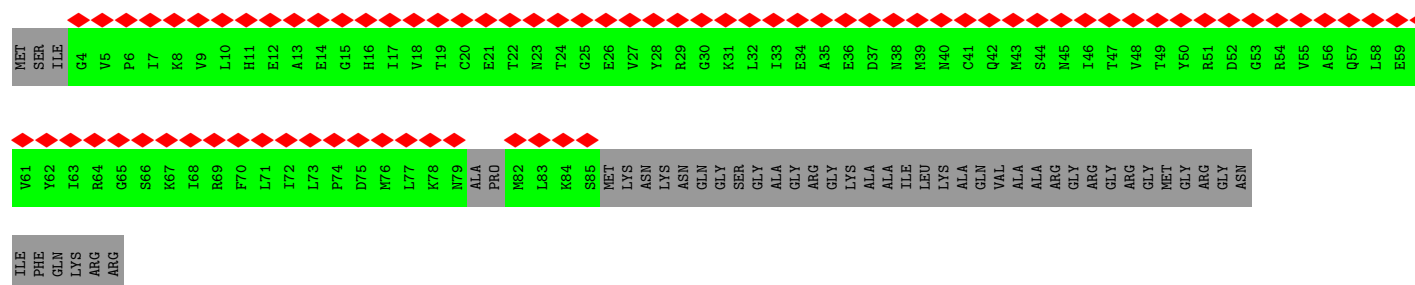




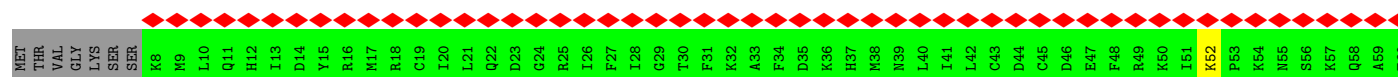
• Molecule 6: Small nuclear ribonucleoprotein Sm D3



• Molecule 6: Small nuclear ribonucleoprotein Sm D3

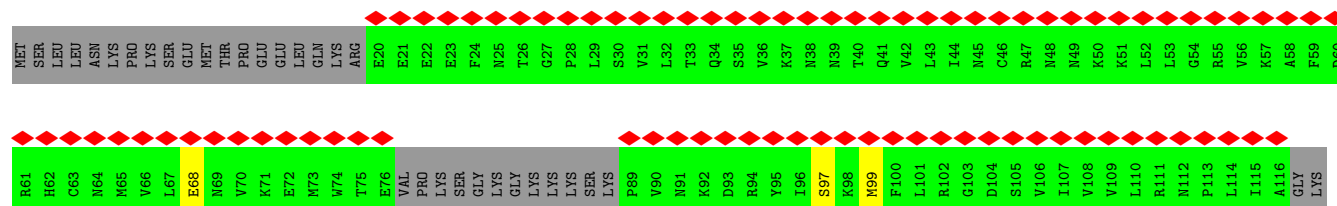


• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

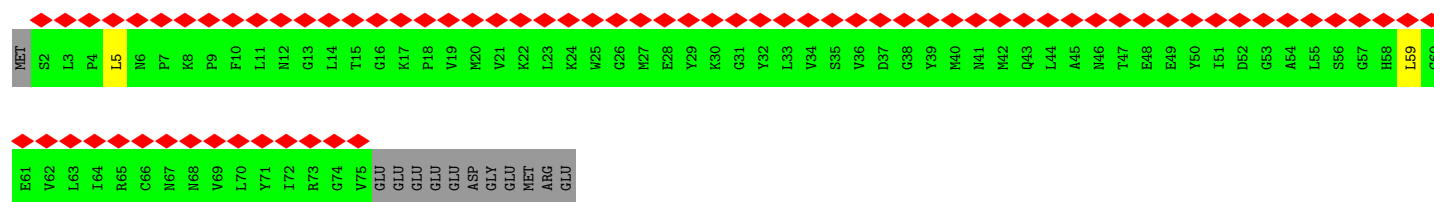
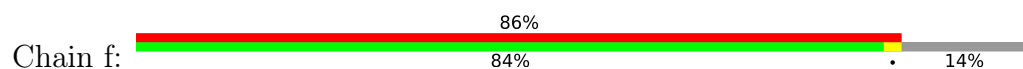




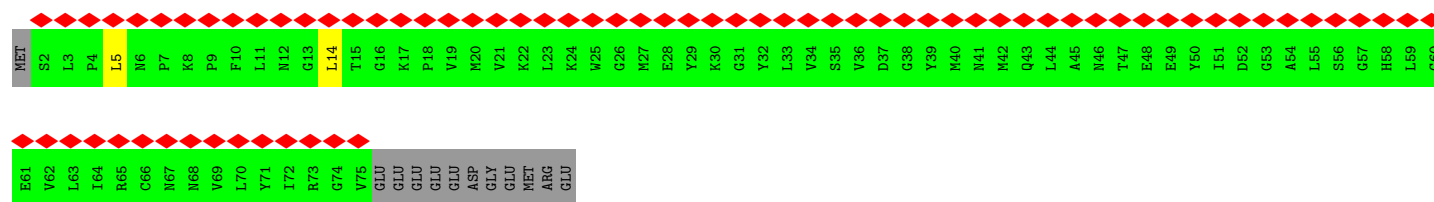
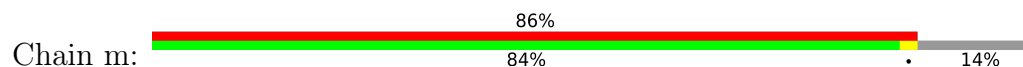
• Molecule 9: Small nuclear ribonucleoprotein Sm D2



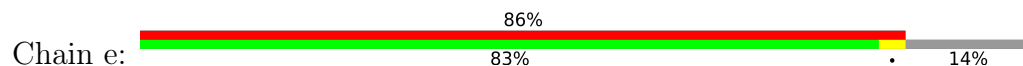
• Molecule 10: Small nuclear ribonucleoprotein F



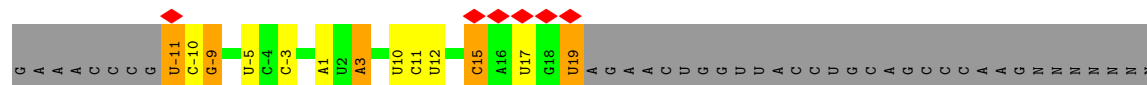
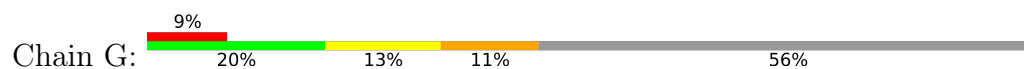
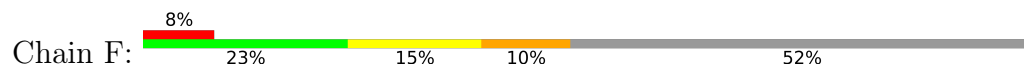
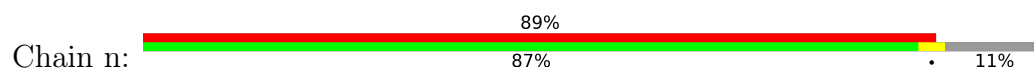
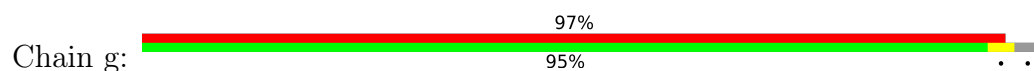
• Molecule 10: Small nuclear ribonucleoprotein F



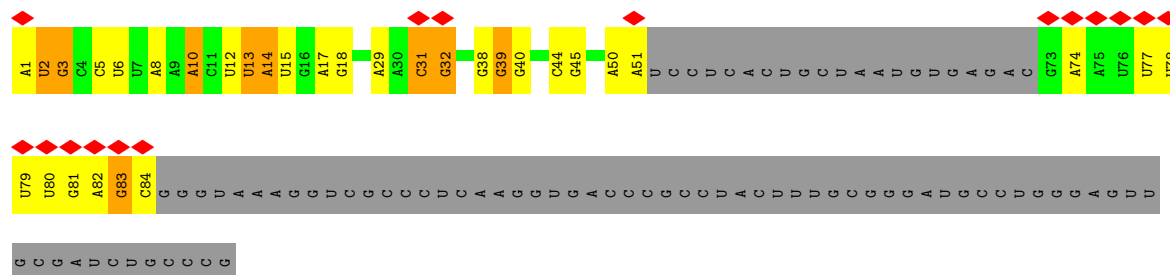
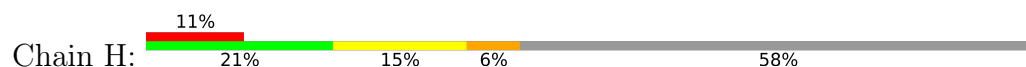
• Molecule 11: Small nuclear ribonucleoprotein E



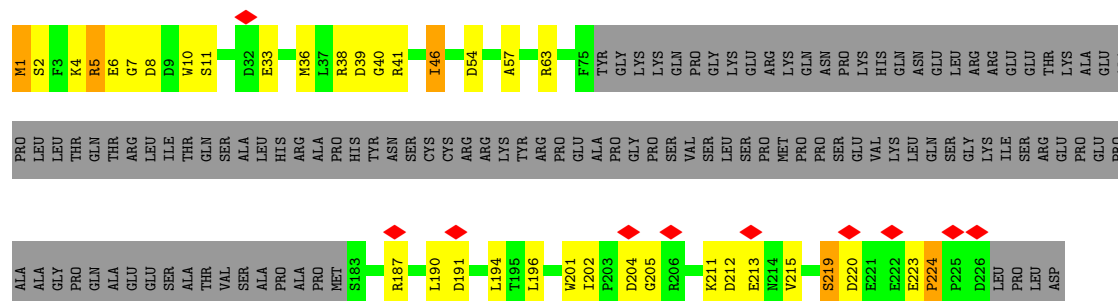
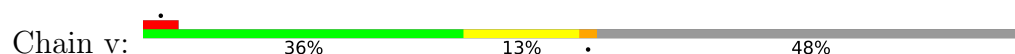
Chain 1: 86% 84% 14%



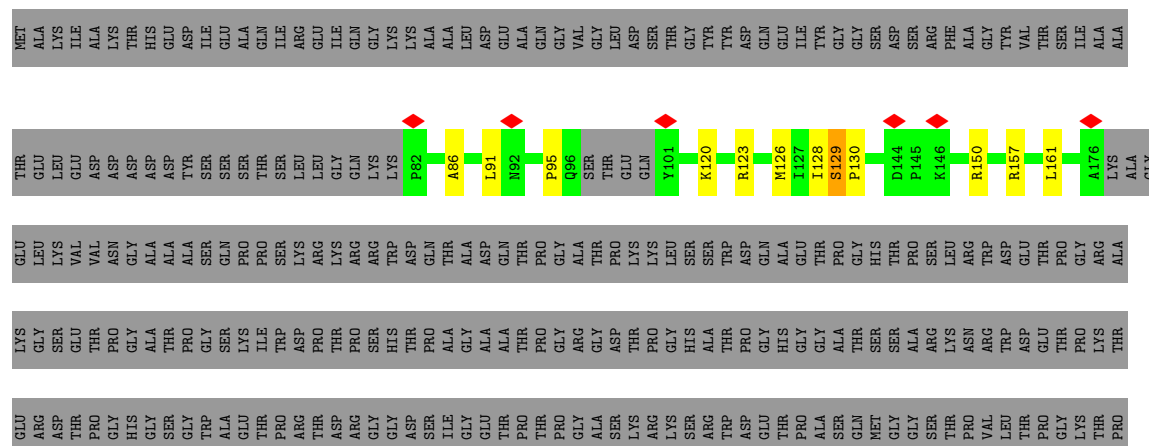
- Molecule 15: U12 snRNA

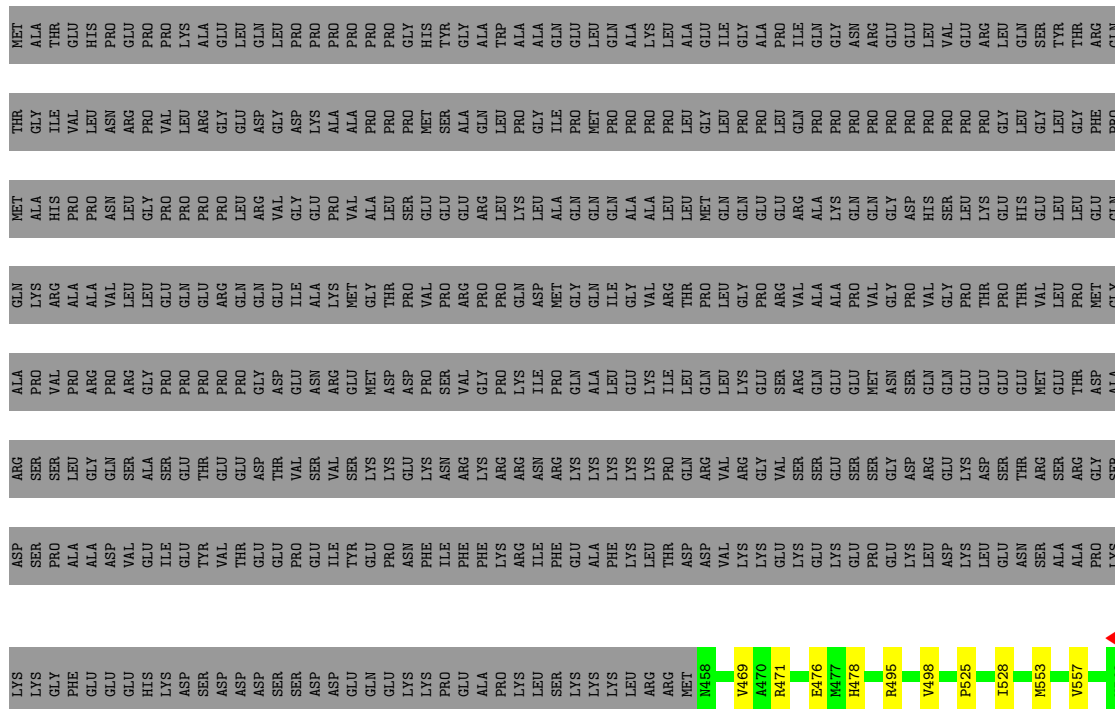


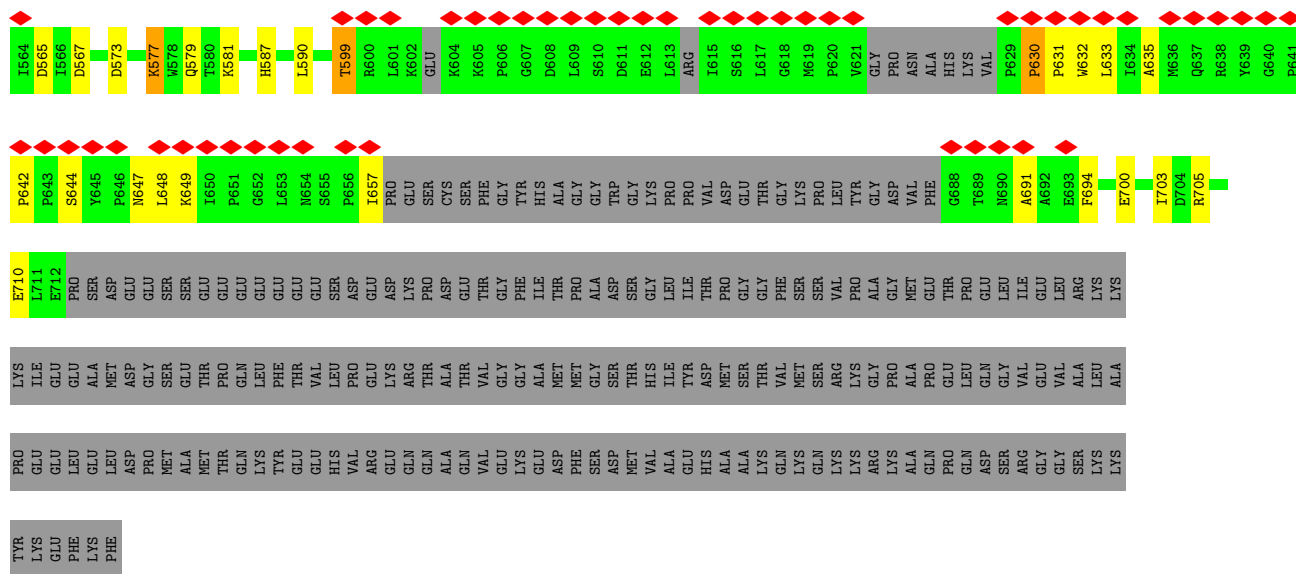
- Molecule 16: Sodium channel modifier 1



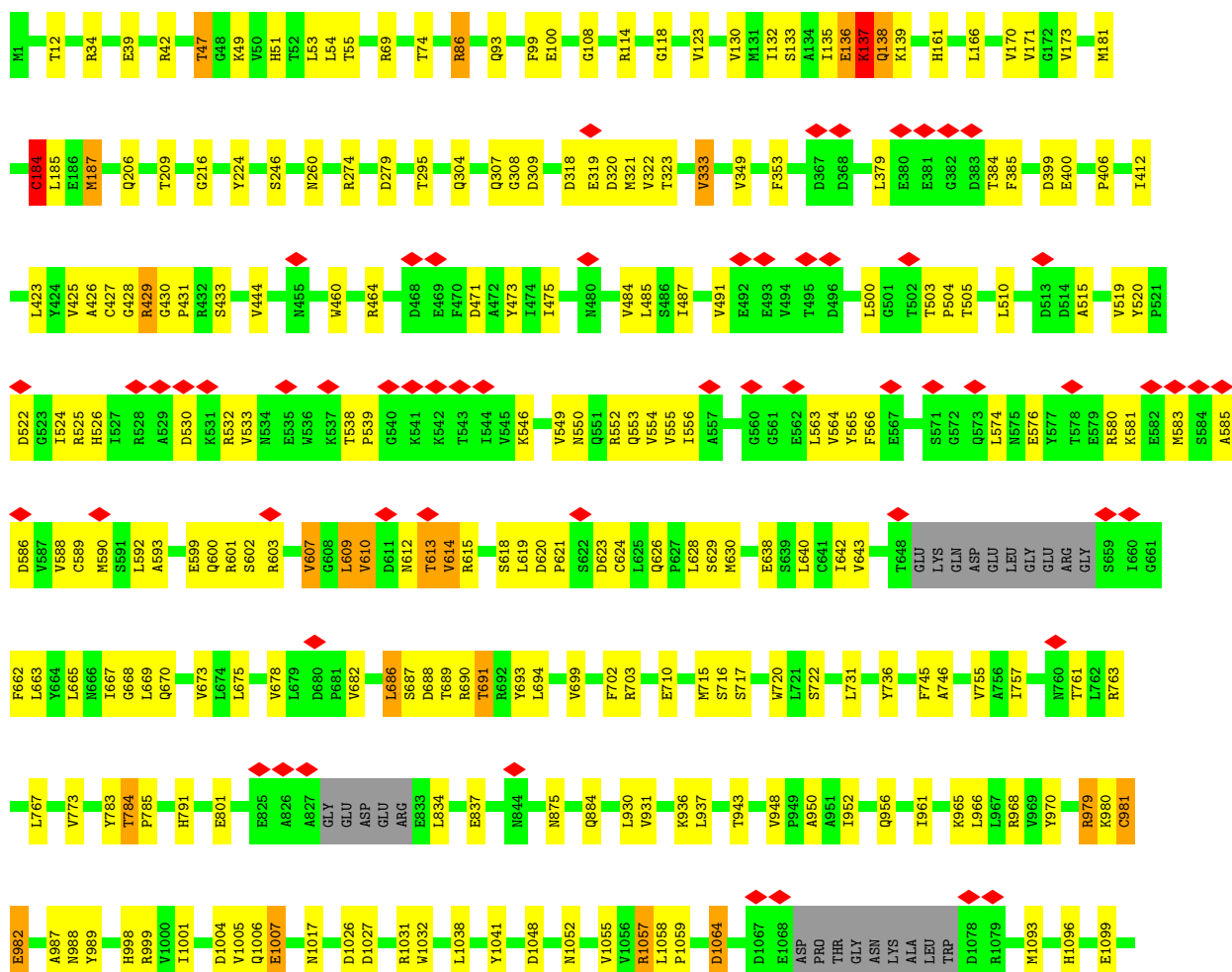
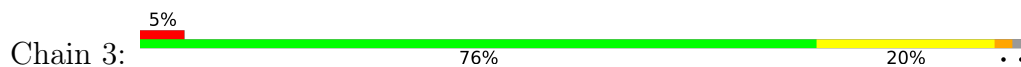
- Molecule 17: Splicing factor 3B subunit 1





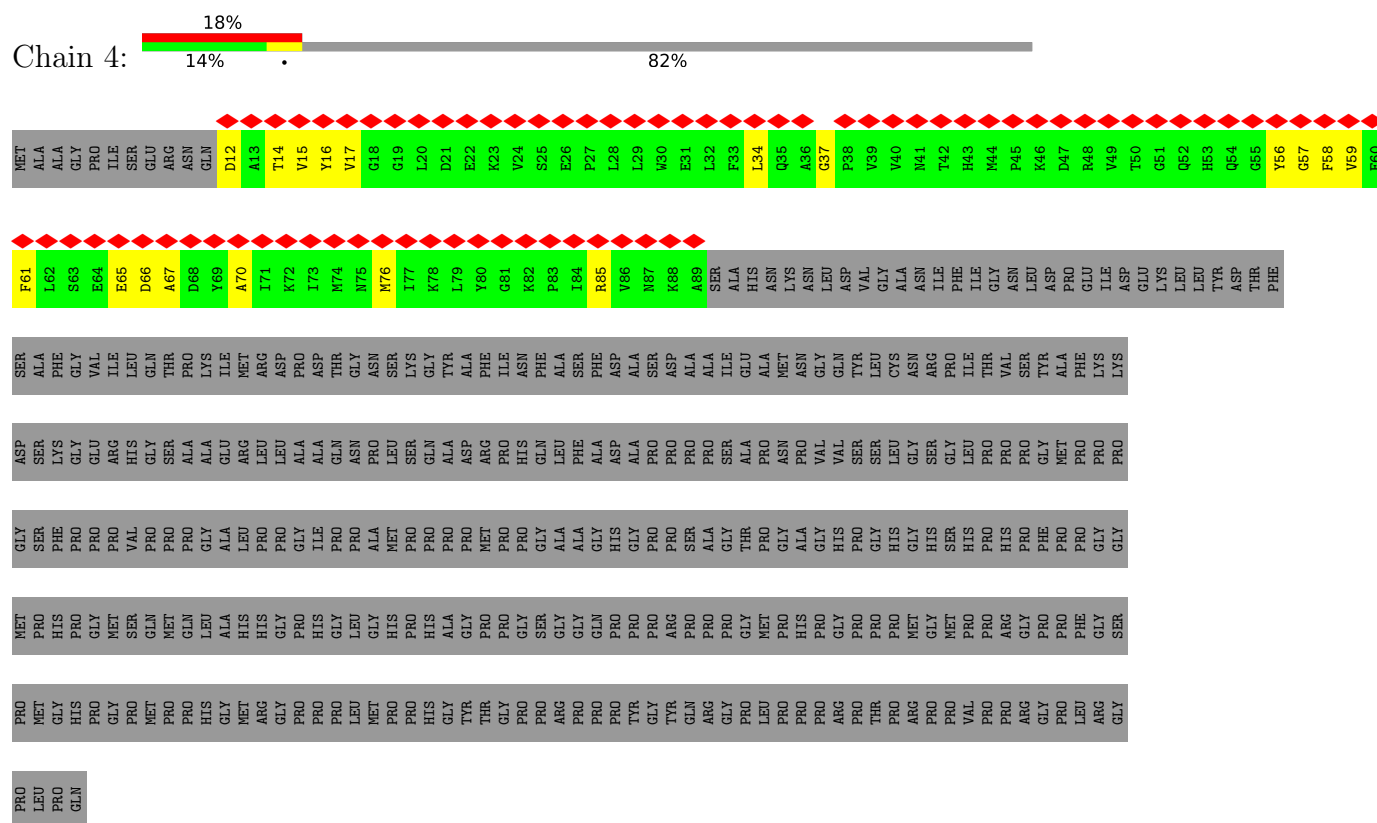


• Molecule 19: Splicing factor 3B subunit 3

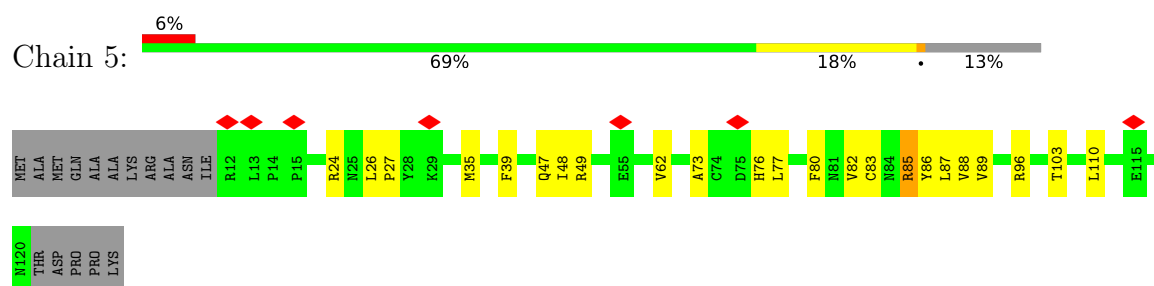




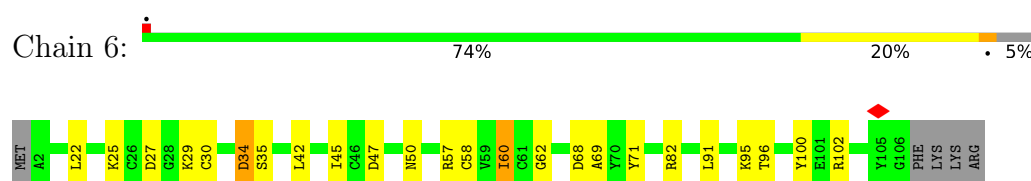
• Molecule 20: Splicing factor 3B subunit 4



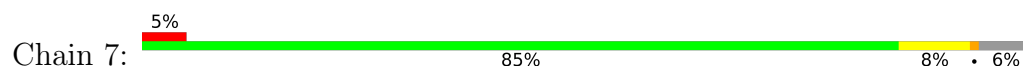
• Molecule 21: Splicing factor 3B subunit 6

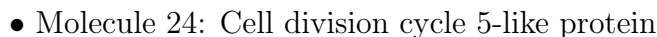


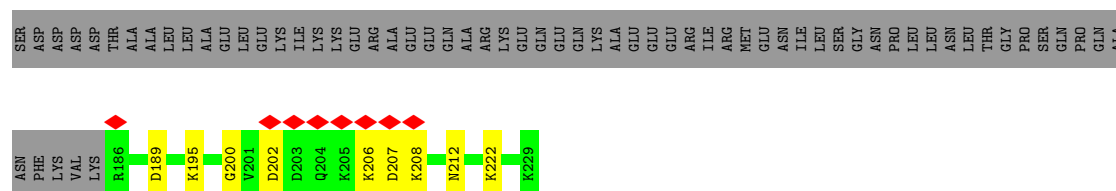
• Molecule 22: PHD finger-like domain-containing protein 5A



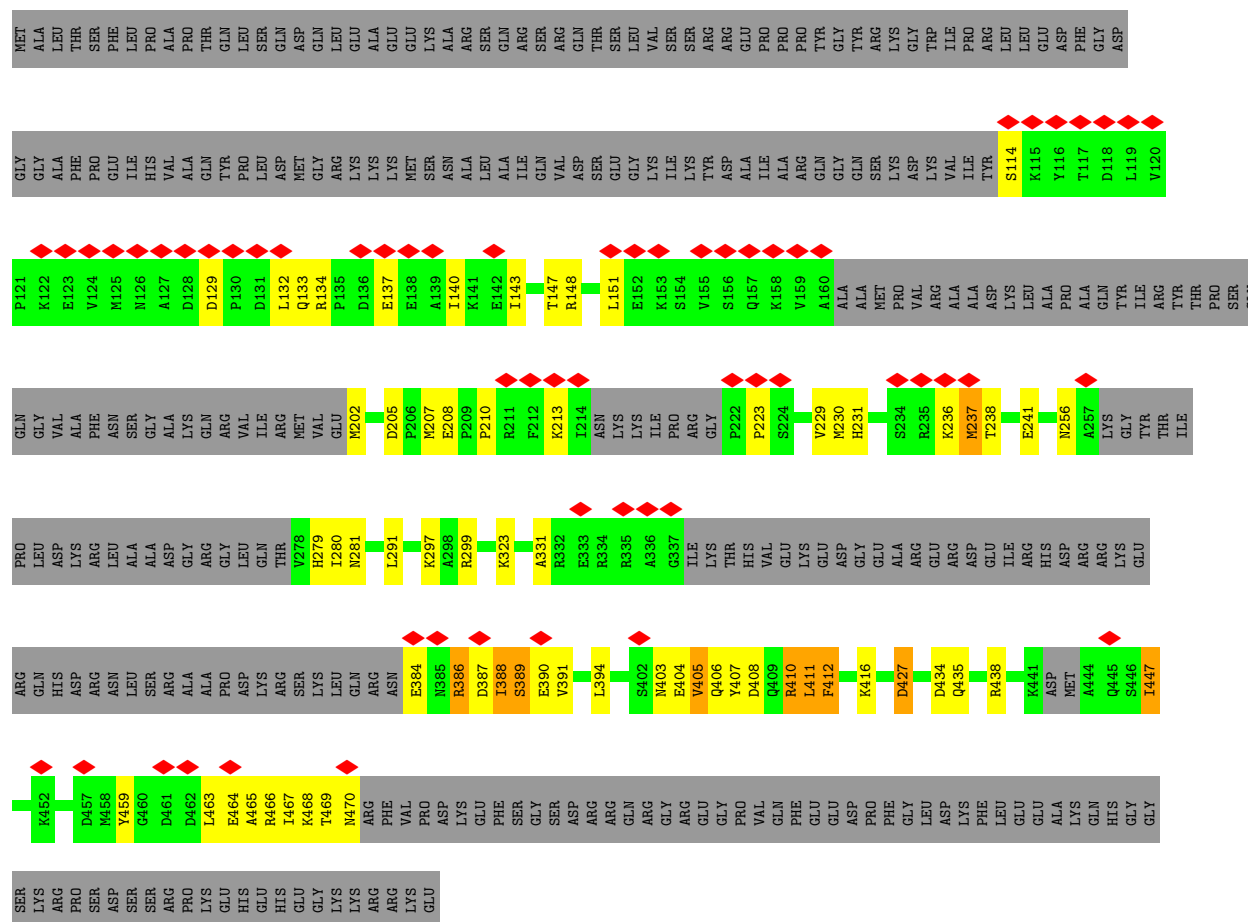
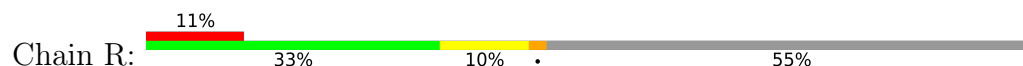
• Molecule 23: Splicing factor 3B subunit 5



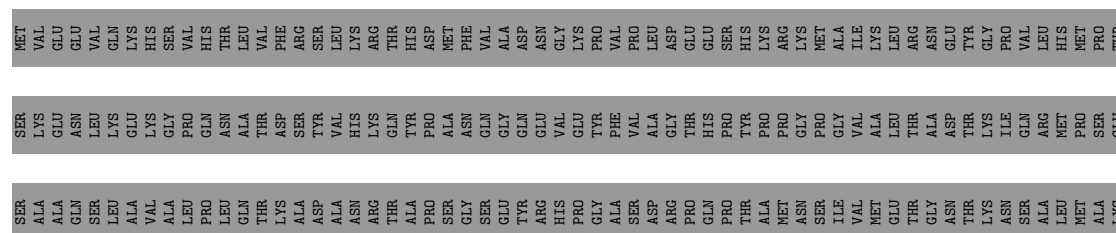


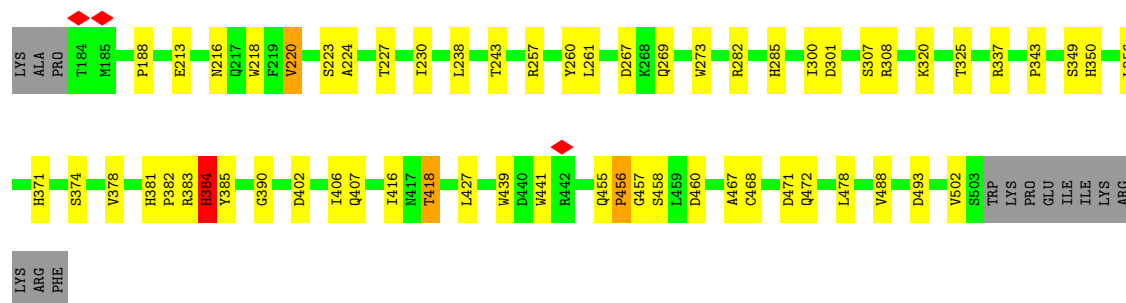


• Molecule 27: SNW domain-containing protein 1

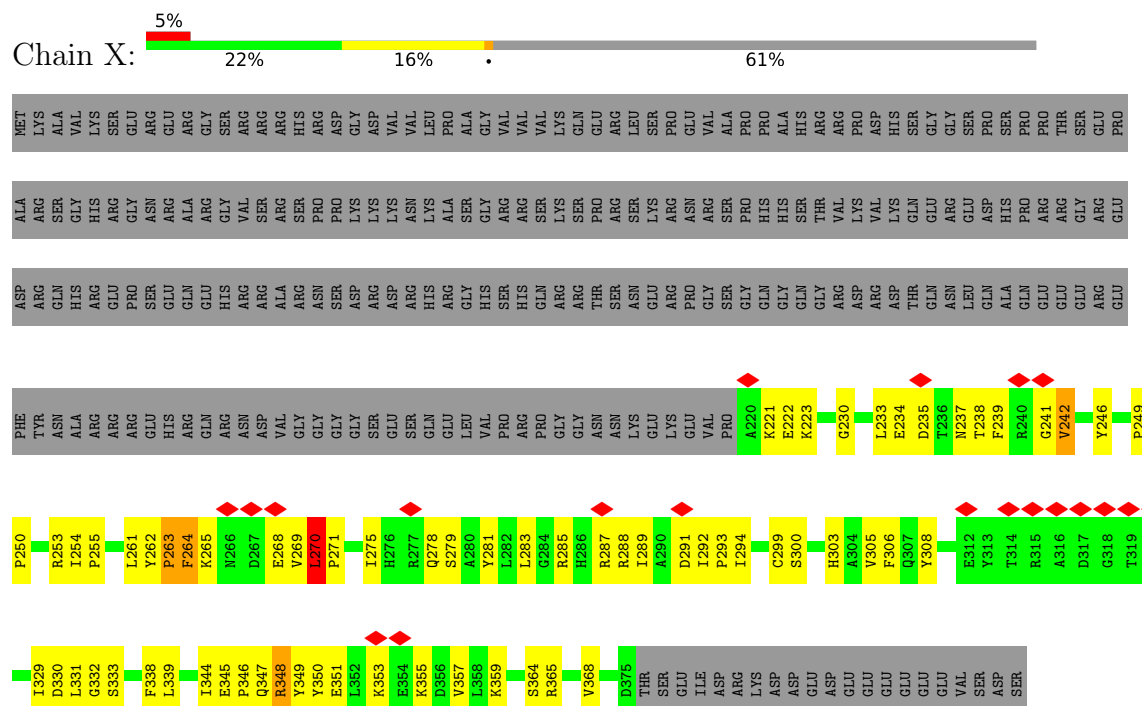


• Molecule 28: Pleiotropic regulator 1

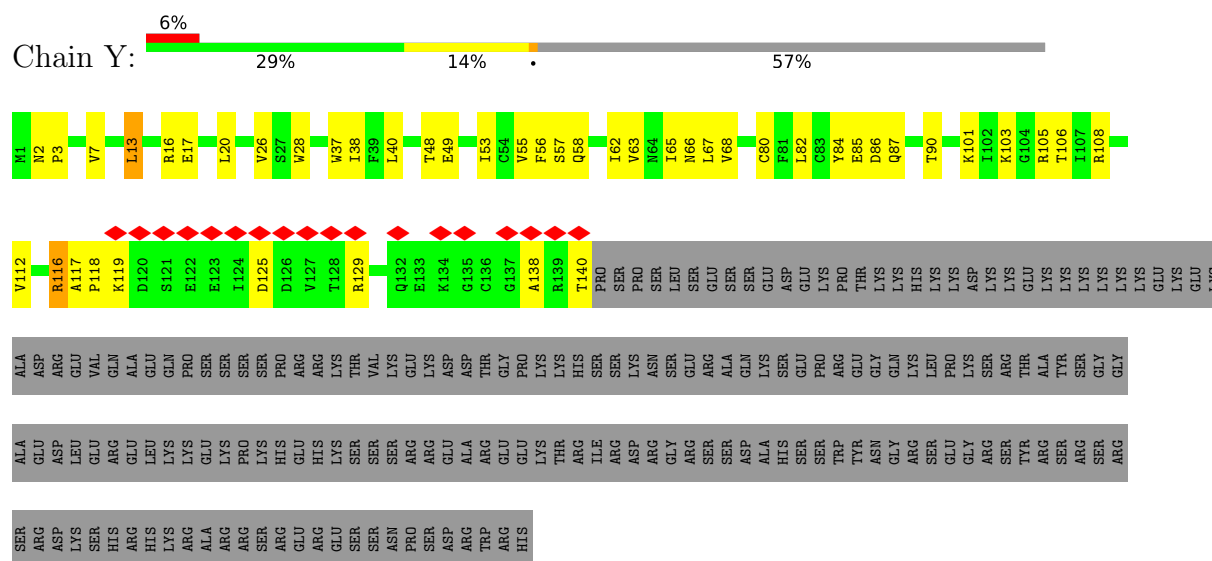




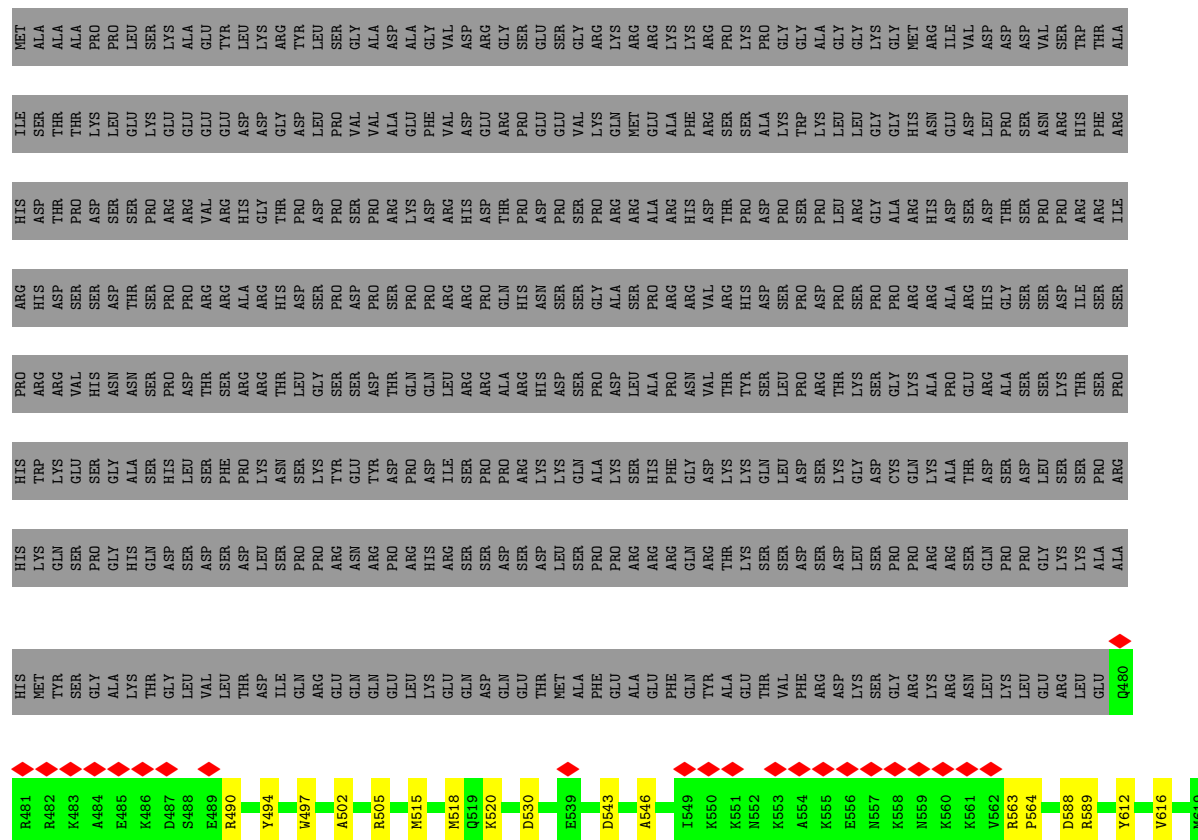
• Molecule 29: Smad nuclear-interacting protein 1



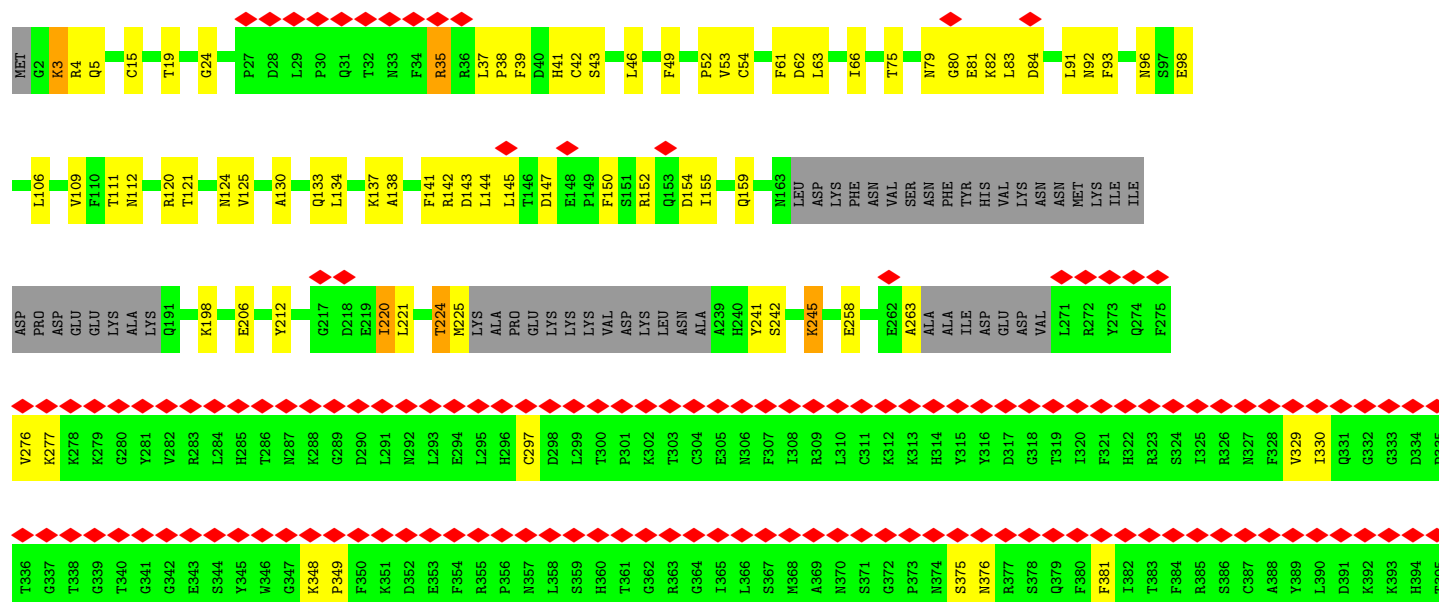
• Molecule 30: RNA-binding motif protein, X-linked 2



Chain Z: 20% 77%



Chain 9:











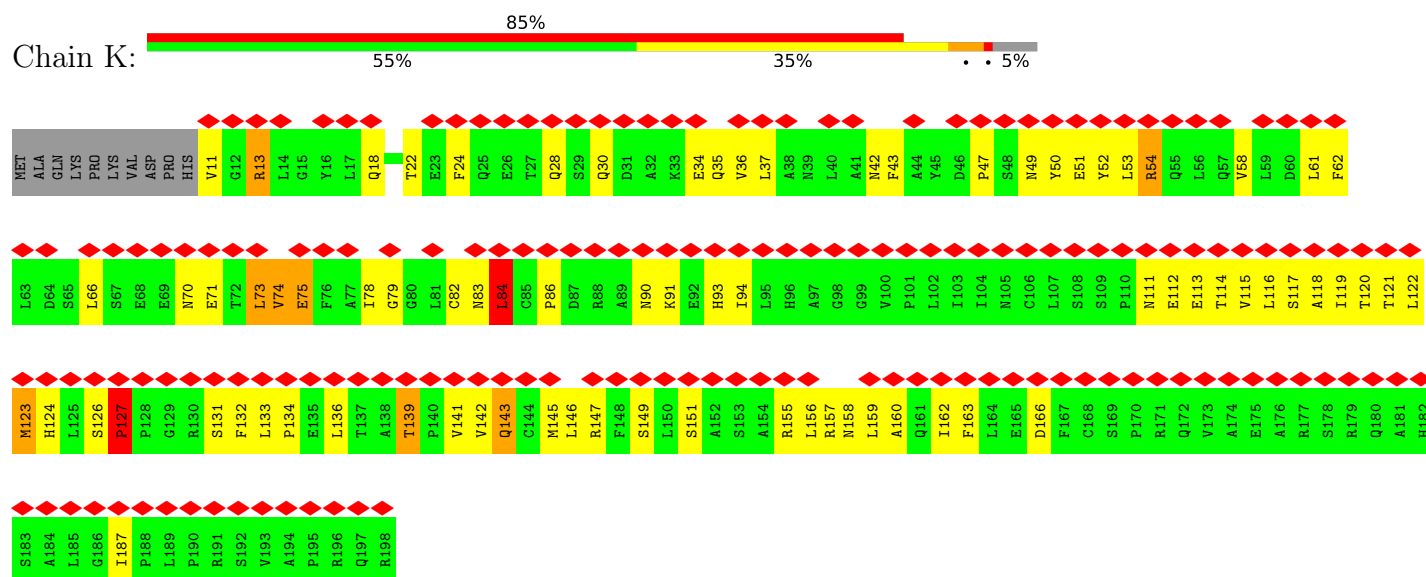
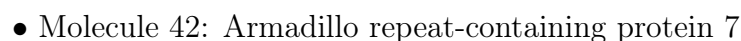
GLY	SER	ALA	PRO	THR	SER
ARG	SER	LEU	THR	THR	SER
ARG	ARG	PRO	ALA	PRO	SER
GLY	GLY	PRO	LYS	LYS	SER
GLN	ARG	ALA	ARG	ARG	SER
ARG	GLY	SER	SER	LYS	SER
GLY	ASP	PRO	ARG	ARG	SER
SER	SER	LYS	SER	SER	SER
ARG	ARG	PRO	SER	SER	SER
SER	SER	PRO	SER	SER	SER
PRO	SER	PRO	SER	SER	SER
GLY	SER	GLY	SER	SER	SER
HIS	SER	GLU	SER	SER	SER
LYS	ARG	ARG	SER	SER	SER
ARG	ARG	SER	SER	SER	SER
ARG	ARG	SER	SER	SER	SER
GLU	GLU	ARG	SER	SER	GLY
THR	THR	SER	SER	SER	SER
PRO	PRO	ARG	SER	SER	SER
SER	SER	LYS	SER	SER	SER
PRO	PRO	PRO	SER	SER	SER
ARG	ARG	ILE	SER	SER	ASP
ARG	ARG	ASP	SER	SER	SER
PRO	MET	SER	SER	SER	GLU
PRO	ARG	LEU	SER	SER	GLY
HIS	HIS	ARG	SER	SER	SER
ARG	ARG	ASP	SER	SER	SER
SER	SER	SER	SER	SER	LEU
ARG	ARG	ARG	SER	SER	VAL
SER	SER	ARG	SER	SER	GLN
ARG	ARG	LEU	SER	SER	PRO
PRO	PRO	TYR	SER	SER	GLU
		SER	SER	SER	VAL
		PRO	SER	SER	ALA
		VAL	SER	SER	LEU
		GLU	SER	SER	LYS
		ARG	SER	SER	ARG
		ARG	SER	SER	VAL
		ARG	SER	SER	PRO
		PRO	SER	SER	PRO
		SER	SER	SER	THR
		GLN	SER	SER	PRO
		PRO	SER	SER	ALA
		SER	SER	SER	PRO
		PRO	SER	SER	LYS
		ARG	SER	SER	GLU
		ASP	PRO	SER	ALA
		GLN	SER	SER	VAL
		GLN	PRO	SER	ARG
		SER	ALA	GLU	GLU
		SER	LYS	GLY	GLU
		SER	PRO	ARG	PRO
		SER	SER	GLY	ARG
		SER	PRO	PRO	GLU
		GLU	ARG	GLN	ARG

- Molecule 38: Pre-mRNA-splicing factor CWC22 homolog

[illegible]

E362	G301	F241	I181	GLU
D363	L302	R242	I182	LEU
D364	K303	R243	Q183	ASP
Q365	L304	Q244	E184	PRO
F366	T305	Y245	L185	LEU
T367	Q306	R246	L186	THR
H368	V307	R247	E187	ARG
K369	S308	W248	E188	GLY
L370	P309	D249	M189	GLY
P371	R310	K250	I190	ALA
L372	G311	Q251	V191	TYR
E373	I312	L252	R192	ILE
D374	N313	C253	G193	PRO
D375	A314	L254	R194	PRO
Y376	I315	T255	G195	LVS
N377	F316	A256	L196	LEU
P378	E317	S257	L197	ARG
E379	R318	K258	S198	MET
D380	L319	F259	R199	GLN
V381	R320	W260	S200	GLN
L382	N321	A261	V201	ILE
N383	I322	H262	L202	THR
F384	E325	L263	Q203	ASP
F385	S326	L264	A204	K149
K386	E327	M265	Q205	N150
N387	I328	Q266	S206	S151
D388	D329	M267	A207	L152
P389	K330	W268	S208	A153
N390	R331	A269	P209	Y154
F391	V332	H270	I210	Q155
K392	Q333	E271	F211	R156
N393	Y334	L272	T212	M157
N394	M335	L273	H213	W158
E395	I336	C274	V214	W159
E396	E337	L275	Y215	E160
K397	V338	E276	A216	L162
Y398	M339	M277	A217	K163
K399	F340	L278	L218	K164
A400	A341	T279	V219	S165
I401	V342	L280	A220	I166
K402	R343	L281	I221	M167
K403	K344	L282	T222	G168
E404	D345	E283	M223	L169
I405	G346	R284	S224	I170
L406	F347	P285	K225	M171
ASP	F347	T286	F226	K172
GLU	K348	D287	P227	V173
GLY	D349	D288	Q228	M174
ASP	H350	S289	I229	I175
THR	P351	V290	Q230	S176
THR	ASP	I352	E231	M177
ASP	ASN	N291	L232	I178
THR	I353	E292	T233	N177
ASP	L354	A293	L234	I179
GLN	E355	T294	K235	N180
ASP	G356	G295	R236	
ALA	L357	F296	L237	
GLY	D358	L297	T238	
GLY	L359	K298	L239	
SER	V360	E299	N240	
	E361	G300		

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101443	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	644.52, 644.52, 644.52	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, K, GTP, SEP, TPO, MG, G5J, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.19	3/18863 (0.0%)	0.89	21/25599 (0.1%)
2	B	0.29	0/2115	0.37	0/3284
3	C	0.99	0/7287	0.86	8/9902 (0.1%)
4	D	0.53	0/9225	1.11	37/12826 (0.3%)
5	E	0.81	0/2390	1.00	8/3238 (0.2%)
6	a	0.71	0/397	0.93	0/549
6	h	0.78	0/390	0.99	0/539
7	b	0.84	0/404	1.12	2/561 (0.4%)
7	i	0.84	0/421	1.15	3/583 (0.5%)
8	c	0.88	0/405	1.12	0/563
8	j	0.87	0/405	1.11	0/563
9	d	1.09	0/479	1.22	1/666 (0.2%)
9	k	1.11	0/420	1.20	1/583 (0.2%)
10	f	1.20	0/360	1.25	0/497
10	m	1.21	1/360 (0.3%)	1.24	0/497
11	e	1.03	0/390	1.24	1/542 (0.2%)
11	l	1.02	0/390	1.24	0/542
12	g	0.86	0/362	1.08	1/501 (0.2%)
12	n	0.85	0/332	1.09	1/458 (0.2%)
13	F	0.26	0/1449	0.26	0/2257
14	G	0.26	0/1445	0.42	1/2238 (0.0%)
15	H	0.32	0/1511	0.36	0/2351
16	v	0.95	0/984	0.76	3/1326 (0.2%)
17	1	1.13	0/8025	0.87	10/10859 (0.1%)
18	2	0.98	0/1710	0.88	5/2306 (0.2%)
19	3	1.00	1/9531 (0.0%)	0.81	10/12931 (0.1%)
20	4	0.94	0/382	1.12	0/529
21	5	0.77	0/925	0.79	0/1247
22	6	1.09	0/825	1.01	4/1106 (0.4%)
23	7	1.27	0/688	0.92	2/930 (0.2%)
24	L	1.22	0/864	0.85	1/1165 (0.1%)
25	J	0.29	0/3494	0.64	4/4743 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	P	1.07	0/391	0.76	0/517
27	R	0.76	1/1954 (0.1%)	0.70	5/2622 (0.2%)
28	T	1.25	0/2574	0.95	2/3511 (0.1%)
29	X	0.25	0/1304	0.66	3/1760 (0.2%)
30	Y	1.05	0/1113	0.80	0/1501
31	Z	1.01	0/1153	0.80	0/1548
32	9	0.59	0/2732	0.80	4/3733 (0.1%)
33	z	1.05	0/1434	0.79	0/1941
34	x	0.57	1/2996 (0.0%)	0.80	10/4142 (0.2%)
35	y	0.21	0/107	0.45	0/141
36	M	0.97	0/1609	0.77	0/2164
37	U	0.92	0/196	0.80	0/265
38	V	0.92	1/3042 (0.0%)	0.95	0/4152
39	8	0.92	0/1028	0.85	0/1379
40	0	1.00	0/782	0.78	0/1043
41	I	0.33	0/1083	0.53	0/1454
42	K	0.34	0/1333	0.85	6/1826 (0.3%)
All	All	0.93	8/102059 (0.0%)	0.87	154/140180 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TYR	CA-C	-7.21	1.41	1.52
1	A	797	ASP	CA-C	-6.95	1.41	1.52
34	x	926	GLU	CA-CB	-5.71	1.45	1.53
38	V	562	TRP	CA-C	-5.43	1.45	1.52
1	A	333	HIS	C-N	-5.34	1.25	1.33
27	R	435	GLN	CA-CB	-5.26	1.43	1.54
19	3	784	THR	C-N	-5.15	1.28	1.33
10	m	14	LEU	CA-C	5.05	1.59	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	102	TYR	N-CA-C	9.87	122.12	111.36
22	6	60	ILE	N-CA-C	8.66	119.46	110.62
27	R	405	VAL	N-CA-C	8.64	120.62	109.30
27	R	412	PHE	N-CA-C	8.31	121.25	110.53
18	2	642	PRO	CA-C-N	8.25	128.21	119.05
18	2	642	PRO	C-N-CA	8.25	128.21	119.05
32	9	376	ASN	N-CA-C	8.21	120.23	111.28
25	J	358	GLU	N-CA-C	8.20	122.00	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	545	ARG	N-CA-C	8.18	120.19	111.28
42	K	84	LEU	N-CA-C	8.12	119.92	111.14
4	D	1642	GLN	N-CA-C	7.79	119.85	111.36
42	K	187	ILE	CA-C-N	7.68	127.44	119.76
42	K	187	ILE	C-N-CA	7.68	127.44	119.76
4	D	789	MET	N-CA-C	7.52	119.11	111.07
14	G	-11	U	C2'-C3'-O3'	7.47	120.71	109.50
17	1	1262	ARG	N-CA-C	7.30	118.88	111.07
4	D	1044	VAL	CA-C-N	7.13	126.62	118.85
4	D	1044	VAL	C-N-CA	7.13	126.62	118.85
4	D	422	PHE	N-CA-C	7.08	120.81	111.75
4	D	533	VAL	N-CA-C	6.99	118.86	112.29
25	J	338	GLU	N-CA-C	-6.96	103.30	111.03
19	3	981	CYS	N-CA-C	6.94	120.97	111.39
32	9	436	ASP	CA-C-N	6.93	126.75	119.05
32	9	436	ASP	C-N-CA	6.93	126.75	119.05
34	x	821	ASP	CA-C-N	6.69	126.47	119.05
34	x	821	ASP	C-N-CA	6.69	126.47	119.05
3	C	779	LEU	N-CA-C	6.62	118.15	111.07
19	3	137	LYS	N-CA-C	6.59	120.90	112.86
17	1	1250	CYS	N-CA-C	6.53	118.39	111.28
1	A	205	ASP	N-CA-C	6.51	118.38	111.28
25	J	340	GLN	CA-C-N	6.47	126.24	119.05
25	J	340	GLN	C-N-CA	6.47	126.24	119.05
27	R	411	LEU	N-CA-C	6.47	118.33	111.28
17	1	844	VAL	N-CA-C	6.46	118.04	111.00
1	A	204	LEU	N-CA-C	6.38	118.24	111.28
19	3	979	ARG	N-CA-C	6.28	119.89	109.46
5	E	322	LYS	N-CA-C	-6.25	98.08	108.34
3	C	567	GLU	CA-C-N	6.24	125.98	119.05
3	C	567	GLU	C-N-CA	6.24	125.98	119.05
5	E	156	SER	N-CA-C	6.19	118.26	108.79
4	D	103	LYS	CA-C-N	6.18	127.56	119.84
4	D	103	LYS	C-N-CA	6.18	127.56	119.84
1	A	207	PHE	N-CA-C	6.12	118.74	111.33
12	g	67	ILE	CB-CA-C	-6.08	104.67	111.23
4	D	108	GLU	N-CA-C	-6.05	104.68	111.28
4	D	1006	LYS	CA-C-N	6.02	126.19	119.32
4	D	1006	LYS	C-N-CA	6.02	126.19	119.32
17	1	1003	VAL	N-CA-C	6.02	116.80	110.72
34	x	821	ASP	O-C-N	6.01	127.29	121.28
1	A	210	HIS	N-CA-C	-5.88	99.61	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	n	67	ILE	CB-CA-C	-5.87	104.89	111.23
4	D	1135	LEU	CA-C-N	5.81	125.75	119.76
4	D	1135	LEU	C-N-CA	5.81	125.75	119.76
1	A	2199	ILE	CB-CA-C	-5.80	104.42	112.02
1	A	1719	PHE	CB-CA-C	5.79	117.93	109.48
19	3	1172	ASN	N-CA-C	5.79	119.54	111.90
29	X	270	LEU	CA-C-N	5.75	127.03	119.84
29	X	270	LEU	C-N-CA	5.75	127.03	119.84
4	D	124	LEU	N-CA-C	5.74	117.62	111.36
22	6	47	ASP	N-CA-C	5.74	118.00	111.11
19	3	184	CYS	N-CA-C	5.73	118.11	109.23
5	E	309	VAL	CB-CA-C	-5.72	104.03	110.96
4	D	1291	LEU	CA-C-N	5.72	126.04	119.92
4	D	1291	LEU	C-N-CA	5.72	126.04	119.92
32	9	329	VAL	N-CA-C	5.68	116.91	109.58
1	A	2153	THR	N-CA-C	-5.67	101.78	109.95
4	D	127	GLN	CA-C-N	-5.65	113.96	119.78
4	D	127	GLN	C-N-CA	-5.65	113.96	119.78
4	D	1624	LEU	N-CA-C	5.64	118.50	110.10
3	C	532	ILE	N-CA-C	-5.63	98.32	106.88
19	3	320	ASP	N-CA-C	5.62	117.40	111.28
1	A	1317	TYR	N-CA-C	5.59	118.31	111.82
1	A	1053	LEU	CA-C-N	-5.59	116.53	122.67
1	A	1053	LEU	C-N-CA	-5.59	116.53	122.67
7	i	52	LYS	CA-C-N	-5.58	114.18	119.76
7	i	52	LYS	C-N-CA	-5.58	114.18	119.76
3	C	221	ILE	N-CA-CB	-5.56	102.73	112.08
7	b	52	LYS	CA-C-N	-5.55	114.21	119.76
7	b	52	LYS	C-N-CA	-5.55	114.21	119.76
1	A	1775	GLN	N-CA-C	5.54	118.47	110.28
4	D	1048	VAL	N-CA-C	-5.54	106.41	113.22
34	x	443	ASN	N-CA-C	5.53	117.31	111.28
22	6	71	TYR	N-CA-C	-5.52	101.87	110.42
1	A	2225	LEU	N-CA-C	5.51	117.77	109.23
7	i	5	LYS	N-CA-C	5.50	118.20	111.82
5	E	237	SER	N-CA-C	5.46	118.00	110.35
1	A	2203	ASN	N-CA-C	5.46	120.74	109.11
1	A	2241	ASN	N-CA-C	5.46	118.23	110.10
5	E	281	VAL	N-CA-C	5.45	116.16	108.36
24	L	54	LEU	N-CA-C	5.45	119.77	113.18
18	2	630	PRO	CA-C-N	5.45	125.10	119.05
18	2	630	PRO	C-N-CA	5.45	125.10	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1228	VAL	CB-CA-C	-5.44	104.91	112.04
28	T	384	HIS	N-CA-C	5.44	119.91	113.16
34	x	508	GLU	CA-C-N	5.41	125.05	119.05
34	x	508	GLU	C-N-CA	5.41	125.05	119.05
42	K	166	ASP	N-CA-C	5.39	117.23	111.36
18	2	647	ASN	N-CA-C	5.38	119.95	113.17
17	1	556	ILE	CA-C-N	-5.37	111.11	121.58
17	1	556	ILE	C-N-CA	-5.37	111.11	121.58
29	X	242	VAL	CB-CA-C	-5.35	106.71	111.74
34	x	783	PRO	CA-C-N	5.34	125.89	120.38
34	x	783	PRO	C-N-CA	5.34	125.89	120.38
1	A	2100	THR	N-CA-C	-5.34	106.76	113.28
4	D	1228	VAL	N-CA-C	5.32	116.69	110.62
1	A	1018	ASN	N-CA-C	5.32	117.09	108.26
4	D	1693	ARG	CA-C-N	5.29	125.09	119.28
4	D	1693	ARG	C-N-CA	5.29	125.09	119.28
22	6	34	ASP	N-CA-C	5.28	118.91	111.52
19	3	1130	VAL	N-CA-C	5.28	113.64	107.89
16	v	224	PRO	CA-C-N	5.26	125.17	119.85
16	v	224	PRO	C-N-CA	5.26	125.17	119.85
1	A	901	LEU	CA-C-N	5.25	131.57	121.54
1	A	901	LEU	C-N-CA	5.25	131.57	121.54
4	D	2096	ALA	CA-C-N	5.25	125.46	120.31
4	D	2096	ALA	C-N-CA	5.25	125.46	120.31
23	7	57	GLU	CA-C-N	-5.25	114.15	122.23
23	7	57	GLU	C-N-CA	-5.25	114.15	122.23
17	1	941	ASN	CA-C-N	-5.24	113.57	123.27
17	1	941	ASN	C-N-CA	-5.24	113.57	123.27
19	3	884	GLN	CA-C-N	-5.24	114.39	123.25
19	3	884	GLN	C-N-CA	-5.24	114.39	123.25
34	x	877	ASP	CA-C-N	-5.24	113.26	120.28
34	x	877	ASP	C-N-CA	-5.24	113.26	120.28
5	E	163	GLY	CA-C-N	-5.24	114.56	119.85
5	E	163	GLY	C-N-CA	-5.24	114.56	119.85
4	D	1127	CYS	CA-C-N	5.23	125.54	119.47
4	D	1127	CYS	C-N-CA	5.23	125.54	119.47
4	D	1852	ALA	N-CA-C	5.23	117.04	110.24
4	D	488	LEU	N-CA-C	5.23	119.76	113.17
4	D	572	ASP	N-CA-C	-5.20	103.28	110.35
27	R	407	TYR	CA-C-N	-5.20	111.62	122.07
27	R	407	TYR	C-N-CA	-5.20	111.62	122.07
3	C	533	SER	N-CA-C	5.19	117.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	260	TYR	N-CA-C	5.19	118.20	109.95
17	1	567	VAL	N-CA-CB	-5.16	105.41	112.28
16	v	219	SER	N-CA-C	5.16	116.90	111.28
1	A	1000	ILE	N-CA-C	5.15	118.11	112.96
1	A	57	GLN	N-CA-C	5.13	116.97	107.73
9	d	99	MET	N-CA-C	5.12	116.85	108.76
1	A	1525	GLY	N-CA-C	-5.11	105.75	111.63
9	k	99	MET	N-CA-C	5.10	116.82	108.76
4	D	574	GLN	N-CA-C	5.09	117.95	111.69
11	e	85	THR	N-CA-C	-5.09	105.92	112.68
17	1	1251	LEU	N-CA-C	5.07	121.61	110.80
4	D	1329	ASN	CA-C-N	-5.07	113.50	119.84
4	D	1329	ASN	C-N-CA	-5.07	113.50	119.84
4	D	1875	VAL	CA-C-N	5.04	124.48	119.24
4	D	1875	VAL	C-N-CA	5.04	124.48	119.24
19	3	333	VAL	N-CA-C	-5.04	103.32	109.01
3	C	139	HIS	N-CA-C	5.04	118.54	111.74
3	C	834	VAL	N-CA-C	5.03	115.09	107.75
42	K	127	PRO	CA-C-N	5.03	124.96	119.78
42	K	127	PRO	C-N-CA	5.03	124.96	119.78

There are no chirality outliers.

There are no planarity outliers.

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	A	18354	0	18179	405	0
2	B	1898	0	963	37	0
3	C	7125	0	7130	127	0
4	D	9215	0	4458	175	0
5	E	2337	0	2272	198	0
6	a	399	0	173	1	0
6	h	392	0	168	0	0
7	b	405	0	170	0	0
7	i	422	0	177	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	c	406	0	170	0	0
8	j	406	0	170	0	0
9	d	480	0	200	3	0
9	k	422	0	175	1	0
10	f	361	0	158	2	0
10	m	361	0	158	1	0
11	e	391	0	163	2	0
11	l	391	0	163	2	0
12	g	363	0	160	1	0
12	n	334	0	143	1	0
13	F	1294	0	650	44	0
14	G	1303	0	667	47	0
15	H	1350	0	679	31	0
16	v	963	0	945	56	0
17	1	7879	0	8044	173	0
18	2	1674	0	1580	43	0
19	3	9352	0	9273	230	0
20	4	383	0	173	24	0
21	5	906	0	913	32	0
22	6	811	0	788	21	0
23	7	669	0	631	7	0
24	L	843	0	852	17	0
25	J	3457	0	2537	161	0
26	P	384	0	382	11	0
27	R	1923	0	1889	124	0
28	T	2507	0	2451	40	0
29	X	1271	0	1252	93	0
30	Y	1095	0	1083	63	0
31	Z	1129	0	1077	23	0
32	9	2691	0	2121	93	0
33	z	1400	0	1344	13	0
34	x	3007	0	1453	18	0
35	y	105	0	107	2	0
36	M	1572	0	1483	40	0
37	U	193	0	196	3	0
38	V	3008	0	2291	18	0
39	8	1011	0	1035	20	0
40	0	770	0	778	28	0
41	I	1062	0	1067	67	0
42	K	1314	0	1177	99	0
43	A	36	0	6	0	0
44	C	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	1	0	0	0	0
45	F	4	0	0	0	0
46	F	2	0	0	0	0
47	F	33	0	0	3	0
48	0	2	0	0	0	0
48	6	3	0	0	0	0
48	M	1	0	0	0	0
48	v	1	0	0	0	0
49	C	3	0	0	0	0
All	All	99906	0	84286	2250	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 12.

All (2250) 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)
17:1:641:ILE:HD11	17:1:675:MET:CE	1.58	1.34
20:4:14:THR:HA	20:4:59:VAL:O	1.32	1.30
5:E:62:LEU:HD12	5:E:351:LEU:CD1	1.66	1.26
25:J:337:MET:HE3	25:J:346:TRP:CH2	1.70	1.25
5:E:62:LEU:CD1	5:E:351:LEU:HD12	1.68	1.23
5:E:326:HIS:CE1	5:E:346:SER:HB3	1.73	1.22
32:9:3:LYS:HD3	32:9:5:GLN:HB2	1.20	1.18
29:X:345:GLU:OE2	29:X:348:ARG:HD2	1.44	1.17
25:J:337:MET:CE	25:J:346:TRP:CZ3	2.29	1.15
16:v:190:LEU:HD21	18:2:691:ALA:HB1	1.27	1.14
5:E:74:PHE:CE1	5:E:81:LEU:HD21	1.81	1.13
24:L:77:LEU:HD21	32:9:221:LEU:HD11	1.30	1.13
1:A:2168:TYR:CZ	1:A:2298:LEU:HD11	1.83	1.12
25:J:316:TYR:HE1	25:J:332:VAL:HG21	1.15	1.12
34:x:664:PRO:O	34:x:667:ALA:HB3	1.46	1.11
4:D:176:GLY:O	4:D:179:ILE:HG22	1.47	1.11
16:v:191:ASP:OD1	18:2:694:PHE:HE2	1.32	1.11
16:v:223:GLU:CG	16:v:224:PRO:HD2	1.81	1.11
17:1:641:ILE:CD1	17:1:675:MET:CE	2.27	1.11
20:4:12:ASP:CB	20:4:67:ALA:HB1	1.80	1.10
5:E:60:MET:SD	5:E:99:CYS:SG	2.50	1.09
19:3:950:ALA:HB2	19:3:989:TYR:OH	1.53	1.08
16:v:187:ARG:CZ	18:2:694:PHE:HE1	1.66	1.08
42:K:119:ILE:HG23	42:K:163:PHE:HD2	1.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:31:ARG:HB3	41:I:31:ARG:HH11	1.16	1.07
19:3:630:MET:CE	36:M:287:LEU:HD21	1.83	1.07
1:A:1838:LYS:HE3	1:A:1865:ARG:CZ	1.83	1.07
17:1:641:ILE:HD11	17:1:675:MET:HE3	1.09	1.07
5:E:119:THR:HG21	5:E:161:ARG:HB2	1.37	1.06
20:4:17:VAL:HA	20:4:85:ARG:O	1.53	1.06
16:v:223:GLU:HG3	16:v:224:PRO:CD	1.85	1.05
39:8:56:VAL:HG21	39:8:68:ILE:HD13	1.39	1.05
5:E:132:THR:CG2	5:E:146:ARG:HB2	1.86	1.04
5:E:258:THR:HG21	5:E:260:ARG:HH11	1.11	1.04
27:R:279:HIS:HA	32:9:224:THR:CG2	1.87	1.04
14:G:222:U:C6	30:Y:119:LYS:HE2	1.91	1.04
19:3:687:SER:O	36:M:306:VAL:HG21	1.55	1.04
25:J:337:MET:HE2	25:J:346:TRP:CZ3	1.92	1.04
29:X:265:LYS:HG3	29:X:364:SER:OG	1.58	1.03
4:D:406:ARG:CB	4:D:955:ASP:HA	1.87	1.03
5:E:326:HIS:CE1	5:E:346:SER:CB	2.40	1.03
27:R:386:ARG:HH12	29:X:353:LYS:HG3	1.20	1.03
5:E:88:ARG:HG2	5:E:110:GLY:O	1.57	1.03
5:E:260:ARG:HD2	5:E:276:ILE:HG12	1.34	1.03
4:D:164:THR:HA	4:D:168:ARG:NH1	1.73	1.03
1:A:2325:VAL:HG13	4:D:788:GLY:O	1.59	1.03
1:A:2325:VAL:HG13	4:D:788:GLY:C	1.83	1.03
27:R:279:HIS:HA	32:9:224:THR:HG23	1.37	1.02
5:E:193:THR:HG23	5:E:194:TYR:CD1	1.94	1.02
27:R:387:ASP:HB2	29:X:351:GLU:HB2	1.36	1.02
17:1:971:MET:HE1	17:1:1003:VAL:HG11	1.40	1.02
29:X:241:GLY:HA2	29:X:288:ARG:NH2	1.74	1.01
27:R:280:ILE:H	32:9:224:THR:CG2	1.72	1.01
25:J:359:VAL:HG21	25:J:389:HIS:NE2	1.77	1.00
13:F:18:A:H61	16:v:2:SER:HB3	1.26	1.00
1:A:1122:ASN:HB2	32:9:35:ARG:HH21	1.27	0.99
17:1:641:ILE:HG13	17:1:675:MET:HE1	1.43	0.98
19:3:630:MET:HE1	36:M:287:LEU:HD21	1.41	0.98
19:3:1130:VAL:CG1	19:3:1215:TYR:CE1	2.46	0.98
25:J:337:MET:CE	25:J:346:TRP:CH2	2.45	0.97
4:D:120:ILE:HD12	4:D:161:LEU:CD2	1.93	0.97
1:A:1122:ASN:HB2	32:9:35:ARG:NH2	1.79	0.97
17:1:613:MET:HE1	17:1:635:VAL:HG11	1.45	0.97
13:F:18:A:N6	16:v:2:SER:HB3	1.80	0.96
4:D:148:LEU:CD2	4:D:152:GLU:HB3	1.93	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:47:THR:CG2	19:3:49:LYS:HG2	1.96	0.96
19:3:630:MET:SD	36:M:287:LEU:HD21	2.04	0.96
1:A:265:THR:HG23	1:A:327:VAL:HG22	1.48	0.96
17:1:641:ILE:CG1	17:1:675:MET:CE	2.45	0.95
21:5:39:PHE:HE1	21:5:77:LEU:HD21	1.28	0.95
19:3:54:LEU:HD23	19:3:99:PHE:CE2	2.00	0.95
42:K:149:SER:O	42:K:157:ARG:HG2	1.65	0.95
5:E:147:LEU:HD13	5:E:179:TRP:CG	1.99	0.95
41:I:37:LYS:HD3	41:I:39:TYR:CZ	2.01	0.94
1:A:2103:THR:HG21	1:A:2260:GLN:OE1	1.66	0.94
5:E:260:ARG:CD	5:E:276:ILE:HG12	1.96	0.94
17:1:641:ILE:CD1	17:1:675:MET:HE3	1.93	0.94
27:R:386:ARG:NH1	29:X:353:LYS:HG3	1.83	0.94
1:A:1307:MET:SD	1:A:1547:VAL:HG11	2.07	0.94
1:A:2219:THR:HG23	1:A:2224:THR:HG22	1.47	0.94
25:J:316:TYR:CE1	25:J:332:VAL:HG21	2.03	0.94
1:A:1092:ILE:HG22	1:A:1093:ASP:H	1.31	0.93
16:v:190:LEU:HD22	18:2:694:PHE:CD2	2.04	0.93
16:v:191:ASP:OD1	18:2:694:PHE:CE2	2.22	0.92
20:4:12:ASP:CB	20:4:67:ALA:CB	2.47	0.92
25:J:232:GLU:HA	25:J:235:ILE:CG2	2.00	0.92
25:J:313:TRP:CZ3	25:J:336:TRP:NE1	2.37	0.92
39:8:56:VAL:HG21	39:8:68:ILE:CD1	1.98	0.92
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	1.52	0.92
42:K:119:ILE:HG23	42:K:163:PHE:CD2	2.05	0.91
19:3:170:VAL:HG22	19:3:184:CYS:SG	2.10	0.91
25:J:333:PHE:CD1	25:J:349:TYR:CD1	2.58	0.91
19:3:1130:VAL:CG1	19:3:1215:TYR:CZ	2.53	0.91
5:E:62:LEU:HD12	5:E:351:LEU:HD12	0.91	0.91
19:3:586:ASP:OD1	19:3:610:VAL:HG11	1.71	0.91
1:A:1921:ASP:HB3	1:A:1966:HIS:ND1	1.86	0.91
19:3:1004:ASP:OD2	19:3:1007:GLU:HB2	1.70	0.91
19:3:429:ARG:HG2	19:3:429:ARG:HH21	1.35	0.91
5:E:258:THR:HG21	5:E:260:ARG:NH1	1.86	0.90
1:A:2284:MET:SD	1:A:2287:ARG:HD2	2.10	0.90
16:v:187:ARG:CZ	18:2:694:PHE:CE1	2.55	0.90
17:1:1004:ILE:HD11	17:1:1009:MET:SD	2.12	0.90
42:K:78:ILE:HG21	42:K:114:THR:HG23	1.54	0.90
29:X:253:ARG:HH21	29:X:253:ARG:HG3	1.36	0.90
16:v:223:GLU:HG3	16:v:224:PRO:HD2	0.94	0.90
4:D:131:ILE:CG1	4:D:697:ALA:HB1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:258:THR:HG22	5:E:260:ARG:HG2	1.53	0.90
27:R:280:ILE:H	32:9:224:THR:HG22	1.35	0.89
4:D:126:ASP:OD2	4:D:1075:PHE:CB	2.20	0.89
42:K:24:PHE:HB2	42:K:36:VAL:HG11	1.53	0.89
5:E:193:THR:CG2	5:E:194:TYR:CD1	2.55	0.89
19:3:1057:ARG:HG3	19:3:1057:ARG:HH11	1.38	0.89
25:J:337:MET:HE3	25:J:346:TRP:CZ2	2.07	0.89
1:A:591:MET:HB3	1:A:598:LEU:CD2	2.02	0.88
27:R:391:VAL:HA	29:X:347:GLN:O	1.72	0.88
17:1:614:ARG:O	17:1:614:ARG:HD2	1.74	0.88
42:K:78:ILE:HG12	42:K:117:SER:HB2	1.54	0.88
30:Y:67:LEU:HA	30:Y:80:CYS:HB2	1.56	0.88
1:A:976:MET:HE2	1:A:1098:PHE:HD1	1.38	0.88
29:X:241:GLY:HA2	29:X:288:ARG:CZ	2.04	0.88
29:X:345:GLU:OE2	29:X:348:ARG:CD	2.22	0.88
32:9:3:LYS:CD	32:9:5:GLN:HB2	2.04	0.88
3:C:779:LEU:HD21	3:C:912:LEU:HD11	1.56	0.88
32:9:220:ILE:H	32:9:220:ILE:HD12	1.37	0.87
34:x:664:PRO:O	34:x:667:ALA:CB	2.22	0.87
27:R:438:ARG:HG3	27:R:438:ARG:HH21	1.35	0.87
5:E:145:LYS:HE2	5:E:184:LYS:HE2	1.56	0.87
1:A:2117:ILE:HD11	1:A:2147:MET:HE2	1.57	0.87
29:X:241:GLY:HA3	29:X:289:ILE:HD11	1.56	0.87
19:3:49:LYS:HG3	19:3:51:HIS:CE1	2.10	0.86
4:D:1589:PHE:O	4:D:1642:GLN:CB	2.23	0.86
5:E:193:THR:CG2	5:E:194:TYR:CE1	2.58	0.86
5:E:326:HIS:ND1	5:E:346:SER:CB	2.38	0.86
4:D:123:ALA:HB3	4:D:161:LEU:HD11	1.56	0.86
5:E:193:THR:HG23	5:E:194:TYR:HD1	1.37	0.86
1:A:1976:TRP:HA	1:A:1979:VAL:CG2	2.05	0.86
4:D:148:LEU:HD21	4:D:152:GLU:HB3	1.55	0.86
18:2:657:ILE:O	18:2:657:ILE:HG22	1.73	0.86
19:3:1130:VAL:HG11	19:3:1215:TYR:CE2	2.09	0.86
1:A:1639:VAL:HG12	1:A:1655:THR:CG2	2.05	0.86
32:9:3:LYS:HD3	32:9:5:GLN:CB	2.04	0.85
1:A:2219:THR:HG23	1:A:2224:THR:CG2	2.05	0.85
4:D:800:LEU:O	4:D:805:HIS:CB	2.24	0.85
25:J:247:LYS:NZ	25:J:247:LYS:HB3	1.92	0.85
19:3:1130:VAL:HG11	19:3:1215:TYR:CD2	2.11	0.85
1:A:1092:ILE:HG22	1:A:1093:ASP:N	1.91	0.85
19:3:1130:VAL:HG13	19:3:1215:TYR:CE1	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:VAL:HA	4:D:145:ASN:ND2	1.90	0.85
1:A:1762:TYR:O	1:A:2008:ARG:HD3	1.77	0.84
4:D:120:ILE:HD12	4:D:161:LEU:HD21	1.55	0.84
20:4:61:PHE:CB	20:4:66:ASP:CB	2.54	0.84
21:5:39:PHE:HE1	21:5:77:LEU:CD2	1.90	0.84
42:K:133:LEU:N	42:K:134:PRO:HD2	1.92	0.84
1:A:2090:ILE:HD12	1:A:2263:LEU:HD11	1.59	0.84
4:D:120:ILE:CD1	4:D:161:LEU:HD22	2.06	0.84
1:A:1122:ASN:HB3	32:9:35:ARG:HD3	1.59	0.84
1:A:2090:ILE:CD1	1:A:2263:LEU:CD1	2.54	0.84
21:5:27:PRO:HG2	21:5:83:CYS:HB3	1.60	0.84
41:I:31:ARG:HH11	41:I:31:ARG:CB	1.90	0.84
25:J:245:TRP:CZ3	25:J:264:ILE:HG23	2.11	0.84
1:A:2168:TYR:CE2	1:A:2298:LEU:HD11	2.13	0.84
1:A:2310:ARG:HG2	1:A:2313:HIS:ND1	1.93	0.84
16:v:190:LEU:CD2	18:2:691:ALA:HB1	2.06	0.83
30:Y:67:LEU:HA	30:Y:80:CYS:CB	2.08	0.83
25:J:246:ILE:HD12	25:J:281:LYS:HG3	1.60	0.83
19:3:968:ARG:HG2	19:3:982:GLU:HB2	1.60	0.83
42:K:37:LEU:HD12	42:K:73:LEU:HG	1.60	0.83
1:A:1385:VAL:CG1	1:A:1419:ILE:HD11	2.09	0.83
1:A:1402:ARG:HD3	27:R:408:ASP:HB3	1.61	0.83
19:3:630:MET:HE2	36:M:287:LEU:HD11	1.59	0.82
19:3:47:THR:HG22	19:3:49:LYS:HG2	1.58	0.82
1:A:1018:ASN:HB2	1:A:1023:ASN:HB3	1.59	0.82
21:5:73:ALA:O	21:5:77:LEU:HB3	1.77	0.82
3:C:262:ARG:HD2	3:C:266:GLU:OE2	1.80	0.82
4:D:131:ILE:HG13	4:D:697:ALA:HB1	1.59	0.82
42:K:158:ASN:O	42:K:162:ILE:HG12	1.80	0.82
1:A:1122:ASN:CB	32:9:35:ARG:HD3	2.09	0.82
1:A:2306:HIS:HE1	1:A:2308:VAL:HG23	1.44	0.82
40:0:93:THR:CG2	40:0:98:GLN:HE22	1.93	0.82
17:1:641:ILE:CG1	17:1:675:MET:HE1	2.08	0.82
5:E:74:PHE:CE2	5:E:343:ILE:HG12	2.15	0.81
5:E:193:THR:HG22	5:E:194:TYR:CE1	2.15	0.81
25:J:238:ASN:HB3	25:J:240:THR:HG22	1.62	0.81
1:A:2090:ILE:HD11	1:A:2263:LEU:CD1	2.10	0.81
1:A:2310:ARG:CG	1:A:2313:HIS:ND1	2.43	0.81
5:E:132:THR:HG21	5:E:146:ARG:HD2	1.60	0.81
5:E:165:GLN:O	5:E:166:LEU:HD23	1.79	0.81
5:E:326:HIS:ND1	5:E:346:SER:HB3	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:585:ALA:HB3	19:3:609:LEU:CD2	2.10	0.81
42:K:66:LEU:HA	42:K:74:VAL:HG23	1.60	0.81
25:J:236:ARG:NH1	25:J:236:ARG:O	2.14	0.81
4:D:148:LEU:CD2	4:D:152:GLU:CB	2.59	0.81
26:P:212:ASN:HD22	28:T:458:SER:HB3	1.46	0.81
19:3:699:VAL:HG12	19:3:716:SER:HB2	1.63	0.81
27:R:387:ASP:HB2	29:X:351:GLU:CB	2.12	0.80
16:v:201:TRP:CE2	16:v:224:PRO:HB3	2.15	0.80
5:E:74:PHE:CE1	5:E:81:LEU:CD2	2.62	0.80
25:J:359:VAL:CG2	25:J:389:HIS:NE2	2.43	0.80
41:I:139:LYS:HZ3	41:I:139:LYS:HB3	1.45	0.80
17:1:641:ILE:HD11	17:1:675:MET:HE2	1.62	0.80
17:1:1058:ILE:HD13	17:1:1058:ILE:O	1.81	0.80
19:3:1130:VAL:HG11	19:3:1215:TYR:CZ	2.15	0.80
5:E:74:PHE:CZ	5:E:81:LEU:HD21	2.16	0.80
5:E:248:SER:HB2	5:E:249:TYR:CD1	2.17	0.80
5:E:265:ARG:H	5:E:272:ARG:NH2	1.80	0.80
27:R:237:MET:CE	27:R:237:MET:H	1.95	0.80
29:X:241:GLY:CA	29:X:288:ARG:NH2	2.44	0.80
27:R:237:MET:H	27:R:237:MET:HE2	1.46	0.80
39:8:56:VAL:CG2	39:8:68:ILE:CD1	2.60	0.80
5:E:174:GLY:HA3	5:E:192:ASN:O	1.82	0.80
17:1:971:MET:HE1	17:1:1003:VAL:CG1	2.12	0.80
17:1:1260:LYS:O	17:1:1264:VAL:HG12	1.82	0.79
1:A:2219:THR:CG2	1:A:2224:THR:CG2	2.60	0.79
4:D:150:ASP:OD1	17:1:879:LEU:HD22	1.81	0.79
16:v:201:TRP:NE1	16:v:224:PRO:HB3	1.96	0.79
27:R:280:ILE:N	32:9:224:THR:CG2	2.45	0.79
1:A:1385:VAL:CG1	1:A:1419:ILE:CD1	2.61	0.79
5:E:147:LEU:HD13	5:E:179:TRP:CD2	2.17	0.79
27:R:280:ILE:H	32:9:224:THR:HG21	1.47	0.79
4:D:129:ARG:HG2	4:D:841:TRP:HE1	1.45	0.79
1:A:2166:HIS:CD2	1:A:2272:MET:HE1	2.18	0.79
20:4:12:ASP:C	20:4:67:ALA:CB	2.56	0.79
5:E:310:TYR:CE1	5:E:322:LYS:HD2	2.18	0.78
15:H:77:U:H5''	15:H:78:U:H5'	1.64	0.78
27:R:467:ILE:HG23	31:Z:515:MET:HE2	1.65	0.78
20:4:17:VAL:O	20:4:56:TYR:HA	1.83	0.78
21:5:39:PHE:CE1	21:5:77:LEU:HD21	2.18	0.78
25:J:232:GLU:HA	25:J:235:ILE:HG22	1.64	0.78
1:A:2219:THR:HG21	1:A:2224:THR:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:GLU:OE1	3:C:76:GLU:N	2.16	0.78
27:R:403:ASN:HB2	29:X:250:PRO:O	1.82	0.78
41:I:128:VAL:HA	42:K:158:ASN:OD1	1.84	0.78
4:D:123:ALA:CB	4:D:161:LEU:HD11	2.13	0.78
19:3:429:ARG:HG2	19:3:429:ARG:NH2	1.97	0.77
36:M:249:TYR:HB3	40:0:72:TYR:OH	1.83	0.77
1:A:2306:HIS:CE1	1:A:2308:VAL:HG23	2.18	0.77
1:A:2090:ILE:HD11	1:A:2263:LEU:HD13	1.67	0.77
17:1:614:ARG:HD2	17:1:614:ARG:C	2.07	0.77
28:T:282:ARG:HB2	28:T:320:LYS:HD3	1.67	0.77
1:A:2117:ILE:HD11	1:A:2147:MET:CE	2.15	0.77
5:E:119:THR:CG2	5:E:161:ARG:HB2	2.12	0.77
5:E:148:LYS:O	5:E:179:TRP:HH2	1.67	0.77
25:J:299:TRP:HB3	25:J:316:TYR:HD2	1.47	0.77
42:K:120:THR:HG22	42:K:124:HIS:CD2	2.19	0.77
1:A:598:LEU:HD11	1:A:637:TRP:HZ3	1.50	0.77
1:A:2219:THR:CG2	1:A:2224:THR:HG21	2.15	0.77
5:E:231:MET:HE1	5:E:250:LEU:HD21	1.65	0.77
1:A:1639:VAL:CG1	1:A:1655:THR:HG23	2.15	0.77
19:3:1130:VAL:HG11	19:3:1215:TYR:CG	2.20	0.77
21:5:27:PRO:HG3	21:5:85:ARG:HD2	1.65	0.77
25:J:236:ARG:HH11	25:J:236:ARG:CA	1.98	0.77
5:E:74:PHE:CD1	5:E:81:LEU:CD2	2.67	0.76
19:3:539:PRO:HG2	19:3:580:ARG:HH22	1.48	0.76
30:Y:140:THR:HG22	31:Z:563:ARG:HG3	1.65	0.76
4:D:173:VAL:CG1	4:D:177:LYS:HE2	2.15	0.76
16:v:1:MET:HB3	18:2:557:VAL:HG11	1.67	0.76
25:J:337:MET:HE3	25:J:346:TRP:CZ3	2.08	0.76
5:E:61:LEU:HD13	5:E:352:TYR:CE1	2.20	0.76
5:E:231:MET:HB3	5:E:262:TRP:CZ3	2.21	0.76
19:3:47:THR:HG21	19:3:49:LYS:HG2	1.67	0.76
19:3:675:LEU:CD2	19:3:691:THR:HG22	2.15	0.76
4:D:120:ILE:HG21	4:D:136:ALA:HB2	1.65	0.76
5:E:277:PHE:HE2	5:E:300:ILE:CD1	1.98	0.76
4:D:151:LYS:HE2	4:D:151:LYS:HA	1.65	0.75
30:Y:138:ALA:HB1	31:Z:564:PRO:HD2	1.68	0.75
1:A:2325:VAL:CG1	4:D:788:GLY:O	2.34	0.75
27:R:387:ASP:H	29:X:351:GLU:HB3	1.51	0.75
4:D:120:ILE:HD12	4:D:161:LEU:HD22	1.65	0.75
32:9:277:LYS:O	32:9:437:PRO:CB	2.35	0.75
1:A:2090:ILE:HG22	1:A:2223:CYS:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:783:ALA:O	4:D:809:LEU:HA	1.85	0.75
25:J:337:MET:CE	25:J:346:TRP:CE3	2.70	0.75
41:I:26:LYS:HG3	41:I:28:ARG:H	1.52	0.75
1:A:1275:ARG:HD2	1:A:1375:TRP:NE1	2.02	0.75
29:X:238:THR:O	29:X:238:THR:HG23	1.85	0.75
5:E:287:ASN:O	5:E:289:LEU:HD23	1.87	0.74
19:3:1057:ARG:HG3	19:3:1057:ARG:NH1	1.97	0.74
20:4:12:ASP:C	20:4:67:ALA:HB2	2.12	0.74
5:E:250:LEU:HD12	5:E:250:LEU:O	1.87	0.74
5:E:326:HIS:CE1	5:E:346:SER:OG	2.39	0.74
25:J:270:ASP:OD1	27:R:223:PRO:CD	2.35	0.74
5:E:62:LEU:HB2	5:E:351:LEU:HB2	1.69	0.74
19:3:630:MET:HE1	36:M:287:LEU:CD2	2.17	0.74
14:G:222:U:C6	30:Y:119:LYS:CE	2.71	0.74
1:A:1639:VAL:HG12	1:A:1655:THR:HG23	1.69	0.74
5:E:132:THR:HG23	5:E:146:ARG:HB2	1.67	0.74
32:9:220:ILE:HD12	32:9:220:ILE:N	2.02	0.74
41:I:37:LYS:CD	41:I:39:TYR:CZ	2.71	0.74
1:A:1838:LYS:HE3	1:A:1865:ARG:NE	2.03	0.74
19:3:662:PHE:CE2	19:3:678:VAL:HG13	2.23	0.74
27:R:410:ARG:HH21	27:R:410:ARG:HG3	1.52	0.74
27:R:410:ARG:HG3	27:R:410:ARG:NH2	2.03	0.74
25:J:238:ASN:HB3	25:J:240:THR:CG2	2.17	0.74
25:J:333:PHE:CD1	25:J:349:TYR:HD1	2.03	0.73
39:8:56:VAL:CG2	39:8:68:ILE:HD11	2.17	0.73
1:A:976:MET:HE2	1:A:1098:PHE:CD1	2.23	0.73
1:A:228:TRP:CH2	1:A:413:LEU:HD11	2.23	0.73
1:A:1923:TRP:O	1:A:1927:ILE:HG12	1.87	0.73
14:G:213:C:C4'	14:G:214:C:OP2	2.37	0.73
27:R:387:ASP:CB	29:X:351:GLU:HB2	2.18	0.73
4:D:154:ARG:HH22	4:D:166:ASP:HA	1.53	0.73
19:3:1130:VAL:CG1	19:3:1215:TYR:CD1	2.71	0.73
1:A:51:PHE:CZ	5:E:66:GLU:OE1	2.42	0.73
3:C:81:VAL:HB	26:P:208:LYS:NZ	2.03	0.73
4:D:747:THR:CB	4:D:750:LEU:CB	2.67	0.73
5:E:133:VAL:O	5:E:146:ARG:HA	1.89	0.73
17:1:721:ILE:HD12	17:1:721:ILE:O	1.88	0.73
17:1:968:GLU:HA	17:1:971:MET:HG2	1.71	0.73
38:V:536:ILE:HG23	38:V:544:LEU:HD11	1.71	0.73
19:3:662:PHE:HE2	19:3:678:VAL:HG13	1.53	0.72
1:A:2069:SER:CB	1:A:2072:GLU:OE1	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:73:ALA:O	21:5:77:LEU:CB	2.37	0.72
25:J:340:GLN:HG3	25:J:372:VAL:HG21	1.69	0.72
34:x:640:ARG:CB	34:x:667:ALA:HA	2.20	0.72
27:R:394:LEU:CD1	29:X:331:LEU:HD22	2.20	0.72
27:R:438:ARG:HG3	27:R:438:ARG:NH2	2.00	0.72
30:Y:17:GLU:OE1	30:Y:28:TRP:HD1	1.71	0.72
1:A:829:PRO:HB3	21:5:86:TYR:CE2	2.25	0.72
3:C:683:ASN:ND2	3:C:683:ASN:H	1.85	0.72
5:E:148:LYS:O	5:E:179:TRP:CH2	2.43	0.72
34:x:515:SER:O	34:x:546:LEU:HA	1.87	0.72
5:E:260:ARG:CD	5:E:276:ILE:CG1	2.68	0.72
4:D:109:THR:HG22	4:D:180:THR:OG1	1.90	0.72
19:3:1165:SER:OG	19:3:1170:VAL:HG23	1.90	0.72
25:J:231:PHE:O	25:J:235:ILE:HG22	1.89	0.72
1:A:1774:ASN:OD1	1:A:1775:GLN:N	2.23	0.72
1:A:1298:ARG:NH2	2:B:39:C:H3'	2.05	0.71
1:A:2168:TYR:CE1	1:A:2298:LEU:HD11	2.24	0.71
38:V:536:ILE:HD12	38:V:544:LEU:CD1	2.19	0.71
1:A:1122:ASN:CB	32:9:35:ARG:HH21	2.01	0.71
14:G:206:C:O2'	14:G:207:A:OP2	2.07	0.71
19:3:47:THR:CG2	19:3:49:LYS:HE3	2.20	0.71
41:I:37:LYS:HD3	41:I:39:TYR:CE1	2.25	0.71
1:A:2324:GLU:HG2	1:A:2330:ARG:HH12	1.54	0.71
5:E:74:PHE:HE2	5:E:343:ILE:HG12	1.54	0.71
5:E:133:VAL:HB	5:E:147:LEU:HG	1.72	0.71
1:A:2074:ARG:NH2	4:D:1044:VAL:O	2.22	0.71
1:A:2090:ILE:HD12	1:A:2263:LEU:CD1	2.18	0.71
4:D:161:LEU:HD12	4:D:161:LEU:O	1.91	0.71
1:A:481:PHE:CZ	27:R:205:ASP:HB3	2.26	0.71
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.55	0.71
25:J:313:TRP:CE3	25:J:336:TRP:CE2	2.78	0.71
41:I:28:ARG:HH12	42:K:11:VAL:CG2	2.03	0.71
5:E:268:ALA:HB1	5:E:269:PRO:HD2	1.70	0.71
14:G:213:C:H4'	14:G:214:C:H5'	1.72	0.71
17:1:1075:ARG:HA	17:1:1078:VAL:HG22	1.72	0.71
27:R:386:ARG:HH11	27:R:386:ARG:HG3	1.53	0.71
1:A:1536:LEU:HG	1:A:1572:SER:HB3	1.72	0.71
4:D:121:GLN:HG2	4:D:132:LEU:HD21	1.73	0.71
19:3:550:ASN:HB2	19:3:592:LEU:HD23	1.71	0.71
5:E:74:PHE:CE2	5:E:343:ILE:CG1	2.73	0.70
30:Y:65:ILE:HD13	30:Y:82:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:37:LYS:CD	41:I:39:TYR:CE1	2.74	0.70
18:2:644:SER:CB	20:4:65:GLU:CB	2.69	0.70
29:X:265:LYS:HG3	29:X:364:SER:HG	1.54	0.70
1:A:1921:ASP:HB3	1:A:1966:HIS:CG	2.26	0.70
17:1:1109:ARG:HA	17:1:1112:THR:CG2	2.21	0.70
42:K:51:GLU:HA	42:K:54:ARG:NH2	2.06	0.70
22:6:27:ASP:OD2	40:0:20:LYS:CE	2.38	0.70
25:J:386:GLU:O	25:J:390:ALA:N	2.24	0.70
27:R:386:ARG:NH1	27:R:386:ARG:HG3	2.03	0.70
42:K:78:ILE:HD11	42:K:118:ALA:CA	2.21	0.70
19:3:1130:VAL:HG11	19:3:1215:TYR:CD1	2.27	0.70
19:3:585:ALA:HB3	19:3:609:LEU:HD23	1.73	0.70
29:X:345:GLU:OE2	29:X:348:ARG:NH1	2.25	0.70
1:A:2319:LEU:HD22	4:D:1070:LEU:HA	1.72	0.70
4:D:1671:GLY:O	4:D:1885:ASN:CB	2.40	0.70
19:3:1130:VAL:HG11	19:3:1215:TYR:CE1	2.25	0.70
25:J:261:ALA:HA	25:J:264:ILE:HD12	1.73	0.70
24:L:73:HIS:CD2	32:9:220:ILE:HD13	2.26	0.70
25:J:358:GLU:HG2	25:J:361:ARG:HD3	1.73	0.70
41:I:128:VAL:CA	42:K:158:ASN:OD1	2.40	0.70
1:A:409:ARG:HG2	1:A:410:PRO:HA	1.74	0.70
5:E:326:HIS:ND1	5:E:346:SER:OG	2.25	0.70
5:E:264:VAL:HA	5:E:272:ARG:NH2	2.07	0.69
32:9:349:PRO:CB	32:9:375:SER:HA	2.22	0.69
40:0:93:THR:CG2	40:0:98:GLN:NE2	2.55	0.69
1:A:1385:VAL:HG21	1:A:1414:ARG:HB3	1.74	0.69
4:D:1850:SER:O	4:D:1855:TYR:CB	2.40	0.69
17:1:1100:ASN:O	17:1:1103:VAL:HG23	1.92	0.69
1:A:977:LEU:C	1:A:977:LEU:HD12	2.17	0.69
1:A:2072:GLU:O	1:A:2076:ARG:HG3	1.92	0.69
1:A:2146:VAL:HG22	1:A:2272:MET:HB2	1.74	0.69
29:X:253:ARG:HG3	29:X:253:ARG:NH2	2.08	0.69
1:A:482:PHE:HZ	27:R:207:MET:HE2	1.57	0.69
1:A:2117:ILE:CD1	1:A:2147:MET:HE2	2.21	0.69
1:A:2127:TYR:OH	1:A:2159:LEU:CD1	2.40	0.69
14:G:215:U:H2'	30:Y:2:ASN:ND2	2.07	0.69
15:H:1:A:H3'	15:H:1:A:N3	2.08	0.69
19:3:138:GLN:HG3	19:3:161:HIS:CE1	2.27	0.69
19:3:1055:VAL:HG23	19:3:1093:MET:HE3	1.73	0.69
4:D:131:ILE:HG12	4:D:697:ALA:HB1	1.74	0.69
3:C:454:THR:HG22	3:C:578:ARG:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:THR:HG22	5:E:146:ARG:HB2	1.72	0.69
42:K:78:ILE:HD11	42:K:118:ALA:N	2.08	0.69
3:C:534:VAL:HB	3:C:537:TYR:O	1.92	0.69
1:A:1275:ARG:HD2	1:A:1375:TRP:CD1	2.28	0.69
5:E:119:THR:HG21	5:E:161:ARG:CB	2.19	0.69
16:v:41:ARG:NH2	16:v:54:ASP:OD1	2.26	0.69
17:1:394:GLU:HG3	17:1:396:ASN:H	1.58	0.69
19:3:54:LEU:HD23	19:3:99:PHE:CD2	2.28	0.69
27:R:280:ILE:N	32:9:224:THR:HG21	2.07	0.69
2:B:23:C:O2	2:B:23:C:H3'	1.93	0.69
5:E:74:PHE:CD1	5:E:81:LEU:HD23	2.28	0.69
25:J:329:ALA:O	25:J:333:PHE:HD2	1.76	0.69
1:A:1385:VAL:HG12	1:A:1419:ILE:HD11	1.73	0.69
4:D:142:VAL:HA	4:D:145:ASN:HD21	1.55	0.69
4:D:423:MET:CB	4:D:878:TYR:CB	2.71	0.69
5:E:243:LEU:HG	5:E:244:SER:O	1.92	0.69
13:F:21:A:C2	24:L:33:ARG:CZ	2.76	0.69
41:I:139:LYS:HB3	41:I:139:LYS:NZ	2.07	0.69
14:G:218:U:C5	30:Y:105:ARG:CZ	2.76	0.68
19:3:586:ASP:OD1	19:3:610:VAL:CG1	2.41	0.68
27:R:134:ARG:HE	28:T:383:ARG:HA	1.55	0.68
1:A:1237:MET:HE1	1:A:1283:GLU:HB3	1.75	0.68
16:v:5:ARG:NH1	16:v:7:GLY:O	2.25	0.68
1:A:598:LEU:HD11	1:A:637:TRP:CZ3	2.27	0.68
1:A:1639:VAL:CG1	1:A:1655:THR:CG2	2.72	0.68
3:C:690:GLU:OE2	3:C:788:LYS:NZ	2.25	0.68
41:I:50:ILE:HG12	41:I:119:VAL:HG12	1.73	0.68
1:A:1307:MET:SD	1:A:1547:VAL:CG1	2.80	0.68
13:F:21:A:H3'	13:F:21:A:N3	2.08	0.68
17:1:641:ILE:CG1	17:1:675:MET:HE2	2.22	0.68
4:D:141:ALA:HA	4:D:182:TYR:OH	1.94	0.68
5:E:178:LEU:CD1	5:E:222:LEU:CD2	2.70	0.68
1:A:1219:GLU:O	1:A:1222:LYS:NZ	2.26	0.68
1:A:1639:VAL:HG12	1:A:1655:THR:HG22	1.74	0.68
1:A:2168:TYR:CZ	1:A:2298:LEU:CD1	2.71	0.68
27:R:390:GLU:OE1	27:R:390:GLU:N	2.20	0.68
34:x:726:ALA:HB1	34:x:732:GLY:HA3	1.75	0.68
1:A:2219:THR:OG1	1:A:2222:SER:HB3	1.93	0.68
41:I:28:ARG:HH12	42:K:11:VAL:HG21	1.58	0.68
4:D:128:PRO:HD2	4:D:131:ILE:HD12	1.75	0.68
31:Z:612:TYR:O	31:Z:616:VAL:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2219:THR:CG2	1:A:2224:THR:HG22	2.23	0.68
4:D:504:PRO:CB	4:D:681:ARG:CB	2.71	0.68
25:J:247:LYS:HB3	25:J:247:LYS:HZ1	1.57	0.68
25:J:307:PRO:HB2	25:J:339:TRP:CZ2	2.29	0.68
19:3:970:TYR:HE1	19:3:979:ARG:HB2	1.57	0.67
27:R:386:ARG:HH21	29:X:339:LEU:HD11	1.59	0.67
32:9:120:ARG:HG2	32:9:120:ARG:HH21	1.59	0.67
19:3:114:ARG:HG3	23:7:41:CYS:SG	2.34	0.67
19:3:761:THR:HG21	19:3:763:ARG:HH21	1.59	0.67
27:R:331:ALA:HB2	29:X:355:LYS:HD2	1.76	0.67
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.75	0.67
5:E:108:HIS:CE1	5:E:128:SER:CB	2.77	0.67
19:3:487:ILE:HA	19:3:491:VAL:HG22	1.76	0.67
5:E:246:GLU:HB2	5:E:248:SER:OG	1.94	0.67
5:E:119:THR:CG2	5:E:161:ARG:CB	2.72	0.67
17:1:632:PHE:HA	17:1:635:VAL:HG13	1.77	0.67
3:C:452:THR:HG22	3:C:577:PHE:HD2	1.58	0.67
30:Y:86:ASP:OD1	31:Z:502:ALA:CB	2.43	0.67
19:3:783:TYR:HB2	19:3:801:GLU:HB3	1.77	0.67
19:3:950:ALA:HB2	19:3:989:TYR:HH	1.60	0.67
1:A:439:GLN:HB3	1:A:443:VAL:CG2	2.25	0.67
2:B:90:U:H5''	6:a:66:SER:CB	2.25	0.67
27:R:394:LEU:HD13	29:X:331:LEU:HD22	1.76	0.67
27:R:394:LEU:HD11	29:X:331:LEU:CD2	2.25	0.67
1:A:173:GLU:OE2	33:z:90:ARG:NH1	2.28	0.67
1:A:1773:SER:O	1:A:1813:ARG:NH1	2.28	0.67
30:Y:67:LEU:CA	30:Y:80:CYS:HB2	2.25	0.67
2:B:35:U:OP1	32:9:15:CYS:HB2	1.95	0.66
5:E:116:HIS:O	5:E:124:LEU:HD12	1.95	0.66
22:6:29:LYS:HD3	22:6:34:ASP:OD1	1.94	0.66
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.78	0.66
42:K:82:CYS:SG	42:K:120:THR:HB	2.36	0.66
15:H:84:C:O5'	15:H:84:C:H6	1.78	0.66
25:J:232:GLU:O	25:J:235:ILE:HG23	1.95	0.66
27:R:388:ILE:HG23	29:X:350:TYR:CD1	2.30	0.66
1:A:1544:ARG:HH21	36:M:183:ILE:HG12	1.61	0.66
19:3:930:LEU:HD12	19:3:937:LEU:HD23	1.77	0.66
4:D:445:VAL:O	4:D:688:THR:CB	2.43	0.66
5:E:178:LEU:HD11	5:E:222:LEU:CD2	2.26	0.66
5:E:258:THR:HG22	5:E:260:ARG:CG	2.25	0.66
5:E:108:HIS:CE1	5:E:128:SER:HB3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TRP:CH2	1:A:413:LEU:CD1	2.78	0.66
4:D:1090:ARG:HG2	4:D:1090:ARG:HH21	1.61	0.66
14:G:210:G:H3'	14:G:210:G:N3	2.11	0.66
17:1:1044:ASP:OD1	17:1:1044:ASP:N	2.28	0.66
19:3:49:LYS:HE2	35:y:29:ARG:NH1	2.11	0.66
19:3:630:MET:CE	36:M:287:LEU:HD11	2.26	0.66
42:K:120:THR:HG22	42:K:124:HIS:HD2	1.60	0.66
5:E:175:THR:CG2	5:E:191:GLN:OE1	2.44	0.65
27:R:281:ASN:O	32:9:221:LEU:HD13	1.96	0.65
5:E:62:LEU:CB	5:E:351:LEU:HB2	2.26	0.65
5:E:268:ALA:HB1	5:E:269:PRO:CD	2.26	0.65
19:3:687:SER:O	36:M:306:VAL:CG2	2.41	0.65
19:3:736:TYR:OH	19:3:763:ARG:NH1	2.28	0.65
4:D:106:THR:HG22	4:D:107:LYS:N	2.09	0.65
13:F:22:G:OP1	24:L:33:ARG:NH1	2.30	0.65
27:R:434:ASP:N	27:R:434:ASP:OD1	2.27	0.65
30:Y:55:VAL:HG13	31:Z:589:ARG:HD2	1.78	0.65
31:Z:530:ASP:OD1	31:Z:530:ASP:N	2.25	0.65
25:J:329:ALA:O	25:J:333:PHE:CD2	2.50	0.65
25:J:340:GLN:HB2	25:J:346:TRP:CZ2	2.31	0.65
41:I:129:GLU:HB2	41:I:133:LYS:HZ3	1.62	0.65
1:A:1975:GLU:O	1:A:1979:VAL:HG22	1.97	0.65
14:G:217:U:H6	14:G:217:U:H5'	1.61	0.65
16:v:187:ARG:NH1	18:2:694:PHE:HE1	1.93	0.65
19:3:586:ASP:O	19:3:610:VAL:HG13	1.97	0.65
25:J:349:TYR:HE2	25:J:365:ILE:HG13	1.61	0.65
1:A:413:LEU:HD13	1:A:415:SER:O	1.97	0.65
32:9:37:LEU:HD12	32:9:38:PRO:HD2	1.78	0.65
1:A:213:LEU:HD12	1:A:230:PHE:CE1	2.31	0.65
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.61	0.65
47:F:207:G5J:O1G	41:I:37:LYS:HE2	1.96	0.65
25:J:340:GLN:HB2	25:J:346:TRP:HZ2	1.61	0.65
1:A:977:LEU:HD12	1:A:977:LEU:O	1.97	0.65
16:v:190:LEU:HD21	18:2:691:ALA:CB	2.16	0.65
25:J:313:TRP:CH2	25:J:336:TRP:CD1	2.85	0.65
27:R:388:ILE:HG23	29:X:350:TYR:CE1	2.30	0.65
30:Y:140:THR:HG22	31:Z:563:ARG:CG	2.25	0.65
14:G:219:U:H6	14:G:219:U:OP1	1.80	0.65
41:I:28:ARG:NH1	42:K:11:VAL:HG21	2.11	0.65
41:I:73:GLU:HB3	41:I:93:LYS:HG2	1.79	0.65
4:D:151:LYS:HE2	4:D:151:LYS:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:1115:ALA:O	17:1:1119:VAL:HG12	1.97	0.64
19:3:1006:GLN:O	19:3:1006:GLN:HG2	1.96	0.64
1:A:228:TRP:CZ2	1:A:413:LEU:HD11	2.32	0.64
5:E:243:LEU:HD21	5:E:247:GLY:HA2	1.79	0.64
25:J:340:GLN:HG3	25:J:372:VAL:CG2	2.28	0.64
42:K:78:ILE:HG12	42:K:117:SER:CB	2.26	0.64
20:4:12:ASP:C	20:4:67:ALA:HB1	2.22	0.64
25:J:359:VAL:HG21	25:J:389:HIS:CE1	2.33	0.64
1:A:661:GLU:O	27:R:213:LYS:HG3	1.97	0.64
1:A:1385:VAL:HG21	1:A:1414:ARG:CB	2.28	0.64
17:1:95:PRO:HB2	27:R:412:PHE:HE2	1.61	0.64
19:3:47:THR:HG22	19:3:49:LYS:H	1.62	0.64
32:9:220:ILE:H	32:9:220:ILE:CD1	2.11	0.64
2:B:102:U:H6	2:B:102:U:O5'	1.81	0.64
5:E:74:PHE:CD1	5:E:81:LEU:HD21	2.29	0.64
18:2:657:ILE:O	18:2:657:ILE:CG2	2.45	0.64
30:Y:116:ARG:HG2	30:Y:116:ARG:HH11	1.63	0.64
1:A:246:LEU:HD11	1:A:411:PHE:CE2	2.32	0.64
17:1:1180:ARG:HH21	17:1:1180:ARG:HB2	1.62	0.64
22:6:27:ASP:OD2	40:0:20:LYS:NZ	2.31	0.64
1:A:2074:ARG:NH1	4:D:1042:GLU:HA	2.12	0.64
27:R:236:LYS:HG2	27:R:237:MET:HE3	1.80	0.64
28:T:381:HIS:ND1	28:T:382:PRO:HD2	2.13	0.64
1:A:1544:ARG:NH2	36:M:183:ILE:HG12	2.14	0.63
17:1:1261:VAL:O	17:1:1264:VAL:HG13	1.98	0.63
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.81	0.63
5:E:178:LEU:HD21	5:E:208:ILE:CD1	2.28	0.63
14:G:222:U:H6	30:Y:119:LYS:HE2	1.59	0.63
24:L:77:LEU:CD2	32:9:221:LEU:HD11	2.20	0.63
39:8:56:VAL:CG2	39:8:68:ILE:HD13	2.22	0.63
13:F:31:U:O2'	13:F:32:C:P	2.56	0.63
17:1:550:HIS:CE1	22:6:96:THR:HG22	2.33	0.63
17:1:1108:ASN:O	17:1:1112:THR:HG22	1.98	0.63
40:0:93:THR:HG22	40:0:98:GLN:HE22	1.62	0.63
42:K:151:SER:HB3	42:K:156:LEU:HD23	1.79	0.63
1:A:51:PHE:O	5:E:88:ARG:NH2	2.31	0.63
1:A:2325:VAL:HG13	4:D:788:GLY:CA	2.27	0.63
2:B:96:A:H3'	2:B:96:A:N3	2.13	0.63
16:v:33:GLU:HG3	16:v:46:ILE:HD11	1.79	0.63
1:A:1777:ILE:HG12	1:A:1860:GLN:HB2	1.80	0.63
4:D:148:LEU:HD22	4:D:153:ARG:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:661:ARG:NH1	17:1:696:ASP:OD2	2.30	0.63
1:A:481:PHE:CE1	27:R:205:ASP:HB3	2.34	0.63
1:A:591:MET:HB3	1:A:598:LEU:HD22	1.81	0.63
1:A:1144:LYS:HG3	32:9:46:LEU:HD22	1.80	0.63
17:1:404:LEU:HD23	21:5:47:GLN:OE1	1.98	0.63
1:A:211:GLN:HB3	1:A:214:ARG:HB2	1.81	0.63
3:C:779:LEU:HD21	3:C:912:LEU:CD1	2.27	0.63
19:3:791:HIS:CE1	19:3:930:LEU:HD23	2.34	0.63
21:5:77:LEU:CD2	21:5:89:VAL:HG11	2.29	0.63
1:A:1541:THR:O	1:A:1544:ARG:HG3	1.99	0.63
1:A:1838:LYS:HG3	1:A:1865:ARG:NH2	2.14	0.63
2:B:43:U:OP2	32:9:3:LYS:HE2	1.99	0.63
27:R:280:ILE:HB	32:9:221:LEU:HD22	1.80	0.63
4:D:164:THR:HA	4:D:168:ARG:HH11	1.64	0.62
5:E:251:LEU:HG	5:E:291:CYS:SG	2.39	0.62
17:1:696:ASP:O	17:1:702:ARG:NH1	2.29	0.62
19:3:1164:ARG:O	19:3:1170:VAL:HG22	1.98	0.62
27:R:427:ASP:OD1	27:R:427:ASP:N	2.30	0.62
1:A:2090:ILE:CD1	1:A:2263:LEU:HD13	2.26	0.62
4:D:713:MET:O	4:D:716:ALA:HB2	1.98	0.62
4:D:1948:MET:HA	4:D:1953:MET:O	1.98	0.62
5:E:308:PHE:CE1	5:E:324:PRO:HB3	2.34	0.62
20:4:15:VAL:O	20:4:58:PHE:HA	1.98	0.62
28:T:390:GLY:HA3	28:T:416:ILE:HD11	1.81	0.62
36:M:157:ASN:OD1	36:M:157:ASN:N	2.32	0.62
42:K:82:CYS:SG	42:K:120:THR:CG2	2.87	0.62
1:A:955:TRP:CZ3	1:A:976:MET:HE1	2.34	0.62
4:D:131:ILE:HG21	4:D:701:PHE:CB	2.29	0.62
27:R:404:GLU:N	29:X:253:ARG:HH11	1.97	0.62
32:9:75:THR:HA	32:9:82:LYS:HA	1.81	0.62
41:I:142:VAL:HG11	42:K:86:PRO:HB2	1.79	0.62
5:E:174:GLY:O	5:E:192:ASN:N	2.32	0.62
17:1:1055:TRP:HA	17:1:1058:ILE:HG22	1.81	0.62
25:J:245:TRP:HZ3	25:J:264:ILE:HG23	1.60	0.62
25:J:347:HIS:HA	25:J:350:ILE:HD12	1.81	0.62
29:X:325:LYS:HD3	29:X:351:GLU:OE2	1.99	0.62
13:F:23:G:O2'	13:F:24:U:P	2.57	0.62
17:1:641:ILE:HG13	17:1:675:MET:CE	2.12	0.62
25:J:560:ALA:O	25:J:564:LEU:CB	2.48	0.62
27:R:202:MET:HE1	41:I:113:PHE:HE1	1.64	0.62
32:9:112:ASN:O	32:9:159:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1774:ASN:OD1	1:A:1775:GLN:CG	2.48	0.62
5:E:147:LEU:HD13	5:E:179:TRP:CD1	2.34	0.62
17:1:665:ILE:HG23	17:1:690:ILE:HD12	1.82	0.62
25:J:232:GLU:CA	25:J:235:ILE:HG22	2.30	0.62
29:X:270:LEU:HB3	29:X:271:PRO:HD2	1.81	0.62
1:A:2105:ILE:HD13	1:A:2266:ARG:HH22	1.64	0.62
4:D:406:ARG:CB	4:D:955:ASP:CA	2.71	0.62
13:F:4:U:H5'	41:I:31:ARG:NH2	2.14	0.62
17:1:1083:TYR:CE1	40:0:13:VAL:HG23	2.35	0.62
20:4:12:ASP:O	20:4:67:ALA:CB	2.48	0.62
29:X:233:LEU:HD11	29:X:237:ASN:HD21	1.64	0.62
1:A:2284:MET:HG3	1:A:2284:MET:O	1.99	0.62
18:2:644:SER:HA	20:4:65:GLU:CB	2.30	0.62
19:3:47:THR:HG21	19:3:49:LYS:HE3	1.81	0.62
30:Y:63:VAL:HG11	31:Z:497:TRP:CD1	2.34	0.62
32:9:49:PHE:CD1	32:9:52:PRO:HG3	2.34	0.62
1:A:1385:VAL:HG11	1:A:1419:ILE:CD1	2.29	0.62
3:C:151:GLU:HG2	3:C:158:ARG:HH11	1.64	0.62
30:Y:117:ALA:HB2	31:Z:494:TYR:CE2	2.35	0.62
36:M:127:GLU:O	36:M:136:ARG:NH2	2.30	0.62
42:K:78:ILE:HG21	42:K:114:THR:CG2	2.29	0.62
1:A:1774:ASN:OD1	1:A:1775:GLN:HG2	2.00	0.62
3:C:532:ILE:HD11	3:C:541:VAL:HG11	1.82	0.62
17:1:588:TYR:CZ	22:6:91:LEU:HD21	2.35	0.62
17:1:1109:ARG:O	17:1:1112:THR:HG23	2.00	0.62
19:3:669:LEU:HD12	19:3:673:VAL:HG23	1.82	0.62
27:R:387:ASP:O	29:X:351:GLU:N	2.29	0.62
36:M:279:HIS:ND1	36:M:296:CYS:SG	2.73	0.62
1:A:200:ASP:OD1	1:A:240:ARG:NH2	2.32	0.61
1:A:2328:ALA:CB	4:D:787:ALA:HB3	2.30	0.61
2:B:45:C:C5	32:9:3:LYS:HG3	2.34	0.61
5:E:108:HIS:CE1	5:E:128:SER:HB2	2.35	0.61
13:F:21:A:H2	24:L:33:ARG:CZ	2.13	0.61
4:D:1090:ARG:HH21	4:D:1090:ARG:CG	2.13	0.61
5:E:160:ALA:HB2	5:E:201:PHE:CD2	2.35	0.61
17:1:1224:PRO:HA	17:1:1227:ILE:HG22	1.81	0.61
1:A:213:LEU:HD12	1:A:230:PHE:HE1	1.65	0.61
4:D:502:CYS:CB	4:D:654:THR:HA	2.30	0.61
17:1:971:MET:CE	17:1:1003:VAL:HG11	2.23	0.61
29:X:222:GLU:OE1	29:X:222:GLU:N	2.26	0.61
33:z:56:ARG:HB3	33:z:64:GLN:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:759:THR:HA	19:3:682:VAL:HG21	1.81	0.61
5:E:178:LEU:HD21	5:E:208:ILE:HD13	1.82	0.61
17:1:719:TYR:HB3	19:3:216:GLY:O	2.00	0.61
42:K:132:PHE:C	42:K:134:PRO:HD2	2.24	0.61
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.29	0.61
4:D:149:ARG:HH11	4:D:149:ARG:CG	2.14	0.61
18:2:599:THR:HG23	18:2:599:THR:O	2.00	0.61
4:D:131:ILE:HG12	4:D:697:ALA:O	1.99	0.61
27:R:280:ILE:N	32:9:224:THR:HG22	2.09	0.61
32:9:49:PHE:CE1	32:9:52:PRO:HG3	2.34	0.61
30:Y:7:VAL:HG22	30:Y:108:ARG:HB3	1.83	0.61
1:A:1864:THR:HA	1:A:1890:GLN:HG2	1.83	0.61
5:E:62:LEU:CG	5:E:351:LEU:HB2	2.30	0.61
5:E:260:ARG:HD3	5:E:276:ILE:HD13	1.82	0.61
13:F:3:G:O6	42:K:13:ARG:HD3	2.00	0.61
19:3:93:GLN:NE2	19:3:100:GLU:OE1	2.34	0.61
19:3:1130:VAL:HG13	19:3:1215:TYR:CD1	2.33	0.61
1:A:466:ALA:HB1	2:B:19:A:C8	2.36	0.61
5:E:277:PHE:HE2	5:E:300:ILE:HD12	1.64	0.61
17:1:1018:PRO:HB2	36:M:223:ARG:HG2	1.82	0.61
19:3:406:PRO:HA	19:3:1122:LEU:O	2.00	0.61
38:V:624:THR:HG23	38:V:643:LEU:HD12	1.83	0.61
1:A:1755:SER:O	17:1:942:ASN:HB2	1.99	0.61
1:A:2227:ALA:HB2	1:A:2261:MET:SD	2.40	0.61
4:D:448:PRO:C	4:D:686:GLU:CB	2.73	0.61
14:G:214:C:OP1	30:Y:2:ASN:HB2	2.01	0.61
17:1:602:LYS:NZ	39:8:9:THR:OG1	2.34	0.61
21:5:76:HIS:O	21:5:76:HIS:ND1	2.27	0.61
25:J:236:ARG:HH11	25:J:236:ARG:CG	2.13	0.61
27:R:410:ARG:HH21	27:R:410:ARG:CG	2.14	0.61
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.83	0.60
3:C:167:TYR:CE2	3:C:535:ALA:HB3	2.36	0.60
14:G:213:C:H4'	14:G:214:C:OP2	1.99	0.60
19:3:86:ARG:HD2	19:3:1157:GLY:O	2.01	0.60
25:J:438:TYR:O	25:J:442:ARG:N	2.32	0.60
27:R:391:VAL:HG23	29:X:347:GLN:HB3	1.82	0.60
29:X:357:VAL:HG22	29:X:368:VAL:HG22	1.83	0.60
4:D:1589:PHE:CA	4:D:1642:GLN:CB	2.79	0.60
25:J:231:PHE:HD2	25:J:248:TYR:HD1	1.49	0.60
25:J:265:TYR:CD2	25:J:282:TYR:HD1	2.20	0.60
25:J:333:PHE:CE1	25:J:349:TYR:HD1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2106:LEU:HD12	1:A:2107:PRO:HD2	1.83	0.60
1:A:2117:ILE:CD1	1:A:2147:MET:CE	2.79	0.60
5:E:258:THR:CG2	5:E:260:ARG:HH11	2.01	0.60
1:A:1919:LEU:HD12	1:A:1936:LEU:HD21	1.82	0.60
4:D:129:ARG:HG2	4:D:841:TRP:NE1	2.17	0.60
4:D:173:VAL:HG12	4:D:177:LYS:HE2	1.83	0.60
5:E:114:GLU:CD	5:E:116:HIS:HE2	2.09	0.60
5:E:265:ARG:H	5:E:272:ARG:HH21	1.47	0.60
17:1:129:SEP:O2P	17:1:572:HIS:ND1	2.29	0.60
5:E:233:GLY:O	5:E:260:ARG:NH2	2.35	0.60
17:1:621:ASP:HB2	17:1:624:VAL:HG22	1.82	0.60
18:2:703:ILE:HG21	18:2:705:ARG:HE	1.66	0.60
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.83	0.60
5:E:260:ARG:CD	5:E:276:ILE:CD1	2.79	0.60
19:3:412:ILE:HG12	19:3:423:LEU:HG	1.82	0.60
1:A:481:PHE:CE2	27:R:205:ASP:HB3	2.36	0.60
5:E:145:LYS:HE2	5:E:184:LYS:CE	2.29	0.60
14:G:206:C:O2'	14:G:207:A:P	2.60	0.60
22:6:22:LEU:HD22	22:6:60:ILE:HD12	1.83	0.60
30:Y:117:ALA:HB2	31:Z:494:TYR:CD2	2.37	0.60
32:9:276:VAL:CB	32:9:297:CYS:CB	2.79	0.60
42:K:119:ILE:CG2	42:K:163:PHE:HD2	2.05	0.60
1:A:150:MET:SD	1:A:153:ARG:HD3	2.42	0.60
16:v:1:MET:CB	18:2:557:VAL:HG11	2.31	0.60
25:J:340:GLN:HG2	25:J:340:GLN:O	2.01	0.60
27:R:390:GLU:H	27:R:390:GLU:CD	2.09	0.60
1:A:1762:TYR:O	1:A:2008:ARG:CD	2.50	0.60
3:C:772:TRP:CZ2	32:9:133:GLN:HG3	2.37	0.60
16:v:204:ASP:OD1	16:v:205:GLY:N	2.34	0.59
17:1:549:ARG:NH2	17:1:584:ASP:OD2	2.34	0.59
15:H:31:C:H2'	15:H:32:G:H5''	1.83	0.59
1:A:143:GLN:NE2	1:A:207:PHE:O	2.34	0.59
27:R:279:HIS:CA	32:9:224:THR:CG2	2.73	0.59
29:X:283:LEU:HD11	29:X:292:ILE:HD12	1.83	0.59
3:C:589:LYS:HE2	3:C:940:ARG:HH12	1.67	0.59
17:1:405:ASP:OD1	21:5:49:ARG:NH2	2.35	0.59
19:3:1004:ASP:CG	19:3:1007:GLU:HB2	2.27	0.59
34:x:418:LEU:HA	34:x:567:ALA:HB1	1.84	0.59
1:A:386:PRO:HD2	1:A:389:LYS:HD2	1.85	0.59
1:A:767:VAL:HG11	2:B:39:C:C6	2.37	0.59
1:A:1790:ILE:HG12	1:A:1800:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1976:TRP:CA	1:A:1979:VAL:HG22	2.31	0.59
1:A:2127:TYR:OH	1:A:2159:LEU:HD11	2.02	0.59
5:E:263:ASP:HB3	5:E:274:VAL:HG21	1.84	0.59
25:J:328:GLY:O	25:J:332:VAL:HG23	2.03	0.59
1:A:1092:ILE:CG2	1:A:1093:ASP:N	2.64	0.59
1:A:1921:ASP:HB3	1:A:1966:HIS:CE1	2.38	0.59
27:R:386:ARG:HH11	27:R:386:ARG:CG	2.14	0.59
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.20	0.59
1:A:2090:ILE:HA	1:A:2223:CYS:O	2.03	0.59
41:I:56:VAL:HG23	41:I:58:VAL:HG13	1.84	0.59
3:C:778:PRO:HD3	3:C:817:TYR:CE1	2.38	0.59
17:1:1000:ILE:O	17:1:1004:ILE:HG12	2.03	0.59
17:1:1109:ARG:HA	17:1:1112:THR:HG22	1.83	0.59
5:E:165:GLN:HG3	5:E:181:ILE:HD11	1.85	0.59
3:C:532:ILE:CD1	3:C:541:VAL:HG11	2.33	0.58
4:D:176:GLY:O	4:D:179:ILE:CG2	2.38	0.58
17:1:631:ALA:O	17:1:635:VAL:HG13	2.03	0.58
21:5:24:ARG:HB2	21:5:88:VAL:HB	1.85	0.58
25:J:236:ARG:HH11	25:J:236:ARG:HA	1.68	0.58
29:X:241:GLY:CA	29:X:288:ARG:CZ	2.76	0.58
42:K:62:PHE:O	42:K:66:LEU:HD12	2.03	0.58
19:3:108:GLY:O	22:6:82:ARG:NH1	2.35	0.58
22:6:58:CYS:HB3	22:6:62:GLY:H	1.67	0.58
25:J:333:PHE:CG	25:J:349:TYR:CE1	2.91	0.58
1:A:2319:LEU:HD22	4:D:1070:LEU:CA	2.33	0.58
17:1:1058:ILE:HD13	17:1:1058:ILE:C	2.28	0.58
19:3:471:ASP:OD2	19:3:746:ALA:N	2.34	0.58
29:X:246:TYR:OH	29:X:249:PRO:HD3	2.04	0.58
36:M:296:CYS:SG	36:M:297:TYR:N	2.75	0.58
1:A:855:ARG:HH22	1:A:1522:GLN:HA	1.69	0.58
1:A:1838:LYS:HE3	1:A:1865:ARG:NH2	2.19	0.58
16:v:8:ASP:OD1	16:v:8:ASP:N	2.36	0.58
17:1:774:ILE:HD11	17:1:810:ILE:HD13	1.84	0.58
19:3:585:ALA:HB3	19:3:609:LEU:HD22	1.84	0.58
19:3:675:LEU:HD21	19:3:691:THR:HG22	1.85	0.58
21:5:77:LEU:HD23	21:5:89:VAL:HG11	1.84	0.58
1:A:439:GLN:HB3	1:A:443:VAL:HG21	1.84	0.58
3:C:81:VAL:HB	26:P:208:LYS:HZ2	1.68	0.58
17:1:546:ASP:N	17:1:546:ASP:OD1	2.32	0.58
41:I:128:VAL:CG1	42:K:158:ASN:OD1	2.51	0.58
1:A:1547:VAL:HG12	1:A:1548:TYR:HD1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TRP:O	1:A:212:PRO:HB3	2.02	0.58
1:A:1549:VAL:O	1:A:1549:VAL:HG12	2.04	0.58
4:D:1825:ASN:CB	4:D:1853:ALA:HB3	2.33	0.58
19:3:47:THR:HG23	19:3:49:LYS:HE3	1.85	0.58
41:I:129:GLU:HB2	41:I:133:LYS:NZ	2.18	0.58
5:E:243:LEU:HD11	5:E:247:GLY:HA2	1.83	0.58
5:E:277:PHE:CE2	5:E:300:ILE:CD1	2.85	0.58
5:E:310:TYR:CE1	5:E:322:LYS:CD	2.86	0.58
40:0:93:THR:HB	40:0:98:GLN:NE2	2.19	0.58
42:K:70:ASN:HD22	42:K:73:LEU:HD13	1.69	0.58
4:D:131:ILE:HG23	4:D:698:ILE:HA	1.86	0.58
4:D:1662:ILE:HA	4:D:1703:VAL:O	2.04	0.58
3:C:780:CYS:SG	3:C:782:GLU:CG	2.92	0.58
4:D:131:ILE:HG12	4:D:697:ALA:C	2.29	0.58
42:K:78:ILE:HD11	42:K:118:ALA:HB2	1.85	0.58
1:A:955:TRP:HZ3	1:A:976:MET:HE1	1.68	0.57
1:A:977:LEU:HB2	1:A:1175:VAL:HG22	1.85	0.57
3:C:450:GLU:HA	3:C:457:VAL:HG22	1.86	0.57
4:D:164:THR:HA	4:D:168:ARG:HH12	1.67	0.57
16:v:194:LEU:CD2	19:3:1017:ASN:HB3	2.34	0.57
19:3:429:ARG:HD2	23:7:58:ASN:OD1	2.04	0.57
16:v:38:ARG:NH1	17:1:1179:ASP:OD1	2.33	0.57
16:v:202:ILE:HG22	16:v:204:ASP:H	1.68	0.57
29:X:283:LEU:HG	29:X:292:ILE:HB	1.85	0.57
40:0:97:LYS:O	40:0:97:LYS:HG3	2.04	0.57
42:K:111:ASN:OD1	42:K:112:GLU:N	2.38	0.57
1:A:1052:VAL:O	1:A:1160:ARG:NH1	2.38	0.57
25:J:333:PHE:CG	25:J:349:TYR:CD1	2.92	0.57
41:I:37:LYS:HD2	41:I:39:TYR:CE1	2.37	0.57
1:A:137:GLU:HG3	1:A:424:ILE:HD13	1.87	0.57
3:C:460:ASP:N	3:C:460:ASP:OD1	2.36	0.57
3:C:711:ARG:NH2	3:C:730:ARG:O	2.37	0.57
4:D:120:ILE:CD1	4:D:161:LEU:CD2	2.67	0.57
14:G:217:U:H5'	14:G:217:U:C6	2.39	0.57
19:3:1130:VAL:HG12	19:3:1215:TYR:CZ	2.36	0.57
27:R:237:MET:O	27:R:237:MET:HG2	2.03	0.57
1:A:822:PHE:CE2	1:A:1000:ILE:HD12	2.40	0.57
1:A:1143:MET:O	1:A:1147:VAL:HG22	2.04	0.57
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.87	0.57
4:D:1619:TYR:HA	4:D:1645:VAL:O	2.05	0.57
32:9:143:ASP:OD1	32:9:144:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:141:GLN:NE2	36:M:159:TYR:O	2.38	0.57
41:I:128:VAL:HG12	42:K:158:ASN:OD1	2.03	0.57
42:K:116:LEU:HD23	42:K:159:LEU:HD12	1.85	0.57
17:1:858:LYS:NZ	17:1:894:ASP:OD2	2.37	0.57
21:5:39:PHE:CE1	21:5:77:LEU:CD2	2.80	0.57
19:3:524:ILE:HD11	19:3:556:ILE:HG21	1.87	0.57
5:E:277:PHE:CE2	5:E:300:ILE:HD13	2.40	0.57
28:T:337:ARG:HG3	28:T:378:VAL:HG23	1.86	0.57
34:x:442:THR:O	34:x:446:MET:N	2.37	0.57
42:K:82:CYS:SG	42:K:120:THR:HG21	2.43	0.57
42:K:82:CYS:HA	42:K:121:THR:HG22	1.86	0.57
3:C:357:THR:OG1	3:C:359:LYS:O	2.20	0.57
13:F:2:U:O2	42:K:42:ASN:HB3	2.05	0.57
16:v:36:MET:HE3	16:v:40:GLY:HA2	1.86	0.57
25:J:319:MET:HE3	25:J:323:LEU:HD12	1.87	0.57
25:J:359:VAL:HG11	25:J:389:HIS:CD2	2.40	0.57
25:J:380:ILE:HD13	25:J:414:HIS:ND1	2.19	0.57
1:A:460:LYS:HE2	2:B:49:A:OP2	2.04	0.57
5:E:147:LEU:CD1	5:E:179:TRP:CD1	2.88	0.57
28:T:418:THR:HG21	28:T:467:ALA:HA	1.87	0.57
30:Y:17:GLU:OE1	30:Y:28:TRP:CD1	2.55	0.57
1:A:774:LYS:NZ	15:H:5:C:O2'	2.28	0.56
3:C:618:THR:HB	3:C:630:LEU:HB2	1.87	0.56
4:D:140:LEU:HD23	4:D:144:LYS:HG2	1.87	0.56
5:E:194:TYR:CD1	5:E:194:TYR:N	2.73	0.56
17:1:1045:ARG:NH1	40:0:22:GLY:O	2.37	0.56
30:Y:37:TRP:O	30:Y:112:VAL:HG22	2.04	0.56
39:8:34:LEU:HD22	39:8:82:SER:HB2	1.86	0.56
42:K:127:PRO:HG2	42:K:131:SER:HB3	1.87	0.56
1:A:215:ASP:OD1	1:A:215:ASP:N	2.37	0.56
1:A:1144:LYS:CG	32:9:46:LEU:HD22	2.35	0.56
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.70	0.56
3:C:389:ASP:OD1	3:C:389:ASP:N	2.33	0.56
25:J:301:ARG:O	25:J:304:THR:HB	2.06	0.56
28:T:350:HIS:HA	28:T:374:SER:HB2	1.88	0.56
38:V:536:ILE:HD12	38:V:544:LEU:HD12	1.87	0.56
1:A:683:LEU:HD12	1:A:683:LEU:O	2.06	0.56
1:A:1125:ILE:HD12	32:9:35:ARG:HG3	1.87	0.56
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.35	0.56
15:H:38:G:H2'	15:H:39:G:H5'	1.86	0.56
19:3:549:VAL:HG13	19:3:554:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:THR:HG22	1:A:898:PHE:CD2	2.41	0.56
17:1:1258:ALA:HB3	17:1:1261:VAL:CG1	2.35	0.56
19:3:565:TYR:OH	19:3:624:CYS:SG	2.62	0.56
19:3:1027:ASP:OD2	19:3:1031:ARG:NH1	2.39	0.56
42:K:53:LEU:HD22	42:K:58:VAL:HG11	1.87	0.56
14:G:192:U:H2'	14:G:193:C:C6	2.40	0.56
1:A:50:LYS:HD2	5:E:88:ARG:HH12	1.71	0.56
1:A:1049:ASP:OD1	1:A:1090:ARG:HD3	2.05	0.56
3:C:381:LEU:HD22	3:C:416:LEU:HD21	1.88	0.56
5:E:88:ARG:HD3	5:E:109:SER:O	2.06	0.56
13:F:31:U:O2'	13:F:32:C:OP1	2.24	0.56
15:H:81:G:H2'	15:H:82:A:H5''	1.87	0.56
16:v:1:MET:HB2	36:M:210:PHE:HB2	1.88	0.56
25:J:327:ALA:O	25:J:331:GLN:OE1	2.24	0.56
1:A:682:ASP:OD2	15:H:3:G:O2'	2.23	0.56
1:A:704:ASN:ND2	1:A:706:ALA:HB2	2.21	0.56
25:J:297:ASN:O	25:J:300:ASP:HB3	2.05	0.56
27:R:391:VAL:HG23	29:X:347:GLN:CB	2.35	0.56
28:T:216:ASN:HD21	28:T:472:GLN:HB2	1.70	0.56
42:K:78:ILE:HD13	42:K:114:THR:O	2.06	0.56
1:A:1782:ASP:OD2	1:A:1865:ARG:NH2	2.39	0.56
3:C:735:PHE:CE1	3:C:744:ILE:HG12	2.41	0.56
4:D:141:ALA:CA	4:D:182:TYR:OH	2.54	0.56
4:D:178:LYS:O	4:D:178:LYS:HG2	2.05	0.56
13:F:23:G:O2'	13:F:24:U:OP1	2.23	0.56
19:3:429:ARG:HH21	19:3:429:ARG:CG	2.13	0.56
19:3:1188:ASN:OD1	19:3:1188:ASN:N	2.38	0.56
1:A:774:LYS:HG2	15:H:6:U:C6	2.40	0.55
3:C:709:TRP:HB3	3:C:713:LYS:HE3	1.89	0.55
15:H:38:G:H2'	15:H:39:G:C5'	2.36	0.55
42:K:70:ASN:HB3	42:K:73:LEU:HB2	1.88	0.55
1:A:662:GLY:CA	27:R:213:LYS:NZ	2.69	0.55
1:A:1385:VAL:HG21	1:A:1414:ARG:HG2	1.88	0.55
3:C:81:VAL:HB	26:P:208:LYS:HZ3	1.71	0.55
4:D:502:CYS:O	4:D:676:PHE:O	2.23	0.55
5:E:132:THR:CG2	5:E:146:ARG:HD2	2.33	0.55
17:1:855:ASP:N	17:1:855:ASP:OD1	2.34	0.55
19:3:638:GLU:OE2	19:3:670:GLN:HG3	2.06	0.55
1:A:804:GLU:OE2	32:9:212:TYR:OH	2.22	0.55
1:A:2284:MET:O	1:A:2284:MET:CG	2.55	0.55
4:D:142:VAL:O	4:D:145:ASN:OD1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:613:TPO:HG21	19:3:613:TPO:O1P	2.04	0.55
25:J:403:VAL:HA	25:J:407:GLY:HA3	1.89	0.55
29:X:264:PHE:N	29:X:264:PHE:CD1	2.73	0.55
29:X:268:GLU:H	29:X:268:GLU:CD	2.13	0.55
1:A:1763:LEU:HD22	1:A:2012:LEU:HD13	1.87	0.55
1:A:2310:ARG:HD2	1:A:2313:HIS:CG	2.41	0.55
4:D:505:THR:CB	4:D:854:GLY:HA3	2.35	0.55
30:Y:86:ASP:OD1	31:Z:502:ALA:HB3	2.06	0.55
41:I:41:ILE:HD13	41:I:138:ARG:HD3	1.89	0.55
5:E:131:LYS:HG2	5:E:152:SER:O	2.06	0.55
5:E:174:GLY:O	5:E:192:ASN:CB	2.54	0.55
25:J:327:ALA:HA	25:J:330:ARG:HG3	1.87	0.55
36:M:262:CYS:SG	36:M:263:PHE:N	2.78	0.55
41:I:18:ARG:NH1	42:K:35:GLN:OE1	2.39	0.55
42:K:133:LEU:N	42:K:134:PRO:CD	2.67	0.55
1:A:1405:LEU:HD23	27:R:411:LEU:HD23	1.87	0.55
4:D:1589:PHE:C	4:D:1642:GLN:CB	2.79	0.55
5:E:310:TYR:CZ	5:E:322:LYS:HD2	2.42	0.55
15:H:15:U:H3'	24:L:40:ARG:NH1	2.22	0.55
25:J:340:GLN:N	25:J:341:PRO:HD3	2.22	0.55
27:R:463:LEU:O	27:R:467:ILE:HG12	2.06	0.55
29:X:254:ILE:HD13	29:X:279:SER:HB3	1.88	0.55
2:B:47:A:O4'	37:U:11:ARG:NH1	2.40	0.55
4:D:1048:VAL:O	4:D:1050:GLU:N	2.40	0.55
5:E:108:HIS:ND1	5:E:128:SER:CB	2.70	0.55
19:3:525:ARG:HE	19:3:533:VAL:HG21	1.72	0.55
21:5:76:HIS:HD1	21:5:76:HIS:C	2.13	0.55
22:6:27:ASP:OD2	40:0:20:LYS:HE3	2.07	0.55
1:A:346:ASP:OD1	1:A:346:ASP:N	2.39	0.55
1:A:2306:HIS:HE1	1:A:2308:VAL:CG2	2.19	0.55
4:D:1582:ALA:C	4:D:1584:ILE:H	2.15	0.55
5:E:175:THR:HG22	5:E:191:GLN:CD	2.31	0.55
30:Y:85:GLU:OE2	31:Z:505:ARG:NH2	2.40	0.55
38:V:536:ILE:HD12	38:V:544:LEU:HD11	1.89	0.55
40:0:93:THR:HB	40:0:98:GLN:HE21	1.71	0.55
4:D:1589:PHE:HA	4:D:1642:GLN:CB	2.37	0.55
5:E:269:PRO:HD2	5:E:272:ARG:HG2	1.89	0.55
17:1:508:THR:H	17:1:511:MET:HE3	1.72	0.55
25:J:310:ASN:ND2	25:J:342:GLU:OE1	2.40	0.55
26:P:195:LYS:HD3	32:9:198:LYS:HB3	1.88	0.55
1:A:2320:LEU:HD23	1:A:2322:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:737:PRO:HG3	3:C:774:THR:O	2.07	0.55
4:D:164:THR:HG22	4:D:168:ARG:HH11	1.72	0.55
4:D:991:TYR:O	4:D:1090:ARG:NH2	2.39	0.55
19:3:678:VAL:O	19:3:686:LEU:HA	2.07	0.55
25:J:337:MET:HE1	25:J:346:TRP:CE3	2.42	0.55
32:9:143:ASP:OD1	32:9:145:LEU:N	2.40	0.55
41:I:139:LYS:HD3	42:K:124:HIS:ND1	2.22	0.55
4:D:1825:ASN:CB	4:D:1853:ALA:CB	2.85	0.54
5:E:260:ARG:HD3	5:E:276:ILE:CD1	2.37	0.54
32:9:53:VAL:HG11	32:9:63:LEU:HD13	1.89	0.54
36:M:279:HIS:HD1	36:M:296:CYS:HG	1.50	0.54
13:F:21:A:C2	24:L:33:ARG:NH2	2.75	0.54
19:3:618:SER:HB2	19:3:628:LEU:HD11	1.89	0.54
19:3:1103:SER:O	19:3:1119:TYR:HA	2.08	0.54
19:3:1130:VAL:CG1	19:3:1215:TYR:CE2	2.84	0.54
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.40	0.54
16:v:220:ASP:OD1	16:v:220:ASP:N	2.40	0.54
17:1:1223:SER:HB3	17:1:1226:VAL:CG1	2.37	0.54
19:3:279:ASP:OD2	19:3:307:GLN:NE2	2.40	0.54
26:P:207:ASP:OD1	26:P:208:LYS:N	2.40	0.54
29:X:238:THR:O	29:X:238:THR:CG2	2.54	0.54
31:Z:543:ASP:HB3	31:Z:546:ALA:HB2	1.90	0.54
42:K:93:HIS:C	42:K:93:HIS:CD2	2.85	0.54
1:A:50:LYS:HD2	5:E:88:ARG:NH1	2.22	0.54
1:A:51:PHE:HZ	5:E:66:GLU:OE1	1.91	0.54
5:E:174:GLY:CA	5:E:192:ASN:O	2.54	0.54
9:d:112:ASN:CB	10:f:59:LEU:O	2.54	0.54
1:A:873:ASN:N	1:A:873:ASN:OD1	2.38	0.54
3:C:543:ARG:CG	3:C:543:ARG:HH11	2.19	0.54
5:E:326:HIS:HE1	5:E:346:SER:CB	2.13	0.54
13:F:28:C:OP2	13:F:46:U:O2'	2.21	0.54
14:G:213:C:O4'	14:G:214:C:OP2	2.26	0.54
19:3:1165:SER:HB3	19:3:1169:PRO:HA	1.90	0.54
29:X:300:SER:OG	29:X:303:HIS:ND1	2.28	0.54
41:I:47:TYR:HE1	41:I:93:LYS:HD2	1.72	0.54
42:K:78:ILE:CG2	42:K:114:THR:HG23	2.31	0.54
17:1:1128:VAL:HG23	17:1:1128:VAL:O	2.07	0.54
25:J:270:ASP:OD1	27:R:223:PRO:CG	2.56	0.54
30:Y:101:LYS:HG2	30:Y:106:THR:HG22	1.89	0.54
1:A:1604:LEU:HD11	1:A:1725:LEU:HD22	1.88	0.54
3:C:737:PRO:HG3	3:C:774:THR:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:66:ASN:O	30:Y:80:CYS:HB2	2.08	0.54
3:C:313:GLN:O	3:C:417:ARG:NH1	2.41	0.54
5:E:178:LEU:CD1	5:E:222:LEU:HD22	2.37	0.54
14:G:222:U:H4'	14:G:222:U:OP1	2.08	0.54
16:v:39:ASP:OD1	16:v:39:ASP:N	2.33	0.54
25:J:403:VAL:O	25:J:408:ASP:N	2.38	0.54
5:E:147:LEU:CD1	5:E:179:TRP:CG	2.83	0.54
19:3:304:GLN:HE21	19:3:308:GLY:HA2	1.73	0.54
25:J:259:GLN:OE1	25:J:262:ARG:NH1	2.41	0.54
27:R:394:LEU:CD1	29:X:331:LEU:CD2	2.84	0.54
25:J:236:ARG:NH1	25:J:236:ARG:HG3	2.22	0.54
25:J:274:ARG:NE	27:R:229:VAL:HG22	2.22	0.54
1:A:2117:ILE:O	1:A:2304:PHE:HB2	2.07	0.53
1:A:2319:LEU:HD11	4:D:1071:LYS:CB	2.38	0.53
15:H:10:A:C2'	15:H:10:A:N3	2.72	0.53
18:2:525:PRO:HG2	18:2:528:ILE:HD12	1.89	0.53
19:3:185:LEU:HB3	19:3:206:GLN:HE21	1.73	0.53
19:3:555:VAL:HG22	19:3:565:TYR:HB3	1.90	0.53
19:3:950:ALA:HB2	19:3:989:TYR:CZ	2.42	0.53
25:J:313:TRP:CE3	25:J:336:TRP:NE1	2.76	0.53
1:A:126:ILE:HG21	27:R:207:MET:HE3	1.90	0.53
1:A:651:TRP:CD1	13:F:38:G:H1'	2.42	0.53
1:A:1320:LYS:NZ	1:A:1325:LEU:O	2.37	0.53
13:F:31:U:O2'	13:F:32:C:O5'	2.25	0.53
18:2:567:ASP:OD1	18:2:567:ASP:N	2.40	0.53
21:5:26:LEU:HD21	21:5:35:MET:HE1	1.89	0.53
27:R:279:HIS:HA	32:9:224:THR:HG22	1.86	0.53
41:I:31:ARG:HB3	41:I:31:ARG:NH1	2.01	0.53
41:I:140:ALA:O	41:I:144:LYS:HE2	2.09	0.53
1:A:44:ARG:HA	1:A:49:ARG:NH1	2.23	0.53
1:A:995:ARG:HG3	27:R:291:LEU:HD13	1.89	0.53
1:A:2103:THR:CG2	1:A:2260:GLN:OE1	2.48	0.53
4:D:141:ALA:CB	4:D:182:TYR:OH	2.56	0.53
5:E:229:TYR:CE2	5:E:272:ARG:NH1	2.77	0.53
17:1:550:HIS:CE1	22:6:96:THR:CG2	2.91	0.53
28:T:307:SER:OG	28:T:308:ARG:N	2.39	0.53
14:G:213:C:H4'	14:G:214:C:C5'	2.37	0.53
38:V:466:SER:OG	38:V:472:CYS:HB2	2.08	0.53
1:A:2328:ALA:HB3	4:D:787:ALA:HB3	1.89	0.53
15:H:10:A:N3	15:H:10:A:H3'	2.23	0.53
18:2:469:VAL:HG12	18:2:471:ARG:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2073:TRP:CD1	1:A:2073:TRP:C	2.85	0.53
16:v:1:MET:HB2	36:M:210:PHE:CB	2.39	0.53
28:T:349:SER:OG	28:T:350:HIS:N	2.37	0.53
32:9:106:LEU:HG	32:9:130:ALA:HB2	1.90	0.53
1:A:661:GLU:O	27:R:213:LYS:HA	2.09	0.53
5:E:178:LEU:CD2	5:E:208:ILE:CD1	2.87	0.53
13:F:31:U:C2'	13:F:32:C:O5'	2.56	0.53
17:1:631:ALA:O	17:1:635:VAL:CG1	2.57	0.53
23:7:48:ASP:OD1	23:7:51:ASN:ND2	2.41	0.53
25:J:236:ARG:HH11	25:J:236:ARG:C	2.15	0.53
29:X:347:GLN:N	29:X:347:GLN:NE2	2.56	0.53
30:Y:58:GLN:NE2	31:Z:588:ASP:OD1	2.41	0.53
40:0:93:THR:HG21	40:0:98:GLN:NE2	2.23	0.53
1:A:1762:TYR:HD1	1:A:1762:TYR:H	1.56	0.53
1:A:1949:ARG:CD	27:R:463:LEU:HD13	2.39	0.53
2:B:23:C:O2	2:B:23:C:C3'	2.57	0.53
3:C:778:PRO:HD3	3:C:817:TYR:CD1	2.43	0.53
16:v:11:SER:HB3	17:1:1103:VAL:HG13	1.90	0.53
17:1:1174:GLU:OE1	17:1:1210:HIS:NE2	2.36	0.53
19:3:675:LEU:HD21	19:3:691:THR:CG2	2.39	0.53
25:J:313:TRP:CZ3	25:J:336:TRP:CD1	2.97	0.53
28:T:216:ASN:ND2	28:T:472:GLN:HB2	2.24	0.53
42:K:54:ARG:CB	42:K:54:ARG:CZ	2.86	0.53
1:A:58:LYS:NZ	1:A:479:THR:O	2.42	0.53
1:A:1002:ASP:OD2	1:A:1004:ASN:HB2	2.09	0.53
3:C:484:THR:OG1	3:C:489:GLN:O	2.26	0.53
5:E:325:GLY:O	5:E:352:TYR:CE2	2.62	0.53
14:G:196:A:N3	14:G:196:A:H5''	2.23	0.53
15:H:2:U:OP1	15:H:2:U:H2'	2.09	0.53
19:3:460:TRP:CZ3	19:3:505:THR:HG23	2.44	0.53
4:D:714:GLU:C	4:D:716:ALA:H	2.17	0.53
5:E:260:ARG:NE	5:E:276:ILE:CD1	2.72	0.53
13:F:23:G:C2'	13:F:24:U:O5'	2.57	0.53
13:F:23:G:HO2'	13:F:24:U:P	2.32	0.53
17:1:1054:GLU:OE1	17:1:1057:ARG:NH1	2.42	0.53
1:A:2333:LEU:HD21	4:D:544:MET:HA	1.91	0.52
5:E:263:ASP:O	5:E:272:ARG:NE	2.32	0.52
25:J:355:ARG:HB3	25:J:355:ARG:NH1	2.23	0.52
32:9:43:SER:H	32:9:61:PHE:HB3	1.74	0.52
1:A:2129:TYR:HB3	1:A:2172:MET:HE3	1.90	0.52
4:D:148:LEU:HD23	4:D:152:GLU:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:LEU:HB2	5:E:351:LEU:CB	2.39	0.52
17:1:680:LEU:HB3	17:1:681:PRO:HD3	1.92	0.52
18:2:633:LEU:C	18:2:635:ALA:H	2.16	0.52
19:3:970:TYR:CE1	19:3:979:ARG:HB2	2.42	0.52
19:3:1055:VAL:HB	19:3:1093:MET:HB3	1.91	0.52
1:A:542:ASN:O	1:A:546:LEU:HB2	2.09	0.52
1:A:2074:ARG:HH12	4:D:1042:GLU:HA	1.72	0.52
3:C:828:MET:HA	3:C:905:GLN:O	2.08	0.52
4:D:1090:ARG:HB2	4:D:1090:ARG:CZ	2.38	0.52
4:D:1948:MET:CB	4:D:1953:MET:O	2.57	0.52
5:E:108:HIS:ND1	5:E:128:SER:HB2	2.24	0.52
5:E:232:ARG:O	5:E:262:TRP:HH2	1.91	0.52
15:H:10:A:N3	15:H:10:A:H2'	2.25	0.52
32:9:120:ARG:NH1	32:9:154:ASP:OD1	2.42	0.52
2:B:115:C:O2	2:B:115:C:H2'	2.09	0.52
14:G:19:U:O2	14:G:19:U:H2'	2.09	0.52
16:v:190:LEU:CD2	18:2:694:PHE:CD2	2.86	0.52
17:1:524:ARG:HH11	17:1:566:LEU:HD11	1.74	0.52
19:3:426:ALA:HB1	19:3:785:PRO:CG	2.39	0.52
31:Z:520:LYS:NZ	31:Z:530:ASP:OD2	2.43	0.52
1:A:422:LEU:O	1:A:635:ARG:NE	2.43	0.52
1:A:2133:PRO:HD2	1:A:2139:VAL:HG13	1.92	0.52
3:C:138:LEU:HD11	3:C:179:VAL:HG23	1.91	0.52
3:C:173:THR:O	3:C:177:ARG:HB3	2.09	0.52
5:E:178:LEU:N	5:E:178:LEU:HD23	2.25	0.52
5:E:260:ARG:HD3	5:E:276:ILE:CG1	2.38	0.52
19:3:722:SER:HB3	19:3:731:LEU:HD13	1.92	0.52
25:J:236:ARG:NH1	25:J:236:ARG:HA	2.24	0.52
25:J:368:ARG:HG2	25:J:368:ARG:HH11	1.74	0.52
28:T:381:HIS:CG	28:T:384:HIS:HB2	2.45	0.52
39:8:74:GLN:HB3	39:8:85:MET:HE2	1.91	0.52
1:A:34:ALA:O	5:E:195:GLN:NE2	2.39	0.52
1:A:1838:LYS:CE	1:A:1865:ARG:NE	2.72	0.52
3:C:164:ASP:OD1	3:C:164:ASP:N	2.33	0.52
4:D:538:ILE:O	4:D:585:ILE:HA	2.09	0.52
5:E:250:LEU:HD11	5:E:262:TRP:HB2	1.91	0.52
19:3:1159:ASP:HB3	19:3:1162:SER:HB3	1.92	0.52
25:J:349:TYR:CE2	25:J:365:ILE:HG13	2.43	0.52
30:Y:37:TRP:HB3	30:Y:112:VAL:CG2	2.40	0.52
3:C:390:THR:OG1	3:C:391:SER:N	2.42	0.52
19:3:69:ARG:NH2	19:3:74:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:27:PRO:CG	21:5:83:CYS:HB3	2.35	0.52
27:R:408:ASP:OD2	27:R:410:ARG:NH2	2.43	0.52
4:D:1948:MET:CA	4:D:1953:MET:O	2.57	0.52
16:v:187:ARG:NH2	18:2:694:PHE:CE1	2.77	0.52
17:1:641:ILE:CD1	17:1:675:MET:HE2	2.24	0.52
19:3:209:THR:HA	19:3:224:TYR:O	2.10	0.52
29:X:303:HIS:CE1	29:X:333:SER:HB2	2.44	0.52
1:A:1957:ASP:HB2	1:A:1960:THR:HG23	1.92	0.52
4:D:128:PRO:CD	4:D:131:ILE:HD12	2.39	0.52
4:D:141:ALA:HA	4:D:182:TYR:CZ	2.44	0.52
20:4:16:TYR:HA	20:4:57:GLY:O	2.10	0.52
21:5:77:LEU:HG	21:5:89:VAL:HG11	1.92	0.52
25:J:268:ALA:O	25:J:271:VAL:HG12	2.10	0.52
32:9:92:ASN:OD1	32:9:124:ASN:HA	2.09	0.52
1:A:481:PHE:CD1	27:R:205:ASP:HB3	2.45	0.52
1:A:662:GLY:HA3	27:R:213:LYS:HG3	1.91	0.52
1:A:1848:LEU:HD13	1:A:1914:MET:HE3	1.91	0.52
3:C:765:SER:OG	3:C:766:ILE:N	2.42	0.52
5:E:175:THR:HG22	5:E:191:GLN:OE1	2.10	0.52
14:G:210:G:N3	14:G:210:G:C2'	2.73	0.52
3:C:261:ASP:N	3:C:261:ASP:OD1	2.42	0.51
47:F:207:G5J:O1A	41:I:34:ARG:HG3	2.10	0.51
16:v:1:MET:HG2	16:v:6:GLU:H	1.75	0.51
17:1:968:GLU:OE1	17:1:971:MET:SD	2.69	0.51
27:R:231:HIS:NE2	28:T:371:HIS:O	2.43	0.51
27:R:459:TYR:CE2	27:R:463:LEU:HD12	2.45	0.51
1:A:1330:MET:HE1	1:A:1369:TYR:HB2	1.91	0.51
3:C:85:ASP:OD1	3:C:85:ASP:N	2.40	0.51
17:1:1083:TYR:CZ	40:0:13:VAL:HG23	2.46	0.51
20:4:34:LEU:HA	20:4:37:GLY:O	2.09	0.51
42:K:78:ILE:HD11	42:K:118:ALA:CB	2.40	0.51
1:A:213:LEU:O	1:A:220:VAL:HG22	2.10	0.51
1:A:661:GLU:OE2	27:R:210:PRO:HG2	2.10	0.51
3:C:137:HIS:CE1	3:C:238:ASN:H	2.28	0.51
3:C:682:LYS:HD2	3:C:802:HIS:CD2	2.45	0.51
25:J:386:GLU:OE2	25:J:391:TYR:HB2	2.10	0.51
1:A:466:ALA:HB1	2:B:19:A:N7	2.25	0.51
1:A:2219:THR:HG21	1:A:2224:THR:CG2	2.34	0.51
5:E:231:MET:SD	5:E:262:TRP:CE3	3.04	0.51
14:G:218:U:C6	30:Y:105:ARG:NH1	2.78	0.51
17:1:823:MET:HG2	17:1:833:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:1276:SER:O	17:1:1276:SER:OG	2.19	0.51
18:2:476:GLU:OE1	18:2:478:HIS:NE2	2.43	0.51
19:3:1032:TRP:O	19:3:1048:ASP:HA	2.10	0.51
22:6:22:LEU:HG	22:6:69:ALA:HB2	1.92	0.51
28:T:471:ASP:OD1	28:T:471:ASP:N	2.41	0.51
28:T:478:LEU:HD23	28:T:488:VAL:HG22	1.93	0.51
32:9:121:THR:HG23	32:9:154:ASP:OD2	2.11	0.51
41:I:31:ARG:HH11	41:I:31:ARG:CG	2.24	0.51
1:A:1963:GLU:HB2	1:A:1966:HIS:CD2	2.46	0.51
5:E:132:THR:CG2	5:E:146:ARG:CB	2.75	0.51
25:J:439:ALA:HA	25:J:442:ARG:HB3	1.93	0.51
4:D:179:ILE:HG23	4:D:179:ILE:O	2.11	0.51
19:3:464:ARG:NH2	19:3:473:TYR:OH	2.43	0.51
20:4:12:ASP:O	20:4:67:ALA:HB1	2.08	0.51
28:T:261:LEU:HB3	28:T:273:TRP:HB2	1.92	0.51
32:9:19:THR:HA	32:9:24:GLY:HA3	1.92	0.51
34:x:640:ARG:CB	34:x:667:ALA:CA	2.88	0.51
38:V:536:ILE:HG23	38:V:544:LEU:CD1	2.39	0.51
3:C:134:LEU:O	3:C:205:THR:OG1	2.28	0.51
3:C:735:PHE:HE1	3:C:744:ILE:HG12	1.74	0.51
4:D:106:THR:HG22	4:D:107:LYS:H	1.76	0.51
25:J:336:TRP:CH2	25:J:345:ALA:HB1	2.46	0.51
25:J:349:TYR:CD2	25:J:365:ILE:HG21	2.46	0.51
42:K:50:TYR:CE1	42:K:84:LEU:HD12	2.46	0.51
2:B:111:A:H2'	2:B:112:A:C8	2.46	0.51
4:D:106:THR:CG2	4:D:107:LYS:N	2.73	0.51
5:E:276:ILE:C	5:E:277:PHE:HD1	2.19	0.51
16:v:215:VAL:HG13	19:3:980:LYS:HG3	1.92	0.51
42:K:50:TYR:OH	42:K:83:ASN:O	2.29	0.51
42:K:146:LEU:C	42:K:146:LEU:HD23	2.36	0.51
1:A:2310:ARG:CD	1:A:2313:HIS:ND1	2.73	0.51
4:D:140:LEU:HD23	4:D:140:LEU:O	2.10	0.51
17:1:933:CYS:SG	17:1:970:LEU:HD21	2.51	0.51
1:A:2147:MET:O	1:A:2274:PRO:HD3	2.10	0.51
15:H:12:U:O2'	15:H:13:U:P	2.69	0.51
19:3:522:ASP:O	19:3:538:THR:HG23	2.10	0.51
19:3:678:VAL:HG23	19:3:688:ASP:OD1	2.11	0.51
19:3:703:ARG:HD3	19:3:710:GLU:OE2	2.11	0.51
25:J:236:ARG:HH11	25:J:236:ARG:CB	2.24	0.51
30:Y:87:GLN:O	30:Y:90:THR:OG1	2.25	0.51
34:x:443:ASN:HA	34:x:446:MET:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:288:GLN:HA	36:M:291:ARG:HD3	1.93	0.51
41:I:128:VAL:N	42:K:158:ASN:OD1	2.44	0.51
1:A:837:LYS:HA	1:A:840:ILE:HG22	1.92	0.50
1:A:2115:ILE:HD11	1:A:2223:CYS:SG	2.51	0.50
2:B:113:G:H2'	2:B:114:G:C8	2.46	0.50
3:C:151:GLU:OE1	3:C:417:ARG:NH2	2.37	0.50
17:1:1256:HIS:ND1	17:1:1261:VAL:HG11	2.26	0.50
19:3:623:ASP:HB2	19:3:626:GLN:HG3	1.93	0.50
20:4:14:THR:CA	20:4:59:VAL:O	2.28	0.50
27:R:129:ASP:O	27:R:133:GLN:HG2	2.11	0.50
29:X:278:GLN:HG2	29:X:281:TYR:CZ	2.46	0.50
1:A:266:SER:OG	1:A:271:MET:O	2.26	0.50
17:1:614:ARG:HB3	17:1:615:PRO:HD3	1.93	0.50
19:3:430:GLY:H	19:3:784:THR:HG22	1.77	0.50
34:x:983:TRP:CB	34:x:1003:ILE:O	2.59	0.50
1:A:591:MET:HB3	1:A:598:LEU:HD21	1.87	0.50
2:B:113:G:H2'	2:B:114:G:H8	1.77	0.50
3:C:686:THR:HB	3:C:793:ASP:HB3	1.94	0.50
18:2:633:LEU:C	18:2:635:ALA:N	2.69	0.50
19:3:428:GLY:HA3	19:3:433:SER:HA	1.93	0.50
19:3:564:VAL:HG22	19:3:580:ARG:HG2	1.93	0.50
28:T:460:ASP:OD1	28:T:460:ASP:N	2.45	0.50
42:K:51:GLU:CA	42:K:54:ARG:NH2	2.74	0.50
42:K:83:ASN:OD1	42:K:84:LEU:N	2.44	0.50
1:A:488:ASP:O	1:A:492:VAL:HG23	2.11	0.50
1:A:2127:TYR:OH	1:A:2159:LEU:HD13	2.11	0.50
3:C:142:LYS:N	44:C:1500:GTP:O1B	2.40	0.50
13:F:32:C:H4'	25:J:236:ARG:O	2.12	0.50
18:2:700:GLU:HA	18:2:703:ILE:HD12	1.94	0.50
29:X:345:GLU:CD	29:X:348:ARG:HH11	2.18	0.50
41:I:17:GLN:OE1	41:I:17:GLN:N	2.45	0.50
5:E:158:TYR:HB2	5:E:199:VAL:O	2.12	0.50
13:F:32:C:O2'	13:F:33:C:OP2	2.27	0.50
19:3:589:CYS:SG	19:3:640:LEU:HD12	2.52	0.50
42:K:82:CYS:SG	42:K:120:THR:CB	2.99	0.50
1:A:344:ASP:OD1	1:A:344:ASP:N	2.35	0.50
2:B:110:C:H2'	2:B:111:A:H8	1.76	0.50
4:D:134:GLY:O	4:D:138:GLU:HG3	2.12	0.50
5:E:265:ARG:N	5:E:272:ARG:HH21	2.10	0.50
5:E:276:ILE:C	5:E:277:PHE:CD1	2.89	0.50
29:X:305:VAL:HB	29:X:329:ILE:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:118:PRO:O	31:Z:490:ARG:NH1	2.45	0.50
32:9:61:PHE:HE1	32:9:66:ILE:HB	1.77	0.50
42:K:51:GLU:HA	42:K:54:ARG:CZ	2.41	0.50
3:C:841:ASP:N	3:C:841:ASP:OD1	2.43	0.50
11:e:15:VAL:O	12:g:33:GLY:HA3	2.12	0.50
13:F:21:A:N6	27:R:256:ASN:OD1	2.44	0.50
14:G:206:C:H4'	14:G:207:A:O5'	2.11	0.50
17:1:1075:ARG:HA	17:1:1078:VAL:CG2	2.39	0.50
19:3:716:SER:OG	19:3:717:SER:N	2.45	0.50
28:T:406:ILE:HG22	28:T:407:GLN:HB2	1.94	0.50
1:A:80:LYS:HB2	41:I:116:LEU:HD11	1.92	0.50
1:A:1070:ASP:OD1	1:A:1073:SER:OG	2.29	0.50
1:A:1762:TYR:N	1:A:1762:TYR:CD1	2.80	0.50
2:B:101:U:H2'	2:B:102:U:C6	2.47	0.50
4:D:721:VAL:N	4:D:807:GLN:O	2.42	0.50
5:E:194:TYR:CD2	5:E:214:ASP:HB3	2.47	0.50
5:E:194:TYR:CE2	5:E:214:ASP:OD2	2.64	0.50
11:l:15:VAL:O	12:n:33:GLY:HA3	2.12	0.50
16:v:1:MET:HE1	18:2:553:MET:HE3	1.94	0.50
25:J:380:ILE:O	25:J:384:ARG:HD3	2.12	0.50
32:9:93:PHE:CD1	32:9:125:VAL:HG11	2.46	0.50
1:A:213:LEU:CD1	1:A:230:PHE:CE1	2.94	0.50
1:A:780:THR:HG22	1:A:898:PHE:HD2	1.75	0.50
1:A:892:LYS:HD2	1:A:912:GLU:HG3	1.94	0.50
1:A:1790:ILE:HA	1:A:1799:THR:O	2.12	0.50
5:E:250:LEU:HD12	5:E:250:LEU:C	2.37	0.50
13:F:18:A:H4'	13:F:45:A:C2	2.47	0.50
25:J:238:ASN:C	25:J:240:THR:H	2.20	0.50
38:V:617:PRO:O	38:V:624:THR:OG1	2.30	0.50
1:A:2303:GLU:CD	1:A:2303:GLU:H	2.19	0.49
3:C:564:THR:HG21	3:C:576:ILE:HA	1.94	0.49
5:E:164:PRO:O	5:E:166:LEU:HG	2.12	0.49
13:F:32:C:H5'	25:J:237:LYS:O	2.11	0.49
25:J:232:GLU:HA	25:J:235:ILE:HG21	1.88	0.49
25:J:232:GLU:CA	25:J:235:ILE:CG2	2.81	0.49
25:J:318:TYR:CE1	25:J:322:MET:HE3	2.47	0.49
28:T:267:ASP:OD1	28:T:267:ASP:N	2.36	0.49
2:B:96:A:N3	2:B:96:A:C2'	2.74	0.49
17:1:619:ASN:OD1	17:1:620:MET:N	2.45	0.49
19:3:118:GLY:HA2	19:3:132:ILE:HD11	1.94	0.49
28:T:223:SER:OG	28:T:224:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:343:PRO:HG3	28:T:356:LEU:HD23	1.94	0.49
42:K:78:ILE:CG1	42:K:117:SER:HB2	2.35	0.49
2:B:91:U:O5'	2:B:91:U:H6	1.95	0.49
4:D:106:THR:O	4:D:110:ARG:N	2.41	0.49
4:D:116:LEU:HD22	4:D:140:LEU:HD12	1.92	0.49
5:E:74:PHE:HE1	5:E:95:VAL:CG2	2.25	0.49
5:E:277:PHE:CE2	5:E:300:ILE:HD12	2.46	0.49
19:3:384:THR:OG1	19:3:385:PHE:N	2.45	0.49
19:3:546:LYS:HG3	19:3:588:VAL:O	2.13	0.49
19:3:968:ARG:CG	19:3:982:GLU:HB2	2.39	0.49
25:J:280:LEU:O	25:J:284:GLU:HG2	2.13	0.49
27:R:408:ASP:OD1	27:R:408:ASP:N	2.44	0.49
29:X:330:ASP:OD1	29:X:346:PRO:HA	2.12	0.49
32:9:142:ARG:HH11	32:9:147:ASP:HB3	1.76	0.49
42:K:111:ASN:O	42:K:115:VAL:HG23	2.12	0.49
1:A:635:ARG:HH22	2:B:27:U:P	2.34	0.49
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.94	0.49
14:G:218:U:C5	30:Y:105:ARG:NH2	2.81	0.49
18:2:644:SER:CA	20:4:65:GLU:CB	2.91	0.49
42:K:18:GLN:HE21	42:K:22:THR:HG23	1.78	0.49
4:D:1090:ARG:CG	4:D:1090:ARG:NH2	2.73	0.49
5:E:74:PHE:HE1	5:E:95:VAL:HG22	1.76	0.49
14:G:202:A:OP1	17:1:1149:LYS:HE3	2.11	0.49
27:R:237:MET:H	27:R:237:MET:HE3	1.75	0.49
27:R:388:ILE:CG2	29:X:350:TYR:CE1	2.95	0.49
29:X:235:ASP:OD1	30:Y:103:LYS:HD2	2.12	0.49
1:A:1275:ARG:HD2	1:A:1375:TRP:CE2	2.48	0.49
1:A:1403:LEU:HD12	1:A:1407:ASP:OD2	2.13	0.49
3:C:680:ASN:O	3:C:682:LYS:N	2.44	0.49
4:D:149:ARG:CG	4:D:149:ARG:NH1	2.73	0.49
19:3:630:MET:CE	36:M:287:LEU:CD2	2.73	0.49
27:R:205:ASP:OD1	27:R:208:GLU:HG3	2.12	0.49
29:X:241:GLY:CA	29:X:288:ARG:HH21	2.20	0.49
39:8:40:MET:HE3	39:8:45:LEU:HD21	1.95	0.49
42:K:122:LEU:HB2	42:K:163:PHE:HE2	1.78	0.49
1:A:444:ARG:HG3	1:A:444:ARG:HH11	1.77	0.49
1:A:487:LEU:HD12	1:A:492:VAL:HG22	1.95	0.49
1:A:1793:THR:OG1	1:A:1797:ASN:O	2.31	0.49
1:A:2225:LEU:HD13	1:A:2261:MET:CE	2.43	0.49
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.95	0.49
14:G:210:G:N3	14:G:210:G:C3'	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:190:LEU:HG	18:2:691:ALA:HB2	1.95	0.49
17:1:619:ASN:CG	17:1:624:VAL:HG21	2.37	0.49
19:3:318:ASP:HB2	19:3:323:THR:HG21	1.94	0.49
19:3:333:VAL:HG11	19:3:349:VAL:HG21	1.94	0.49
29:X:268:GLU:OE1	29:X:268:GLU:N	2.39	0.49
36:M:274:VAL:N	36:M:308:ASN:O	2.41	0.49
40:0:93:THR:HG21	40:0:98:GLN:HE22	1.72	0.49
1:A:137:GLU:HG2	1:A:410:PRO:HG3	1.95	0.49
3:C:515:THR:HG23	3:C:518:ASP:H	1.77	0.49
17:1:540:MET:HE3	17:1:577:VAL:HG22	1.95	0.49
19:3:552:ARG:HD3	19:3:600:GLN:O	2.12	0.49
25:J:220:LEU:HD11	25:J:224:LYS:HZ3	1.77	0.49
25:J:236:ARG:NH1	25:J:236:ARG:CA	2.73	0.49
32:9:54:CYS:HB2	32:9:91:LEU:HD11	1.94	0.49
34:x:452:GLN:N	34:x:496:MET:O	2.45	0.49
36:M:286:ALA:HA	36:M:289:HIS:HB3	1.95	0.49
1:A:481:PHE:CD2	27:R:205:ASP:HB3	2.47	0.49
2:B:111:A:H2'	2:B:112:A:H8	1.78	0.49
3:C:683:ASN:H	3:C:683:ASN:HD22	1.57	0.49
4:D:148:LEU:CD2	4:D:152:GLU:HB2	2.42	0.49
4:D:720:GLN:H	4:D:824:HIS:CB	2.25	0.49
19:3:530:ASP:OD1	19:3:532:ARG:HG2	2.13	0.49
30:Y:37:TRP:CB	30:Y:112:VAL:CG2	2.91	0.49
1:A:733:THR:HG23	32:9:241:TYR:HA	1.94	0.49
1:A:1644:LEU:O	1:A:1723:LYS:NZ	2.46	0.49
1:A:1776:ILE:HB	1:A:1858:PRO:HA	1.95	0.49
5:E:308:PHE:HE1	5:E:324:PRO:HB3	1.75	0.49
17:1:562:LYS:HA	17:1:562:LYS:HD2	1.60	0.49
17:1:1180:ARG:HH21	17:1:1180:ARG:CB	2.26	0.49
33:z:157:ASN:N	33:z:157:ASN:OD1	2.45	0.49
1:A:213:LEU:HD13	1:A:219:TYR:CB	2.42	0.48
1:A:2314:PHE:HD2	4:D:1123:TRP:CB	2.26	0.48
4:D:713:MET:O	4:D:716:ALA:CB	2.60	0.48
4:D:1308:PRO:C	4:D:1310:SER:H	2.20	0.48
13:F:40:C:O4'	28:T:285:HIS:CE1	2.66	0.48
14:G:197:U:H4'	24:L:12:ARG:HD2	1.95	0.48
14:G:218:U:C5	30:Y:105:ARG:NH1	2.81	0.48
15:H:2:U:O2'	15:H:3:G:P	2.71	0.48
17:1:130:PRO:HG2	17:1:150:ARG:HD2	1.95	0.48
17:1:614:ARG:N	17:1:615:PRO:CD	2.76	0.48
19:3:757:ILE:HG13	19:3:757:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:K:122:LEU:HB2	42:K:163:PHE:CE2	2.47	0.48
1:A:2328:ALA:HB1	4:D:787:ALA:HB3	1.94	0.48
3:C:103:THR:HG22	3:C:171:LEU:HD23	1.96	0.48
5:E:263:ASP:OD1	5:E:272:ARG:HB3	2.13	0.48
14:G:211:U:H2'	14:G:213:C:OP2	2.14	0.48
17:1:671:ILE:HG23	17:1:675:MET:HG3	1.95	0.48
19:3:630:MET:SD	36:M:287:LEU:CD2	2.91	0.48
25:J:282:TYR:CE2	25:J:298:ILE:HG21	2.48	0.48
25:J:495:PHE:O	25:J:499:ARG:N	2.46	0.48
29:X:332:GLY:HA2	29:X:346:PRO:HB3	1.96	0.48
32:9:152:ARG:O	32:9:155:ILE:HG22	2.12	0.48
1:A:2149:PRO:O	1:A:2160:PRO:HD3	2.12	0.48
3:C:564:THR:CG2	3:C:576:ILE:HG22	2.43	0.48
3:C:796:VAL:HB	3:C:803:ARG:HH11	1.78	0.48
4:D:104:PRO:HB2	4:D:110:ARG:HG3	1.95	0.48
4:D:423:MET:CB	4:D:878:TYR:HA	2.43	0.48
16:v:187:ARG:NH1	18:2:694:PHE:CE1	2.75	0.48
25:J:299:TRP:HB3	25:J:316:TYR:CD2	2.39	0.48
25:J:349:TYR:HD2	25:J:365:ILE:HG21	1.77	0.48
1:A:828:PRO:HB2	1:A:882:LYS:HE3	1.95	0.48
1:A:1962:THR:HG22	1:A:1969:PRO:HA	1.94	0.48
4:D:1090:ARG:CZ	4:D:1090:ARG:CB	2.91	0.48
5:E:157:CYS:HA	5:E:168:CYS:O	2.13	0.48
19:3:970:TYR:HE1	19:3:979:ARG:CB	2.25	0.48
25:J:316:TYR:CE1	25:J:332:VAL:CG2	2.89	0.48
28:T:188:PRO:HG2	28:T:502:VAL:HG11	1.96	0.48
28:T:227:THR:HG22	28:T:243:THR:HG22	1.95	0.48
28:T:267:ASP:OD2	28:T:269:GLN:NE2	2.46	0.48
28:T:427:LEU:HB3	28:T:439:TRP:HB2	1.95	0.48
1:A:422:LEU:HD23	1:A:422:LEU:H	1.78	0.48
1:A:545:HIS:HB3	1:A:594:TYR:CZ	2.49	0.48
2:B:102:U:H2'	2:B:103:G:C8	2.48	0.48
5:E:129:THR:HB	5:E:153:PHE:CD1	2.48	0.48
5:E:284:PHE:O	5:E:286:LYS:HG2	2.14	0.48
19:3:54:LEU:CD2	19:3:99:PHE:CD2	2.96	0.48
19:3:138:GLN:HG3	19:3:161:HIS:HE1	1.75	0.48
19:3:720:TRP:CE3	19:3:731:LEU:HG	2.49	0.48
22:6:91:LEU:HD13	39:8:6:PHE:CE2	2.49	0.48
29:X:241:GLY:CA	29:X:289:ILE:HD11	2.36	0.48
41:I:78:LEU:HD23	41:I:78:LEU:H	1.78	0.48
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:190:LEU:HD11	18:2:691:ALA:HA	1.96	0.48
17:1:933:CYS:SG	17:1:970:LEU:HD11	2.54	0.48
19:3:49:LYS:CG	19:3:51:HIS:CE1	2.92	0.48
19:3:123:VAL:HG12	19:3:130:VAL:HG23	1.96	0.48
19:3:1118:VAL:HG22	19:3:1128:ILE:HG22	1.96	0.48
41:I:47:TYR:CE1	41:I:93:LYS:HD2	2.49	0.48
41:I:63:VAL:HG21	41:I:75:TYR:CD2	2.48	0.48
1:A:2252:LEU:HD23	1:A:2253:PRO:HD2	1.96	0.48
4:D:123:ALA:CB	4:D:161:LEU:CD1	2.88	0.48
5:E:175:THR:HG22	5:E:191:GLN:HA	1.95	0.48
5:E:228:THR:HG22	5:E:229:TYR:HD1	1.77	0.48
14:G:215:U:H2'	30:Y:2:ASN:HD21	1.75	0.48
28:T:402:ASP:OD1	28:T:402:ASP:N	2.40	0.48
1:A:2328:ALA:HB1	4:D:787:ALA:CB	2.44	0.48
4:D:721:VAL:O	4:D:808:VAL:HA	2.14	0.48
5:E:62:LEU:HB2	5:E:351:LEU:H	1.79	0.48
5:E:129:THR:HB	5:E:153:PHE:HD1	1.78	0.48
29:X:261:LEU:HG	29:X:275:ILE:HG13	1.95	0.48
32:9:37:LEU:HD12	32:9:38:PRO:CD	2.43	0.48
42:K:54:ARG:HB3	42:K:54:ARG:NH1	2.29	0.48
5:E:178:LEU:CD2	5:E:208:ILE:HD13	2.44	0.48
42:K:78:ILE:CD1	42:K:118:ALA:HB2	2.43	0.48
1:A:439:GLN:O	1:A:444:ARG:NH1	2.47	0.48
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.41	0.48
13:F:21:A:H2	24:L:33:ARG:NH2	2.10	0.48
19:3:952:ILE:HG12	19:3:961:ILE:HG12	1.96	0.48
22:6:22:LEU:CD2	22:6:60:ILE:HD12	2.44	0.48
25:J:260:ARG:O	25:J:264:ILE:HG13	2.13	0.48
25:J:274:ARG:HE	27:R:229:VAL:HG22	1.78	0.48
27:R:403:ASN:HB2	29:X:250:PRO:C	2.39	0.48
29:X:345:GLU:OE2	29:X:348:ARG:CZ	2.62	0.48
32:9:79:ASN:OD1	32:9:80:GLY:N	2.47	0.48
41:I:91:LEU:HD11	41:I:125:PHE:CE2	2.49	0.48
13:F:31:U:HO2'	13:F:32:C:P	2.35	0.47
17:1:936:VAL:CG2	17:1:954:LEU:HD23	2.44	0.47
29:X:285:ARG:N	29:X:300:SER:O	2.45	0.47
32:9:38:PRO:HB2	32:9:41:HIS:ND1	2.29	0.47
41:I:139:LYS:NZ	41:I:139:LYS:CB	2.73	0.47
42:K:54:ARG:HD3	42:K:90:ASN:ND2	2.29	0.47
1:A:1553:VAL:HG13	36:M:196:ASP:HB2	1.95	0.47
4:D:759:THR:HA	19:3:682:VAL:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:1094:LEU:HD22	17:1:1128:VAL:HB	1.96	0.47
25:J:308:ARG:HG3	27:R:231:HIS:O	2.14	0.47
29:X:253:ARG:NH2	29:X:253:ARG:CG	2.73	0.47
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.35	0.47
1:A:2325:VAL:HG22	4:D:788:GLY:O	2.14	0.47
3:C:834:VAL:HG11	3:C:883:PHE:HE2	1.79	0.47
5:E:258:THR:CG2	5:E:260:ARG:CG	2.93	0.47
13:F:32:C:O2'	13:F:33:C:P	2.73	0.47
17:1:929:LEU:HD22	17:1:962:MET:HE2	1.96	0.47
17:1:1033:GLU:OE1	17:1:1070:LYS:HE2	2.15	0.47
25:J:232:GLU:OE1	25:J:235:ILE:HG21	2.14	0.47
25:J:270:ASP:OD1	27:R:223:PRO:HD3	2.15	0.47
29:X:230:GLY:O	29:X:234:GLU:HG3	2.14	0.47
1:A:651:TRP:CG	13:F:38:G:H1'	2.49	0.47
1:A:1385:VAL:HG11	1:A:1419:ILE:HD12	1.94	0.47
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.49	0.47
3:C:811:THR:O	3:C:815:VAL:HG23	2.14	0.47
5:E:258:THR:CG2	5:E:260:ARG:HG2	2.37	0.47
16:v:201:TRP:CH2	16:v:224:PRO:HD3	2.49	0.47
29:X:364:SER:O	29:X:365:ARG:HG2	2.14	0.47
30:Y:37:TRP:HB3	30:Y:112:VAL:HG21	1.96	0.47
33:z:165:GLU:OE2	36:M:104:ARG:NH2	2.47	0.47
34:x:716:LYS:N	34:x:748:GLU:O	2.47	0.47
3:C:780:CYS:SG	3:C:782:GLU:HG3	2.54	0.47
4:D:423:MET:CB	4:D:878:TYR:CA	2.92	0.47
5:E:160:ALA:HB2	5:E:201:PHE:CE2	2.50	0.47
14:G:211:U:O2'	14:G:213:C:OP2	2.25	0.47
25:J:313:TRP:CH2	25:J:339:TRP:CD1	3.03	0.47
29:X:329:ILE:O	29:X:329:ILE:HG23	2.13	0.47
32:9:141:PHE:HB3	32:9:150:PHE:O	2.14	0.47
33:z:150:ASP:N	33:z:154:ARG:O	2.44	0.47
34:x:452:GLN:O	34:x:498:ASP:N	2.44	0.47
1:A:796:LYS:O	32:9:225:MET:HE1	2.14	0.47
1:A:1762:TYR:HD1	1:A:1762:TYR:N	2.12	0.47
1:A:1872:LEU:HD22	1:A:1884:ILE:HG12	1.96	0.47
3:C:478:THR:O	3:C:562:THR:OG1	2.26	0.47
5:E:88:ARG:CG	5:E:110:GLY:O	2.46	0.47
5:E:248:SER:HB2	5:E:249:TYR:HD1	1.75	0.47
17:1:758:ASP:N	17:1:758:ASP:OD1	2.48	0.47
17:1:1124:SER:O	17:1:1127:THR:OG1	2.30	0.47
20:4:67:ALA:O	20:4:70:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:388:ILE:HD13	29:X:350:TYR:HD1	1.79	0.47
41:I:81:TYR:HD2	41:I:89:VAL:HG21	1.79	0.47
1:A:152:ARG:NH2	1:A:618:THR:O	2.47	0.47
1:A:206:TRP:HB2	1:A:212:PRO:HB2	1.95	0.47
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.95	0.47
1:A:1523:ARG:HH22	16:v:4:LYS:HD2	1.79	0.47
14:G:218:U:C4	30:Y:105:ARG:CZ	2.98	0.47
15:H:15:U:H3'	24:L:40:ARG:HH12	1.80	0.47
19:3:399:ASP:OD1	19:3:400:GLU:N	2.48	0.47
19:3:720:TRP:HE3	19:3:731:LEU:HG	1.80	0.47
20:4:12:ASP:O	20:4:67:ALA:HB2	2.10	0.47
21:5:80:PHE:CD2	21:5:82:VAL:HG23	2.50	0.47
22:6:30:CYS:O	22:6:34:ASP:HA	2.15	0.47
28:T:493:ASP:OD1	28:T:493:ASP:N	2.37	0.47
1:A:761:ILE:HD12	1:A:775:ASN:HD22	1.80	0.47
3:C:649:SER:HB3	3:C:651:ILE:HG12	1.95	0.47
3:C:774:THR:HA	3:C:784:ILE:HD12	1.96	0.47
15:H:14:A:C6	16:v:10:TRP:HB3	2.50	0.47
17:1:128:ILE:HB	21:5:96:ARG:HB3	1.97	0.47
17:1:415:LEU:HD23	17:1:415:LEU:HA	1.79	0.47
19:3:629:SER:OG	19:3:686:LEU:HD12	2.15	0.47
19:3:987:ALA:HB3	19:3:1007:GLU:HG2	1.96	0.47
25:J:236:ARG:NH1	25:J:236:ARG:C	2.73	0.47
25:J:276:ILE:HD11	25:J:309:VAL:HG11	1.96	0.47
25:J:303:ILE:HD13	25:J:313:TRP:CD1	2.50	0.47
33:z:13:GLY:HA2	33:z:168:PHE:HD2	1.80	0.47
42:K:120:THR:CG2	42:K:124:HIS:CD2	2.96	0.47
1:A:2148:VAL:O	1:A:2150:GLN:HG2	2.14	0.47
2:B:96:A:N3	2:B:96:A:C3'	2.77	0.47
3:C:543:ARG:CG	3:C:543:ARG:NH1	2.77	0.47
4:D:141:ALA:HB2	4:D:182:TYR:OH	2.15	0.47
5:E:277:PHE:CD1	5:E:277:PHE:N	2.82	0.47
15:H:2:U:O2'	15:H:3:G:OP2	2.26	0.47
19:3:353:PHE:HE2	19:3:429:ARG:NH1	2.13	0.47
19:3:1004:ASP:OD2	19:3:1007:GLU:CB	2.55	0.47
29:X:338:PHE:HD2	29:X:359:LYS:HB3	1.79	0.47
30:Y:65:ILE:CD1	30:Y:82:LEU:HD21	2.44	0.47
1:A:662:GLY:HA3	27:R:213:LYS:NZ	2.30	0.47
1:A:1122:ASN:HB2	32:9:35:ARG:HD3	1.94	0.47
1:A:2121:ARG:O	1:A:2154:HIS:HA	2.15	0.47
4:D:1672:LYS:HA	4:D:1885:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:57:ALA:HB1	24:L:14:THR:HB	1.97	0.47
27:R:389:SER:HB3	29:X:349:TYR:HB2	1.97	0.47
32:9:79:ASN:ND2	32:9:81:GLU:HG2	2.30	0.47
3:C:813:ARG:NH1	32:9:106:LEU:HD22	2.30	0.46
17:1:1032:GLN:O	17:1:1036:ILE:HG22	2.15	0.46
18:2:565:ASP:OD1	18:2:565:ASP:N	2.47	0.46
21:5:77:LEU:CG	21:5:89:VAL:HG11	2.45	0.46
27:R:403:ASN:ND2	27:R:403:ASN:O	2.47	0.46
28:T:381:HIS:HD2	28:T:441:TRP:CE2	2.33	0.46
34:x:640:ARG:CB	34:x:667:ALA:N	2.78	0.46
40:0:82:ILE:HA	40:0:89:LYS:HA	1.98	0.46
42:K:113:GLU:HA	42:K:116:LEU:HD12	1.97	0.46
1:A:642:ARG:HG3	2:B:56:C:H1'	1.97	0.46
1:A:881:ILE:HG23	1:A:918:THR:HG23	1.97	0.46
13:F:17:G:O2'	13:F:18:A:N7	2.46	0.46
14:G:-9:G:N2	37:U:5:ILE:O	2.44	0.46
15:H:13:U:H5'	15:H:14:A:C5'	2.45	0.46
15:H:39:G:H2'	15:H:40:G:O4'	2.15	0.46
25:J:232:GLU:O	25:J:235:ILE:CG2	2.63	0.46
25:J:236:ARG:HH11	25:J:236:ARG:HG3	1.79	0.46
27:R:140:ILE:HA	27:R:143:ILE:HG22	1.97	0.46
32:9:276:VAL:CB	32:9:297:CYS:C	2.89	0.46
33:z:151:ASP:N	33:z:151:ASP:OD1	2.48	0.46
36:M:249:TYR:HB3	40:0:72:TYR:CZ	2.51	0.46
36:M:287:LEU:O	36:M:291:ARG:HG3	2.14	0.46
39:8:51:TRP:HH2	39:8:104:GLU:HG3	1.79	0.46
39:8:56:VAL:HG23	39:8:68:ILE:HD11	1.96	0.46
40:0:93:THR:CB	40:0:98:GLN:NE2	2.78	0.46
1:A:1129:ASN:OD1	1:A:1129:ASN:N	2.46	0.46
1:A:1347:ASP:OD1	1:A:1347:ASP:N	2.35	0.46
4:D:498:ASN:O	4:D:672:GLY:O	2.33	0.46
5:E:243:LEU:HD11	5:E:247:GLY:CA	2.44	0.46
17:1:675:MET:HB2	17:1:679:ILE:HG23	1.97	0.46
20:4:12:ASP:CB	20:4:67:ALA:HB3	2.43	0.46
21:5:48:ILE:HG12	21:5:62:VAL:HG22	1.98	0.46
32:9:52:PRO:HB2	32:9:91:LEU:HB2	1.96	0.46
38:V:469:PHE:CD1	38:V:469:PHE:C	2.93	0.46
41:I:104:LYS:HG3	41:I:119:VAL:HG23	1.98	0.46
1:A:1415:GLY:O	1:A:1418:ARG:NH1	2.47	0.46
1:A:1853:PRO:HD2	1:A:1856:GLU:HG3	1.98	0.46
19:3:1064:ASP:OD1	19:3:1064:ASP:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:48:THR:OG1	30:Y:49:GLU:N	2.46	0.46
1:A:443:VAL:HG11	1:A:614:TYR:CD1	2.51	0.46
4:D:1582:ALA:C	4:D:1584:ILE:N	2.72	0.46
5:E:119:THR:CG2	5:E:161:ARG:HB3	2.46	0.46
5:E:178:LEU:HG	5:E:188:GLN:HB2	1.98	0.46
16:v:194:LEU:HD21	19:3:1017:ASN:HB3	1.97	0.46
19:3:643:VAL:O	19:3:663:LEU:HD12	2.16	0.46
25:J:236:ARG:NH1	25:J:236:ARG:CG	2.73	0.46
25:J:376:VAL:HG23	25:J:415:LEU:HD12	1.97	0.46
27:R:237:MET:HB2	27:R:241:GLU:OE2	2.16	0.46
29:X:344:ILE:HB	29:X:350:TYR:CE2	2.50	0.46
32:9:75:THR:HG22	32:9:82:LYS:HB3	1.97	0.46
41:I:97:LEU:O	41:I:101:ARG:HG3	2.15	0.46
42:K:139:THR:HB	42:K:141:VAL:HG22	1.96	0.46
1:A:1093:ASP:N	1:A:1093:ASP:OD2	2.49	0.46
3:C:506:PRO:HB3	3:C:526:THR:HG22	1.98	0.46
17:1:129:SEP:O3P	17:1:150:ARG:NH2	2.30	0.46
17:1:933:CYS:O	17:1:937:LEU:HB2	2.15	0.46
19:3:1164:ARG:C	19:3:1170:VAL:HG22	2.41	0.46
41:I:123:PRO:O	41:I:126:GLU:HG2	2.16	0.46
1:A:514:ASN:N	1:A:514:ASN:OD1	2.44	0.46
1:A:1260:VAL:HG21	1:A:1325:LEU:HB3	1.97	0.46
1:A:1527:ASN:HB2	36:M:215:ASP:HB3	1.98	0.46
4:D:783:ALA:O	4:D:809:LEU:CA	2.60	0.46
13:F:6:G:H2'	13:F:6:G:N3	2.30	0.46
13:F:23:G:O2'	13:F:24:U:O5'	2.34	0.46
17:1:937:LEU:HD23	17:1:937:LEU:HA	1.78	0.46
19:3:55:THR:O	19:3:55:THR:HG23	2.16	0.46
19:3:515:ALA:HB1	19:3:526:HIS:NE2	2.31	0.46
25:J:308:ARG:HH21	25:J:341:PRO:HB3	1.80	0.46
29:X:332:GLY:CA	29:X:346:PRO:HB3	2.46	0.46
41:I:78:LEU:HD21	41:I:89:VAL:HG12	1.96	0.46
1:A:413:LEU:C	1:A:413:LEU:HD12	2.41	0.46
1:A:1292:GLU:OE2	1:A:1331:GLY:N	2.41	0.46
1:A:1648:SER:HB3	1:A:1883:VAL:HG12	1.97	0.46
4:D:140:LEU:HD23	4:D:140:LEU:C	2.40	0.46
4:D:1349:GLY:HA2	4:D:1491:SER:O	2.16	0.46
5:E:250:LEU:CD1	5:E:262:TRP:HB2	2.45	0.46
15:H:38:G:C2'	15:H:39:G:H5''	2.46	0.46
22:6:45:ILE:HD11	22:6:50:ASN:HB3	1.97	0.46
1:A:662:GLY:CA	27:R:213:LYS:HZ2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	1.96	0.46
5:E:177:LYS:C	5:E:178:LEU:HD23	2.41	0.46
17:1:1250:CYS:HA	17:1:1265:TYR:CE2	2.51	0.46
19:3:519:VAL:HG23	19:3:524:ILE:HG12	1.98	0.46
19:3:950:ALA:CB	19:3:989:TYR:OH	2.44	0.46
25:J:270:ASP:OD1	27:R:223:PRO:HG3	2.16	0.46
25:J:366:TYR:CE2	25:J:382:TYR:HA	2.51	0.46
30:Y:67:LEU:HA	30:Y:80:CYS:HB3	1.92	0.46
1:A:774:LYS:HZ1	15:H:5:C:HO2'	1.58	0.46
1:A:1536:LEU:HD11	1:A:1576:ILE:HD11	1.98	0.46
3:C:683:ASN:ND2	3:C:683:ASN:N	2.60	0.46
5:E:260:ARG:NE	5:E:276:ILE:HD11	2.31	0.46
16:v:190:LEU:CG	18:2:691:ALA:CB	2.94	0.46
18:2:648:LEU:HD12	18:2:649:LYS:H	1.81	0.46
28:T:455:GLN:HG2	28:T:456:PRO:HD2	1.97	0.46
30:Y:67:LEU:CD1	30:Y:80:CYS:HB3	2.45	0.46
38:V:619:ASP:OD1	38:V:620:ASN:N	2.49	0.46
39:8:38:VAL:O	39:8:79:ASN:ND2	2.49	0.46
41:I:28:ARG:HA	41:I:28:ARG:HD2	1.57	0.46
41:I:139:LYS:O	41:I:143:VAL:HG23	2.16	0.46
3:C:126:SER:O	3:C:126:SER:OG	2.25	0.45
4:D:151:LYS:HE2	4:D:151:LYS:N	2.31	0.45
5:E:232:ARG:O	5:E:262:TRP:CH2	2.69	0.45
5:E:274:VAL:C	5:E:275:LYS:HG3	2.39	0.45
19:3:614:VAL:HG11	19:3:667:ILE:HD13	1.98	0.45
25:J:286:GLU:HB3	25:J:295:ALA:HB2	1.97	0.45
25:J:336:TRP:C	25:J:338:GLU:N	2.75	0.45
25:J:436:TYR:CZ	25:J:440:LEU:HD22	2.50	0.45
25:J:439:ALA:O	25:J:443:ILE:HG12	2.15	0.45
42:K:143:GLN:H	42:K:143:GLN:HG3	1.53	0.45
1:A:1385:VAL:HG21	1:A:1414:ARG:CG	2.45	0.45
4:D:500:LEU:O	4:D:674:PHE:O	2.34	0.45
5:E:260:ARG:CD	5:E:276:ILE:HD13	2.45	0.45
14:G:11:C:H2'	14:G:12:U:O4'	2.16	0.45
17:1:577:VAL:O	17:1:577:VAL:HG12	2.17	0.45
17:1:716:ALA:O	17:1:719:TYR:N	2.40	0.45
17:1:902:GLU:OE1	27:R:447:ILE:HD12	2.16	0.45
19:3:137:LYS:O	19:3:137:LYS:HD3	2.15	0.45
29:X:287:ARG:HA	29:X:293:PRO:HB3	1.98	0.45
30:Y:140:THR:CG2	31:Z:563:ARG:CG	2.93	0.45
36:M:225:ASP:N	36:M:225:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.46	0.45
1:A:1404:THR:O	1:A:1407:ASP:OD1	2.35	0.45
1:A:1774:ASN:OD1	1:A:1775:GLN:HG3	2.15	0.45
1:A:1860:GLN:HG2	1:A:1883:VAL:HG22	1.98	0.45
1:A:2196:HIS:HB3	1:A:2230:LEU:HD11	1.98	0.45
3:C:490:PHE:HE2	3:C:612:LYS:HB2	1.80	0.45
19:3:173:VAL:HB	19:3:181:MET:HB2	1.98	0.45
19:3:1004:ASP:OD1	19:3:1005:VAL:N	2.49	0.45
25:J:296:ARG:HG3	25:J:319:MET:HE1	1.97	0.45
25:J:361:ARG:O	25:J:364:THR:OG1	2.28	0.45
27:R:465:ALA:O	27:R:469:THR:HG23	2.16	0.45
28:T:381:HIS:ND1	28:T:384:HIS:HB2	2.32	0.45
32:9:42:CYS:SG	32:9:61:PHE:HB2	2.56	0.45
1:A:635:ARG:NH2	2:B:26:A:O3'	2.49	0.45
1:A:2169:LEU:HD21	1:A:2272:MET:HG3	1.98	0.45
5:E:178:LEU:CD1	5:E:222:LEU:HD21	2.46	0.45
19:3:593:ALA:HB3	19:3:602:SER:OG	2.16	0.45
25:J:223:TYR:HA	25:J:226:ARG:NE	2.32	0.45
1:A:44:ARG:HA	1:A:49:ARG:HH12	1.81	0.45
1:A:79:ARG:O	1:A:82:ARG:HG3	2.16	0.45
1:A:1454:TRP:H	1:A:1454:TRP:CD1	2.33	0.45
2:B:96:A:N3	2:B:96:A:H2'	2.32	0.45
4:D:131:ILE:HG12	4:D:697:ALA:CB	2.46	0.45
17:1:982:LEU:HD12	17:1:1019:ARG:HG2	1.97	0.45
1:A:28:GLU:HG2	1:A:29:LYS:N	2.31	0.45
3:C:676:ALA:HB3	3:C:815:VAL:HG22	1.99	0.45
4:D:831:THR:CB	4:D:871:THR:HA	2.47	0.45
19:3:136:GLU:HB3	19:3:166:LEU:HD23	1.98	0.45
19:3:640:LEU:HD23	19:3:665:LEU:HD11	1.99	0.45
25:J:251:TRP:CZ2	25:J:255:LEU:HD11	2.52	0.45
33:z:38:ARG:HH22	33:z:173:ASP:CG	2.25	0.45
42:K:47:PRO:HA	42:K:50:TYR:CD2	2.52	0.45
1:A:2279:TRP:CD1	1:A:2279:TRP:H	2.34	0.45
5:E:133:VAL:O	5:E:147:LEU:N	2.46	0.45
17:1:641:ILE:HG12	17:1:675:MET:HE2	1.96	0.45
19:3:702:PHE:HE2	19:3:715:MET:SD	2.40	0.45
27:R:391:VAL:O	27:R:391:VAL:HG13	2.17	0.45
27:R:463:LEU:HD21	31:Z:518:MET:HE1	1.99	0.45
32:9:137:LYS:HA	32:9:137:LYS:HD2	1.76	0.45
42:K:112:GLU:HG3	42:K:116:LEU:HD11	1.97	0.45
4:D:126:ASP:O	4:D:127:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:185:LEU:HB3	19:3:206:GLN:NE2	2.32	0.45
19:3:675:LEU:HD23	19:3:691:THR:HA	1.99	0.45
24:L:55:ASP:OD2	24:L:57:SER:OG	2.27	0.45
5:E:193:THR:HG22	5:E:194:TYR:CD1	2.41	0.45
5:E:243:LEU:HD11	5:E:247:GLY:C	2.41	0.45
14:G:222:U:H6	30:Y:119:LYS:CE	2.23	0.45
17:1:1136:TYR:HD1	17:1:1147:VAL:CG2	2.30	0.45
17:1:1303:ILE:HD12	17:1:1303:ILE:HA	1.77	0.45
19:3:444:VAL:HG22	19:3:767:LEU:HD22	1.98	0.45
22:6:57:ARG:HE	39:8:1:MET:HE3	1.82	0.45
3:C:780:CYS:SG	3:C:782:GLU:HB2	2.57	0.45
19:3:491:VAL:O	35:y:20:SER:HA	2.17	0.45
1:A:1332:HIS:CE1	1:A:1359:HIS:HB3	2.52	0.44
1:A:2280:ASN:HB3	1:A:2309:HIS:CD2	2.52	0.44
4:D:102:TYR:HB3	4:D:103:LYS:H	1.61	0.44
4:D:1090:ARG:NH2	4:D:1090:ARG:CB	2.80	0.44
27:R:390:GLU:N	27:R:390:GLU:CD	2.73	0.44
29:X:348:ARG:HH11	29:X:348:ARG:HG3	1.81	0.44
1:A:150:MET:O	1:A:153:ARG:HG2	2.17	0.44
1:A:2320:LEU:HD21	1:A:2322:GLU:CD	2.41	0.44
2:B:39:C:C4'	2:B:40:U:OP1	2.65	0.44
18:2:632:TRP:HB3	20:4:76:MET:CB	2.47	0.44
19:3:638:GLU:OE1	19:3:638:GLU:HA	2.16	0.44
25:J:223:TYR:N	25:J:226:ARG:HH21	2.15	0.44
25:J:303:ILE:HD13	25:J:313:TRP:HD1	1.81	0.44
25:J:340:GLN:N	25:J:341:PRO:CD	2.80	0.44
27:R:297:LYS:HZ1	32:9:206:GLU:HG3	1.82	0.44
27:R:404:GLU:HB3	29:X:253:ARG:NH1	2.32	0.44
29:X:364:SER:OG	29:X:365:ARG:N	2.50	0.44
1:A:203:VAL:O	1:A:203:VAL:HG13	2.17	0.44
3:C:259:LYS:HG2	44:C:1500:GTP:C6	2.53	0.44
3:C:508:LYS:HE3	3:C:510:LEU:HD21	1.99	0.44
5:E:276:ILE:O	5:E:277:PHE:HD1	2.00	0.44
14:G:210:G:N3	14:G:210:G:H2'	2.32	0.44
14:G:219:U:O2	14:G:219:U:O2'	2.31	0.44
17:1:1109:ARG:O	17:1:1112:THR:CG2	2.63	0.44
17:1:1258:ALA:HB3	17:1:1261:VAL:HG12	1.98	0.44
19:3:1052:ASN:OD1	19:3:1052:ASN:N	2.50	0.44
25:J:375:ASP:OD1	25:J:376:VAL:N	2.50	0.44
27:R:132:LEU:O	28:T:385:TYR:HB3	2.18	0.44
1:A:738:MET:HE2	1:A:738:MET:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2156:THR:OG1	1:A:2157:VAL:N	2.50	0.44
4:D:102:TYR:HA	4:D:137:ASP:OD2	2.18	0.44
17:1:770:MET:HE3	17:1:801:VAL:HG11	1.98	0.44
17:1:1044:ASP:HB3	17:1:1083:TYR:CD1	2.52	0.44
17:1:1045:ARG:HH11	40:0:24:ARG:HG3	1.83	0.44
17:1:1287:ILE:HG13	23:7:32:LEU:HD21	2.00	0.44
19:3:485:LEU:HD23	19:3:491:VAL:CG1	2.47	0.44
19:3:1001:ILE:HG13	19:3:1038:LEU:HD11	2.00	0.44
25:J:313:TRP:HH2	25:J:339:TRP:CD1	2.35	0.44
25:J:336:TRP:C	25:J:338:GLU:H	2.26	0.44
29:X:294:ILE:HD12	29:X:299:CYS:SG	2.58	0.44
30:Y:16:ARG:NH1	30:Y:20:LEU:HD11	2.33	0.44
1:A:410:PRO:O	1:A:413:LEU:HG	2.18	0.44
4:D:144:LYS:HD2	4:D:144:LYS:HA	1.42	0.44
5:E:62:LEU:HD13	5:E:351:LEU:HD12	1.85	0.44
17:1:946:LYS:HA	17:1:946:LYS:HD2	1.79	0.44
17:1:1304:LEU:HD23	17:1:1304:LEU:HA	1.82	0.44
19:3:460:TRP:HZ3	19:3:505:THR:HG23	1.82	0.44
29:X:255:PRO:HB3	29:X:308:TYR:CD1	2.52	0.44
30:Y:37:TRP:C	30:Y:112:VAL:HG22	2.42	0.44
30:Y:38:ILE:O	30:Y:38:ILE:HG13	2.17	0.44
30:Y:40:LEU:HD12	30:Y:80:CYS:SG	2.58	0.44
42:K:151:SER:CB	42:K:156:LEU:HD23	2.46	0.44
1:A:543:ALA:HB3	13:F:38:G:OP1	2.18	0.44
1:A:1237:MET:HB3	1:A:1237:MET:HE2	1.73	0.44
2:B:34:U:O4	32:9:4:ARG:NH1	2.51	0.44
17:1:446:MET:HB2	27:R:299:ARG:HG2	2.00	0.44
25:J:241:VAL:HG22	25:J:244:ASN:HB2	1.99	0.44
25:J:265:TYR:HD2	25:J:282:TYR:HD1	1.66	0.44
38:V:599:LEU:O	38:V:603:LEU:HB2	2.17	0.44
40:0:8:LYS:HB3	40:0:8:LYS:HE2	1.80	0.44
1:A:481:PHE:CG	27:R:205:ASP:HB3	2.51	0.44
1:A:1638:ASN:HB3	1:A:1652:MET:O	2.17	0.44
1:A:2078:ILE:HG23	4:D:1047:PRO:CB	2.47	0.44
3:C:590:ILE:HG22	3:C:629:ILE:HB	1.99	0.44
5:E:92:LEU:O	5:E:101:ASN:OD1	2.36	0.44
16:v:190:LEU:CG	18:2:691:ALA:HB2	2.48	0.44
19:3:485:LEU:HD23	19:3:491:VAL:HG12	2.00	0.44
19:3:563:LEU:HD12	19:3:581:LYS:HD3	1.99	0.44
29:X:241:GLY:HA3	29:X:288:ARG:NE	2.32	0.44
29:X:262:TYR:HA	29:X:263:PRO:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:x:953:ARG:N	34:x:960:ARG:O	2.36	0.44
1:A:1421:THR:O	1:A:1424:GLN:HG2	2.18	0.44
5:E:274:VAL:C	5:E:275:LYS:CG	2.91	0.44
17:1:732:TRP:HA	17:1:732:TRP:CE3	2.53	0.44
17:1:936:VAL:HG11	17:1:955:ILE:HG13	2.00	0.44
19:3:12:THR:O	19:3:34:ARG:NH1	2.50	0.44
20:4:12:ASP:CA	20:4:67:ALA:HB1	2.44	0.44
41:I:144:LYS:HB2	41:I:144:LYS:HE3	1.70	0.44
42:K:58:VAL:HG23	42:K:61:LEU:HD13	1.98	0.44
3:C:306:ASN:HA	3:C:433:MET:HG3	2.00	0.44
3:C:847:TYR:CE1	3:C:857:VAL:HG21	2.53	0.44
5:E:237:SER:HB2	5:E:255:MET:HG3	1.98	0.44
5:E:246:GLU:HB2	5:E:248:SER:HG	1.81	0.44
5:E:251:LEU:CG	5:E:291:CYS:SG	3.05	0.44
5:E:277:PHE:CE1	5:E:317:ARG:HG2	2.53	0.44
13:F:39:A:OP2	13:F:39:A:H8	2.01	0.44
17:1:884:ILE:HG23	17:1:888:LEU:HD23	2.00	0.44
19:3:42:ARG:HB2	19:3:53:LEU:HD11	1.99	0.44
19:3:318:ASP:HB2	19:3:323:THR:CG2	2.48	0.44
19:3:1057:ARG:HH11	19:3:1057:ARG:CG	2.13	0.44
25:J:259:GLN:OE1	25:J:259:GLN:HA	2.18	0.44
32:9:106:LEU:HD23	32:9:106:LEU:HA	1.77	0.44
1:A:41:GLN:OE1	1:A:41:GLN:HA	2.18	0.43
1:A:1574:ILE:HG22	36:M:220:LEU:HD22	2.00	0.43
1:A:1673:SER:O	1:A:1673:SER:OG	2.31	0.43
3:C:497:LEU:HD23	3:C:497:LEU:HA	1.78	0.43
4:D:505:THR:CB	4:D:854:GLY:CA	2.96	0.43
4:D:1308:PRO:C	4:D:1310:SER:N	2.75	0.43
4:D:1589:PHE:O	4:D:1642:GLN:N	2.49	0.43
14:G:209:U:H4'	14:G:210:G:C5	2.53	0.43
17:1:524:ARG:HG2	23:7:1:MET:HE2	1.99	0.43
17:1:1262:ARG:NH1	23:7:24:ALA:O	2.47	0.43
18:2:630:PRO:HA	18:2:631:PRO:HD3	1.78	0.43
27:R:466:ARG:HD2	27:R:466:ARG:HA	1.77	0.43
29:X:330:ASP:OD1	29:X:330:ASP:O	2.36	0.43
32:9:134:LEU:O	32:9:138:ALA:HB3	2.17	0.43
33:z:16:LEU:HB3	33:z:165:GLU:HB3	1.99	0.43
34:x:446:MET:HA	34:x:513:SER:O	2.18	0.43
42:K:75:GLU:HA	42:K:78:ILE:HG22	2.00	0.43
1:A:61:MET:HE3	1:A:61:MET:HB3	1.65	0.43
1:A:596:TYR:C	1:A:598:LEU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:LYS:HA	1:A:1344:LYS:HD3	1.78	0.43
1:A:1887:SER:O	1:A:1890:GLN:NE2	2.50	0.43
1:A:2306:HIS:CE1	1:A:2308:VAL:CG2	2.94	0.43
3:C:259:LYS:HD3	44:C:1500:GTP:C4	2.53	0.43
4:D:106:THR:CG2	4:D:107:LYS:H	2.30	0.43
16:v:201:TRP:CZ3	16:v:211:LYS:HG3	2.53	0.43
17:1:731:LEU:HD23	17:1:731:LEU:HA	1.90	0.43
17:1:1109:ARG:CA	17:1:1112:THR:HG22	2.47	0.43
17:1:1183:VAL:HA	17:1:1186:GLN:HG2	2.00	0.43
19:3:553:GLN:NE2	19:3:619:LEU:HD13	2.32	0.43
26:P:189:ASP:OD1	26:P:189:ASP:N	2.34	0.43
29:X:241:GLY:O	29:X:288:ARG:NH2	2.50	0.43
30:Y:38:ILE:HG23	30:Y:90:THR:HG22	1.99	0.43
32:9:245:LYS:HD2	32:9:258:GLU:HG3	2.01	0.43
41:I:128:VAL:O	41:I:131:THR:OG1	2.27	0.43
3:C:758:LEU:HG	3:C:803:ARG:HH12	1.84	0.43
18:2:573:ASP:OD1	18:2:577:LYS:HE3	2.18	0.43
19:3:475:ILE:HD13	19:3:484:VAL:HG23	2.00	0.43
25:J:258:ILE:O	25:J:261:ALA:N	2.51	0.43
25:J:289:ASN:O	25:J:291:GLN:N	2.51	0.43
39:8:86:GLN:HB2	39:8:102:MET:HG3	2.00	0.43
40:0:89:LYS:HE2	40:0:89:LYS:HB3	1.84	0.43
41:I:91:LEU:HD11	41:I:125:PHE:CD2	2.53	0.43
3:C:481:MET:HB3	3:C:481:MET:HE2	1.79	0.43
4:D:140:LEU:CD2	4:D:144:LYS:HG2	2.48	0.43
17:1:150:ARG:HH21	17:1:150:ARG:HD3	1.71	0.43
19:3:520:TYR:CD1	19:3:522:ASP:HB2	2.53	0.43
19:3:566:PHE:HD1	19:3:576:GLU:HA	1.83	0.43
28:T:257:ARG:NH2	28:T:301:ASP:OD1	2.51	0.43
1:A:579:GLN:HB3	1:A:630:TRP:HB3	2.00	0.43
1:A:1551:PHE:CD2	36:M:192:THR:OG1	2.72	0.43
2:B:93:U:H4'	2:B:94:U:H5''	2.00	0.43
19:3:875:ASN:OD1	19:3:875:ASN:N	2.33	0.43
27:R:238:THR:OG1	27:R:241:GLU:HG3	2.18	0.43
27:R:470:ASN:HB3	31:Z:515:MET:HE1	1.99	0.43
28:T:220:VAL:HG13	28:T:230:ILE:HG12	1.99	0.43
33:z:98:LEU:H	33:z:116:THR:HG22	1.83	0.43
38:V:465:SER:OG	38:V:475:LYS:NZ	2.51	0.43
41:I:36:VAL:HG23	41:I:36:VAL:O	2.19	0.43
1:A:829:PRO:HB3	21:5:86:TYR:CD2	2.52	0.43
1:A:834:HIS:CD2	1:A:1432:TYR:CE1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LYS:O	1:A:840:ILE:HG22	2.18	0.43
14:G:217:U:H6	14:G:217:U:C5'	2.29	0.43
15:H:38:G:C2'	15:H:39:G:C5'	2.97	0.43
15:H:83:G:H2'	15:H:84:C:C6	2.54	0.43
17:1:563:LEU:HB3	17:1:566:LEU:HD12	2.00	0.43
18:2:495:ARG:NH2	19:3:1026:ASP:OD2	2.52	0.43
19:3:1120:THR:HG22	19:3:1126:ILE:HG12	2.00	0.43
25:J:222:ASP:C	25:J:226:ARG:HH21	2.26	0.43
32:9:242:SER:HA	32:9:263:ALA:HA	2.01	0.43
42:K:28:GLN:OE1	42:K:28:GLN:N	2.50	0.43
1:A:1768:TYR:CD1	1:A:1768:TYR:C	2.97	0.43
3:C:192:ASP:OD1	3:C:195:GLY:N	2.39	0.43
3:C:854:ARG:HH21	3:C:854:ARG:HD2	1.70	0.43
17:1:563:LEU:H	17:1:563:LEU:HG	1.52	0.43
17:1:971:MET:CE	17:1:1003:VAL:CG1	2.88	0.43
19:3:630:MET:HE1	36:M:287:LEU:CG	2.48	0.43
29:X:241:GLY:C	29:X:288:ARG:HH21	2.27	0.43
41:I:138:ARG:HH21	42:K:83:ASN:HB2	1.83	0.43
1:A:1676:ILE:HD13	1:A:1706:ASP:HB2	2.01	0.43
1:A:1949:ARG:NE	27:R:463:LEU:HD13	2.33	0.43
1:A:2272:MET:HE3	1:A:2296:LEU:HB3	2.01	0.43
3:C:323:PHE:CD2	3:C:373:ILE:HG12	2.53	0.43
4:D:123:ALA:HB1	4:D:161:LEU:CD1	2.48	0.43
4:D:1635:LEU:O	4:D:1640:ALA:N	2.51	0.43
14:G:218:U:H3'	30:Y:3:PRO:HG2	2.00	0.43
17:1:885:ASP:OD1	17:1:885:ASP:N	2.50	0.43
19:3:47:THR:CG2	19:3:49:LYS:CG	2.84	0.43
19:3:956:GLN:HE22	19:3:998:HIS:CE1	2.37	0.43
21:5:76:HIS:ND1	21:5:76:HIS:C	2.73	0.43
27:R:148:ARG:HG3	28:T:300:ILE:HG23	2.01	0.43
41:I:67:ALA:HB2	41:I:72:ILE:HD12	2.01	0.43
1:A:1681:ARG:HG3	1:A:1715:TYR:CZ	2.53	0.43
3:C:758:LEU:HD11	3:C:798:GLN:HA	2.00	0.43
13:F:10:G:H1	14:G:10:U:H3	1.67	0.43
16:v:190:LEU:HD11	18:2:691:ALA:CB	2.48	0.43
19:3:406:PRO:O	19:3:427:CYS:CB	2.67	0.43
19:3:603:ARG:NH1	19:3:620:ASP:HB2	2.33	0.43
19:3:669:LEU:HD12	19:3:673:VAL:CG2	2.47	0.43
25:J:358:GLU:HG2	25:J:361:ARG:HH11	1.83	0.43
30:Y:53:ILE:O	30:Y:57:SER:OG	2.23	0.43
42:K:53:LEU:O	42:K:58:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ILE:CD1	32:9:35:ARG:HG3	2.49	0.43
1:A:1499:GLU:OE2	1:A:1928:SER:OG	2.34	0.43
1:A:1639:VAL:O	1:A:1654:SER:HB3	2.19	0.43
1:A:2074:ARG:H	1:A:2074:ARG:HG2	1.54	0.43
3:C:602:LYS:HD2	3:C:651:ILE:HD11	2.00	0.43
3:C:634:GLU:OE2	3:C:882:GLY:N	2.49	0.43
4:D:434:SER:HA	4:D:446:HIS:O	2.19	0.43
16:v:212:ASP:OD1	16:v:213:GLU:N	2.52	0.43
17:1:1023:ILE:O	17:1:1023:ILE:HG22	2.19	0.43
17:1:1050:VAL:HG21	17:1:1055:TRP:CZ2	2.53	0.43
18:2:632:TRP:CB	20:4:76:MET:CB	2.97	0.43
19:3:931:VAL:HG23	19:3:936:LYS:HB3	2.01	0.43
25:J:336:TRP:HE1	25:J:341:PRO:HG3	1.83	0.43
41:I:135:LEU:HD23	41:I:135:LEU:HA	1.81	0.43
1:A:444:ARG:HG3	1:A:444:ARG:NH1	2.33	0.42
1:A:796:LYS:CG	32:9:225:MET:HE1	2.49	0.42
1:A:976:MET:HE2	1:A:976:MET:HB2	1.93	0.42
2:B:36:C:O2	37:U:11:ARG:NH2	2.51	0.42
4:D:109:THR:CG2	4:D:180:THR:OG1	2.63	0.42
4:D:406:ARG:CB	4:D:955:ASP:CB	2.97	0.42
5:E:323:LEU:HA	5:E:324:PRO:HD2	1.88	0.42
17:1:550:HIS:CG	22:6:100:TYR:CD2	3.06	0.42
17:1:1129:LEU:HD23	17:1:1129:LEU:HA	1.75	0.42
17:1:1291:ASP:N	17:1:1291:ASP:OD1	2.51	0.42
17:1:1302:TYR:OH	23:7:57:GLU:OE2	2.37	0.42
19:3:965:LYS:HG3	19:3:966:LEU:HD12	2.00	0.42
25:J:287:MET:HE3	25:J:319:MET:HG3	2.01	0.42
25:J:438:TYR:CE2	25:J:442:ARG:HD2	2.54	0.42
28:T:213:GLU:HG3	28:T:218:TRP:CZ2	2.54	0.42
32:9:61:PHE:CE1	32:9:66:ILE:HB	2.53	0.42
1:A:946:GLU:OE1	1:A:954:LYS:HD2	2.19	0.42
1:A:2216:CYS:HA	1:A:2225:LEU:HB3	2.01	0.42
2:B:44:A:N7	32:9:3:LYS:NZ	2.62	0.42
2:B:101:U:H6	2:B:101:U:O5'	2.02	0.42
3:C:929:LEU:HD23	3:C:929:LEU:HA	1.78	0.42
4:D:119:PHE:CD1	4:D:119:PHE:C	2.97	0.42
4:D:831:THR:CB	4:D:871:THR:CB	2.96	0.42
5:E:348:ASP:C	5:E:348:ASP:OD1	2.62	0.42
9:k:68:GLU:HA	9:k:97:SER:O	2.19	0.42
17:1:1083:TYR:CZ	40:0:13:VAL:CG2	3.02	0.42
24:L:77:LEU:O	24:L:79:PRO:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:246:ILE:O	25:J:250:GLN:HG2	2.19	0.42
30:Y:13:LEU:HD12	30:Y:13:LEU:HA	1.85	0.42
32:9:277:LYS:H	32:9:437:PRO:CB	2.32	0.42
34:x:561:SER:O	34:x:566:ASP:N	2.42	0.42
42:K:34:GLU:HG2	42:K:73:LEU:HD12	2.00	0.42
1:A:38:GLN:HB2	5:E:195:GLN:HE21	1.85	0.42
1:A:92:LEU:HD13	1:A:503:MET:HB3	2.00	0.42
3:C:377:LEU:HD12	3:C:377:LEU:HA	1.88	0.42
3:C:480:LYS:HA	3:C:480:LYS:HD2	1.84	0.42
4:D:149:ARG:NH1	4:D:149:ARG:HG3	2.34	0.42
5:E:114:GLU:CD	5:E:116:HIS:NE2	2.76	0.42
15:H:74:A:H5'	15:H:80:U:OP2	2.18	0.42
25:J:340:GLN:CG	25:J:372:VAL:HG21	2.43	0.42
30:Y:116:ARG:HH11	30:Y:116:ARG:CG	2.30	0.42
30:Y:117:ALA:HA	30:Y:118:PRO:HD3	1.86	0.42
32:9:112:ASN:HA	32:9:159:GLN:HE22	1.84	0.42
39:8:63:GLU:OE1	39:8:63:GLU:N	2.51	0.42
40:0:79:LYS:HB2	40:0:79:LYS:HE2	1.84	0.42
1:A:829:PRO:HA	21:5:86:TYR:HE2	1.83	0.42
15:H:50:A:H2'	15:H:51:A:C8	2.55	0.42
17:1:1119:VAL:HA	17:1:1122:THR:HG22	2.01	0.42
19:3:274:ARG:NH2	19:3:309:ASP:OD1	2.53	0.42
19:3:583:MET:HE1	19:3:607:VAL:HG21	2.02	0.42
25:J:245:TRP:O	25:J:245:TRP:HE3	2.02	0.42
38:V:600:ASN:OD1	38:V:604:LYS:NZ	2.53	0.42
41:I:37:LYS:CD	41:I:39:TYR:OH	2.67	0.42
41:I:65:ARG:O	41:I:68:LEU:HB3	2.19	0.42
1:A:246:LEU:HD11	1:A:411:PHE:HE2	1.82	0.42
1:A:662:GLY:CA	27:R:213:LYS:HZ3	2.31	0.42
1:A:1017:ILE:O	1:A:1023:ASN:HA	2.19	0.42
3:C:333:ASP:OD1	3:C:333:ASP:N	2.50	0.42
19:3:678:VAL:HB	19:3:687:SER:HB3	2.00	0.42
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.82	0.42
1:A:1678:ARG:HA	1:A:1678:ARG:HD2	1.80	0.42
1:A:1954:LEU:HA	1:A:1954:LEU:HD23	1.84	0.42
3:C:140:HIS:CD2	3:C:230:ASP:HB2	2.55	0.42
3:C:469:ASP:N	3:C:469:ASP:OD1	2.52	0.42
3:C:506:PRO:HA	3:C:526:THR:HA	2.01	0.42
3:C:737:PRO:HB3	3:C:775:ARG:HB2	2.01	0.42
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.19	0.42
17:1:551:LEU:HA	17:1:551:LEU:HD23	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:572:HIS:HB2	17:1:612:THR:HG23	2.01	0.42
17:1:1206:ASP:N	17:1:1206:ASP:OD1	2.50	0.42
25:J:358:GLU:CG	25:J:361:ARG:HD3	2.46	0.42
26:P:222:LYS:HA	26:P:222:LYS:HD2	1.89	0.42
27:R:147:THR:HG22	27:R:151:LEU:HD23	2.01	0.42
27:R:405:VAL:O	27:R:405:VAL:HG13	2.18	0.42
27:R:464:GLU:O	27:R:468:LYS:HG2	2.19	0.42
36:M:279:HIS:CE1	36:M:298:VAL:HB	2.55	0.42
40:O:98:GLN:H	40:O:98:GLN:HG2	1.54	0.42
1:A:596:TYR:C	1:A:598:LEU:N	2.76	0.42
3:C:454:THR:CG2	3:C:578:ARG:HG3	2.49	0.42
4:D:445:VAL:O	4:D:688:THR:CA	2.67	0.42
5:E:62:LEU:HG	5:E:351:LEU:HB2	2.01	0.42
5:E:174:GLY:O	5:E:192:ASN:CA	2.67	0.42
9:d:68:GLU:HA	9:d:97:SER:O	2.19	0.42
13:F:26:A:H2'	13:F:27:G:O4'	2.20	0.42
17:1:1125:PRO:O	17:1:1129:LEU:HB2	2.19	0.42
29:X:275:ILE:HG21	29:X:306:PHE:CE2	2.55	0.42
29:X:285:ARG:NH1	29:X:299:CYS:O	2.52	0.42
30:Y:66:ASN:C	30:Y:80:CYS:HB2	2.45	0.42
32:9:62:ASP:OD1	32:9:63:LEU:N	2.53	0.42
39:8:115:ASN:OD1	39:8:116:ILE:N	2.53	0.42
42:K:51:GLU:HG3	42:K:52:TYR:N	2.35	0.42
42:K:83:ASN:O	42:K:86:PRO:HD2	2.20	0.42
3:C:785:ARG:HH11	3:C:785:ARG:HD2	1.68	0.42
4:D:1661:VAL:O	4:D:1702:CYS:HA	2.19	0.42
18:2:710:GLU:OE2	19:3:1057:ARG:NH2	2.53	0.42
19:3:429:ARG:NH2	19:3:429:ARG:CG	2.73	0.42
25:J:274:ARG:NE	27:R:229:VAL:CG2	2.82	0.42
27:R:470:ASN:CB	31:Z:515:MET:HE1	2.50	0.42
29:X:221:LYS:O	29:X:223:LYS:HG3	2.19	0.42
38:V:461:LEU:HD13	38:V:461:LEU:HA	1.88	0.42
1:A:1189:MET:HE2	1:A:1189:MET:HB2	1.90	0.42
1:A:1425:LYS:HD2	1:A:1425:LYS:O	2.19	0.42
1:A:1580:HIS:O	1:A:1584:LYS:HD3	2.20	0.42
1:A:2112:LYS:HE2	1:A:2112:LYS:HB3	1.67	0.42
3:C:190:LEU:O	3:C:197:SER:HA	2.19	0.42
3:C:510:LEU:HB2	3:C:564:THR:HG23	2.01	0.42
3:C:934:MET:HE3	3:C:934:MET:HB3	1.66	0.42
17:1:123:ARG:HA	17:1:126:MET:HE2	2.01	0.42
17:1:721:ILE:HG12	17:1:757:MET:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:34:ARG:HE	19:3:39:GLU:CD	2.28	0.42
19:3:520:TYR:CE1	19:3:522:ASP:HB2	2.55	0.42
19:3:601:ARG:NH2	19:3:621:PRO:HD3	2.35	0.42
19:3:610:VAL:O	19:3:610:VAL:HG23	2.20	0.42
21:5:110:LEU:HA	21:5:110:LEU:HD13	1.87	0.42
25:J:248:TYR:CE2	25:J:264:ILE:HG12	2.54	0.42
25:J:421:LYS:O	25:J:424:GLU:HB3	2.20	0.42
30:Y:7:VAL:CG2	30:Y:108:ARG:HB3	2.49	0.42
30:Y:117:ALA:CB	31:Z:494:TYR:CE2	3.00	0.42
33:z:52:THR:HG22	33:z:68:PRO:HA	2.01	0.42
41:I:48:LEU:HD12	41:I:48:LEU:HA	1.89	0.42
42:K:50:TYR:CE1	42:K:84:LEU:HA	2.55	0.42
42:K:127:PRO:CG	42:K:131:SER:HB3	2.48	0.42
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.89	0.42
1:A:2111:LEU:HD21	1:A:2225:LEU:HD21	2.02	0.42
1:A:2272:MET:HE3	1:A:2272:MET:HB3	1.75	0.42
3:C:916:ILE:HD13	3:C:928:HIS:HB3	2.02	0.42
13:F:6:G:HI'	14:G:15:C:O2	2.20	0.42
17:1:1114:VAL:O	17:1:1118:ILE:HG12	2.20	0.42
19:3:532:ARG:HE	19:3:532:ARG:HB2	1.68	0.42
42:K:18:GLN:O	42:K:18:GLN:NE2	2.50	0.42
42:K:126:SER:HA	42:K:127:PRO:HD3	1.80	0.42
1:A:137:GLU:O	1:A:141:ILE:HG13	2.20	0.41
1:A:1501:LEU:HD22	1:A:1753:LEU:CD1	2.49	0.41
1:A:1782:ASP:N	1:A:1782:ASP:OD1	2.52	0.41
1:A:2125:ALA:O	1:A:2150:GLN:NE2	2.51	0.41
1:A:2310:ARG:CD	1:A:2313:HIS:CG	3.02	0.41
3:C:607:LEU:HD23	3:C:607:LEU:HA	1.86	0.41
3:C:799:GLU:HG3	3:C:802:HIS:H	1.85	0.41
4:D:148:LEU:HD23	4:D:152:GLU:HB2	2.02	0.41
17:1:505:LYS:HE3	17:1:505:LYS:HB3	1.87	0.41
27:R:388:ILE:HD13	29:X:350:TYR:CD1	2.55	0.41
32:9:98:GLU:H	32:9:98:GLU:CD	2.28	0.41
36:M:131:GLN:O	36:M:135:GLU:HG2	2.20	0.41
38:V:530:LYS:HG2	38:V:567:CYS:SG	2.60	0.41
41:I:27:TYR:HE2	42:K:36:VAL:HG22	1.85	0.41
42:K:30:GLN:O	42:K:34:GLU:HG3	2.20	0.41
42:K:127:PRO:HB2	42:K:131:SER:HB3	2.02	0.41
1:A:78:ASN:HB3	1:A:80:LYS:HG2	2.01	0.41
1:A:977:LEU:CB	1:A:1175:VAL:HG22	2.48	0.41
1:A:1023:ASN:OD1	1:A:1023:ASN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.55	0.41
1:A:2117:ILE:HG21	1:A:2301:PRO:HB2	2.02	0.41
1:A:2120:LEU:HD12	1:A:2120:LEU:N	2.35	0.41
3:C:230:ASP:CG	3:C:259:LYS:HE3	2.45	0.41
4:D:1589:PHE:CB	4:D:1642:GLN:CB	2.98	0.41
47:F:207:G5J:O1B	41:I:39:TYR:OH	2.27	0.41
17:1:793:LYS:HG3	17:1:839:GLU:HG3	2.02	0.41
17:1:1133:MET:HG2	17:1:1172:LEU:HD22	2.02	0.41
19:3:47:THR:HG21	19:3:49:LYS:CG	2.44	0.41
19:3:628:LEU:O	36:M:309:PRO:HG3	2.20	0.41
19:3:988:ASN:HB2	19:3:1004:ASP:OD1	2.21	0.41
19:3:1099:GLU:HG3	19:3:1121:THR:HG21	2.01	0.41
25:J:423:GLU:HA	25:J:426:GLN:HB3	2.02	0.41
29:X:270:LEU:CB	29:X:271:PRO:HD2	2.47	0.41
1:A:769:LYS:HB3	1:A:1249:MET:HG2	2.01	0.41
1:A:2073:TRP:CD1	1:A:2073:TRP:O	2.73	0.41
1:A:2121:ARG:HD2	1:A:2121:ARG:HA	1.55	0.41
3:C:491:HIS:CB	3:C:551:LEU:HD22	2.50	0.41
3:C:914:LYS:NZ	3:C:946:ASP:OD1	2.43	0.41
4:D:148:LEU:HD22	4:D:152:GLU:C	2.45	0.41
5:E:62:LEU:HD12	5:E:351:LEU:HB2	2.02	0.41
16:v:1:MET:HG2	16:v:6:GLU:HB3	2.02	0.41
16:v:33:GLU:HB3	16:v:63:ARG:HH22	1.86	0.41
19:3:430:GLY:HA3	19:3:431:PRO:HD2	1.84	0.41
19:3:503:THR:OG1	19:3:504:PRO:HD2	2.21	0.41
25:J:364:THR:O	25:J:367:GLU:HB3	2.20	0.41
36:M:250:GLU:OE2	40:0:88:LYS:HG2	2.20	0.41
41:I:40:THR:CG2	42:K:79:GLY:HA2	2.50	0.41
4:D:148:LEU:HD22	4:D:152:GLU:CB	2.49	0.41
4:D:722:LEU:HA	4:D:809:LEU:O	2.19	0.41
4:D:1580:CYS:O	4:D:1585:GLN:O	2.38	0.41
5:E:132:THR:HG21	5:E:146:ARG:CD	2.41	0.41
5:E:237:SER:HB2	5:E:255:MET:CG	2.51	0.41
13:F:6:G:N7	41:I:31:ARG:CZ	2.84	0.41
17:1:1014:LYS:HD2	40:0:91:LEU:HD21	2.02	0.41
19:3:563:LEU:HD21	19:3:590:MET:HE1	2.02	0.41
24:L:12:ARG:HH21	24:L:12:ARG:HD3	1.75	0.41
30:Y:55:VAL:HG22	31:Z:589:ARG:CZ	2.50	0.41
3:C:130:ARG:HE	3:C:435:VAL:HA	1.84	0.41
3:C:311:SER:HB3	3:C:316:ILE:HB	2.03	0.41
3:C:676:ALA:HB1	3:C:814:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1481:ILE:C	4:D:1483:ARG:H	2.28	0.41
5:E:147:LEU:N	5:E:147:LEU:HD23	2.35	0.41
17:1:1118:ILE:HG23	40:0:13:VAL:HG13	2.02	0.41
19:3:187:MET:HE3	19:3:187:MET:HB2	1.67	0.41
19:3:246:SER:O	19:3:260:ASN:ND2	2.53	0.41
19:3:642:ILE:HG22	19:3:663:LEU:HD11	2.02	0.41
21:5:27:PRO:HG3	21:5:85:ARG:CD	2.44	0.41
25:J:338:GLU:O	25:J:340:GLN:OE1	2.38	0.41
27:R:391:VAL:CG2	29:X:347:GLN:HB3	2.50	0.41
33:z:67:ASP:OD2	33:z:72:GLY:N	2.47	0.41
39:8:24:LEU:HD23	39:8:24:LEU:HA	1.88	0.41
1:A:384:VAL:O	3:C:354:ARG:NH2	2.50	0.41
1:A:537:LYS:HE2	1:A:537:LYS:HB2	1.86	0.41
3:C:781:ASP:HB2	3:C:943:LEU:HD21	2.02	0.41
15:H:17:A:H1'	22:6:102:ARG:HH12	1.86	0.41
17:1:929:LEU:HA	17:1:929:LEU:HD23	1.84	0.41
19:3:694:LEU:HD12	19:3:694:LEU:O	2.20	0.41
19:3:745:PHE:HB2	19:3:755:VAL:HG23	2.03	0.41
25:J:313:TRP:CE3	25:J:336:TRP:CZ2	3.08	0.41
27:R:387:ASP:H	29:X:351:GLU:CB	2.29	0.41
30:Y:37:TRP:CB	30:Y:112:VAL:HG22	2.50	0.41
30:Y:56:PHE:O	30:Y:84:TYR:OH	2.32	0.41
41:I:139:LYS:HD2	42:K:86:PRO:HB3	2.03	0.41
42:K:49:ASN:O	42:K:53:LEU:HG	2.20	0.41
42:K:120:THR:O	42:K:124:HIS:CD2	2.73	0.41
1:A:1665:GLN:HG3	1:A:1702:LEU:HD21	2.02	0.41
3:C:123:MET:HE2	3:C:123:MET:HB3	1.93	0.41
3:C:412:ILE:HD13	3:C:412:ILE:HA	1.87	0.41
3:C:836:VAL:HG22	3:C:897:SER:HB3	2.02	0.41
4:D:128:PRO:HG2	4:D:131:ILE:HD12	2.02	0.41
13:F:45:A:OP2	14:G:3:A:O2'	2.34	0.41
14:G:207:A:O4'	22:6:102:ARG:HG3	2.21	0.41
15:H:79:U:C3'	15:H:80:U:H5'	2.51	0.41
16:v:196:LEU:O	16:v:201:TRP:HB2	2.20	0.41
17:1:1200:TYR:CD1	17:1:1239:VAL:O	2.74	0.41
17:1:1245:ARG:O	17:1:1249:TYR:HD1	2.04	0.41
19:3:834:LEU:O	19:3:837:GLU:HB3	2.21	0.41
19:3:1052:ASN:HB3	19:3:1096:HIS:HA	2.03	0.41
22:6:29:LYS:HA	22:6:35:SER:O	2.20	0.41
25:J:440:LEU:HG	25:J:445:LYS:HE2	2.02	0.41
38:V:517:LEU:HD23	38:V:517:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2200:MET:HE2	1:A:2200:MET:HB3	1.65	0.41
3:C:85:ASP:HB3	28:T:238:LEU:HG	2.03	0.41
9:d:62:HIS:O	9:d:103:GLY:HA3	2.21	0.41
16:v:194:LEU:HA	16:v:194:LEU:HD23	1.85	0.41
17:1:619:ASN:ND2	17:1:624:VAL:HG21	2.35	0.41
19:3:138:GLN:HA	19:3:161:HIS:ND1	2.35	0.41
19:3:379:LEU:HD21	19:3:384:THR:HA	2.03	0.41
19:3:574:LEU:HA	19:3:574:LEU:HD23	1.78	0.41
21:5:83:CYS:O	21:5:83:CYS:SG	2.79	0.41
25:J:252:GLU:OE1	25:J:252:GLU:HA	2.21	0.41
26:P:200:GLY:C	26:P:202:ASP:H	2.29	0.41
26:P:206:LYS:HD2	26:P:206:LYS:N	2.35	0.41
29:X:223:LYS:HG3	29:X:223:LYS:H	1.63	0.41
34:x:558:ALA:O	34:x:561:SER:N	2.54	0.41
1:A:193:LEU:O	1:A:195:LEU:HD12	2.20	0.41
1:A:259:ASP:OD1	1:A:259:ASP:N	2.48	0.41
1:A:265:THR:HG23	1:A:327:VAL:CG2	2.35	0.41
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.89	0.41
1:A:534:GLU:OE2	13:F:11:A:H5'	2.20	0.41
1:A:1112:ARG:HH11	1:A:1112:ARG:HD3	1.71	0.41
1:A:1425:LYS:HB3	27:R:416:LYS:HA	2.03	0.41
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.27	0.41
3:C:205:THR:HB	3:C:215:VAL:HG22	2.02	0.41
5:E:90:ILE:HB	5:E:105:LEU:HB2	2.03	0.41
14:G:211:U:C2'	14:G:213:C:OP2	2.69	0.41
17:1:157:ARG:NH1	21:5:103:THR:OG1	2.54	0.41
17:1:1167:TYR:CZ	18:2:581:LYS:HE2	2.56	0.41
19:3:1194:SER:HB2	19:3:1199:ARG:O	2.20	0.41
25:J:423:GLU:HB2	25:J:432:VAL:HG22	2.03	0.41
27:R:280:ILE:CG2	32:9:221:LEU:HD22	2.50	0.41
33:z:148:ASP:O	33:z:156:HIS:N	2.53	0.41
38:V:604:LYS:HE3	38:V:604:LYS:HB3	1.86	0.41
39:8:82:SER:HB3	39:8:106:TRP:CH2	2.56	0.41
41:I:98:GLN:HA	41:I:101:ARG:HD3	2.01	0.41
42:K:50:TYR:HE1	42:K:84:LEU:HA	1.86	0.41
1:A:829:PRO:HA	21:5:86:TYR:CE2	2.56	0.41
1:A:1655:THR:OG1	1:A:1656:THR:N	2.54	0.41
4:D:117:LEU:HA	4:D:120:ILE:HG22	2.03	0.41
4:D:121:GLN:HG2	4:D:132:LEU:CD2	2.48	0.41
4:D:144:LYS:HE2	4:D:179:ILE:CG2	2.51	0.41
14:G:197:U:H4'	24:L:12:ARG:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:476:ASP:N	17:1:476:ASP:OD1	2.51	0.41
19:3:510:LEU:HG	19:3:510:LEU:O	2.20	0.41
19:3:999:ARG:NH1	19:3:1041:TYR:O	2.54	0.41
19:3:1161:LEU:O	19:3:1165:SER:OG	2.29	0.41
21:5:87:LEU:HA	21:5:87:LEU:HD12	1.86	0.41
22:6:42:LEU:HD11	22:6:68:ASP:HB3	2.03	0.41
24:L:72:LEU:HA	24:L:72:LEU:HD23	1.85	0.41
25:J:270:ASP:OD1	27:R:223:PRO:HD2	2.17	0.41
25:J:289:ASN:C	25:J:291:GLN:H	2.28	0.41
32:9:96:ASN:HD21	32:9:109:VAL:HG22	1.86	0.41
32:9:330:ILE:O	32:9:381:PHE:CB	2.69	0.41
36:M:288:GLN:O	36:M:291:ARG:HB2	2.21	0.41
1:A:957:GLN:OE1	1:A:957:GLN:HA	2.21	0.40
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.56	0.40
1:A:1753:LEU:HD23	1:A:1753:LEU:HA	1.87	0.40
1:A:2259:VAL:HG22	1:A:2260:GLN:H	1.86	0.40
4:D:642:THR:C	4:D:644:GLU:H	2.30	0.40
4:D:686:GLU:O	4:D:866:GLU:HA	2.21	0.40
4:D:861:TYR:O	19:3:599:GLU:HG3	2.22	0.40
10:m:5:LEU:O	11:l:49:GLY:HA3	2.21	0.40
17:1:397:ARG:HD3	17:1:398:PRO:HD2	2.04	0.40
17:1:648:LEU:HA	17:1:648:LEU:HD12	1.90	0.40
17:1:844:VAL:HG11	17:1:848:GLU:HG2	2.03	0.40
17:1:1002:ASN:HD22	17:1:1002:ASN:HA	1.50	0.40
25:J:333:PHE:CB	25:J:349:TYR:CE1	3.04	0.40
27:R:137:GLU:HA	27:R:140:ILE:HG12	2.03	0.40
27:R:237:MET:CE	27:R:237:MET:N	2.75	0.40
28:T:468:CYS:HA	28:T:478:LEU:O	2.21	0.40
29:X:278:GLN:NE2	29:X:291:ASP:OD2	2.54	0.40
29:X:346:PRO:C	29:X:347:GLN:HE21	2.29	0.40
30:Y:125:ASP:O	30:Y:129:ARG:HG3	2.20	0.40
42:K:13:ARG:HD3	42:K:13:ARG:HA	1.73	0.40
3:C:200:PHE:HD1	3:C:200:PHE:HA	1.80	0.40
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.56	0.40
5:E:248:SER:HB2	5:E:249:TYR:CE1	2.53	0.40
13:F:33:C:H2'	13:F:34:C:O4'	2.21	0.40
16:v:33:GLU:OE1	16:v:33:GLU:N	2.55	0.40
17:1:403:GLU:O	17:1:406:ALA:HB3	2.20	0.40
17:1:997:LEU:HD12	17:1:997:LEU:HA	1.81	0.40
19:3:133:SER:HB2	19:3:139:LYS:HG2	2.02	0.40
19:3:500:LEU:HB2	19:3:525:ARG:HH11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:673:VAL:HG12	19:3:693:TYR:HA	2.03	0.40
19:3:1129:LEU:HD23	19:3:1129:LEU:HA	1.93	0.40
27:R:114:SER:N	27:R:230:MET:HE1	2.36	0.40
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.87	0.40
1:A:767:VAL:HG21	2:B:39:C:C2	2.56	0.40
1:A:1157:ILE:HD13	1:A:1157:ILE:HA	1.92	0.40
1:A:1256:PHE:CE2	1:A:1303:LEU:HD21	2.56	0.40
1:A:1501:LEU:HD22	1:A:1753:LEU:HD11	2.02	0.40
3:C:461:LEU:HD23	3:C:461:LEU:HA	1.91	0.40
4:D:448:PRO:O	4:D:686:GLU:HA	2.21	0.40
4:D:577:LYS:O	4:D:581:SER:N	2.54	0.40
5:E:178:LEU:CD2	5:E:208:ILE:HD11	2.51	0.40
5:E:307:ARG:HB3	5:E:326:HIS:O	2.22	0.40
13:F:51:G:H4'	13:F:52:A:OP1	2.20	0.40
16:v:1:MET:CG	16:v:6:GLU:HB3	2.51	0.40
17:1:86:ALA:HB3	17:1:91:LEU:HD11	2.03	0.40
17:1:860:GLU:HG2	30:Y:26:VAL:HG11	2.03	0.40
17:1:1120:ALA:HB2	17:1:1128:VAL:HG21	2.02	0.40
25:J:228:ARG:HG3	25:J:228:ARG:HH11	1.86	0.40
29:X:329:ILE:HB	29:X:349:TYR:CE1	2.57	0.40
32:9:111:THR:HG22	32:9:112:ASN:N	2.36	0.40
39:8:110:LEU:HD23	39:8:110:LEU:HA	1.91	0.40
41:I:38:VAL:HA	42:K:42:ASN:HD21	1.86	0.40
3:C:780:CYS:SG	3:C:780:CYS:O	2.79	0.40
4:D:991:TYR:O	4:D:1090:ARG:HG2	2.22	0.40
5:E:283:ASN:OD1	5:E:283:ASN:C	2.65	0.40
10:f:5:LEU:O	11:e:49:GLY:HA3	2.22	0.40
13:F:2:U:O2'	42:K:43:PHE:CE1	2.73	0.40
19:3:981:CYS:SG	19:3:981:CYS:O	2.79	0.40
25:J:367:GLU:O	25:J:371:LEU:HG	2.21	0.40
25:J:419:PHE:CE2	25:J:435:ILE:HG21	2.56	0.40
27:R:280:ILE:CB	32:9:221:LEU:HD22	2.48	0.40
32:9:39:PHE:HB3	32:9:159:GLN:OE1	2.21	0.40
32:9:83:LEU:HD12	32:9:84:ASP:N	2.36	0.40
38:V:603:LEU:HD12	38:V:603:LEU:HA	1.79	0.40
42:K:24:PHE:HD2	42:K:61:LEU:HD11	1.86	0.40
42:K:123:MET:O	42:K:126:SER:HB3	2.20	0.40
1:A:221:ASN:OD1	1:A:222:GLY:N	2.55	0.40
1:A:686:ARG:NH1	15:H:3:G:H4'	2.37	0.40
1:A:686:ARG:HE	1:A:710:LEU:HD13	1.86	0.40
3:C:476:CYS:HB3	3:C:565:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:738:ASP:OD1	3:C:738:ASP:N	2.33	0.40
4:D:128:PRO:CG	4:D:131:ILE:HD12	2.51	0.40
17:1:157:ARG:O	17:1:161:LEU:HB2	2.22	0.40
17:1:675:MET:HB2	17:1:679:ILE:CG2	2.51	0.40
17:1:1045:ARG:NH1	40:0:24:ARG:HG3	2.35	0.40
19:3:137:LYS:O	19:3:137:LYS:CG	2.70	0.40
19:3:668:GLY:HA3	19:3:699:VAL:HG23	2.03	0.40
19:3:1058:LEU:HA	19:3:1059:PRO:HD3	1.98	0.40
25:J:433:ARG:HD2	25:J:433:ARG:HA	1.87	0.40
26:P:212:ASN:H	28:T:457:GLY:HA3	1.87	0.40
41:I:31:ARG:NH1	41:I:31:ARG:CG	2.80	0.40
42:K:149:SER:HA	42:K:160:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2213/2335 (95%)	2146 (97%)	66 (3%)	1 (0%)	100	100
3	C	900/972 (93%)	862 (96%)	38 (4%)	0	100	100
4	D	1799/2136 (84%)	1710 (95%)	84 (5%)	5 (0%)	36	65
5	E	297/357 (83%)	278 (94%)	19 (6%)	0	100	100
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
6	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
7	b	80/240 (33%)	78 (98%)	2 (2%)	0	100	100
7	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
8	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
8	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
9	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
10	f	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
10	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
11	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
12	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
16	v	115/230 (50%)	113 (98%)	2 (2%)	0	100	100
17	1	977/1304 (75%)	961 (98%)	16 (2%)	0	100	100
18	2	206/895 (23%)	198 (96%)	8 (4%)	0	100	100
19	3	1184/1217 (97%)	1136 (96%)	48 (4%)	0	100	100
20	4	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
21	5	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
22	6	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
23	7	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
24	L	99/802 (12%)	93 (94%)	6 (6%)	0	100	100
25	J	483/848 (57%)	447 (92%)	36 (8%)	0	100	100
26	P	42/229 (18%)	37 (88%)	5 (12%)	0	100	100
27	R	229/536 (43%)	219 (96%)	10 (4%)	0	100	100
28	T	318/514 (62%)	310 (98%)	8 (2%)	0	100	100
29	X	154/396 (39%)	137 (89%)	16 (10%)	1 (1%)	21	51
30	Y	138/322 (43%)	135 (98%)	3 (2%)	0	100	100
31	Z	138/619 (22%)	137 (99%)	1 (1%)	0	100	100
32	9	401/520 (77%)	382 (95%)	18 (4%)	1 (0%)	43	72
33	z	175/472 (37%)	169 (97%)	6 (3%)	0	100	100
34	x	575/1041 (55%)	554 (96%)	21 (4%)	0	100	100
35	y	11/476 (2%)	11 (100%)	0	0	100	100
36	M	185/343 (54%)	172 (93%)	13 (7%)	0	100	100
37	U	24/2752 (1%)	24 (100%)	0	0	100	100
38	V	464/908 (51%)	457 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	8	124/904 (14%)	124 (100%)	0	0	100	100
40	0	98/101 (97%)	98 (100%)	0	0	100	100
41	I	124/367 (34%)	120 (97%)	4 (3%)	0	100	100
42	K	186/198 (94%)	183 (98%)	2 (1%)	1 (0%)	24	54
All	All	13111/24253 (54%)	12617 (96%)	485 (4%)	9 (0%)	49	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1584	ILE
4	D	1864	GLU
1	A	1092	ILE
29	X	263	PRO
42	K	127	PRO
4	D	1859	PRO
32	9	348	LYS
4	D	745	LYS
4	D	1583	ASP

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	
1	A	1979/2108 (94%)	1915 (97%)	64 (3%)	34	68
3	C	798/866 (92%)	781 (98%)	17 (2%)	47	77
4	D	76/1908 (4%)	56 (74%)	20 (26%)	0	2
5	E	255/300 (85%)	243 (95%)	12 (5%)	23	56
16	v	104/199 (52%)	100 (96%)	4 (4%)	29	64
17	1	854/1103 (77%)	809 (95%)	45 (5%)	20	52
18	2	163/776 (21%)	157 (96%)	6 (4%)	30	64
19	3	1031/1050 (98%)	997 (97%)	34 (3%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	5	97/109 (89%)	96 (99%)	1 (1%)	68	89
22	6	90/95 (95%)	88 (98%)	2 (2%)	45	77
23	7	72/77 (94%)	72 (100%)	0	100	100
24	L	87/709 (12%)	85 (98%)	2 (2%)	44	76
25	J	203/751 (27%)	194 (96%)	9 (4%)	25	59
26	P	42/203 (21%)	42 (100%)	0	100	100
27	R	206/459 (45%)	196 (95%)	10 (5%)	22	54
28	T	273/441 (62%)	268 (98%)	5 (2%)	51	80
29	X	134/349 (38%)	128 (96%)	6 (4%)	24	58
30	Y	117/291 (40%)	113 (97%)	4 (3%)	32	66
31	Z	110/545 (20%)	110 (100%)	0	100	100
32	9	195/456 (43%)	190 (97%)	5 (3%)	40	73
33	z	152/416 (36%)	152 (100%)	0	100	100
34	x	14/897 (2%)	14 (100%)	0	100	100
35	y	11/397 (3%)	11 (100%)	0	100	100
36	M	168/294 (57%)	165 (98%)	3 (2%)	51	80
37	U	21/2432 (1%)	20 (95%)	1 (5%)	23	55
38	V	193/838 (23%)	187 (97%)	6 (3%)	35	69
39	8	111/831 (13%)	111 (100%)	0	100	100
40	0	86/87 (99%)	82 (95%)	4 (5%)	23	56
41	I	112/326 (34%)	108 (96%)	4 (4%)	31	65
42	K	119/171 (70%)	102 (86%)	17 (14%)	3	11
All	All	7873/19484 (40%)	7592 (96%)	281 (4%)	32	65

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	203	VAL
1	A	204	LEU
1	A	211	GLN
1	A	227	ARG
1	A	258	PHE
1	A	327	VAL

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Mol	Chain	Res	Type
1	A	419	ARG
1	A	420	ARG
1	A	422	LEU
1	A	426	LEU
1	A	546	LEU
1	A	606	LYS
1	A	635	ARG
1	A	658	ARG
1	A	683	LEU
1	A	779	LEU
1	A	818	GLU
1	A	840	ILE
1	A	873	ASN
1	A	894	VAL
1	A	977	LEU
1	A	978	GLU
1	A	1017	ILE
1	A	1018	ASN
1	A	1022	MET
1	A	1094	ARG
1	A	1230	LEU
1	A	1231	ARG
1	A	1370	ARG
1	A	1403	LEU
1	A	1419	ILE
1	A	1425	LYS
1	A	1499	GLU
1	A	1526	LEU
1	A	1553	VAL
1	A	1630	LEU
1	A	1639	VAL
1	A	1693	SER
1	A	1745	GLU
1	A	1753	LEU
1	A	1762	TYR
1	A	1764	SER
1	A	1840	LYS
1	A	1883	VAL
1	A	1889	LEU
1	A	1891	LEU
1	A	1919	LEU
1	A	1921	ASP

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Mol	Chain	Res	Type
1	A	1959	THR
1	A	2073	TRP
1	A	2074	ARG
1	A	2087	THR
1	A	2139	VAL
1	A	2193	VAL
1	A	2194	THR
1	A	2226	THR
1	A	2254	SER
1	A	2258	ARG
1	A	2259	VAL
1	A	2268	LEU
1	A	2273	VAL
1	A	2303	GLU
1	A	2333	LEU
3	C	57	VAL
3	C	80	ILE
3	C	148	CYS
3	C	152	GLN
3	C	153	THR
3	C	307	VAL
3	C	308	CYS
3	C	527	VAL
3	C	543	ARG
3	C	551	LEU
3	C	683	ASN
3	C	714	LEU
3	C	738	ASP
3	C	767	VAL
3	C	788	LYS
3	C	878	ILE
3	C	934	MET
4	D	103	LYS
4	D	108	GLU
4	D	110	ARG
4	D	114	GLU
4	D	126	ASP
4	D	142	VAL
4	D	144	LYS
4	D	146	GLU
4	D	148	LEU
4	D	149	ARG

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Mol	Chain	Res	Type
4	D	153	ARG
4	D	154	ARG
4	D	155	LYS
4	D	157	ILE
4	D	161	LEU
4	D	167	THR
4	D	168	ARG
4	D	171	VAL
4	D	992	TYR
4	D	1090	ARG
5	E	62	LEU
5	E	74	PHE
5	E	102	TYR
5	E	150	HIS
5	E	152	SER
5	E	156	SER
5	E	178	LEU
5	E	194	TYR
5	E	215	ASN
5	E	229	TYR
5	E	248	SER
5	E	289	LEU
16	v	1	MET
16	v	5	ARG
16	v	46	ILE
16	v	219	SER
17	1	120	LYS
17	1	412	TYR
17	1	479	LEU
17	1	487	LEU
17	1	531	LEU
17	1	562	LYS
17	1	563	LEU
17	1	564	ASP
17	1	614	ARG
17	1	624	VAL
17	1	635	VAL
17	1	651	VAL
17	1	674	LEU
17	1	675	MET
17	1	677	CYS
17	1	680	LEU

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Mol	Chain	Res	Type
17	1	721	ILE
17	1	872	ILE
17	1	909	VAL
17	1	936	VAL
17	1	976	VAL
17	1	997	LEU
17	1	1002	ASN
17	1	1003	VAL
17	1	1024	LEU
17	1	1038	LEU
17	1	1050	VAL
17	1	1058	ILE
17	1	1061	GLU
17	1	1112	THR
17	1	1113	THR
17	1	1119	VAL
17	1	1127	THR
17	1	1128	VAL
17	1	1180	ARG
17	1	1182	LEU
17	1	1184	HIS
17	1	1226	VAL
17	1	1227	ILE
17	1	1239	VAL
17	1	1260	LYS
17	1	1261	VAL
17	1	1264	VAL
17	1	1277	GLN
17	1	1303	ILE
18	2	498	VAL
18	2	577	LYS
18	2	579	GLN
18	2	587	HIS
18	2	590	LEU
18	2	599	THR
19	3	47	THR
19	3	86	ARG
19	3	135	ILE
19	3	136	GLU
19	3	137	LYS
19	3	138	GLN
19	3	171	VAL

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Mol	Chain	Res	Type
19	3	184	CYS
19	3	187	MET
19	3	295	THR
19	3	319	GLU
19	3	321	MET
19	3	322	VAL
19	3	425	VAL
19	3	429	ARG
19	3	607	VAL
19	3	609	LEU
19	3	610	VAL
19	3	612	ASN
19	3	614	VAL
19	3	615	ARG
19	3	686	LEU
19	3	689	THR
19	3	690	ARG
19	3	691	THR
19	3	773	VAL
19	3	943	THR
19	3	948	VAL
19	3	982	GLU
19	3	1007	GLU
19	3	1057	ARG
19	3	1064	ASP
19	3	1165	SER
19	3	1214	ARG
21	5	85	ARG
22	6	25	LYS
22	6	95	LYS
24	L	54	LEU
24	L	77	LEU
25	J	235	ILE
25	J	236	ARG
25	J	242	ILE
25	J	245	TRP
25	J	247	LYS
25	J	337	MET
25	J	338	GLU
25	J	359	VAL
25	J	360	ASP
27	R	237	MET

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Mol	Chain	Res	Type
27	R	323	LYS
27	R	384	GLU
27	R	386	ARG
27	R	388	ILE
27	R	389	SER
27	R	406	GLN
27	R	410	ARG
27	R	427	ASP
27	R	447	ILE
28	T	220	VAL
28	T	325	THR
28	T	384	HIS
28	T	418	THR
28	T	456	PRO
29	X	239	PHE
29	X	242	VAL
29	X	264	PHE
29	X	269	VAL
29	X	270	LEU
29	X	348	ARG
30	Y	13	LEU
30	Y	62	ILE
30	Y	68	VAL
30	Y	116	ARG
32	9	3	LYS
32	9	35	ARG
32	9	220	ILE
32	9	224	THR
32	9	245	LYS
36	M	103	THR
36	M	157	ASN
36	M	226	TYR
37	U	20	GLN
38	V	461	LEU
38	V	467	LEU
38	V	469	PHE
38	V	471	GLU
38	V	477	LEU
38	V	536	ILE
40	0	14	ILE
40	0	74	GLN
40	0	98	GLN

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Mol	Chain	Res	Type
40	0	100	SER
41	I	31	ARG
41	I	37	LYS
41	I	105	ARG
41	I	139	LYS
42	K	13	ARG
42	K	54	ARG
42	K	71	GLU
42	K	73	LEU
42	K	74	VAL
42	K	75	GLU
42	K	84	LEU
42	K	91	LYS
42	K	94	ILE
42	K	123	MET
42	K	136	LEU
42	K	139	THR
42	K	142	VAL
42	K	143	GLN
42	K	145	MET
42	K	147	ARG
42	K	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	483	GLN
1	A	675	GLN
1	A	704	ASN
1	A	1042	GLN
1	A	1373	GLN
1	A	1424	GLN
1	A	1487	HIS
1	A	1615	HIS
1	A	1995	ASN
1	A	2089	HIS
1	A	2123	GLN
1	A	2155	GLN
1	A	2291	ASN
3	C	139	HIS
3	C	175	GLN

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Mol	Chain	Res	Type
3	C	437	HIS
3	C	477	HIS
3	C	683	ASN
3	C	706	GLN
3	C	807	GLN
4	D	127	GLN
5	E	65	HIS
5	E	101	ASN
5	E	108	HIS
5	E	253	ASN
16	v	214	ASN
17	1	92	ASN
17	1	473	GLN
17	1	698	GLN
17	1	817	HIS
17	1	1026	ASN
17	1	1225	HIS
17	1	1252	GLN
17	1	1283	HIS
17	1	1293	ASN
18	2	490	HIS
18	2	587	HIS
19	3	21	ASN
19	3	51	HIS
19	3	206	GLN
19	3	219	HIS
19	3	304	GLN
19	3	394	ASN
24	L	99	HIS
25	J	347	HIS
27	R	133	GLN
27	R	157	GLN
27	R	329	GLN
27	R	470	ASN
28	T	283	HIS
28	T	285	HIS
28	T	324	HIS
29	X	307	GLN
29	X	347	GLN
30	Y	66	ASN
32	9	140	ASN
33	z	39	ASN

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Mol	Chain	Res	Type
33	z	64	GLN
37	U	3	ASN
38	V	445	HIS
38	V	629	ASN
39	8	19	ASN
40	0	98	GLN
41	I	51	GLN
42	K	18	GLN
42	K	49	ASN
42	K	70	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	58/124 (46%)	14 (24%)	3 (5%)
14	G	62/142 (43%)	22 (35%)	5 (8%)
15	H	61/150 (40%)	14 (22%)	0
2	B	87/117 (74%)	21 (24%)	2 (2%)
All	All	268/533 (50%)	71 (26%)	10 (3%)

All (71) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	21	A
2	B	22	U
2	B	24	G
2	B	25	C
2	B	28	A
2	B	35	U
2	B	39	C
2	B	40	U
2	B	45	C
2	B	71	C
2	B	86	C
2	B	88	A
2	B	89	U
2	B	90	U
2	B	94	U
2	B	95	G
2	B	97	G

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Mol	Chain	Res	Type
2	B	98	G
2	B	115	C
2	B	116	U
13	F	5	U
13	F	6	G
13	F	15	G
13	F	18	A
13	F	24	U
13	F	25	U
13	F	27	G
13	F	32	C
13	F	33	C
13	F	39	A
13	F	46	U
13	F	47	G
13	F	50	A
13	F	52	A
14	G	-10	C
14	G	-9	G
14	G	-5	U
14	G	-3	C
14	G	1	A
14	G	3	A
14	G	15	C
14	G	17	U
14	G	19	U
14	G	196	A
14	G	203	A
14	G	207	A
14	G	208	U
14	G	210	G
14	G	211	U
14	G	214	C
14	G	216	U
14	G	217	U
14	G	218	U
14	G	219	U
14	G	220	U
14	G	222	U
15	H	2	U
15	H	3	G
15	H	8	A

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Mol	Chain	Res	Type
15	H	10	A
15	H	13	U
15	H	14	A
15	H	18	G
15	H	29	A
15	H	31	C
15	H	32	G
15	H	39	G
15	H	44	C
15	H	45	G
15	H	83	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C
2	B	96	A
13	F	23	G
13	F	31	U
13	F	51	G
14	G	-11	U
14	G	206	C
14	G	213	C
14	G	217	U
14	G	219	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z > 2$
19	TPO	3	613	19	8,10,11	0.91	0	10,14,16	1.77	2 (20%)
17	SEP	1	129	17	8,9,10	1.11	1 (12%)	7,12,14	1.51	2 (28%)

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
19	TPO	3	613	19	-	1/9/11/13	-
17	SEP	1	129	17	-	5/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	129	SEP	P-O1P	2.22	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	613	TPO	P-OG1-CB	-4.97	109.83	123.33
19	3	613	TPO	O-C-CA	-2.26	118.95	124.77
17	1	129	SEP	O3P-P-OG	2.24	112.52	106.67
17	1	129	SEP	OG-CB-CA	2.09	110.18	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	129	SEP	N-CA-CB-OG
17	1	129	SEP	C-CA-CB-OG
17	1	129	SEP	CB-OG-P-O1P
17	1	129	SEP	CB-OG-P-O2P
17	1	129	SEP	CB-OG-P-O3P
19	3	613	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	613	TPO	1	0
17	1	129	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 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$
43	IHP	A	3000	-	36,36,36	1.16	3 (8%)	60,60,60	1.14	4 (6%)
47	G5J	F	207	13	35,35,35	1.45	4 (11%)	44,55,55	0.94	2 (4%)
44	GTP	C	1500	45	33,34,34	2.08	12 (36%)	50,54,54	1.96	12 (24%)

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
43	IHP	A	3000	-	-	1/30/54/54	0/1/1/1
47	G5J	F	207	13	-	6/25/41/41	0/3/3/3
44	GTP	C	1500	45	-	4/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	207	G5J	C5-C4	5.20	1.46	1.38
44	C	1500	GTP	PB-O3A	-4.17	1.55	1.59
47	F	207	G5J	C4-N9	-3.78	1.33	1.37
44	C	1500	GTP	C5-N7	-3.57	1.31	1.39
44	C	1500	GTP	PA-O3A	-3.55	1.55	1.59
44	C	1500	GTP	PB-O3B	-3.18	1.56	1.59
44	C	1500	GTP	C5-C6	-2.69	1.34	1.44
44	C	1500	GTP	O4'-C4'	-2.60	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	1500	GTP	C6-N1	-2.47	1.34	1.38
44	C	1500	GTP	PG-O2G	-2.44	1.45	1.54
44	C	1500	GTP	PG-O3G	-2.41	1.45	1.54
47	F	207	G5J	C5-N7	-2.28	1.34	1.39
44	C	1500	GTP	C2'-C3'	-2.22	1.47	1.53
43	A	3000	IHP	P4-O34	-2.13	1.46	1.54
43	A	3000	IHP	P5-O45	-2.11	1.47	1.54
47	F	207	G5J	C4-N3	-2.10	1.33	1.37
44	C	1500	GTP	PB-O2B	-2.08	1.45	1.55
43	A	3000	IHP	P1-O31	-2.07	1.47	1.54
44	C	1500	GTP	O3'-C3'	-2.05	1.37	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	1500	GTP	C5-C4-N3	-5.45	119.71	128.39
44	C	1500	GTP	C2-N3-C4	4.78	120.53	112.30
44	C	1500	GTP	C2-N1-C6	-4.36	117.20	125.11
43	A	3000	IHP	C5-C6-C1	-3.74	102.23	110.43
44	C	1500	GTP	O2B-PB-O3B	3.54	116.83	107.27
44	C	1500	GTP	C5-C6-N1	3.46	122.07	113.25
44	C	1500	GTP	N9-C8-N7	-3.22	107.42	113.40
43	A	3000	IHP	C6-C1-C2	-3.22	103.37	110.43
44	C	1500	GTP	O3'-C3'-C2'	-3.03	102.10	111.82
44	C	1500	GTP	N9-C4-N3	3.03	132.01	125.95
44	C	1500	GTP	O6-C6-C5	-2.91	118.84	126.53
43	A	3000	IHP	P1-O11-C1	-2.79	115.98	123.43
43	A	3000	IHP	O14-C4-C5	-2.73	102.96	108.76
44	C	1500	GTP	O2A-PA-O3A	2.72	114.62	107.27
44	C	1500	GTP	C8-N7-C5	2.69	109.05	104.26
47	F	207	G5J	C4-C5-N7	-2.23	106.36	109.26
44	C	1500	GTP	O3'-C3'-C4'	-2.14	104.95	111.08
47	F	207	G5J	C8-N9-C4	2.06	108.41	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	O4'-C4'-C5'-O5'
47	F	207	G5J	C5'-O5'-PA-O3A
47	F	207	G5J	O4'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'

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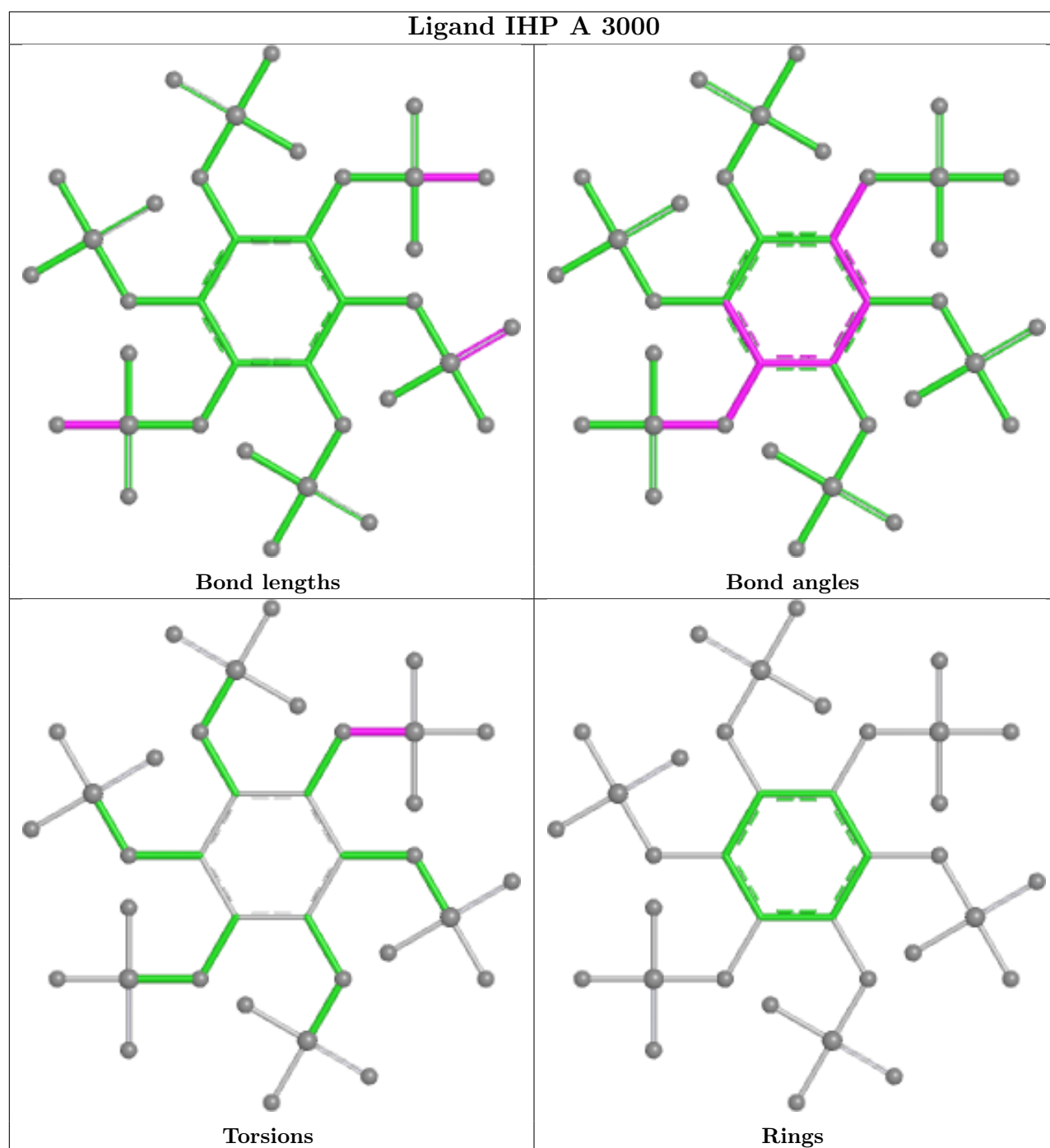
Mol	Chain	Res	Type	Atoms
47	F	207	G5J	C3'-C4'-C5'-O5'
47	F	207	G5J	C3G-O3G-PG-O1G
44	C	1500	GTP	PG-O3B-PB-O1B
47	F	207	G5J	C5'-O5'-PA-O1A
47	F	207	G5J	C3G-O3G-PG-O2G
44	C	1500	GTP	PG-O3B-PB-O2B
43	A	3000	IHP	C4-O14-P4-O44

There are no ring outliers.

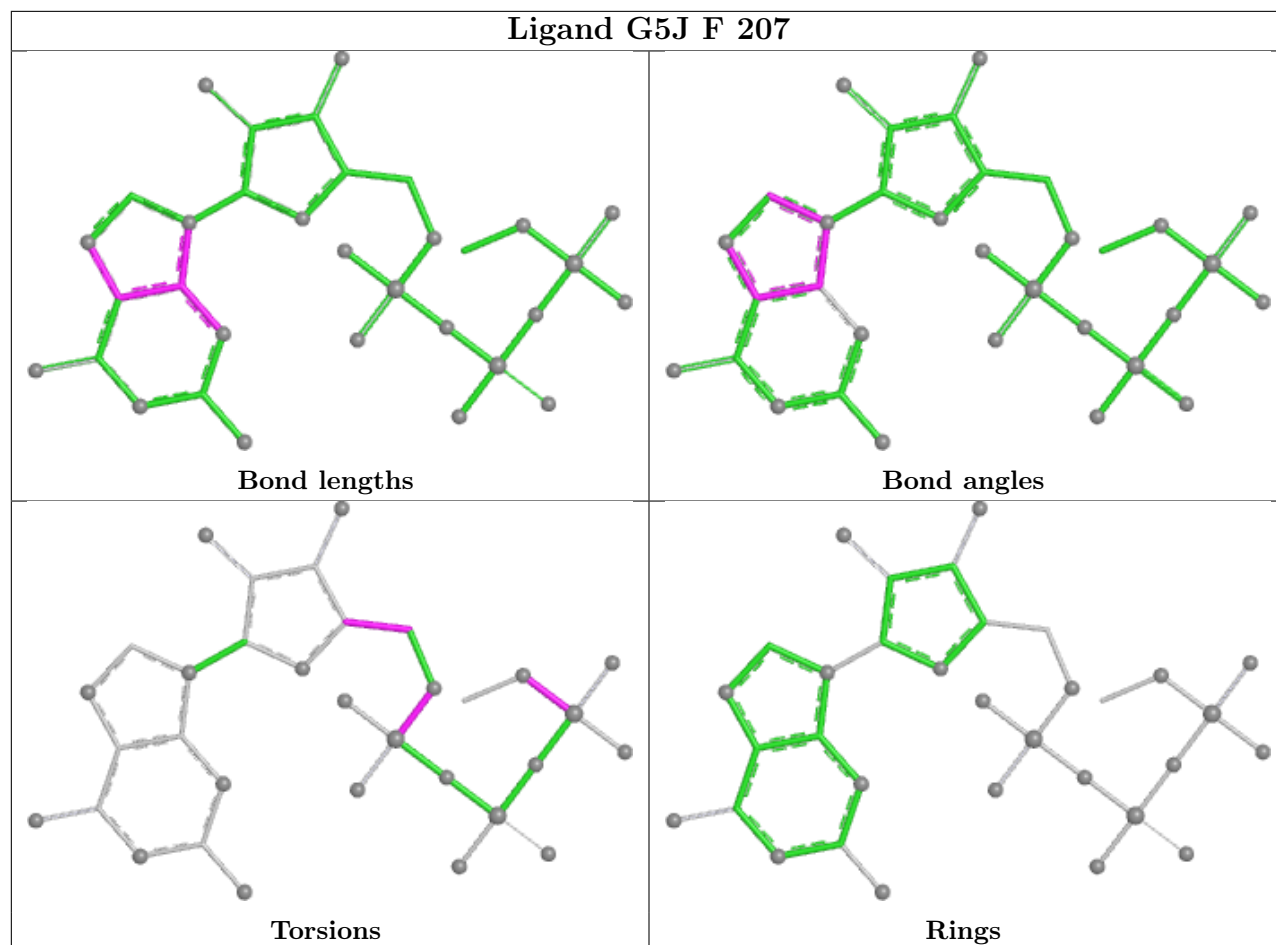
2 monomers are involved in 6 short contacts:

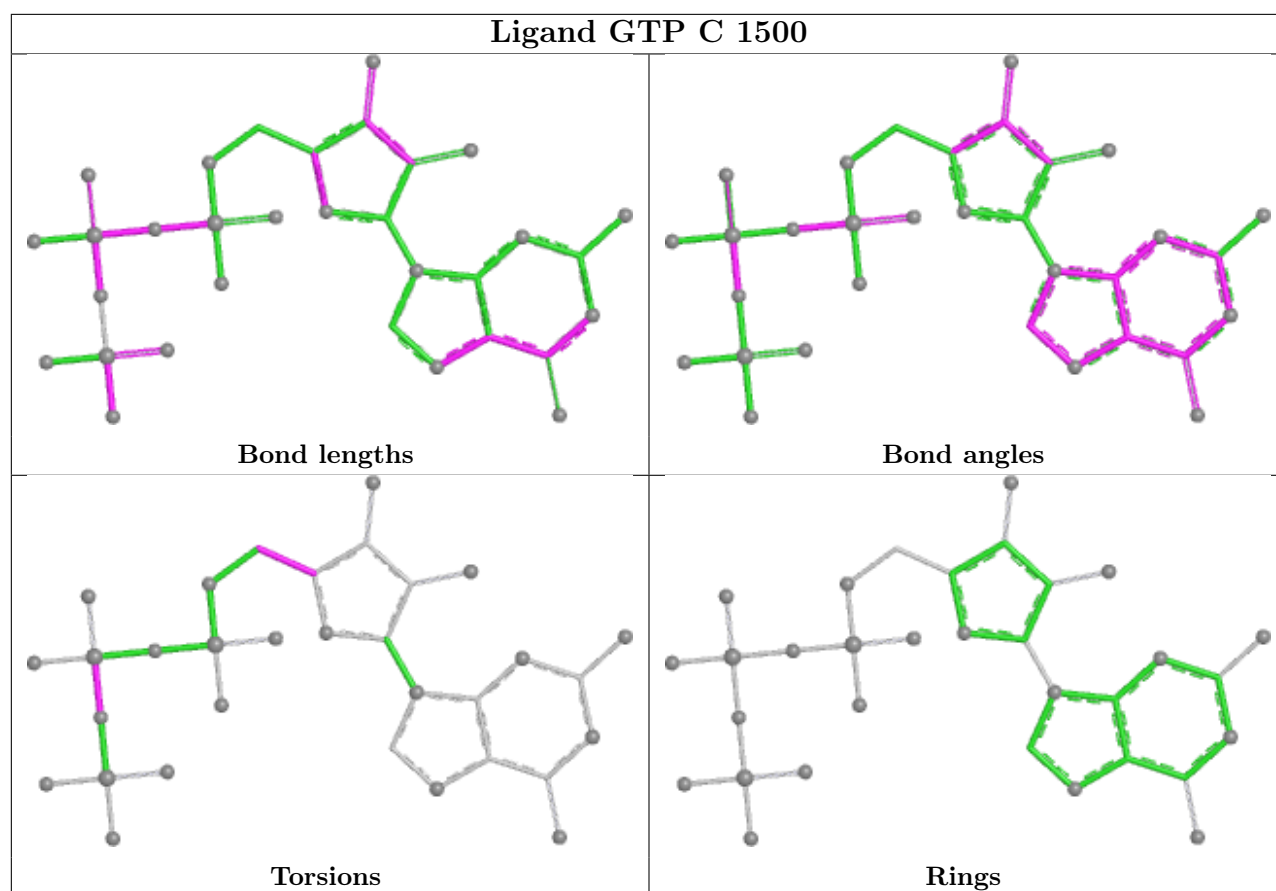
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	F	207	G5J	3	0
44	C	1500	GTP	3	0

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 G5J F 207





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

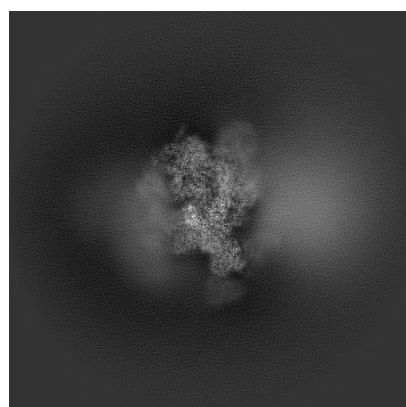
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30875. These allow visual inspection of the internal detail of the map and identification of artifacts.

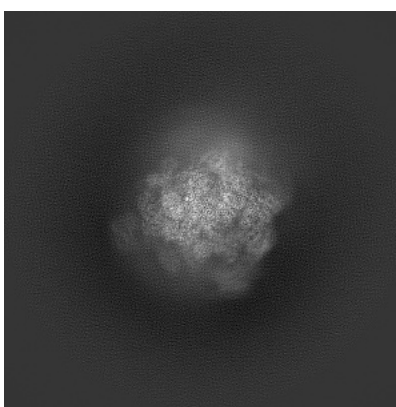
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

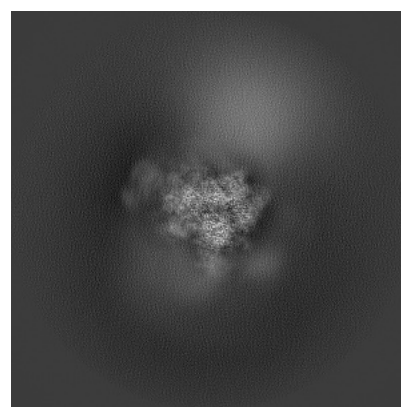
6.1.1 Primary map



X



Y

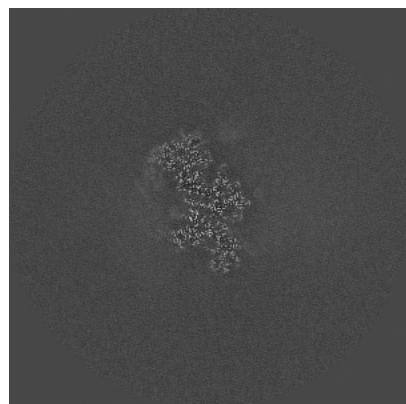


Z

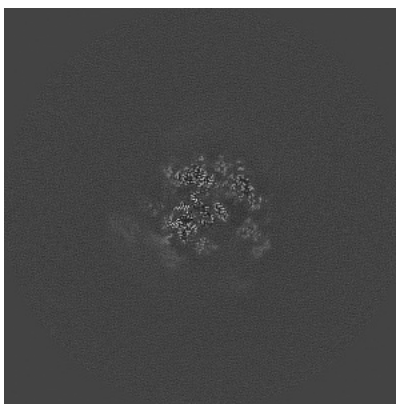
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

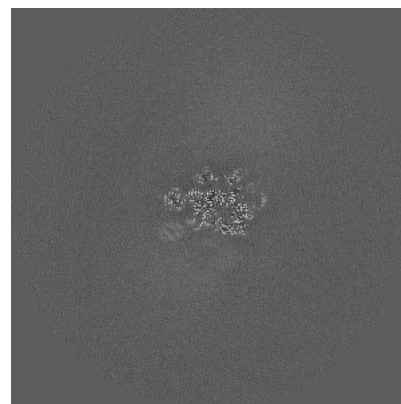
6.2.1 Primary map



X Index: 300



Y Index: 300

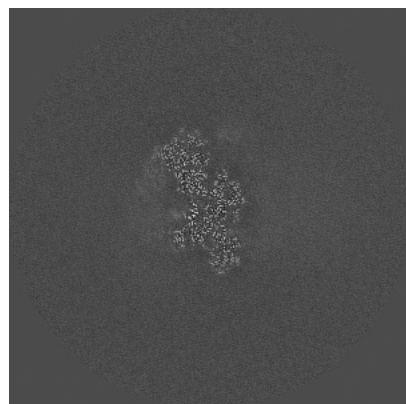


Z Index: 300

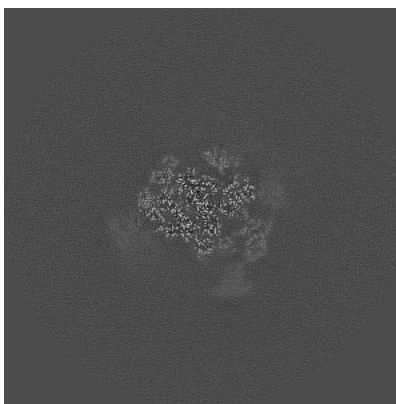
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 304



Y Index: 316

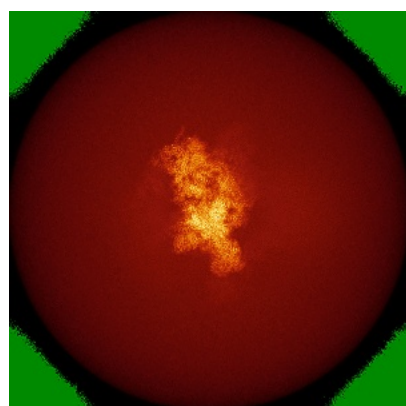


Z Index: 284

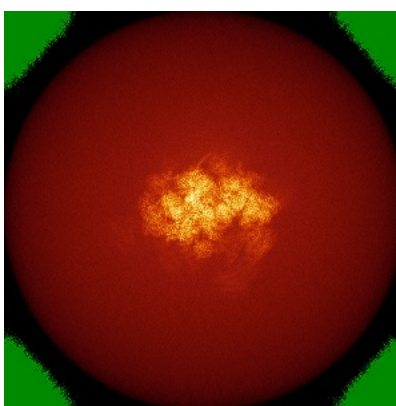
The images above show the largest variance slices of the map in three orthogonal directions.

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

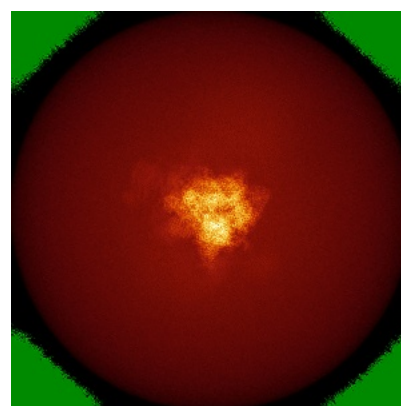
6.4.1 Primary map



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

This section was not generated.

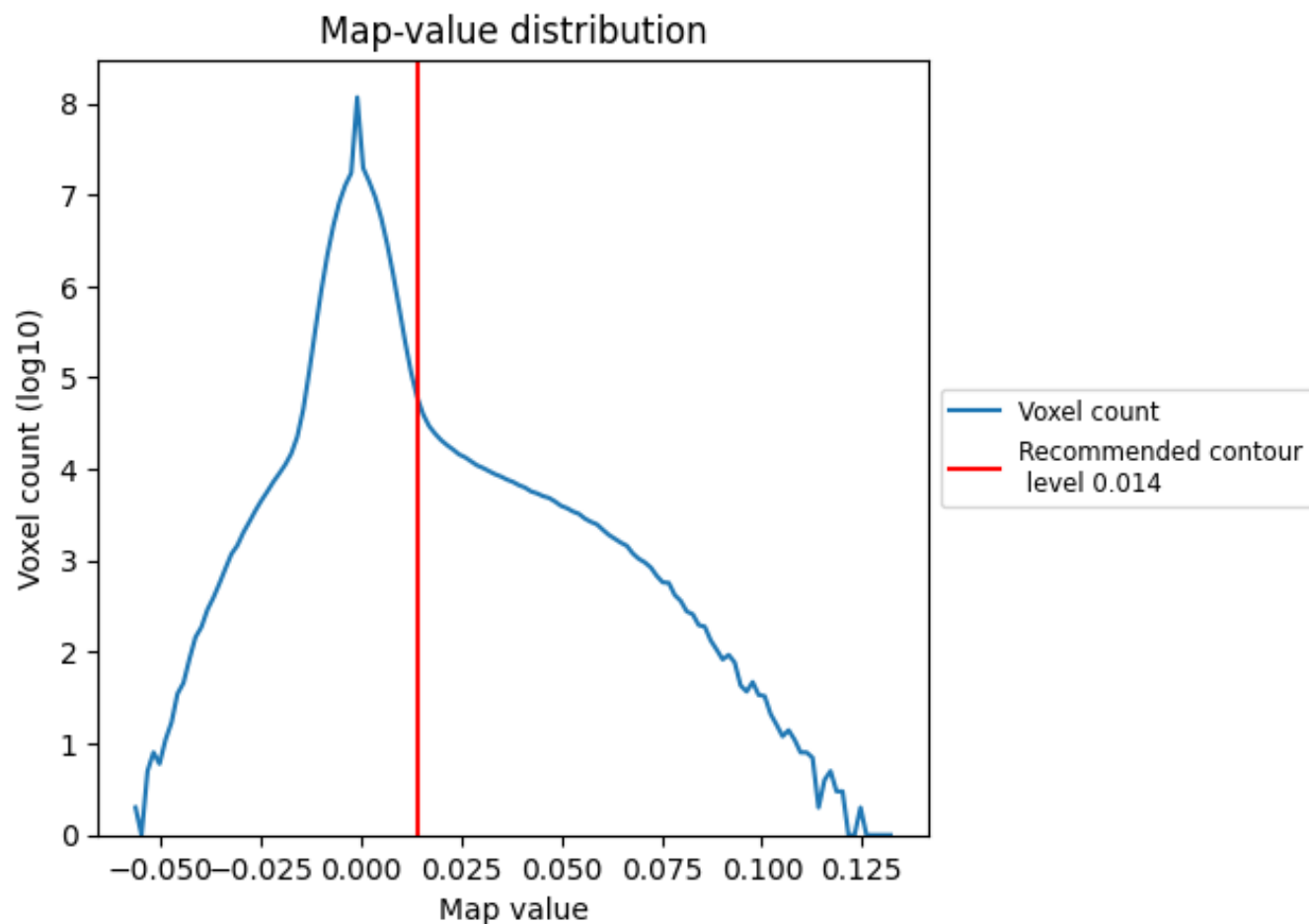
6.6 Mask visualisation

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

7 Map analysis [i](#)

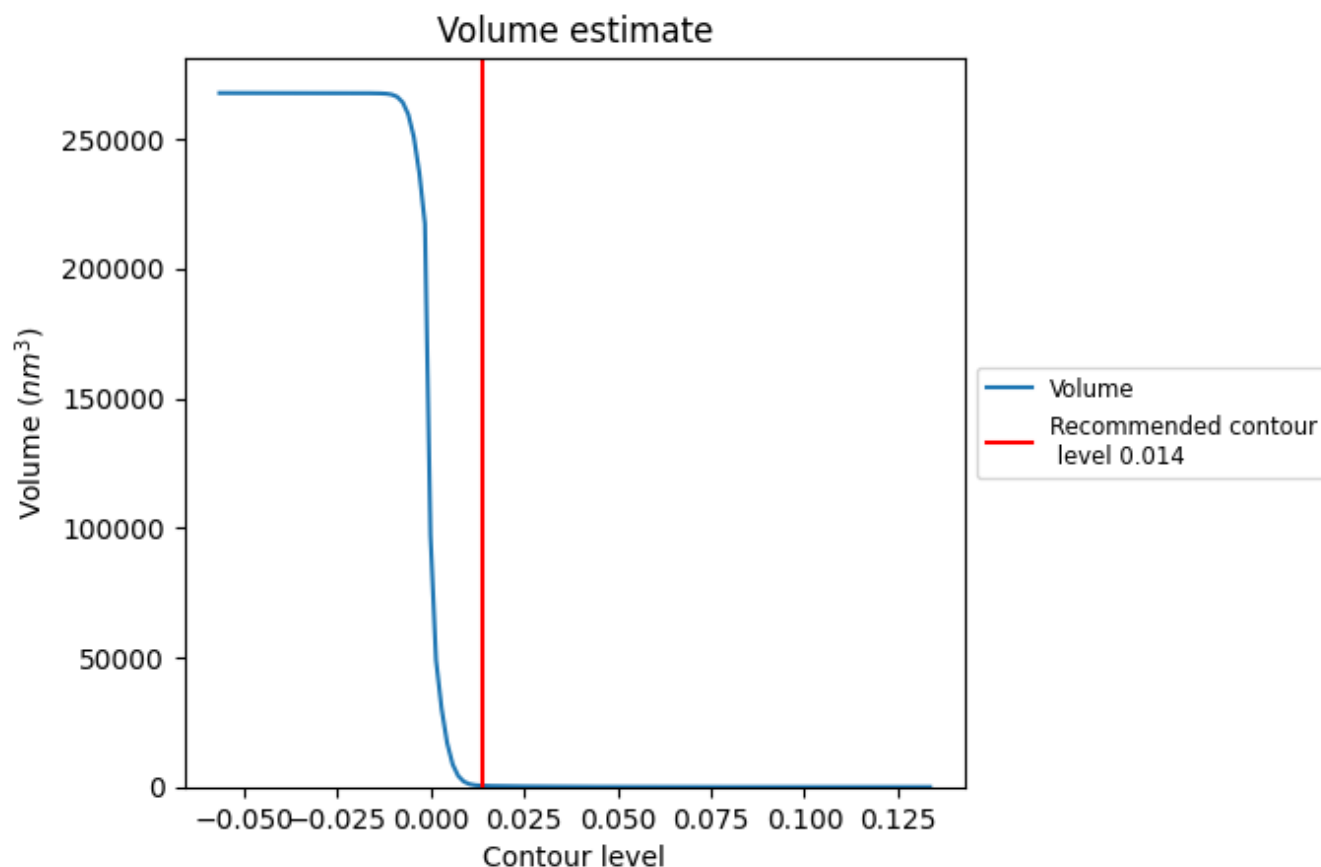
This section contains the results of statistical analysis of the map.

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.

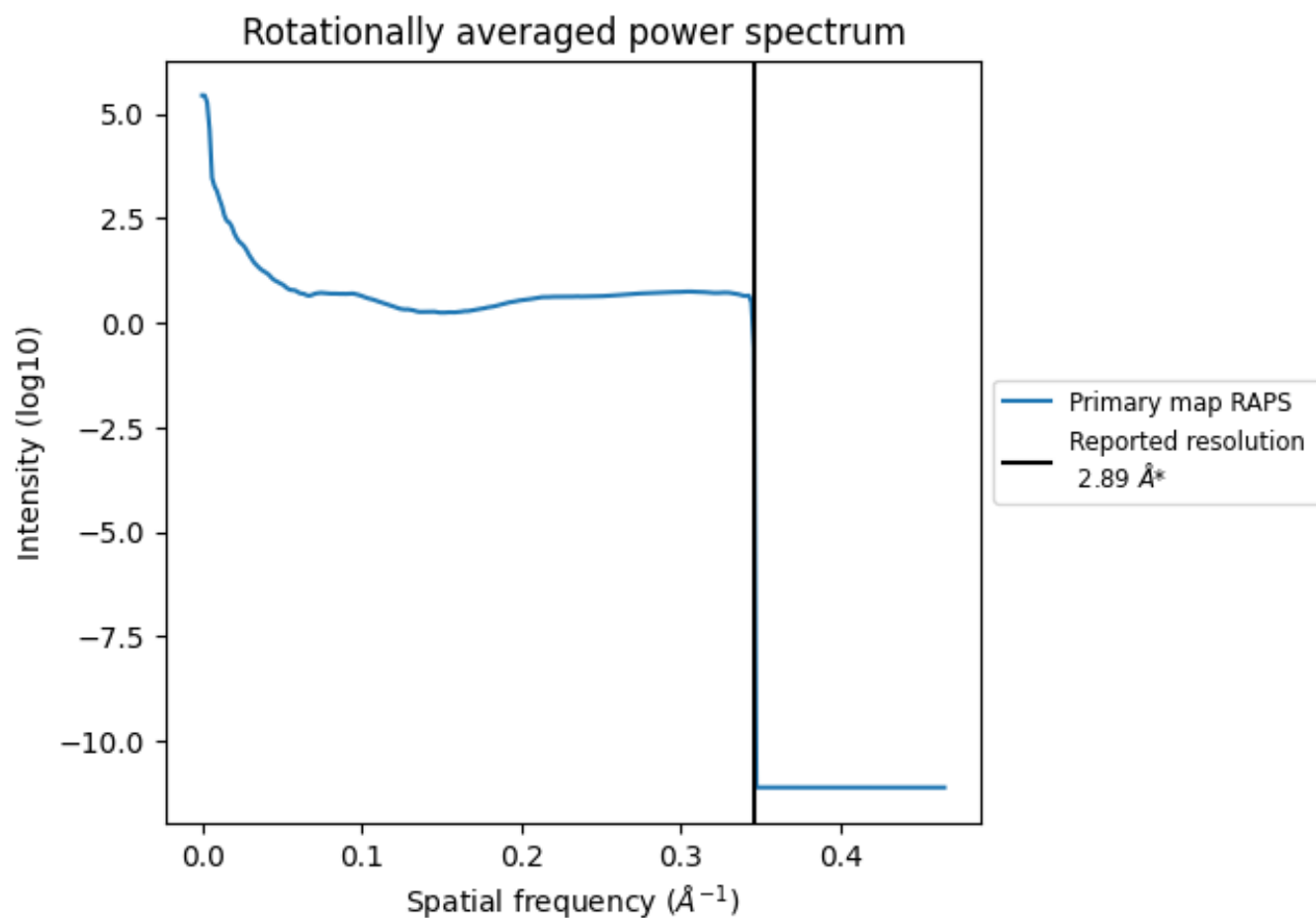
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 486 nm^3 ; this corresponds to an approximate mass of 439 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 0.346 Å⁻¹

8 Fourier-Shell correlation

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

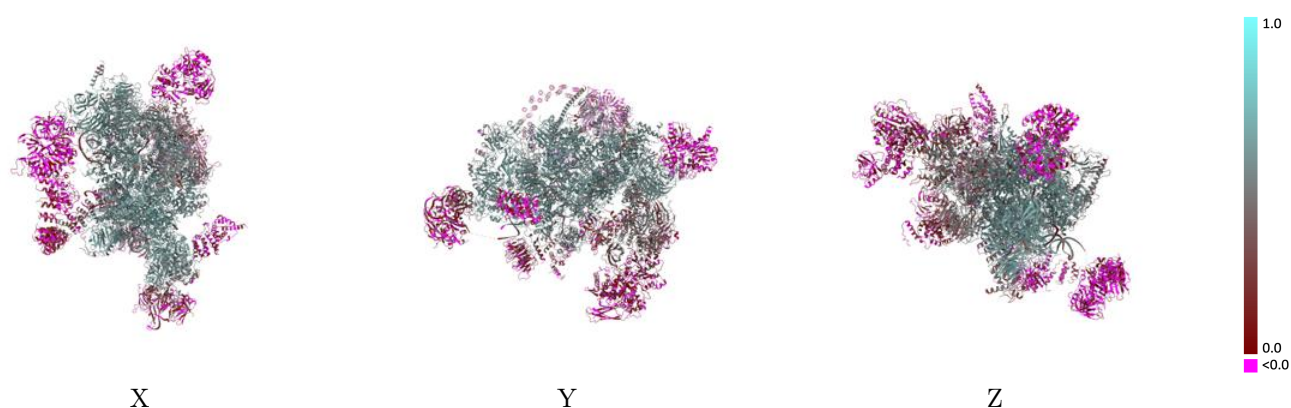
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30875 and PDB model 7DVQ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

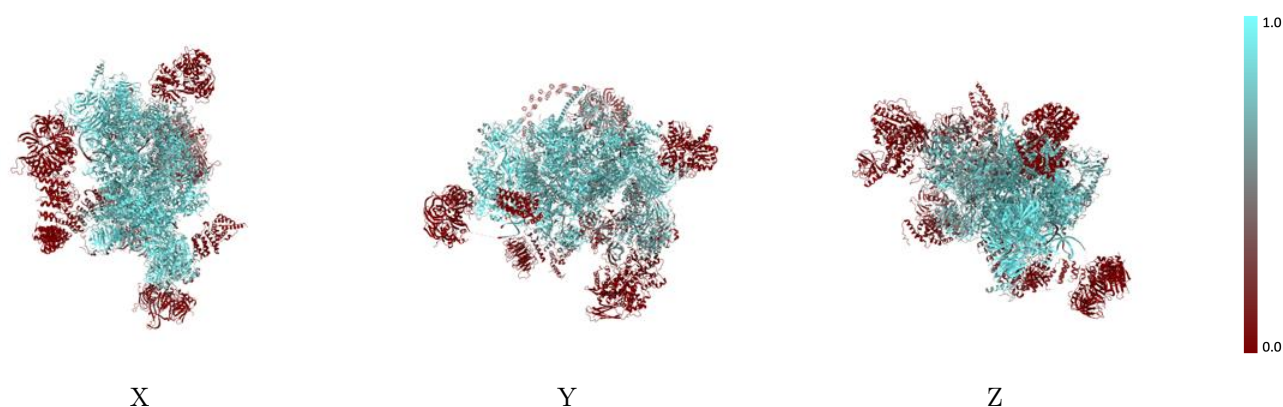
This section was not generated.

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



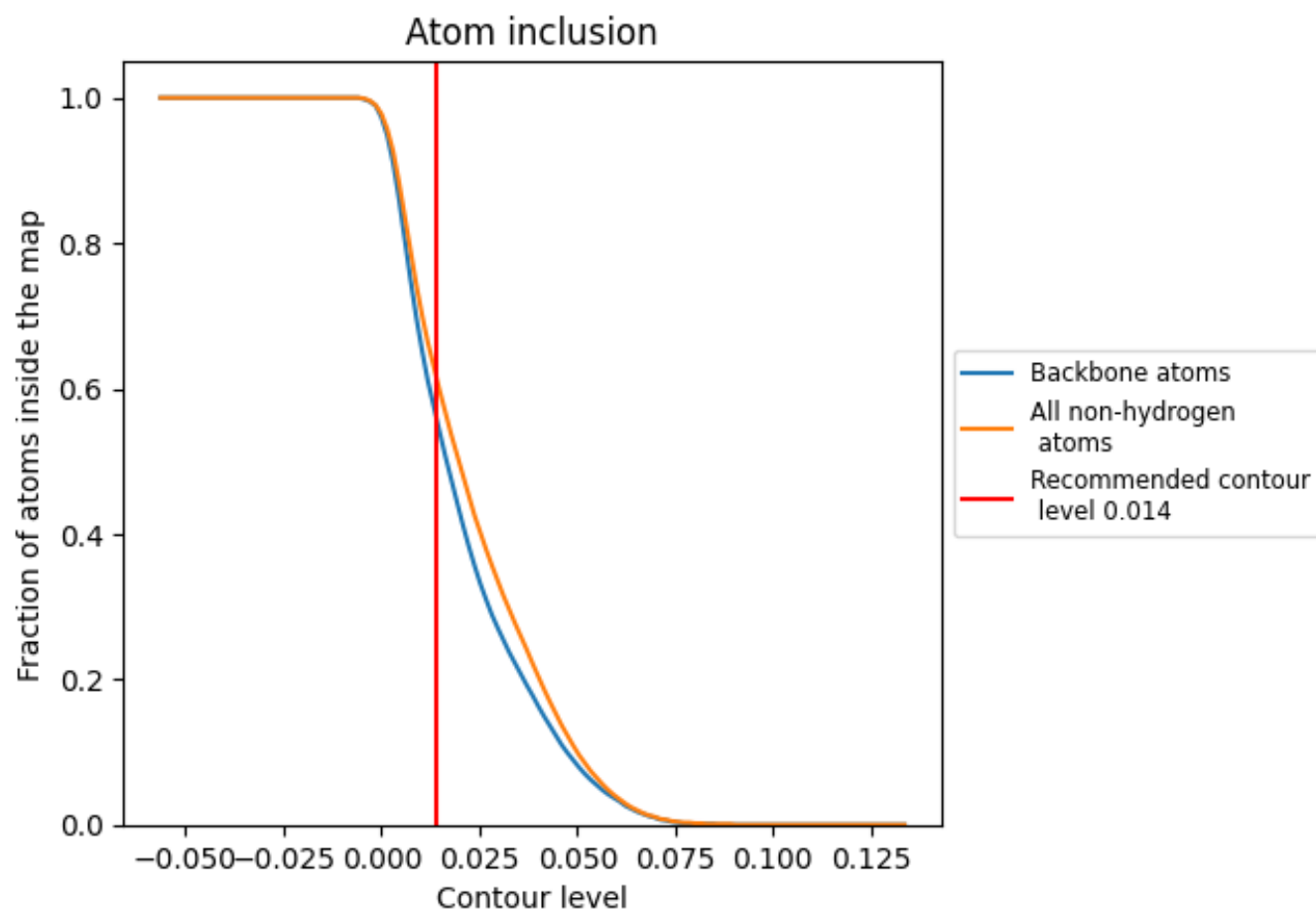
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 62% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.4320
0	 0.8640	 0.6050
1	 0.8840	 0.5900
2	 0.7180	 0.5030
3	 0.8240	 0.5400
4	 0.0500	 0.0180
5	 0.7480	 0.5010
6	 0.9240	 0.6120
7	 0.8850	 0.5890
8	 0.8130	 0.5490
9	 0.5000	 0.3510
A	 0.8240	 0.5630
B	 0.6310	 0.4010
C	 0.8440	 0.5630
D	 0.3160	 0.2360
E	 0.0330	 0.1220
F	 0.7790	 0.4750
G	 0.7180	 0.4570
H	 0.6700	 0.4050
I	 0.4980	 0.3360
J	 0.0750	 0.2170
K	 0.1660	 0.1400
L	 0.8980	 0.5950
M	 0.6270	 0.4630
P	 0.7410	 0.5350
R	 0.6330	 0.5000
T	 0.9430	 0.6110
U	 0.9250	 0.6080
V	 0.4990	 0.3300
X	 0.6770	 0.4420
Y	 0.8180	 0.5610
Z	 0.7390	 0.5420
a	 0.0880	 0.2650
b	 0.0320	 0.1610
c	 0.0200	 0.0820



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Chain	Atom inclusion	Q-score
d	 0.0150	 0.0700
e	 0.0080	 0.0930
f	 0.0050	 0.0620
g	 0.0140	 0.1750
h	 0.0000	 -0.0340
i	 0.0020	 -0.0230
j	 0.0000	 0.0510
k	 0.0020	 0.0090
l	 0.0030	 -0.0030
m	 0.0030	 0.0080
n	 0.0030	 -0.0330
v	 0.8140	 0.5130
x	 0.0320	 0.0370
y	 0.3030	 0.2890
z	 0.8920	 0.5800