



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 7YEV / pdb_00007yev
EMDB ID : EMD-33778
Title : In situ structure of polymerase complex of mammalian reovirus in the pre-elongation state
Authors : Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.
Deposited on : 2022-07-06
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

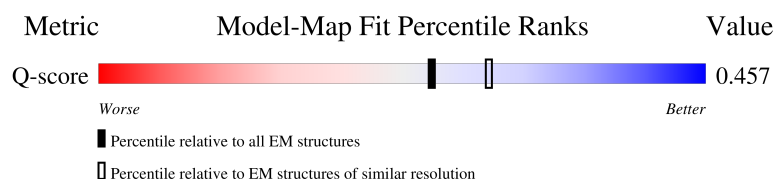
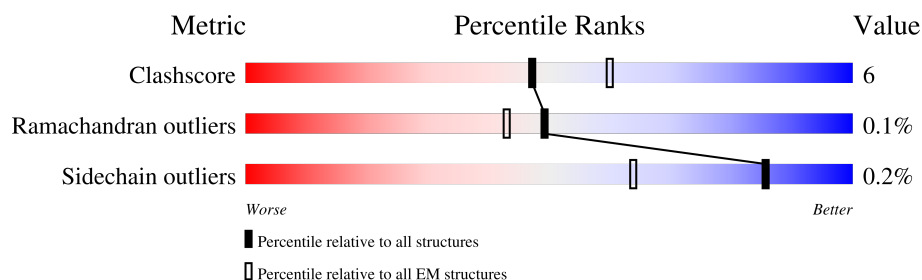
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



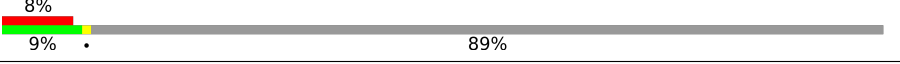
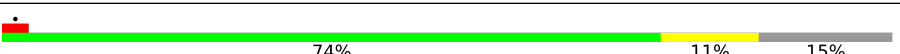
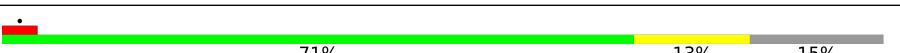
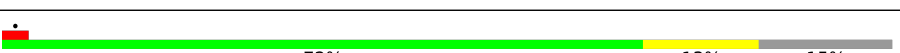
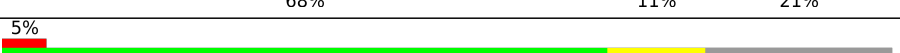
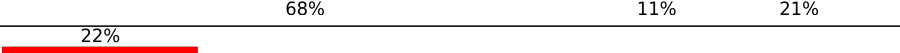
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1	1275	 9% . 89%
1	2	1275	 10% . 89%
1	3	1275	 10% . 89%
1	4	1275	 9% . 90%

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Mol	Chain	Length	Quality of chain
1	5	1275	
1	A	1275	
1	B	1275	
1	C	1275	
1	D	1275	
1	E	1275	
1	a	1275	
1	b	1275	
1	c	1275	
1	d	1275	
1	e	1275	
2	H	1289	
2	I	1289	
2	J	1289	
2	K	1289	
2	L	1289	
3	R	1267	
4	U	736	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SAM	H	1301	-	-	X	-
6	SAM	H	1302	-	-	X	-
6	SAM	I	1301	-	-	X	-
6	SAM	I	1302	-	-	X	-
6	SAM	J	1301	-	-	X	-
6	SAM	J	1302	-	-	X	-
6	SAM	K	1301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SAM	K	1302	-	-	X	-
6	SAM	L	1301	-	-	X	-
6	SAM	L	1302	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 146613 atoms, of which 220 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 RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	140	Total	C	N	O	S	0	0
			1041	619	198	221	3		
1	2	139	Total	C	N	O	S	0	0
			1035	616	197	219	3		
1	3	138	Total	C	N	O	S	0	0
			1030	613	196	218	3		
1	4	131	Total	C	N	O	S	0	0
			967	574	183	207	3		
1	5	140	Total	C	N	O	S	0	0
			1041	619	198	221	3		
1	A	1128	Total	C	N	O	S	0	0
			8868	5654	1510	1651	53		
1	B	1073	Total	C	N	O	S	0	0
			8442	5389	1431	1571	51		
1	C	1088	Total	C	N	O	S	0	0
			8583	5480	1454	1598	51		
1	D	1050	Total	C	N	O	S	0	0
			8300	5306	1403	1542	49		
1	E	1061	Total	C	N	O	S	0	0
			8385	5356	1420	1560	49		
1	a	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		
1	b	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		
1	c	1082	Total	C	N	O	S	0	0
			8539	5455	1452	1581	51		
1	d	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		
1	e	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		

- Molecule 2 is a protein called Lambda-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	I	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	J	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	K	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		
2	L	1024	Total	C	N	O	S	0	0
			8073	5150	1375	1519	29		

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	1253	Total	C	N	O	S	0	0
			9913	6327	1697	1824	65		

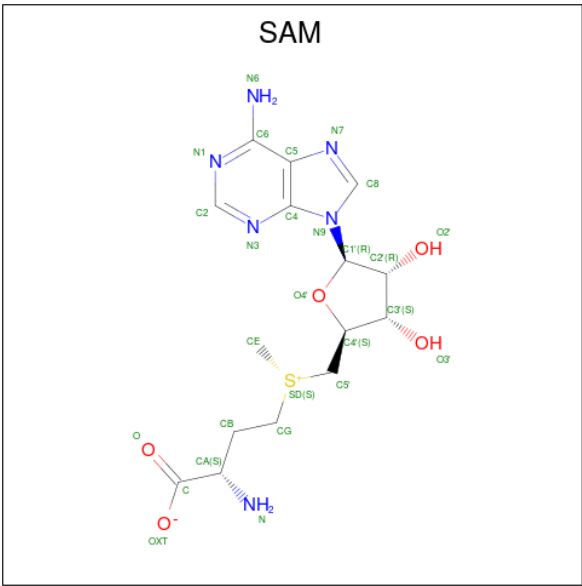
- Molecule 4 is a protein called Mu-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	668	Total	C	N	O	S	0	0
			5322	3413	901	979	29		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	a	1	Total	Zn	0
			1	1	
5	b	1	Total	Zn	0
			1	1	
5	c	1	Total	Zn	0
			1	1	
5	d	1	Total	Zn	0
			1	1	
5	e	1	Total	Zn	0
			1	1	

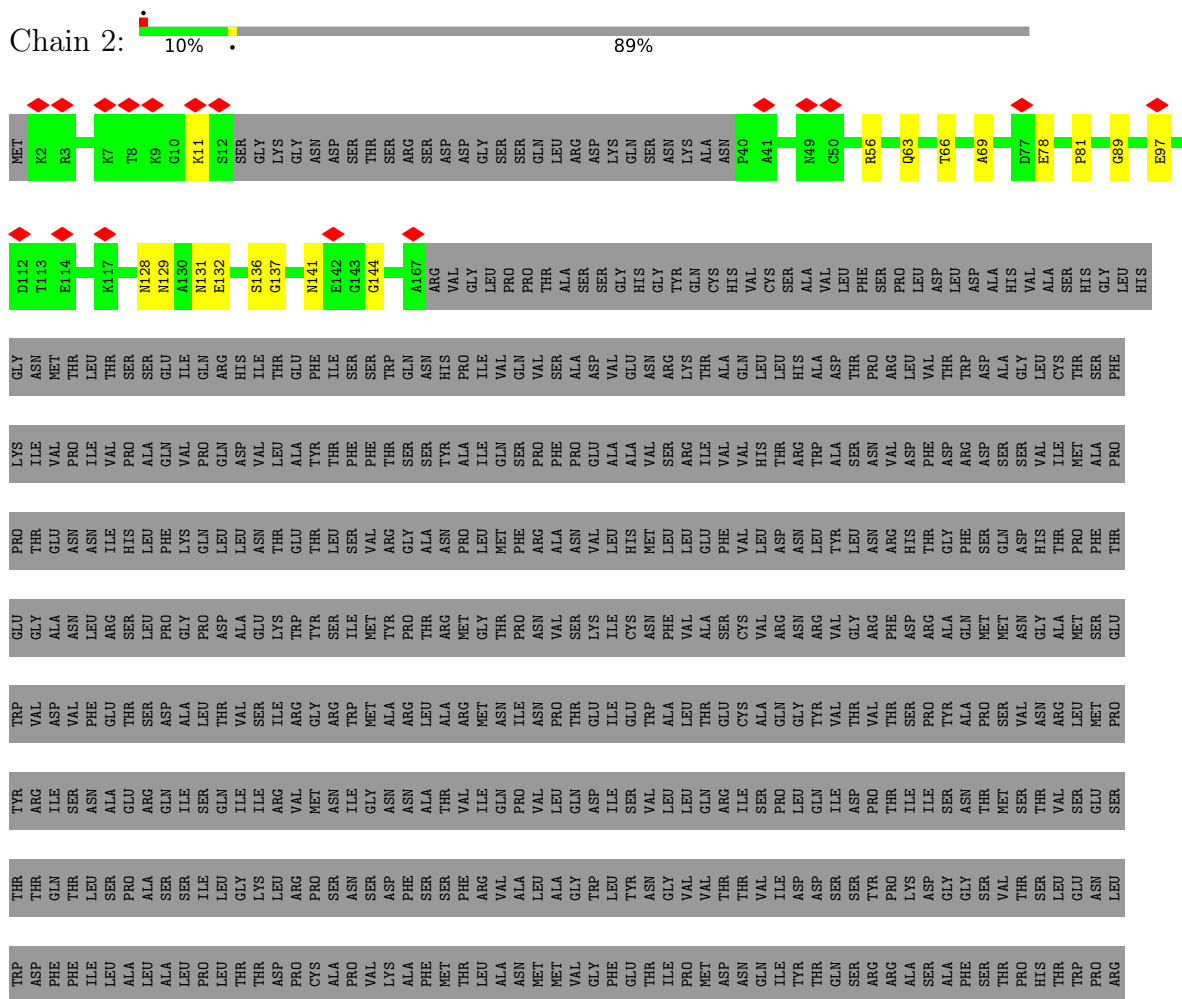
- Molecule 6 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms						AltConf
6	H	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	H	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	I	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	I	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	J	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	J	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	K	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	K	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	L	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
6	L	1	Total 49	C 15	H 22	N 6	O 5	S 1	0

[illegible]

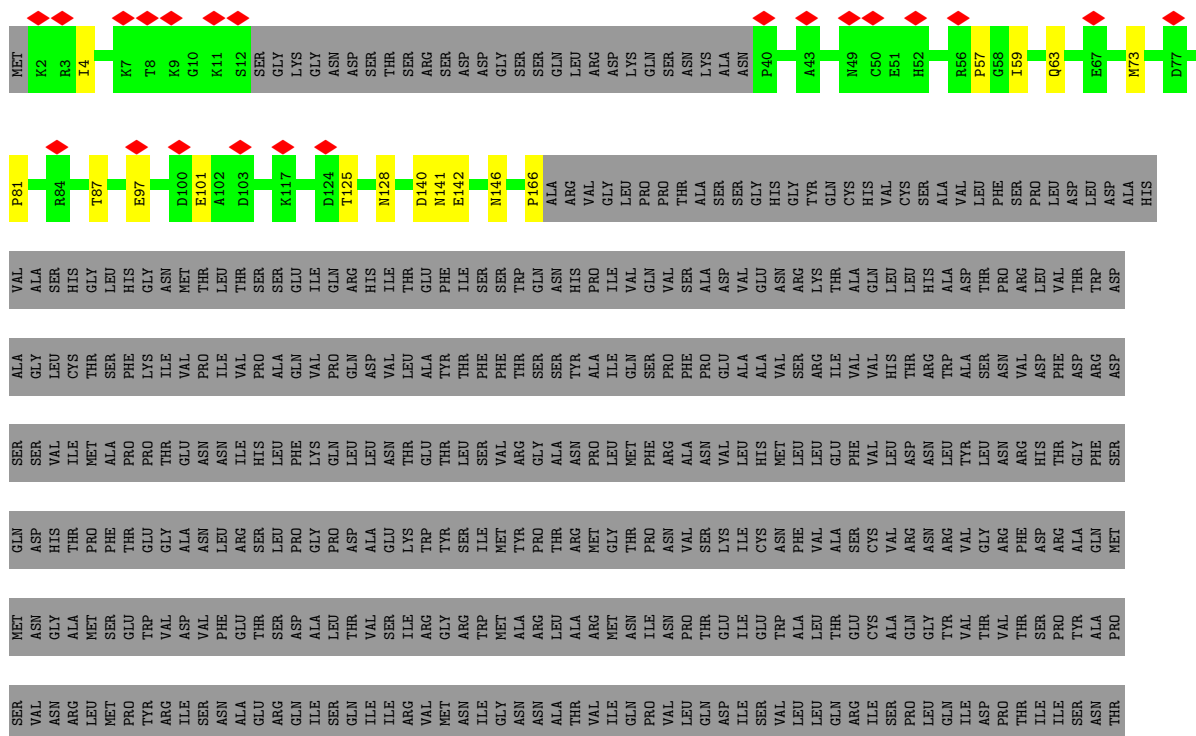
- Molecule 1: RNA helicase



[illegible]

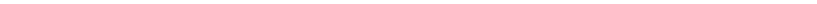
- Molecule 1: RNA helicase

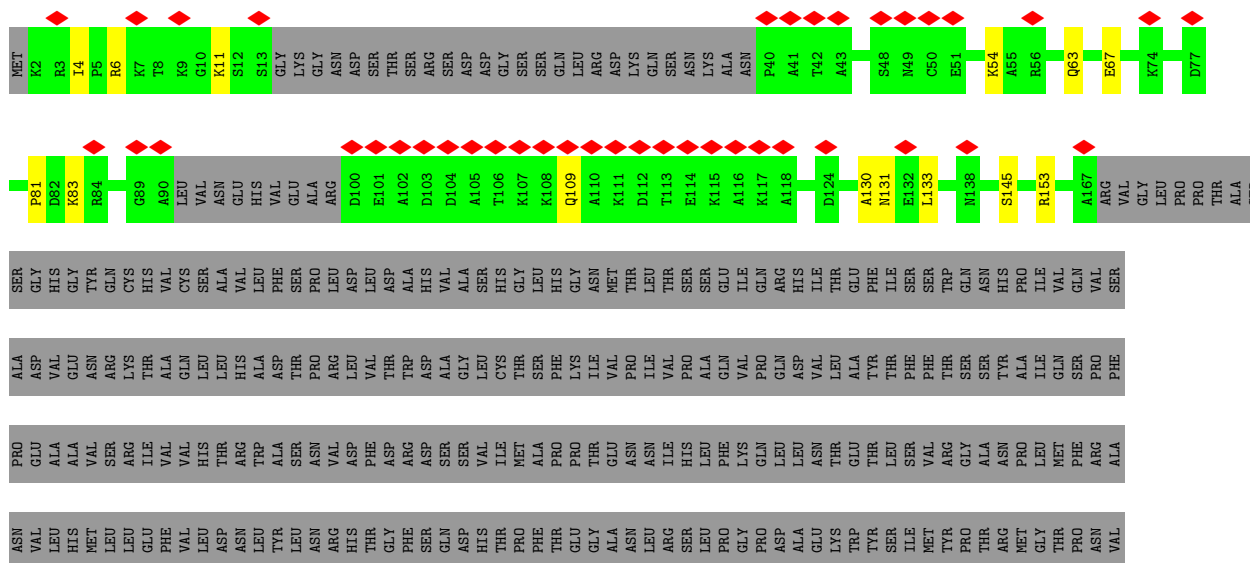
Chain 3: 10% 89%



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

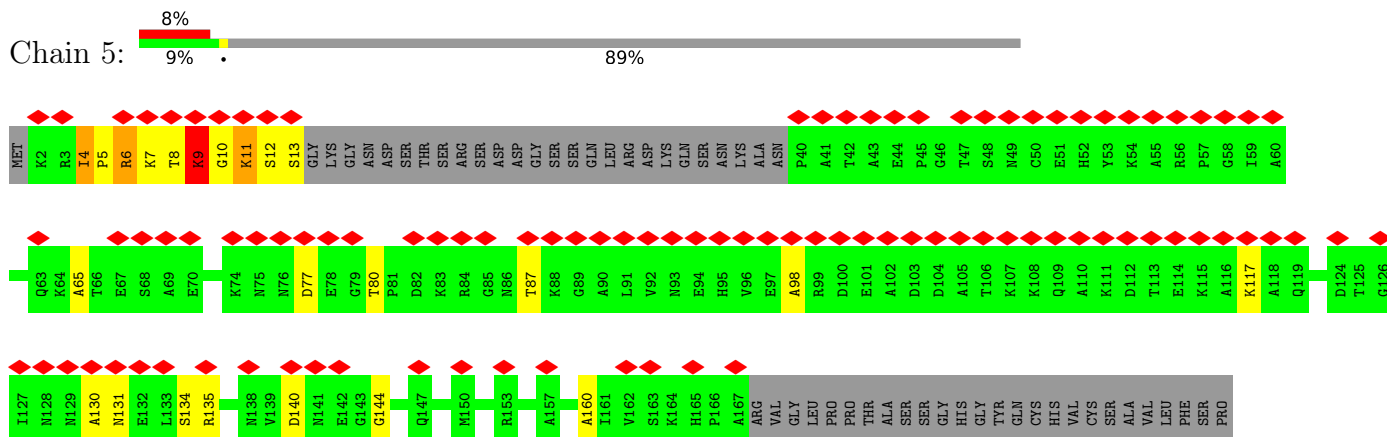
- Molecule 1: RNA helicase

Chain 4:  9% 90%

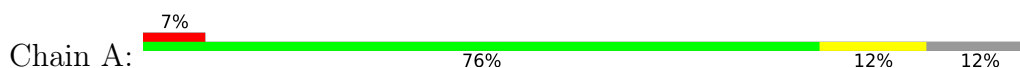


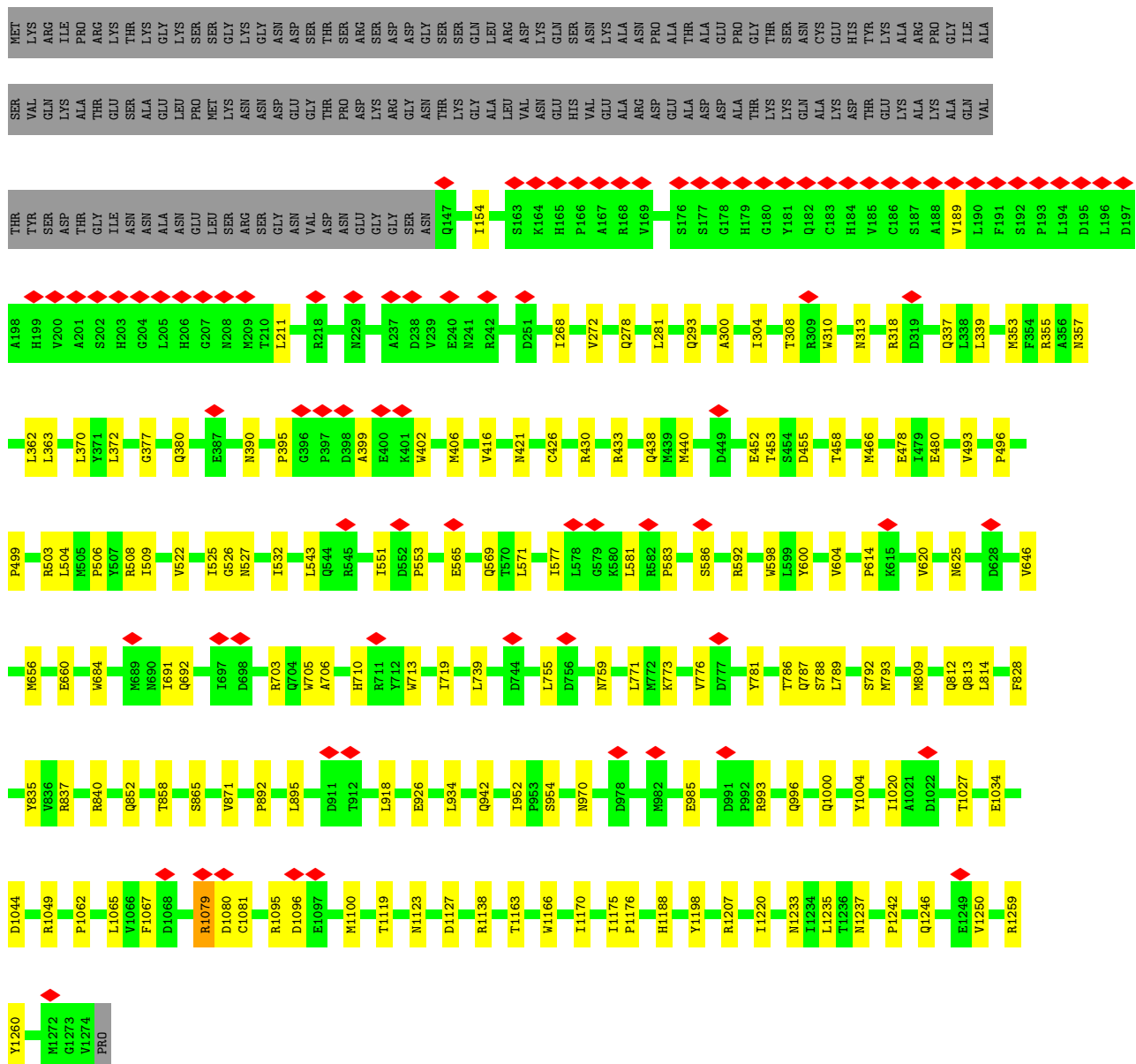
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- Molecule 1: RNA helicase

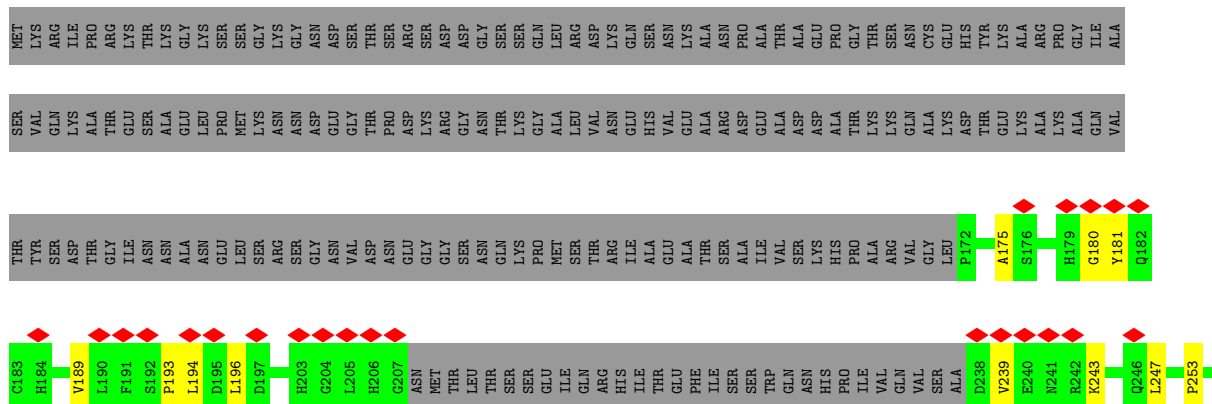


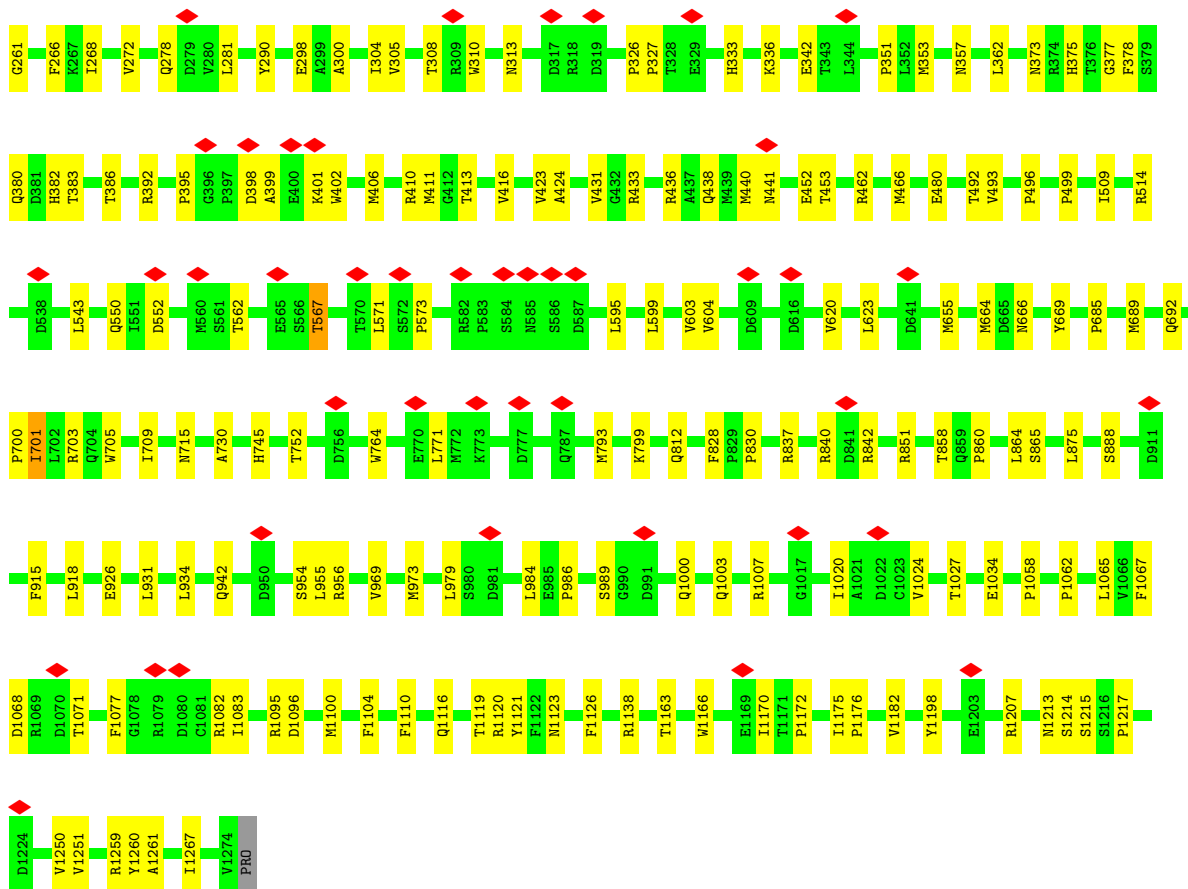
- Molecule 1: RNA helicase



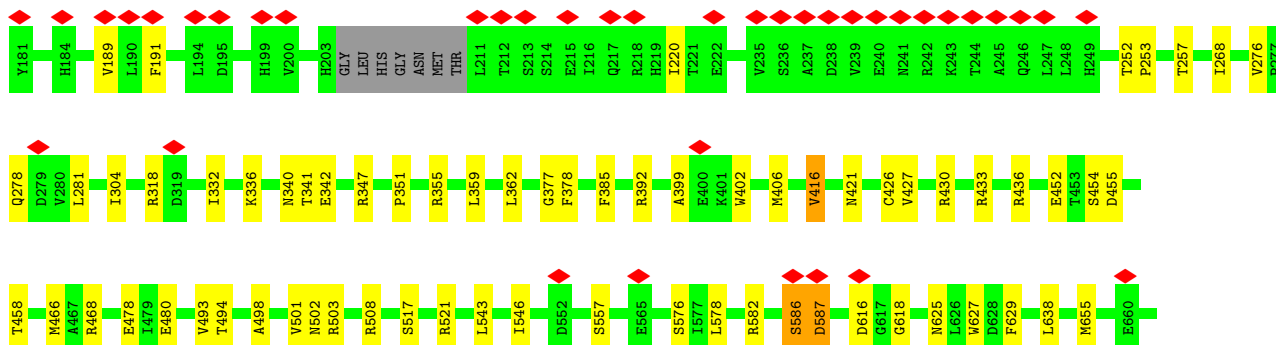
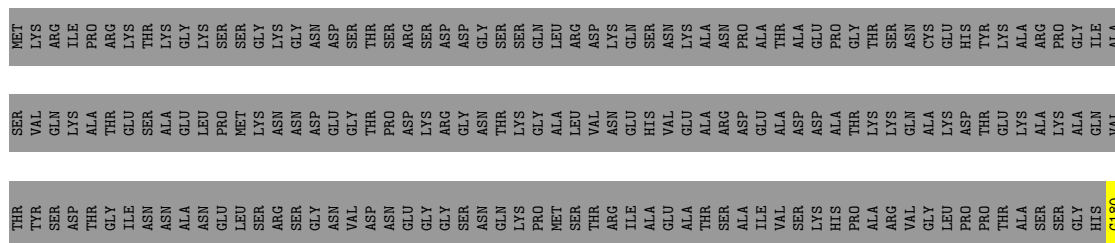


- Molecule 1: RNA helicase





- Molecule 1: RNA helicase

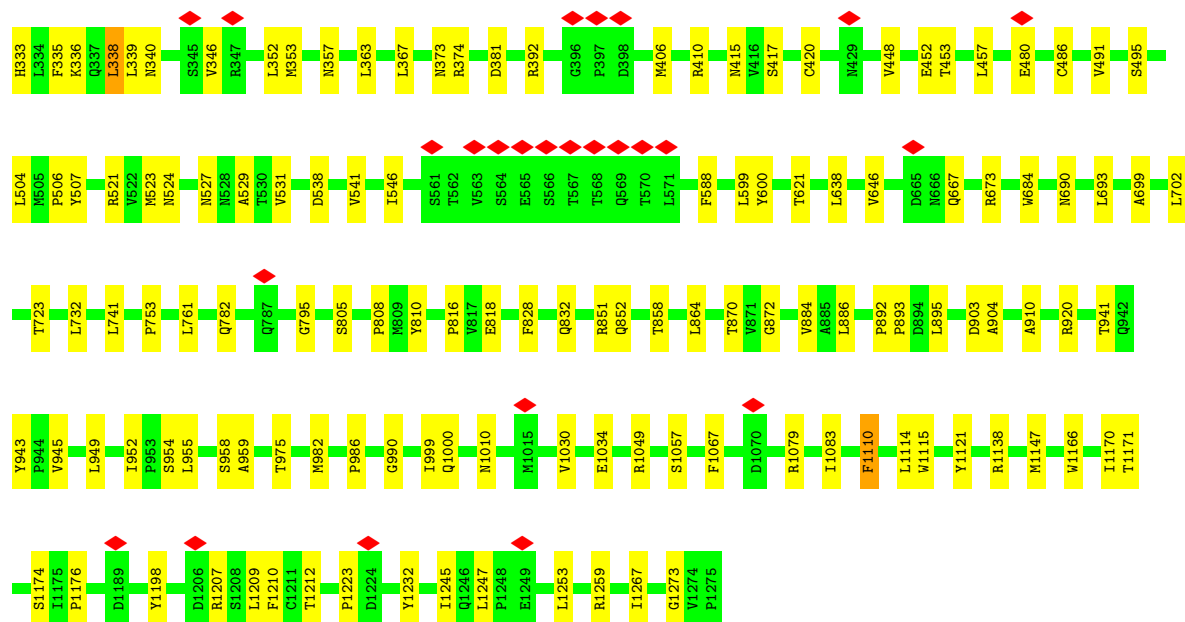


Frequency	Percentage
Daily	71%
Weekly	12%
Monthly	17%



Frequency	Percentage
Daily	73%
Weekly	12%
Monthly	15%





- Molecule 1: RNA helicase

Chain b:

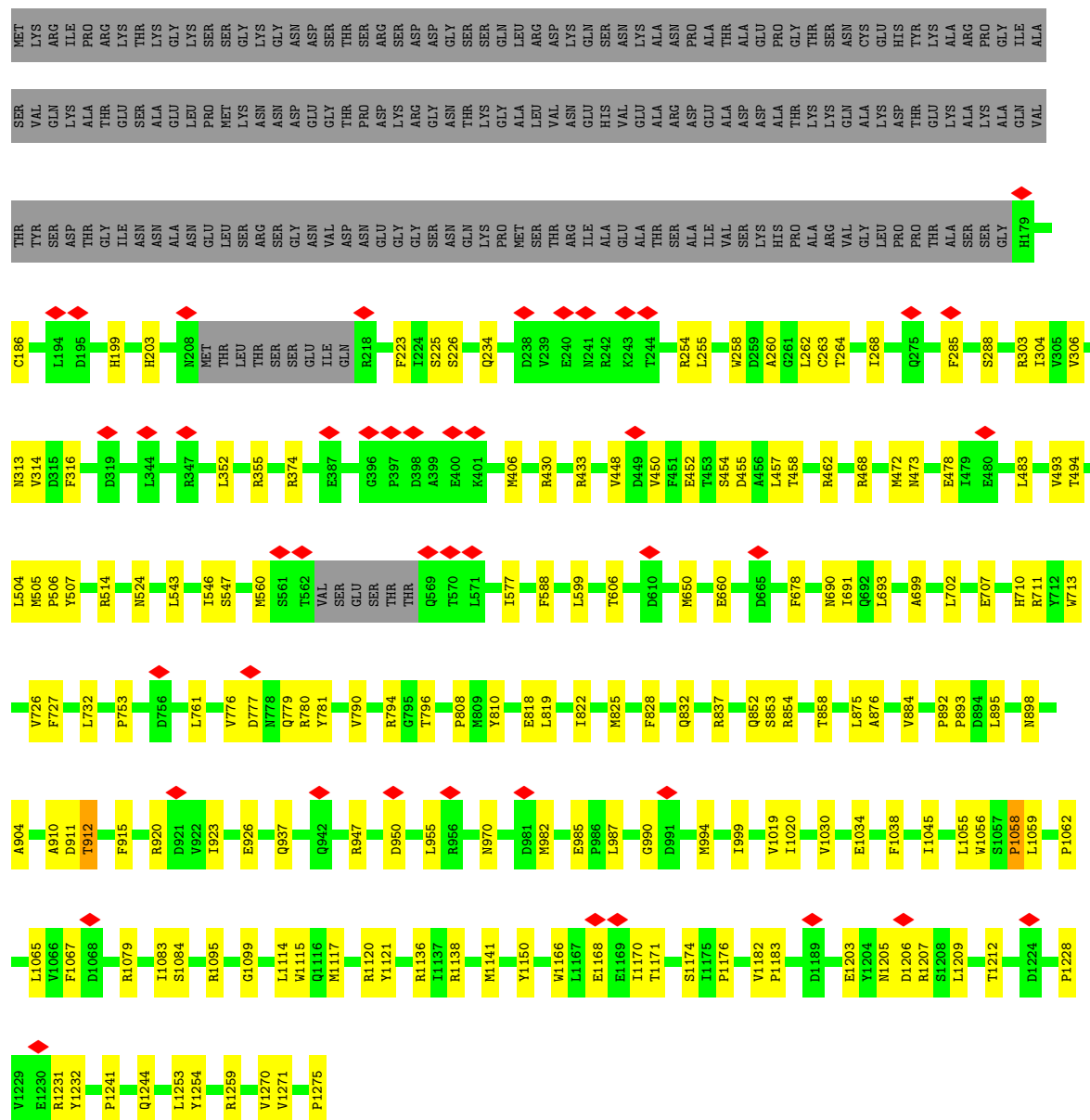
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K801	P808	L819	A820	W821	1822	F828	R837	T850	T870	W871	0872	L875	K890	T891	P892	R893	D894	L895	I905	F915	R920	L931	L934	Q942	V945	Y948	L949	I952	L955	A963	M982	L983	L984	L987	Q990				
V563	S564	E565	S566	T567	T568	Q569	T570	L571	Y600	V603	T606	D609	P614	M625	D641	M656	V657	E660	M680	L693	W705	W713	T723	F726	W727	G728	N731	L732	P736	E737	V738	N749	L761	E770	L771	W773	K773		
P383	P384	F385	T386	E387	G396	P397	D398	K401	M415	R430	R433	F434	D435	R436	V448	E452	A456	V459	M466	A467	R468	M472	E478	A482	L483	V493	L504	M505	P506	Y507	R508	R514	I520	I525	D538	D552	T562		
S187	L194	D195	V200	L205	W208	ME1	THR	THR	THR	SER	SER	GLU	ILE	GLN	R218	T221	D238	V239	E240	Q246	F266	V272	V280	F285	A300	V301	D319	H333	K336	Q337	L338	L339	L344	S345	V346	R347	L352	N373	E378



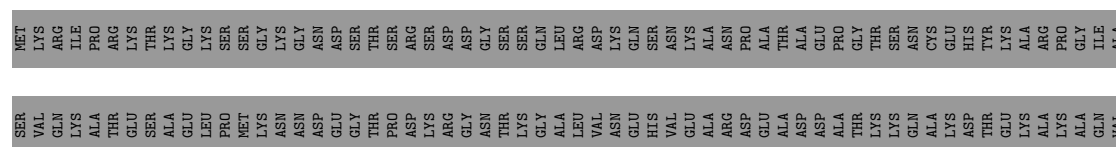
• Molecule 1: RNA helicase

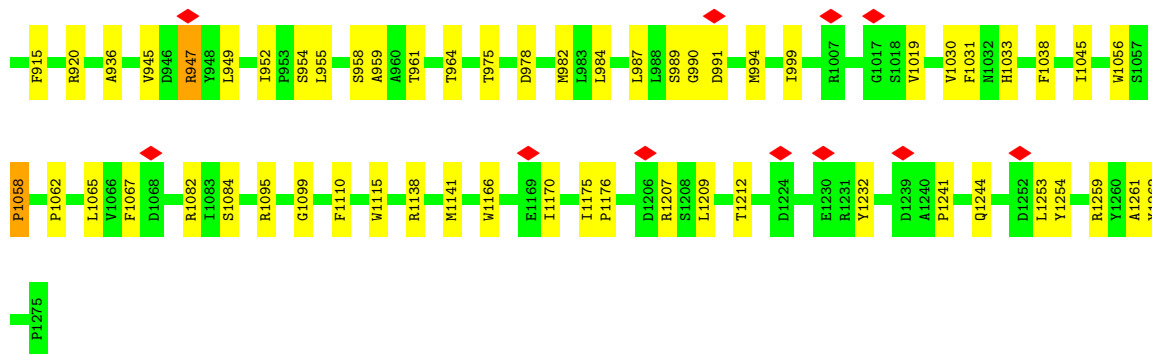
Chain c: 71% 13% 15%



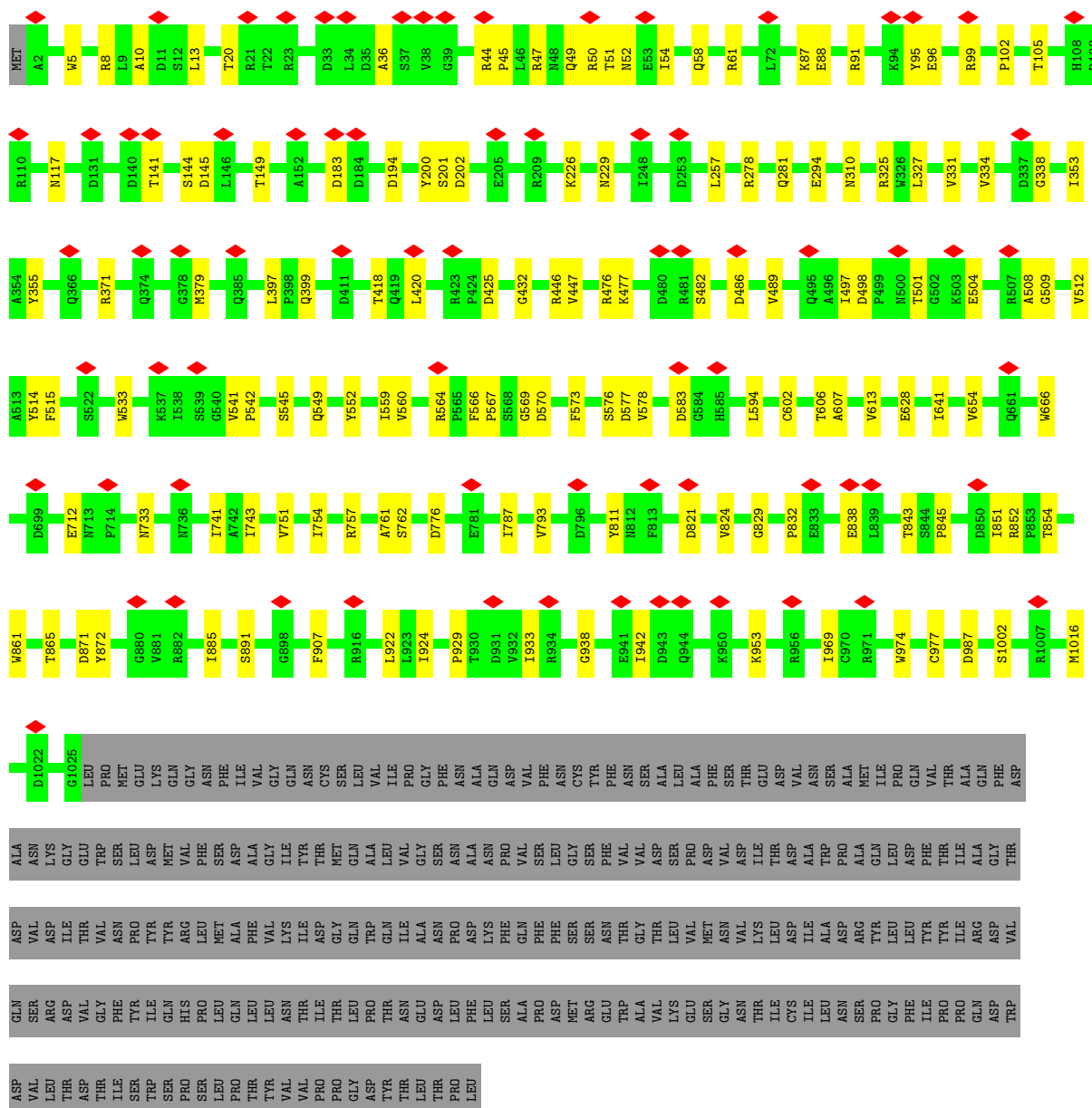
• Molecule 1: RNA helicase

Chain d: 74% 11% 15%

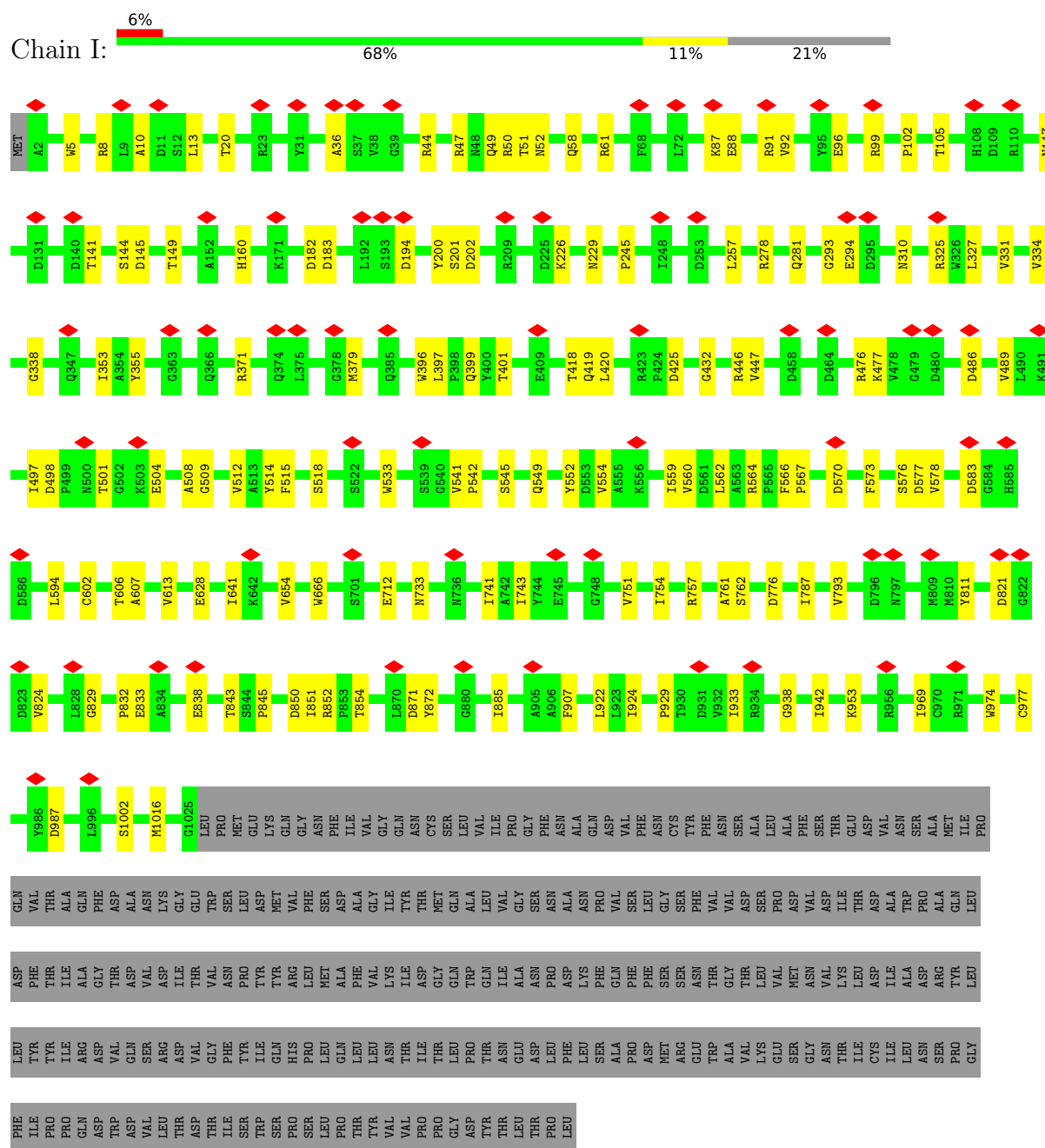




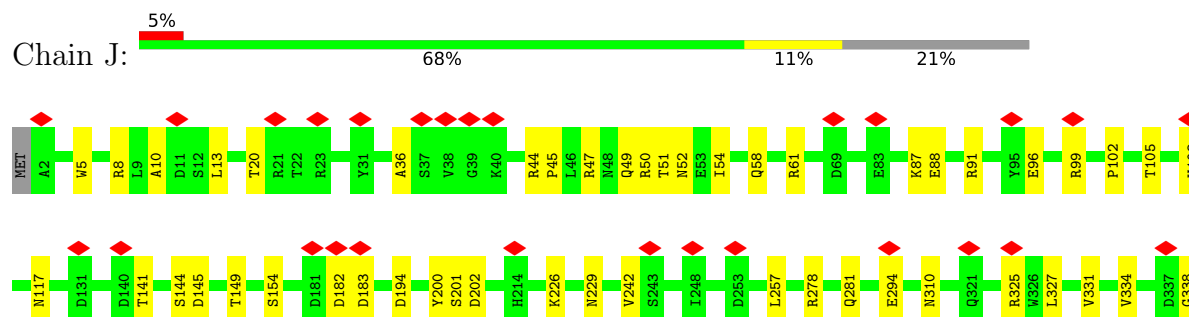
• Molecule 2: Lambda-2 protein



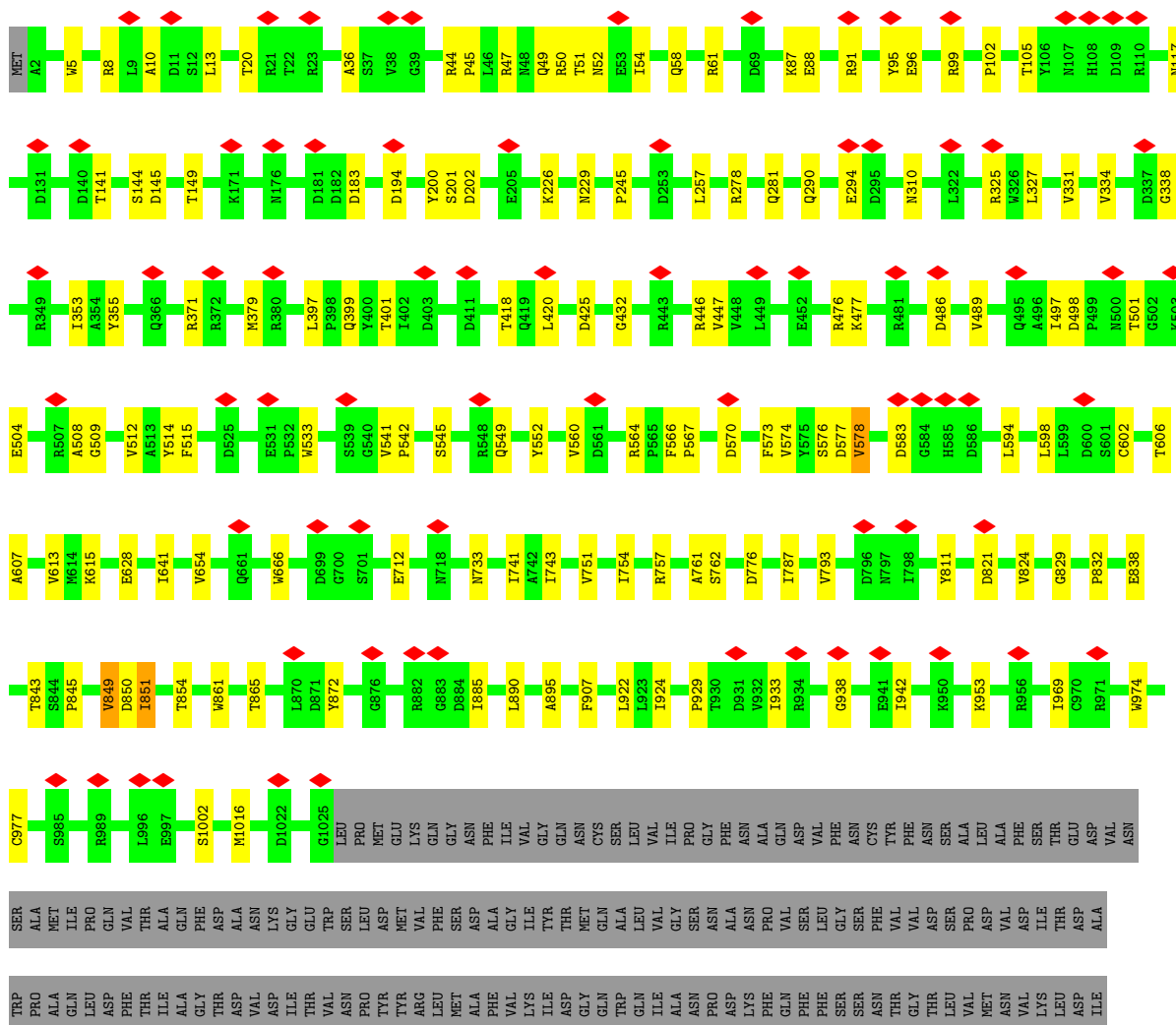
- Molecule 2: Lambda-2 protein



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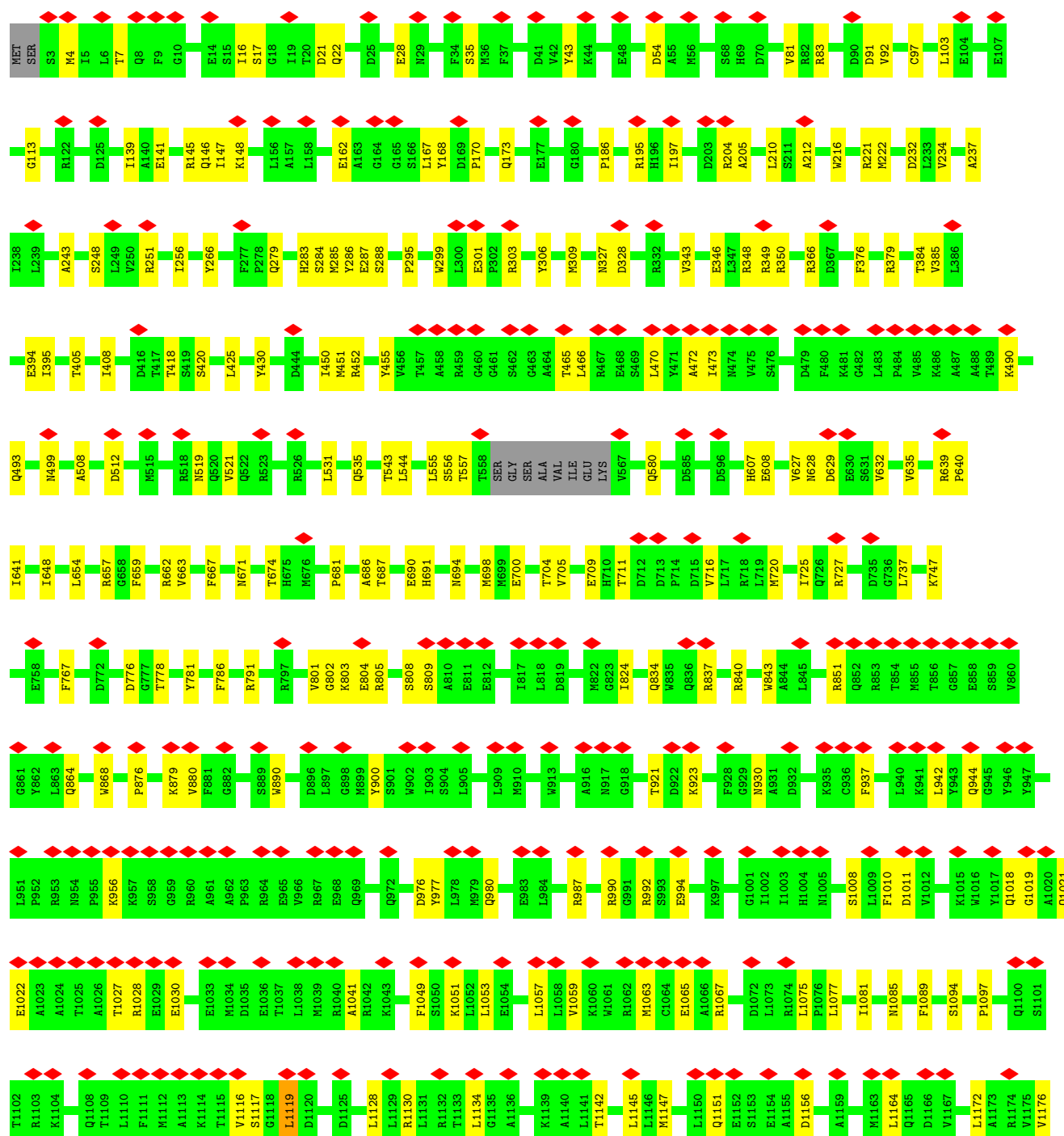
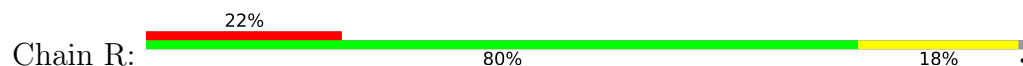


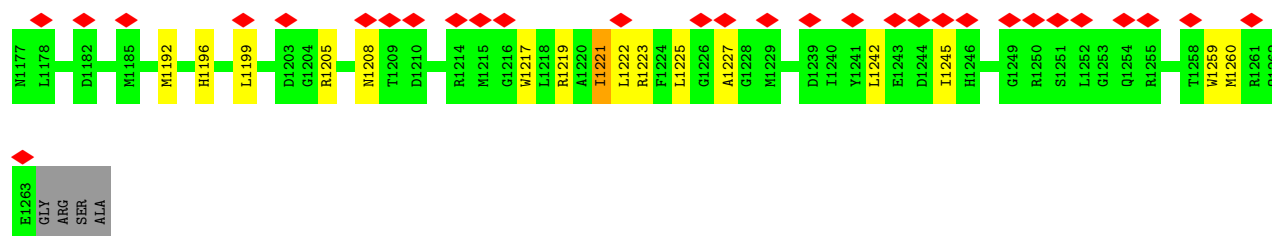
- Molecule 2: Lambda-2 protein



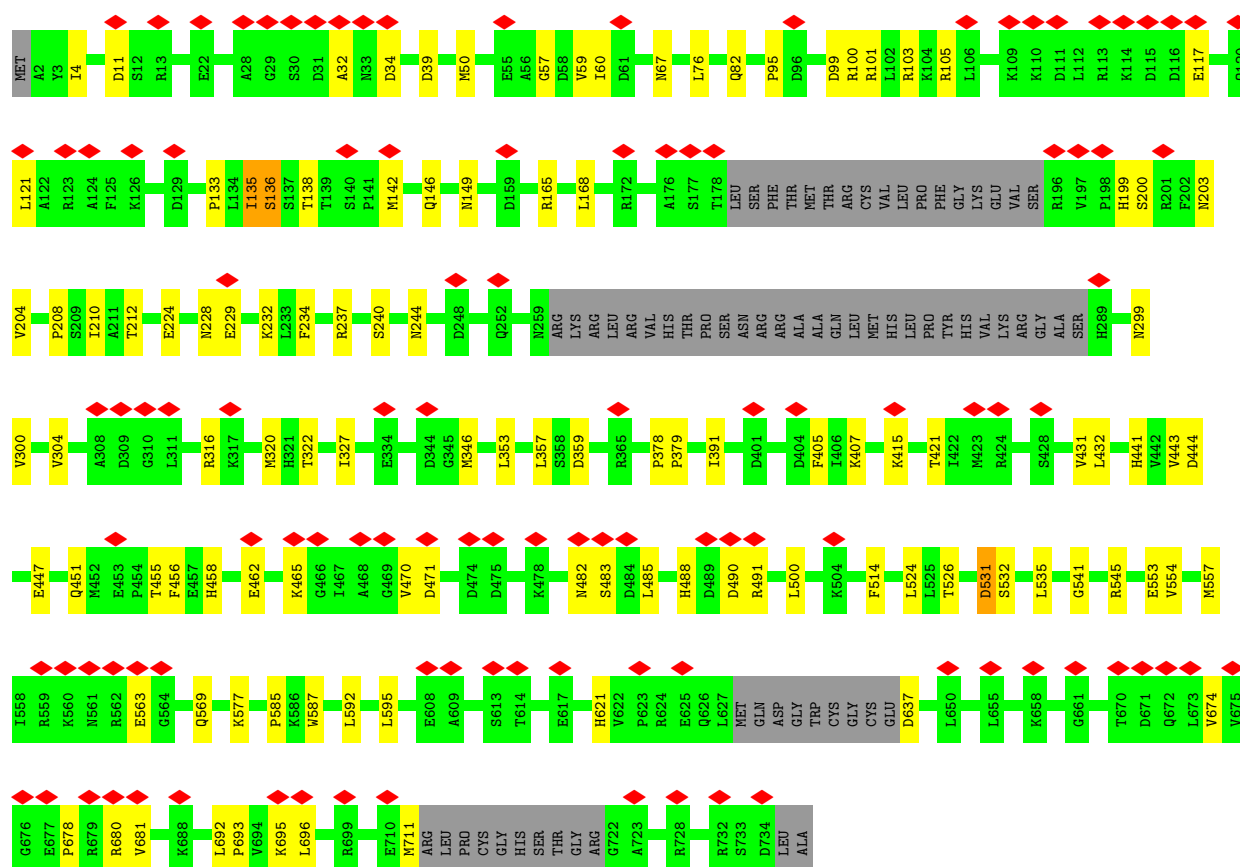
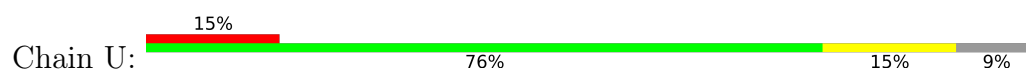
ALA	ASP	ARG	TYR	LEU	LEU	TYR	TYR	ILE	ASP	ASP	VAL	GLN	SER	ASP	VAL	ASP	GLY	PHE	TYR	ILE	THR	GLN	HIS	PRO	SER	PRO	LEU	GLN	LEU	LEU	ASN	VAL	THR	THR	ILE	THR	THR	GLY	ASP	PRO	THR	THR	ASN	GLU	ASP	PHE	LEU	SER	SER	ALA	PRO	ASP	MET	ARG	GLU	TRP	ALA	VAL	LYS	GLU	SER	GLY	ASN	THR	ILE	CYS	ILE
LEU	ASN	SER	PRO	GLY	PHE	ILE	PRO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

• Molecule 3: RNA-directed RNA polymerase





• Molecule 4: Mu-2 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45544	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.634	Depositor
Minimum map value	-1.369	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.24	0/1052	0.55	0/1413
1	2	0.22	0/1046	0.52	0/1405
1	3	0.25	0/1041	0.56	0/1398
1	4	0.24	0/976	0.60	0/1308
1	5	0.31	0/1052	0.81	6/1413 (0.4%)
1	A	0.28	0/9107	0.59	7/12474 (0.1%)
1	B	0.28	0/8671	0.59	2/11878 (0.0%)
1	C	0.28	0/8814	0.58	1/12074 (0.0%)
1	D	0.27	0/8526	0.57	4/11680 (0.0%)
1	E	0.27	0/8612	0.57	0/11798
1	a	0.27	0/8804	0.58	2/12061 (0.0%)
1	b	0.25	0/8804	0.53	0/12061
1	c	0.27	0/8772	0.55	0/12015
1	d	0.26	1/8804 (0.0%)	0.53	0/12061
1	e	0.26	0/8804	0.56	0/12061
2	H	0.22	0/8275	0.55	2/11284 (0.0%)
2	I	0.22	0/8275	0.55	2/11284 (0.0%)
2	J	0.22	0/8275	0.56	2/11284 (0.0%)
2	K	0.22	0/8275	0.55	2/11284 (0.0%)
2	L	0.24	0/8275	0.57	3/11284 (0.0%)
3	R	0.28	0/10166	0.65	6/13806 (0.0%)
4	U	0.30	0/5439	0.69	10/7385 (0.1%)
All	All	0.26	1/149865 (0.0%)	0.57	49/204711 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	2
1	a	0	3
1	b	0	2
1	c	0	1
1	d	0	4
1	e	0	2
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
3	R	0	3
4	U	0	3
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	242	ARG	CA-CB	5.12	1.62	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	9	LYS	N-CA-C	10.83	123.09	111.28
4	U	210	ILE	N-CA-C	-9.43	103.21	112.17
1	5	4	ILE	CA-C-N	8.50	128.94	120.52
1	5	4	ILE	C-N-CA	8.50	128.94	120.52
3	R	1011	ASP	CA-C-N	7.75	125.12	120.24
3	R	1011	ASP	C-N-CA	7.75	125.12	120.24
1	5	4	ILE	N-CA-C	7.45	115.95	109.02
1	5	11	LYS	N-CA-C	6.80	118.69	111.28
1	a	308	THR	CA-C-N	6.56	134.07	121.54
1	a	308	THR	C-N-CA	6.56	134.07	121.54
3	R	1176	VAL	N-CA-C	-6.28	107.17	113.20
1	B	308	THR	CA-C-N	5.94	132.89	121.54
1	B	308	THR	C-N-CA	5.94	132.89	121.54
4	U	82	GLN	N-CA-C	-5.87	107.11	114.56
2	J	294	GLU	CA-C-N	5.73	133.42	123.91
2	J	294	GLU	C-N-CA	5.73	133.42	123.91
2	H	294	GLU	CA-C-N	5.73	133.41	123.91
2	H	294	GLU	C-N-CA	5.73	133.41	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	294	GLU	CA-C-N	5.71	133.39	123.91
2	K	294	GLU	C-N-CA	5.71	133.39	123.91
2	I	294	GLU	CA-C-N	5.71	133.39	123.91
2	I	294	GLU	C-N-CA	5.71	133.39	123.91
2	L	294	GLU	CA-C-N	5.70	133.38	123.91
2	L	294	GLU	C-N-CA	5.70	133.38	123.91
3	R	285	MET	CA-C-N	5.55	132.13	121.54
3	R	285	MET	C-N-CA	5.55	132.13	121.54
3	R	555	LEU	CA-CB-CG	5.51	135.60	116.30
4	U	228	ASN	CA-C-N	5.45	131.96	121.54
4	U	228	ASN	C-N-CA	5.45	131.96	121.54
4	U	482	ASN	CA-C-N	5.36	131.78	121.54
4	U	482	ASN	C-N-CA	5.36	131.78	121.54
2	L	849	VAL	N-CA-C	5.31	115.77	108.12
1	A	308	THR	CA-C-N	5.29	131.64	121.54
1	A	308	THR	C-N-CA	5.29	131.64	121.54
1	A	1246	GLN	CA-C-N	5.28	126.69	120.09
1	A	1246	GLN	C-N-CA	5.28	126.69	120.09
1	D	714	PRO	CA-C-N	5.26	136.22	120.69
1	D	714	PRO	C-N-CA	5.26	136.22	120.69
4	U	32	ALA	CA-C-N	5.18	131.44	121.54
4	U	32	ALA	C-N-CA	5.18	131.44	121.54
1	5	8	THR	N-CA-C	5.17	117.67	109.50
1	A	1079	ARG	CA-C-N	5.15	127.49	120.54
1	A	1079	ARG	C-N-CA	5.15	127.49	120.54
4	U	470	VAL	CA-C-N	5.15	131.37	121.54
4	U	470	VAL	C-N-CA	5.15	131.37	121.54
1	C	587	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	1119	THR	N-CA-C	5.02	117.14	111.02
1	D	984	LEU	CA-C-N	5.01	126.36	120.09
1	D	984	LEU	C-N-CA	5.01	126.36	120.09

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	793	MET	Peptide
1	C	276	VAL	Peptide
1	E	376	THR	Peptide
1	E	981	ASP	Peptide
2	H	1002	SER	Peptide
2	I	1002	SER	Peptide

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Mol	Chain	Res	Type	Group
2	J	1002	SER	Peptide
2	K	1002	SER	Peptide
2	L	1002	SER	Peptide
3	R	1065	GLU	Peptide
3	R	1119	LEU	Peptide
3	R	97	CYS	Peptide
4	U	135	ILE	Peptide
4	U	378	PRO	Peptide
4	U	483	SER	Peptide
1	a	1110	PHE	Peptide
1	a	285	PHE	Peptide
1	a	945	VAL	Peptide
1	b	1110	PHE	Peptide
1	b	945	VAL	Peptide
1	c	912	THR	Peptide
1	d	1110	PHE	Peptide
1	d	342	GLU	Peptide
1	d	375	HIS	Peptide
1	d	945	VAL	Peptide
1	e	1110	PHE	Peptide
1	e	947	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1041	0	1024	16	0
1	2	1035	0	1019	15	0
1	3	1030	0	1014	13	0
1	4	967	0	951	13	0
1	5	1041	0	1024	44	0
1	A	8868	0	8762	94	0
1	B	8442	0	8328	106	0
1	C	8583	0	8470	83	0
1	D	8300	0	8200	88	0
1	E	8385	0	8286	99	0
1	a	8571	0	8453	92	0
1	b	8571	0	8453	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	8539	0	8421	99	0
1	d	8571	0	8453	84	0
1	e	8571	0	8453	120	0
2	H	8073	0	7925	146	0
2	I	8073	0	7925	141	0
2	J	8073	0	7925	126	0
2	K	8073	0	7925	147	0
2	L	8073	0	7925	118	0
3	R	9913	0	9836	138	0
4	U	5322	0	5341	59	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0
5	d	1	0	0	0	0
5	e	1	0	0	0	0
6	H	54	44	41	66	0
6	I	54	44	42	55	0
6	J	54	44	44	43	0
6	K	54	44	44	65	0
6	L	54	44	44	37	0
All	All	146393	220	144328	1747	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 6.

All (1747) 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)
2:I:851:ILE:HG23	6:I:1301:SAM:C2	1.44	1.43
2:H:577:ASP:O	6:H:1301:SAM:CE	1.66	1.41
2:I:552:TYR:CE2	6:I:1302:SAM:C5	2.05	1.40
2:H:552:TYR:HB2	6:H:1301:SAM:O2'	1.21	1.33
2:K:872:TYR:CE1	6:K:1302:SAM:C2	2.11	1.33
2:J:552:TYR:CE2	6:J:1302:SAM:C5	2.12	1.31
2:H:872:TYR:CD1	6:H:1302:SAM:C2	2.14	1.29
2:K:851:ILE:HG23	6:K:1302:SAM:C2	1.61	1.29
2:I:851:ILE:CG2	6:I:1301:SAM:C2	2.12	1.26
2:H:851:ILE:HG23	6:H:1302:SAM:N3	1.53	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:552:TYR:CZ	6:I:1302:SAM:C6	2.22	1.23
2:J:872:TYR:CE1	6:J:1301:SAM:C2	2.23	1.21
2:L:552:TYR:HB2	6:L:1302:SAM:O2'	1.37	1.19
2:K:872:TYR:CD1	6:K:1302:SAM:C2	2.26	1.19
2:H:552:TYR:CE2	6:H:1301:SAM:C5	2.27	1.18
2:L:552:TYR:CE2	6:L:1302:SAM:C5	2.26	1.17
2:I:851:ILE:HG23	6:I:1301:SAM:N3	1.58	1.17
2:K:850:ASP:CG	6:K:1302:SAM:O2'	1.87	1.17
2:K:850:ASP:OD1	6:K:1302:SAM:H1'	1.42	1.17
2:K:552:TYR:CE2	6:K:1301:SAM:C5	2.27	1.16
2:K:552:TYR:CE2	6:K:1301:SAM:C4	2.29	1.16
2:I:518:SER:OG	6:I:1302:SAM:O	1.58	1.15
2:J:552:TYR:CE2	6:J:1302:SAM:C4	2.28	1.15
2:J:552:TYR:CZ	6:J:1302:SAM:C6	2.29	1.15
2:I:577:ASP:O	6:I:1302:SAM:CE	1.97	1.13
2:J:872:TYR:CD1	6:J:1301:SAM:C2	2.30	1.13
2:I:552:TYR:HB2	6:I:1302:SAM:O2'	1.48	1.13
2:J:552:TYR:CD2	6:J:1302:SAM:C4	2.32	1.12
2:H:872:TYR:CE1	6:H:1302:SAM:N3	2.18	1.12
2:I:577:ASP:O	6:I:1302:SAM:HE1	1.51	1.10
2:K:552:TYR:CZ	6:K:1301:SAM:C5	2.35	1.08
2:K:552:TYR:CZ	6:K:1301:SAM:C6	2.38	1.07
2:J:872:TYR:HE1	6:J:1301:SAM:N3	1.51	1.06
2:H:552:TYR:CZ	6:H:1301:SAM:C6	2.38	1.06
1:5:9:LYS:O	1:e:319:ASP:OD2	1.73	1.04
2:I:552:TYR:OH	6:I:1302:SAM:N6	1.89	1.04
2:H:577:ASP:OD2	6:H:1301:SAM:O	1.76	1.03
2:H:872:TYR:HE1	6:H:1302:SAM:N3	1.56	1.02
2:I:872:TYR:CD1	6:I:1301:SAM:C2	2.41	1.02
2:K:850:ASP:OD1	6:K:1302:SAM:C1'	2.06	1.02
2:K:850:ASP:OD2	6:K:1302:SAM:O2'	1.77	1.02
2:H:577:ASP:O	6:H:1301:SAM:HE1	1.58	1.01
2:K:850:ASP:OD2	6:K:1302:SAM:O3'	1.76	1.01
2:K:552:TYR:OH	6:K:1301:SAM:C6	2.08	1.00
2:K:872:TYR:HE1	6:K:1302:SAM:N3	1.57	1.00
1:5:11:LYS:HB2	1:e:319:ASP:O	1.61	1.00
2:H:872:TYR:CE1	6:H:1302:SAM:C2	2.43	0.99
2:H:851:ILE:HG23	6:H:1302:SAM:C2	1.92	0.99
2:J:552:TYR:OH	6:J:1302:SAM:C6	2.10	0.99
2:I:552:TYR:OH	6:I:1302:SAM:C6	2.12	0.98
2:K:552:TYR:CD2	6:K:1301:SAM:C4	2.47	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:552:TYR:CD2	6:I:1302:SAM:C4	2.46	0.98
2:H:552:TYR:HB2	6:H:1301:SAM:HO2'	1.21	0.97
2:K:872:TYR:HE1	6:K:1302:SAM:C2	1.65	0.97
2:K:851:ILE:CG2	6:K:1302:SAM:C2	2.42	0.96
2:H:851:ILE:CG2	6:H:1302:SAM:C2	2.43	0.96
2:J:872:TYR:CE1	6:J:1301:SAM:N3	2.33	0.96
2:L:552:TYR:CD2	6:L:1302:SAM:C4	2.48	0.95
2:I:851:ILE:CG2	6:I:1301:SAM:N1	2.29	0.95
1:5:11:LYS:N	1:e:319:ASP:OD2	2.00	0.95
2:L:552:TYR:CE2	6:L:1302:SAM:C6	2.50	0.94
2:L:552:TYR:H	6:L:1302:SAM:H8	1.31	0.94
2:H:552:TYR:CB	6:H:1301:SAM:O2'	2.16	0.94
2:K:872:TYR:CD1	6:K:1302:SAM:H2	2.02	0.94
2:I:872:TYR:CE1	6:I:1301:SAM:C2	2.51	0.93
2:H:851:ILE:HG23	6:H:1302:SAM:C4	1.97	0.93
2:I:850:ASP:OD2	6:I:1301:SAM:O3'	1.86	0.93
2:L:552:TYR:CZ	6:L:1302:SAM:C5	2.51	0.93
2:K:552:TYR:OH	6:K:1301:SAM:N6	2.01	0.93
2:K:850:ASP:OD1	6:K:1302:SAM:O2'	1.80	0.93
2:I:872:TYR:HE1	6:I:1301:SAM:C4	1.82	0.93
2:L:552:TYR:CE2	6:L:1302:SAM:C4	2.52	0.93
2:L:552:TYR:CZ	6:L:1302:SAM:C6	2.52	0.92
6:J:1302:SAM:CG	6:J:1302:SAM:O	2.17	0.92
2:L:552:TYR:OH	6:L:1302:SAM:N6	2.02	0.92
2:I:552:TYR:CE2	6:I:1302:SAM:C4	2.53	0.92
2:K:850:ASP:CG	6:K:1302:SAM:HO2'	1.69	0.91
1:5:10:GLY:HA3	1:e:975:THR:CG2	2.00	0.91
2:H:872:TYR:HE1	6:H:1302:SAM:C4	1.83	0.91
2:H:872:TYR:HD1	6:H:1302:SAM:C2	1.77	0.90
2:I:872:TYR:HE1	6:I:1301:SAM:N3	1.69	0.90
2:H:872:TYR:HD1	6:H:1302:SAM:H2	1.35	0.90
2:K:872:TYR:HD1	6:K:1302:SAM:H2	1.36	0.89
2:J:552:TYR:CZ	6:J:1302:SAM:C5	2.54	0.89
1:5:10:GLY:CA	1:e:319:ASP:OD2	2.19	0.89
2:H:872:TYR:CD1	6:H:1302:SAM:H2	2.06	0.89
2:H:552:TYR:OH	6:H:1301:SAM:C6	2.21	0.89
2:H:552:TYR:CD2	6:H:1301:SAM:C4	2.56	0.88
2:H:871:ASP:OD1	6:H:1302:SAM:N6	2.05	0.88
2:J:872:TYR:CD1	6:J:1301:SAM:H2	2.05	0.88
2:K:518:SER:OG	6:K:1301:SAM:N	2.05	0.88
1:5:10:GLY:C	1:e:319:ASP:OD2	2.17	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:552:TYR:CE2	6:H:1301:SAM:C4	2.56	0.88
2:K:872:TYR:CE1	6:K:1302:SAM:N1	2.41	0.87
2:I:577:ASP:O	6:I:1302:SAM:HE2	1.74	0.87
2:I:552:TYR:CE2	6:I:1302:SAM:N7	2.43	0.86
2:K:518:SER:HB3	6:K:1301:SAM:HN2	1.39	0.86
2:H:829:GLY:O	6:H:1302:SAM:HB1	1.77	0.85
2:I:872:TYR:CE1	6:I:1301:SAM:N3	2.45	0.84
2:K:850:ASP:CG	6:K:1302:SAM:H1'	2.02	0.84
2:H:578:VAL:HG23	6:H:1301:SAM:N9	1.92	0.84
1:5:6:ARG:NH1	1:e:316:PHE:CZ	2.45	0.84
2:I:552:TYR:CE2	6:I:1302:SAM:C6	2.53	0.83
2:H:552:TYR:CZ	6:H:1301:SAM:N1	2.45	0.83
1:5:10:GLY:HA3	1:e:319:ASP:OD2	1.78	0.83
6:J:1302:SAM:O	6:J:1302:SAM:HG2	1.78	0.83
2:J:552:TYR:OH	6:J:1302:SAM:N6	2.09	0.83
2:I:829:GLY:O	6:I:1301:SAM:N	2.11	0.83
2:K:851:ILE:HG23	6:K:1302:SAM:N3	1.95	0.82
2:J:552:TYR:CZ	6:J:1302:SAM:N1	2.48	0.82
2:J:872:TYR:HD1	6:J:1301:SAM:H2	1.41	0.82
2:J:552:TYR:CE1	6:J:1302:SAM:C2	2.63	0.81
2:H:872:TYR:CE1	6:H:1302:SAM:C4	2.60	0.81
2:H:552:TYR:OH	6:H:1301:SAM:N6	2.15	0.80
2:K:552:TYR:CE2	6:K:1301:SAM:C6	2.63	0.79
1:5:11:LYS:H	1:e:319:ASP:CG	1.89	0.79
2:J:552:TYR:CD2	6:J:1302:SAM:N9	2.51	0.79
2:H:552:TYR:CE2	6:H:1301:SAM:C6	2.64	0.79
2:J:889:MET:HB2	6:J:1301:SAM:O	1.83	0.79
2:H:578:VAL:HG23	6:H:1301:SAM:C8	2.13	0.78
2:K:518:SER:CB	6:K:1301:SAM:HN2	1.96	0.78
2:I:552:TYR:CZ	6:I:1302:SAM:N1	2.52	0.78
2:H:578:VAL:HG23	6:H:1301:SAM:C4	2.15	0.77
2:L:552:TYR:N	6:L:1302:SAM:H8	1.99	0.77
2:I:552:TYR:HE2	6:I:1302:SAM:N7	1.83	0.77
2:K:552:TYR:H	6:K:1301:SAM:H8	1.49	0.76
2:I:872:TYR:HD1	6:I:1301:SAM:C2	1.97	0.76
2:K:552:TYR:CD2	6:K:1301:SAM:N9	2.52	0.76
1:5:10:GLY:CA	1:e:975:THR:CG2	2.62	0.76
2:L:577:ASP:O	2:L:615:LYS:HD3	1.84	0.76
2:K:518:SER:CB	6:K:1301:SAM:N	2.48	0.76
2:I:851:ILE:HG22	6:I:1301:SAM:C2	2.13	0.76
1:5:10:GLY:HA3	1:e:975:THR:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:850:ASP:OD2	6:K:1302:SAM:C2'	2.33	0.75
2:K:578:VAL:HG23	6:K:1301:SAM:C4	2.15	0.75
1:5:11:LYS:N	1:e:319:ASP:CG	2.43	0.75
2:L:578:VAL:HG11	2:L:598:LEU:HD22	1.69	0.75
1:5:10:GLY:CA	1:e:975:THR:HG21	2.18	0.74
2:J:552:TYR:HE2	6:J:1302:SAM:C5	1.96	0.74
2:L:552:TYR:CB	6:L:1302:SAM:O2'	2.29	0.74
1:e:723:THR:O	1:e:727:PHE:HB2	1.86	0.74
2:K:850:ASP:OD1	6:K:1302:SAM:C2'	2.36	0.74
2:I:872:TYR:CE1	6:I:1301:SAM:C4	2.71	0.73
2:H:851:ILE:CG2	6:H:1302:SAM:N3	2.43	0.73
1:E:436:ARG:HG3	1:d:859:GLN:HE22	1.52	0.73
1:D:776:VAL:HA	1:D:782:GLN:HE22	1.53	0.73
2:H:851:ILE:HG12	6:H:1302:SAM:O2'	1.88	0.73
2:J:552:TYR:CE2	6:J:1302:SAM:N7	2.57	0.72
1:5:6:ARG:NH1	1:5:6:ARG:HB3	2.04	0.72
1:5:10:GLY:HA3	1:e:975:THR:HG21	1.70	0.72
2:H:577:ASP:C	6:H:1301:SAM:CE	2.60	0.71
2:K:851:ILE:CG2	6:K:1302:SAM:N1	2.52	0.71
2:J:872:TYR:HE1	6:J:1301:SAM:C4	2.02	0.71
2:H:872:TYR:CD1	6:H:1302:SAM:N3	2.52	0.71
2:I:552:TYR:HE2	6:I:1302:SAM:C5	1.92	0.71
2:K:850:ASP:OD2	6:K:1302:SAM:C3'	2.38	0.71
1:4:131:ASN:HD21	1:E:503:ARG:HH12	1.39	0.70
2:K:872:TYR:HE1	6:K:1302:SAM:C4	2.05	0.70
2:L:552:TYR:OH	6:L:1302:SAM:C6	2.39	0.70
3:R:283:HIS:ND1	3:R:776:ASP:OD2	2.25	0.70
2:I:851:ILE:HG23	6:I:1301:SAM:C4	2.22	0.69
2:L:851:ILE:HG12	6:L:1301:SAM:N3	2.07	0.69
2:K:552:TYR:CE2	6:K:1301:SAM:N3	2.60	0.69
1:B:380:GLN:HE21	1:a:958:SER:HB2	1.57	0.69
1:C:336:LYS:HA	1:C:340:ASN:HD22	1.56	0.69
1:e:1232:TYR:HE1	1:e:1253:LEU:HB2	1.57	0.69
2:L:872:TYR:HE1	6:L:1301:SAM:C4	2.06	0.69
2:I:552:TYR:CZ	6:I:1302:SAM:C5	2.59	0.69
1:d:1232:TYR:HE1	1:d:1253:LEU:HB2	1.58	0.69
2:K:851:ILE:HG23	6:K:1302:SAM:N1	2.08	0.68
2:H:851:ILE:CG2	6:H:1302:SAM:C4	2.71	0.68
2:L:552:TYR:H	6:L:1302:SAM:C8	2.06	0.68
1:4:83:LYS:HE2	1:d:971:THR:HG21	1.75	0.68
1:3:97:GLU:O	1:3:101:GLU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:552:TYR:CE1	6:H:1301:SAM:C2	2.76	0.68
2:K:516:GLY:O	6:K:1301:SAM:HB2	1.93	0.68
2:L:552:TYR:HB2	6:L:1302:SAM:C2'	2.24	0.68
1:A:380:GLN:HE21	1:e:958:SER:HB2	1.60	0.67
1:E:426:CYS:SG	1:E:427:VAL:N	2.67	0.67
2:L:552:TYR:CD2	6:L:1302:SAM:N9	2.62	0.67
1:5:10:GLY:CA	1:e:975:THR:HG23	2.25	0.67
1:a:1115:TRP:HE1	1:a:1170:ILE:HG21	1.59	0.67
2:K:577:ASP:OD2	6:K:1301:SAM:OXT	2.13	0.67
2:K:850:ASP:CG	6:K:1302:SAM:C2'	2.68	0.67
2:K:872:TYR:CE1	6:K:1302:SAM:N3	2.42	0.66
2:L:552:TYR:HD2	6:L:1302:SAM:H2'	1.60	0.66
1:b:1115:TRP:HE1	1:b:1170:ILE:HG21	1.59	0.66
1:E:630:PHE:HB2	1:E:772:MET:HE1	1.77	0.66
1:E:761:LEU:HB2	1:E:808:PRO:HB3	1.77	0.66
2:H:578:VAL:CG2	6:H:1301:SAM:C5	2.73	0.66
2:I:552:TYR:CD2	6:I:1302:SAM:N9	2.64	0.66
2:L:552:TYR:CD2	6:L:1302:SAM:C5	2.75	0.66
3:R:148:LYS:HE3	3:R:824:ILE:HD11	1.78	0.66
2:H:871:ASP:OD1	6:H:1302:SAM:C6	2.42	0.66
1:c:987:LEU:HD13	1:c:994:MET:HE1	1.78	0.66
1:5:4:ILE:HG23	1:5:5:PRO:HD2	1.76	0.66
2:K:578:VAL:CG2	6:K:1301:SAM:C4	2.75	0.65
2:H:578:VAL:CG2	6:H:1301:SAM:C4	2.75	0.65
2:H:482:SER:CB	6:H:1301:SAM:OXT	2.45	0.65
3:R:210:LEU:HD23	3:R:212:ALA:H	1.62	0.65
2:K:577:ASP:OD2	6:K:1301:SAM:HB1	1.97	0.65
2:J:514:TYR:OH	6:J:1302:SAM:OXT	2.15	0.65
1:e:373:ASN:HB3	1:e:1259:ARG:HD3	1.77	0.65
1:D:656:MET:HB2	1:D:659:PHE:HB2	1.79	0.64
1:D:858:THR:HG23	1:D:942:GLN:HB2	1.79	0.64
2:J:552:TYR:CE1	6:J:1302:SAM:N1	2.65	0.64
2:L:552:TYR:CG	6:L:1302:SAM:C8	2.80	0.64
1:B:604:VAL:HG13	1:B:875:LEU:HD13	1.78	0.64
1:E:560:MET:SD	1:E:799:LYS:NZ	2.71	0.64
1:a:1034:GLU:HG2	1:a:1207:ARG:HE	1.62	0.64
2:H:829:GLY:O	6:H:1302:SAM:CB	2.46	0.64
2:K:577:ASP:O	6:K:1301:SAM:HG2	1.98	0.64
1:d:569:GLN:HE22	1:d:787:GLN:HG2	1.62	0.64
2:H:851:ILE:HG22	6:H:1302:SAM:C2	2.27	0.64
2:J:889:MET:CB	6:J:1301:SAM:O	2.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:1232:TYR:HE1	1:c:1253:LEU:HB2	1.63	0.64
1:D:399:ALA:HA	1:D:402:TRP:HD1	1.62	0.64
1:D:979:LEU:HD11	1:D:983:LEU:HD23	1.80	0.64
2:H:552:TYR:HE2	6:H:1301:SAM:C5	2.06	0.64
2:J:552:TYR:HE2	6:J:1302:SAM:N7	1.94	0.63
1:a:338:LEU:HD23	1:a:339:LEU:HG	1.81	0.63
2:L:578:VAL:HG22	2:L:598:LEU:HD11	1.80	0.63
2:K:552:TYR:HE2	6:K:1301:SAM:C2	2.12	0.63
1:b:373:ASN:HB3	1:b:1259:ARG:HD3	1.80	0.63
1:c:852:GLN:HG3	1:c:858:THR:HG21	1.80	0.63
1:B:261:GLY:H	1:B:392:ARG:HH22	1.47	0.62
1:A:526:GLY:HA2	1:A:871:VAL:HG13	1.81	0.62
4:U:199:HIS:HB2	4:U:203:ASN:HD21	1.63	0.62
1:5:6:ARG:HB3	1:5:6:ARG:CZ	2.28	0.62
1:B:1120:ARG:NH1	1:b:187:SER:OG	2.32	0.62
1:E:559:THR:HB	1:E:799:LYS:HZ3	1.65	0.62
3:R:657:ARG:NH2	4:U:541:GLY:O	2.32	0.62
1:e:1033:HIS:O	1:e:1207:ARG:NH1	2.32	0.62
2:L:895:ALA:HB2	6:L:1301:SAM:N7	2.14	0.62
3:R:490:LYS:NZ	3:R:531:LEU:O	2.32	0.62
1:e:892:PRO:HD2	1:e:895:LEU:HD12	1.82	0.62
1:5:117:LYS:NZ	3:R:711:THR:O	2.32	0.62
2:L:933:ILE:HG21	2:L:942:ILE:HD13	1.82	0.62
1:a:892:PRO:HD2	1:a:895:LEU:HD12	1.82	0.62
1:4:81:PRO:HG3	1:d:963:ALA:HB1	1.82	0.62
1:d:949:LEU:HD13	1:d:952:ILE:HD12	1.82	0.62
2:K:552:TYR:HH	6:K:1301:SAM:C6	2.11	0.61
1:a:330:ASN:HA	1:a:1147:MET:HE1	1.82	0.61
1:A:993:ARG:HH22	1:a:753:PRO:HA	1.66	0.61
1:c:473:ASN:HA	1:c:506:PRO:HA	1.82	0.61
2:K:933:ILE:HG21	2:K:942:ILE:HD13	1.82	0.61
1:C:761:LEU:HB3	1:C:808:PRO:HB3	1.81	0.61
1:B:562:THR:HB	1:B:799:LYS:HZ2	1.65	0.61
1:5:6:ARG:HH11	1:5:6:ARG:CG	2.13	0.61
1:E:438:GLN:H	1:d:859:GLN:HE21	1.49	0.61
2:I:578:VAL:HG23	6:I:1302:SAM:N9	2.15	0.61
3:R:944:GLN:NE2	3:R:1041:ALA:O	2.34	0.61
1:C:931:LEU:HD22	1:C:984:LEU:HD21	1.83	0.61
3:R:103:LEU:HD21	3:R:113:GLY:HA3	1.82	0.61
2:H:933:ILE:HG21	2:H:942:ILE:HD13	1.82	0.60
1:b:280:VAL:H	1:b:415:ASN:HD21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ILE:O	1:A:703:ARG:NH1	2.35	0.60
1:E:620:VAL:O	1:E:782:GLN:NE2	2.33	0.60
2:I:933:ILE:HG21	2:I:942:ILE:HD13	1.82	0.60
2:H:871:ASP:OD1	6:H:1302:SAM:N1	2.34	0.60
2:K:552:TYR:CG	6:K:1301:SAM:C8	2.84	0.60
1:d:777:ASP:OD1	1:d:794:ARG:NH2	2.32	0.60
1:e:920:ARG:NH2	1:e:982:MET:O	2.33	0.60
2:I:578:VAL:HG23	6:I:1302:SAM:C4	2.30	0.60
1:5:6:ARG:HH11	1:5:6:ARG:HG2	1.65	0.60
2:J:552:TYR:CZ	6:J:1302:SAM:C2	2.84	0.60
1:A:583:PRO:HG2	1:A:586:SER:HA	1.81	0.60
2:L:890:LEU:HB3	6:L:1301:SAM:HB1	1.82	0.60
2:L:872:TYR:CD1	6:L:1301:SAM:C2	2.85	0.60
1:C:480:GLU:HG3	1:C:493:VAL:HG23	1.84	0.60
3:R:580:GLN:HE21	3:R:747:LYS:HE2	1.66	0.59
1:c:777:ASP:OD1	1:c:794:ARG:NH2	2.35	0.59
1:E:455:ASP:HB3	1:E:458:THR:HG22	1.85	0.59
2:L:578:VAL:HG13	2:L:598:LEU:HD13	1.85	0.59
1:B:851:ARG:NH1	1:B:989:SER:OG	2.36	0.59
1:E:237:ALA:HB2	3:R:405:THR:HG21	1.84	0.59
1:C:618:GLY:HA3	1:C:655:MET:HG2	1.82	0.59
1:D:600:TYR:OH	1:D:828:PHE:O	2.19	0.59
2:I:577:ASP:C	6:I:1302:SAM:HE1	2.26	0.59
3:R:1027:THR:HG22	3:R:1028:ARG:HE	1.68	0.59
1:b:468:ARG:HB2	1:b:1019:VAL:HG11	1.85	0.59
2:J:933:ILE:HG21	2:J:942:ILE:HD13	1.82	0.59
1:A:509:ILE:HG12	1:A:918:LEU:HD23	1.85	0.59
1:B:333:HIS:HA	1:B:336:LYS:HG2	1.85	0.59
1:5:4:ILE:CG2	1:5:5:PRO:HD2	2.33	0.59
4:U:532:SER:HA	4:U:535:LEU:HB2	1.84	0.59
1:a:1067:PHE:O	1:a:1138:ARG:NH1	2.35	0.59
1:d:186:CYS:SG	1:d:199:HIS:NE2	2.73	0.59
1:E:1202:THR:HG23	1:E:1203:GLU:HG3	1.83	0.59
3:R:425:LEU:HD12	3:R:698:MET:HE3	1.85	0.59
4:U:39:ASP:OD2	4:U:165:ARG:NH2	2.36	0.59
1:d:468:ARG:HB2	1:d:1019:VAL:HG21	1.83	0.59
1:A:211:LEU:HD12	3:R:1063:MET:HE1	1.84	0.59
3:R:452:ARG:HH12	3:R:980:GLN:HB2	1.67	0.59
2:H:50:ARG:HG3	2:H:51:THR:HG23	1.85	0.58
2:H:851:ILE:HG12	6:H:1302:SAM:C2'	2.33	0.58
2:J:50:ARG:HG3	2:J:51:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:834:GLN:HG3	3:R:1085:ASN:HD21	1.67	0.58
1:A:1123:ASN:O	1:A:1127:ASP:HB2	2.03	0.58
1:D:1067:PHE:O	1:D:1138:ARG:NH1	2.35	0.58
2:J:578:VAL:HG23	6:J:1302:SAM:N9	2.18	0.58
2:L:743:ILE:H	2:L:787:ILE:HB	1.68	0.58
1:e:949:LEU:HD13	1:e:952:ILE:HD12	1.83	0.58
1:b:1241:PRO:HG2	1:b:1244:GLN:HB2	1.86	0.58
1:2:129:ASN:ND2	1:2:132:GLU:OE1	2.37	0.58
1:d:536:LEU:HD11	1:d:604:VAL:HG11	1.84	0.58
1:d:544:GLN:OE1	1:d:545:ARG:NH1	2.33	0.58
1:B:247:LEU:HD21	1:B:828:PHE:HB2	1.86	0.58
1:E:280:VAL:HG11	1:E:1188:HIS:HB3	1.84	0.58
2:H:743:ILE:H	2:H:787:ILE:HB	1.68	0.58
2:L:8:ARG:HH12	2:L:10:ALA:HB2	1.69	0.58
4:U:142:MET:HE3	4:U:146:GLN:HE22	1.68	0.58
2:H:8:ARG:HH12	2:H:10:ALA:HB2	1.69	0.58
2:H:891:SER:HB3	6:H:1302:SAM:HG2	1.85	0.58
3:R:956:LYS:HA	3:R:1030:GLU:HG3	1.86	0.58
2:H:578:VAL:HG21	6:H:1301:SAM:C5	2.33	0.58
2:I:577:ASP:C	6:I:1302:SAM:CE	2.75	0.58
2:J:552:TYR:CD1	6:J:1302:SAM:C2	2.87	0.58
3:R:956:LYS:NZ	3:R:1021:GLN:O	2.37	0.58
1:c:1241:PRO:HG2	1:c:1244:GLN:HB2	1.85	0.58
1:A:1207:ARG:HH22	1:A:1250:VAL:HG12	1.67	0.58
1:c:1045:ILE:HG12	1:c:1141:MET:HE1	1.86	0.58
1:e:455:ASP:HB3	1:e:1253:LEU:HD23	1.84	0.58
2:I:8:ARG:HH12	2:I:10:ALA:HB2	1.69	0.58
6:J:1302:SAM:O	6:J:1302:SAM:HG1	2.02	0.58
2:L:50:ARG:HG3	2:L:51:THR:HG23	1.85	0.58
3:R:248:SER:OG	3:R:350:ARG:NH1	2.37	0.58
4:U:553:GLU:OE2	4:U:577:LYS:NZ	2.36	0.58
1:C:426:CYS:SG	1:C:427:VAL:N	2.76	0.57
1:E:430:ARG:HH12	1:E:1242:PRO:HG3	1.69	0.57
2:I:743:ILE:H	2:I:787:ILE:HB	1.68	0.57
2:J:743:ILE:H	2:J:787:ILE:HB	1.68	0.57
2:K:8:ARG:HH12	2:K:10:ALA:HB2	1.69	0.57
1:d:851:ARG:NH1	1:d:990:GLY:O	2.37	0.57
1:e:524:ASN:ND2	1:e:982:MET:SD	2.77	0.57
1:C:430:ARG:HH12	1:C:1242:PRO:HG3	1.68	0.57
2:H:482:SER:HB2	6:H:1301:SAM:OXT	2.04	0.57
2:J:552:TYR:CD2	6:J:1302:SAM:N3	2.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:50:ARG:HG3	2:K:51:THR:HG23	1.85	0.57
2:K:552:TYR:CE2	6:K:1301:SAM:C2	2.87	0.57
1:a:732:LEU:HD13	1:a:999:ILE:HG21	1.85	0.57
1:e:383:THR:HG22	1:e:385:PHE:H	1.69	0.57
1:A:551:ILE:HD11	1:A:592:ARG:HH12	1.68	0.57
1:C:433:ARG:HD2	1:C:436:ARG:HB3	1.86	0.57
2:I:50:ARG:HG3	2:I:51:THR:HG23	1.85	0.57
3:R:687:THR:O	3:R:691:HIS:ND1	2.35	0.57
1:e:732:LEU:HD13	1:e:999:ILE:HG21	1.85	0.57
2:H:577:ASP:OD2	6:H:1301:SAM:C	2.53	0.57
2:J:8:ARG:HH12	2:J:10:ALA:HB2	1.69	0.57
2:K:830:THR:O	6:K:1302:SAM:HG1	2.04	0.57
1:c:1115:TRP:HE1	1:c:1170:ILE:HG21	1.69	0.57
2:K:743:ILE:H	2:K:787:ILE:HB	1.68	0.57
4:U:229:GLU:HA	4:U:232:LYS:HB3	1.86	0.57
1:1:4:ILE:HD13	1:a:254:ARG:HH22	1.69	0.57
1:A:1067:PHE:O	1:A:1138:ARG:NH1	2.37	0.57
3:R:704:THR:HG23	3:R:705:VAL:HG23	1.87	0.57
1:c:1067:PHE:O	1:c:1138:ARG:NH1	2.38	0.57
1:d:732:LEU:HD13	1:d:999:ILE:HG21	1.86	0.57
1:B:452:GLU:OE2	1:B:1259:ARG:NH2	2.30	0.57
2:I:425:ASP:HB3	2:I:793:VAL:HG12	1.87	0.57
4:U:100:ARG:HH22	1:d:564:SER:HA	1.68	0.57
2:J:355:TYR:O	2:J:371:ARG:NH2	2.38	0.57
3:R:54:ASP:O	3:R:251:ARG:NH1	2.38	0.57
1:e:527:ASN:ND2	1:e:864:LEU:O	2.38	0.57
1:e:562:THR:HG23	1:e:563:VAL:HG13	1.87	0.57
1:C:359:LEU:HD21	1:C:937:GLN:HB2	1.87	0.57
2:H:355:TYR:O	2:H:371:ARG:NH2	2.38	0.57
2:I:567:PRO:HA	2:J:832:PRO:HB2	1.86	0.57
2:L:355:TYR:O	2:L:371:ARG:NH2	2.38	0.57
2:H:577:ASP:OD2	6:H:1301:SAM:HB2	2.05	0.57
2:K:761:ALA:HB1	2:K:838:GLU:HB3	1.87	0.57
2:J:567:PRO:HA	2:K:832:PRO:HB2	1.87	0.56
3:R:195:ARG:HG3	3:R:204:ARG:HH22	1.68	0.56
1:b:514:ARG:NH1	1:b:728:GLY:O	2.38	0.56
1:e:478:GLU:OE1	1:e:508:ARG:NH2	2.38	0.56
2:I:761:ALA:HB1	2:I:838:GLU:HB3	1.87	0.56
1:a:392:ARG:HB3	1:a:406:MET:HE1	1.87	0.56
1:1:87:THR:OG1	1:1:146:ASN:ND2	2.38	0.56
1:5:144:GLY:HA3	1:A:377:GLY:HA2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:THR:HG23	1:A:942:GLN:HB2	1.86	0.56
2:I:850:ASP:OD2	6:I:1301:SAM:C3'	2.53	0.56
3:R:659:PHE:HE2	3:R:681:PRO:HD3	1.70	0.56
3:R:1051:LYS:HD2	3:R:1259:TRP:HD1	1.70	0.56
4:U:678:PRO:HG2	4:U:680:ARG:HD2	1.86	0.56
1:b:482:ALA:HA	1:b:723:THR:HG21	1.86	0.56
1:d:221:THR:HG22	1:d:1267:ILE:HB	1.88	0.56
1:C:421:ASN:OD1	1:b:1082:ARG:NH1	2.39	0.56
1:E:919:GLN:OE1	4:U:244:ASN:ND2	2.39	0.56
2:J:872:TYR:CE1	6:J:1301:SAM:N1	2.73	0.56
1:e:186:CYS:SG	1:e:199:HIS:NE2	2.70	0.56
2:I:552:TYR:CE1	6:I:1302:SAM:C2	2.88	0.56
2:J:200:TYR:HE2	2:J:229:ASN:HB2	1.71	0.56
1:c:524:ASN:ND2	1:c:982:MET:SD	2.79	0.56
2:I:200:TYR:HE2	2:I:229:ASN:HB2	1.71	0.56
2:I:355:TYR:O	2:I:371:ARG:NH2	2.38	0.56
2:I:578:VAL:HG23	6:I:1302:SAM:C8	2.36	0.56
2:I:851:ILE:CG2	6:I:1301:SAM:C6	2.83	0.56
2:L:425:ASP:HB3	2:L:793:VAL:HG12	1.87	0.56
1:e:851:ARG:NH1	1:e:990:GLY:O	2.38	0.56
1:C:749:ASN:HD21	2:J:154:SER:H	1.54	0.56
3:R:328:ASP:OD1	3:R:348:ARG:NH1	2.39	0.56
4:U:95:PRO:O	4:U:103:ARG:NH2	2.39	0.56
1:d:440:MET:HG2	1:d:445:SER:HA	1.88	0.56
1:B:692:GLN:HG3	2:I:245:PRO:HB3	1.87	0.56
3:R:1059:VAL:HA	3:R:1245:ILE:HA	1.88	0.56
1:3:81:PRO:HD3	1:3:141:ASN:HD21	1.70	0.56
2:I:562:LEU:HG	6:I:1302:SAM:H2	1.86	0.56
2:L:200:TYR:HE2	2:L:229:ASN:HB2	1.71	0.56
3:R:450:ILE:HG12	3:R:1116:VAL:HB	1.88	0.56
1:A:399:ALA:HA	1:A:402:TRP:HD1	1.71	0.56
1:D:480:GLU:HG3	1:D:493:VAL:HG23	1.87	0.56
2:H:552:TYR:CZ	6:H:1301:SAM:C2	2.88	0.56
2:J:425:ASP:HB3	2:J:793:VAL:HG12	1.87	0.56
1:B:956:ARG:NH2	1:b:749:ASN:OD1	2.39	0.55
1:D:618:GLY:HA3	1:D:655:MET:HA	1.86	0.55
2:K:355:TYR:O	2:K:371:ARG:NH2	2.38	0.55
2:K:577:ASP:CG	6:K:1301:SAM:HB1	2.31	0.55
1:B:715:ASN:OD1	1:B:837:ARG:NH1	2.39	0.55
1:B:1034:GLU:HG2	1:B:1207:ARG:HE	1.71	0.55
2:K:552:TYR:N	6:K:1301:SAM:H8	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1232:TYR:HE1	1:a:1253:LEU:HB2	1.72	0.55
1:e:440:MET:HG2	1:e:445:SER:HA	1.87	0.55
2:H:567:PRO:HA	2:I:832:PRO:HB2	1.88	0.55
2:H:761:ALA:HB1	2:H:838:GLU:HB3	1.87	0.55
2:I:88:GLU:OE1	2:I:91:ARG:NH2	2.40	0.55
2:L:761:ALA:HB1	2:L:838:GLU:HB3	1.87	0.55
1:b:552:ASP:OD1	1:b:890:LYS:NZ	2.40	0.55
1:A:504:LEU:HD23	1:A:506:PRO:HD3	1.89	0.55
1:B:375:HIS:HB3	1:B:1261:ALA:HB2	1.89	0.55
1:C:392:ARG:NH2	1:C:406:MET:SD	2.80	0.55
1:C:993:ARG:HH22	1:c:753:PRO:HA	1.71	0.55
1:D:452:GLU:OE2	1:D:1259:ARG:NH2	2.36	0.55
2:J:761:ALA:HB1	2:J:838:GLU:HB3	1.87	0.55
2:K:432:GLY:O	2:K:476:ARG:NH2	2.39	0.55
3:R:499:ASN:ND2	3:R:976:ASP:OD2	2.38	0.55
1:B:865:SER:HA	1:B:1000:GLN:HE22	1.72	0.55
1:B:1119:THR:O	1:B:1123:ASN:ND2	2.40	0.55
1:D:603:VAL:HG23	1:D:604:VAL:HG23	1.87	0.55
1:E:324:MET:HE1	1:E:1038:PHE:HA	1.89	0.55
1:E:480:GLU:HG3	1:E:493:VAL:HG23	1.88	0.55
2:J:552:TYR:CG	6:J:1302:SAM:N3	2.74	0.55
2:K:564:ARG:HH21	2:L:776:ASP:HB2	1.71	0.55
3:R:1208:ASN:HB3	3:R:1245:ILE:H	1.72	0.55
1:a:1209:LEU:HD21	1:a:1212:THR:HG23	1.87	0.55
1:B:1163:THR:HG21	1:B:1198:TYR:HB2	1.89	0.55
1:E:224:ILE:HB	4:U:379:PRO:HG2	1.89	0.55
2:J:432:GLY:O	2:J:476:ARG:NH2	2.39	0.55
2:K:200:TYR:HE2	2:K:229:ASN:HB2	1.71	0.55
3:R:170:PRO:O	3:R:173:GLN:NE2	2.39	0.55
1:5:130:ALA:HB3	1:A:496:PRO:HG3	1.89	0.55
2:H:425:ASP:HB3	2:H:793:VAL:HG12	1.87	0.55
2:I:872:TYR:HD1	6:I:1301:SAM:H2	1.68	0.55
2:L:432:GLY:O	2:L:476:ARG:NH2	2.39	0.55
2:L:577:ASP:O	2:L:578:VAL:C	2.48	0.55
1:D:1267:ILE:HA	1:D:1270:VAL:HG12	1.89	0.55
2:I:552:TYR:CE1	6:I:1302:SAM:N1	2.75	0.55
2:I:851:ILE:HG21	6:I:1301:SAM:C6	2.36	0.55
2:K:88:GLU:OE1	2:K:91:ARG:NH2	2.40	0.55
3:R:148:LYS:HG2	3:R:803:LYS:HB2	1.88	0.55
3:R:186:PRO:HB2	3:R:237:ALA:HB2	1.88	0.55
1:a:527:ASN:ND2	1:a:864:LEU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ALA:O	1:A:710:HIS:ND1	2.31	0.55
1:c:263:CYS:SG	1:c:462:ARG:NH1	2.80	0.55
2:K:425:ASP:HB3	2:K:793:VAL:HG12	1.87	0.54
3:R:147:ILE:HA	3:R:802:GLY:HA2	1.89	0.54
1:A:421:ASN:OD1	1:e:1082:ARG:NH1	2.40	0.54
1:B:1116:GLN:HB3	1:B:1172:PRO:HA	1.89	0.54
2:L:88:GLU:OE1	2:L:91:ARG:NH2	2.40	0.54
3:R:690:GLU:OE2	3:R:694:ASN:ND2	2.40	0.54
1:B:189:VAL:O	3:R:879:LYS:NZ	2.39	0.54
2:J:88:GLU:OE1	2:J:91:ARG:NH2	2.40	0.54
1:a:309:ARG:O	1:a:311:ALA:N	2.38	0.54
1:A:268:ILE:HG12	1:A:304:ILE:HG22	1.89	0.54
1:B:858:THR:HG23	1:B:942:GLN:HB2	1.90	0.54
1:E:858:THR:HG23	1:E:942:GLN:HB2	1.89	0.54
2:K:872:TYR:CD1	6:K:1302:SAM:N1	2.70	0.54
1:C:268:ILE:HG12	1:C:304:ILE:HG22	1.90	0.54
1:E:1067:PHE:O	1:E:1138:ARG:NH1	2.40	0.54
2:H:200:TYR:HE2	2:H:229:ASN:HB2	1.71	0.54
2:K:850:ASP:CG	6:K:1302:SAM:C1'	2.70	0.54
3:R:395:ILE:HG23	3:R:767:PHE:HA	1.90	0.54
1:d:333:HIS:HA	1:d:336:LYS:HG2	1.88	0.54
1:A:1081:CYS:HA	1:A:1095:ARG:HB3	1.89	0.54
1:D:692:GLN:HE22	2:L:95:TYR:HD2	1.55	0.54
2:I:432:GLY:O	2:I:476:ARG:NH2	2.39	0.54
4:U:455:THR:HG23	4:U:458:HIS:HB2	1.90	0.54
2:L:872:TYR:CE1	6:L:1301:SAM:C5	2.90	0.54
1:c:468:ARG:HB2	1:c:1019:VAL:HG21	1.89	0.54
1:5:11:LYS:CB	1:e:319:ASP:O	2.45	0.54
1:E:268:ILE:HG12	1:E:304:ILE:HG22	1.89	0.54
4:U:60:ILE:HD12	4:U:234:PHE:HD1	1.72	0.54
1:a:333:HIS:HA	1:a:336:LYS:HG2	1.88	0.54
1:a:524:ASN:ND2	1:a:982:MET:SD	2.81	0.54
1:d:657:VAL:HG22	1:d:671:GLN:HG3	1.90	0.54
1:2:56:ARG:NH1	1:B:342:GLU:OE1	2.41	0.54
1:C:455:ASP:HB3	1:C:458:THR:HG22	1.89	0.54
2:I:578:VAL:HA	6:I:1302:SAM:HE1	1.90	0.54
4:U:101:ARG:HG2	4:U:121:LEU:HD21	1.89	0.54
1:a:381:ASP:OD2	1:a:410:ARG:NH1	2.40	0.54
1:c:452:GLU:OE2	1:c:1259:ARG:NH2	2.38	0.54
1:B:860:PRO:O	1:B:864:LEU:HB2	2.08	0.54
1:D:385:PHE:O	1:D:428:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:GLU:OE1	2:H:91:ARG:NH2	2.40	0.54
2:L:552:TYR:CZ	6:L:1302:SAM:N6	2.71	0.54
1:b:850:THR:HB	1:b:998:ALA:HB3	1.90	0.54
1:d:822:ILE:HG12	1:d:908:MET:HE1	1.90	0.54
1:C:466:MET:HG2	1:C:1260:TYR:HE2	1.73	0.53
1:b:892:PRO:HD2	1:b:895:LEU:HD12	1.89	0.53
1:C:452:GLU:OE2	1:C:1259:ARG:NH2	2.33	0.53
2:L:552:TYR:CD2	6:L:1302:SAM:C8	2.92	0.53
3:R:306:TYR:OH	3:R:556:SER:O	2.23	0.53
1:b:466:MET:HG3	1:b:1260:TYR:HE2	1.73	0.53
1:b:1034:GLU:OE2	1:b:1207:ARG:NH2	2.41	0.53
1:3:4:ILE:HG21	1:c:254:ARG:HH22	1.73	0.53
1:C:454:SER:OG	1:C:1255:ASN:OD1	2.25	0.53
1:D:1120:ARG:NH2	1:d:225:SER:O	2.42	0.53
2:K:446:ARG:NH1	2:K:447:VAL:O	2.42	0.53
3:R:472:ALA:HA	4:U:695:LYS:HE2	1.90	0.53
4:U:441:HIS:HB2	4:U:524:LEU:HG	1.90	0.53
1:A:759:ASN:HB2	1:A:812:GLN:HE21	1.72	0.53
2:K:552:TYR:CD2	6:K:1301:SAM:C8	2.90	0.53
1:b:934:LEU:HD11	1:b:1024:VAL:HG11	1.90	0.53
1:C:826:LEU:HD12	1:C:827:PRO:HD2	1.90	0.53
2:H:432:GLY:O	2:H:476:ARG:NH2	2.39	0.53
1:d:351:PRO:HG2	1:d:1116:GLN:HE22	1.73	0.53
1:A:527:ASN:HD21	1:a:795:GLY:HA3	1.73	0.53
1:B:573:PRO:HA	1:B:623:LEU:HD21	1.90	0.53
1:C:1067:PHE:O	1:C:1138:ARG:NH1	2.36	0.53
1:E:1124:GLN:NE2	1:e:182:GLN:OE1	2.39	0.53
2:H:552:TYR:CE1	6:H:1301:SAM:N1	2.76	0.53
1:a:761:LEU:HB2	1:a:808:PRO:HB3	1.91	0.53
1:e:468:ARG:HB2	1:e:1019:VAL:HG21	1.90	0.53
1:e:1209:LEU:HD21	1:e:1212:THR:HG23	1.90	0.53
1:5:10:GLY:HA2	1:e:975:THR:CG2	2.39	0.53
1:A:1062:PRO:HG2	1:A:1065:LEU:HD13	1.89	0.53
1:A:1096:ASP:HB3	1:A:1100:MET:H	1.73	0.53
1:D:278:GLN:HE21	1:D:281:LEU:HB3	1.72	0.53
2:H:446:ARG:NH1	2:H:447:VAL:O	2.42	0.53
1:B:181:TYR:HB2	1:B:189:VAL:HB	1.90	0.53
2:H:832:PRO:HB2	2:L:567:PRO:HA	1.91	0.53
1:a:949:LEU:HD13	1:a:952:ILE:HD12	1.91	0.53
1:1:166:PRO:HB3	1:B:290:TYR:HE1	1.74	0.53
1:3:87:THR:OG1	1:3:146:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG12	1:B:243:LYS:HE2	1.91	0.53
1:B:1067:PHE:O	1:B:1138:ARG:NH1	2.36	0.53
1:D:650:MET:HE3	1:D:685:PRO:HG3	1.91	0.53
2:H:570:ASP:OD1	2:I:852:ARG:NH1	2.42	0.53
2:H:852:ARG:NH1	2:L:570:ASP:OD1	2.41	0.53
2:I:160:HIS:O	1:a:667:GLN:NE2	2.42	0.53
2:K:145:ASP:O	2:K:149:THR:HB	2.09	0.53
4:U:444:ASP:HB3	4:U:447:GLU:HG3	1.91	0.53
1:b:1049:ARG:NH1	1:b:1131:LYS:O	2.42	0.53
1:1:122:TYR:HD2	1:a:529:ALA:HB1	1.75	0.53
1:5:6:ARG:CZ	1:5:6:ARG:CB	2.87	0.53
1:a:335:PHE:O	1:a:357:ASN:ND2	2.42	0.53
1:b:920:ARG:NH2	1:b:982:MET:O	2.42	0.53
1:c:430:ARG:O	1:c:1254:TYR:OH	2.26	0.53
1:e:261:GLY:HA3	1:e:312:SER:HA	1.91	0.53
1:A:755:LEU:HA	1:A:809:MET:HE1	1.91	0.52
1:E:478:GLU:OE1	1:E:508:ARG:NH2	2.42	0.52
2:J:145:ASP:O	2:J:149:THR:HB	2.09	0.52
2:J:851:ILE:HG23	6:J:1301:SAM:C2	2.39	0.52
3:R:385:VAL:HG11	3:R:663:VAL:HG21	1.90	0.52
1:e:851:ARG:NH2	1:e:989:SER:OG	2.42	0.52
1:B:705:TRP:HE3	1:B:771:LEU:HD13	1.73	0.52
1:D:1119:THR:O	1:D:1123:ASN:ND2	2.42	0.52
2:H:145:ASP:O	2:H:149:THR:HB	2.09	0.52
2:J:446:ARG:NH1	2:J:447:VAL:O	2.42	0.52
2:K:515:PHE:HB2	2:K:576:SER:HA	1.92	0.52
3:R:543:THR:HB	3:R:686:ALA:HB2	1.91	0.52
4:U:105:ARG:NH2	4:U:117:GLU:OE2	2.37	0.52
1:b:430:ARG:O	1:b:1254:TYR:OH	2.28	0.52
1:d:948:TYR:HE2	1:d:1025:GLN:HB3	1.73	0.52
1:e:314:VAL:HG12	1:e:316:PHE:H	1.73	0.52
1:A:892:PRO:HA	3:R:301:GLU:HG2	1.91	0.52
1:E:732:LEU:HD23	1:E:999:ILE:HG21	1.91	0.52
1:b:272:VAL:HG22	1:b:301:VAL:HG12	1.91	0.52
1:b:452:GLU:OE2	1:b:1259:ARG:NH2	2.42	0.52
1:B:745:HIS:ND1	1:B:812:GLN:O	2.41	0.52
1:E:1080:ASP:OD1	1:E:1095:ARG:NH2	2.43	0.52
2:I:145:ASP:O	2:I:149:THR:HB	2.09	0.52
2:I:446:ARG:NH1	2:I:447:VAL:O	2.42	0.52
2:J:578:VAL:HG23	6:J:1302:SAM:C4	2.40	0.52
3:R:465:THR:OG1	3:R:512:ASP:OD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:546:ILE:HG13	1:c:904:ALA:HB1	1.92	0.52
1:e:504:LEU:HD23	1:e:506:PRO:HD3	1.91	0.52
1:B:931:LEU:HD22	1:B:984:LEU:HD13	1.91	0.52
1:C:189:VAL:O	3:R:930:ASN:ND2	2.43	0.52
2:H:577:ASP:CG	6:H:1301:SAM:HB2	2.34	0.52
2:J:552:TYR:CE2	6:J:1302:SAM:C8	2.92	0.52
3:R:379:ARG:HE	3:R:384:THR:HG22	1.74	0.52
4:U:100:ARG:NH2	1:d:563:VAL:O	2.42	0.52
1:1:6:ARG:NH2	1:a:975:THR:O	2.38	0.52
1:A:713:TRP:O	1:A:837:ARG:NH1	2.43	0.52
1:B:351:PRO:HG3	1:B:1116:GLN:HE22	1.75	0.52
1:B:1062:PRO:HG2	1:B:1065:LEU:HD13	1.91	0.52
1:D:841:ASP:O	1:D:1003:GLN:NE2	2.43	0.52
1:E:438:GLN:NE2	1:E:440:MET:O	2.41	0.52
2:J:861:TRP:CD1	2:J:865:THR:HG1	2.28	0.52
2:L:145:ASP:O	2:L:149:THR:HB	2.09	0.52
2:L:861:TRP:CD1	2:L:865:THR:HG1	2.28	0.52
3:R:81:VAL:HB	3:R:671:ASN:HD21	1.74	0.52
1:a:538:ASP:HA	1:a:541:VAL:HG12	1.91	0.52
1:c:732:LEU:HD13	1:c:999:ILE:HG21	1.91	0.52
1:5:10:GLY:HA2	1:e:975:THR:HG21	1.92	0.52
1:A:339:LEU:HB2	1:A:353:MET:HG2	1.91	0.52
1:B:552:ASP:O	1:B:888:SER:OG	2.27	0.52
1:C:985:GLU:HA	1:C:988:LEU:HD23	1.90	0.52
1:D:546:ILE:HD11	1:D:905:ILE:HG12	1.90	0.52
1:D:801:LYS:HG3	1:D:802:LEU:HG	1.90	0.52
2:L:446:ARG:NH1	2:L:447:VAL:O	2.42	0.52
1:a:852:GLN:HG3	1:a:858:THR:HG21	1.90	0.52
1:b:1057:SER:HB2	1:b:1223:PRO:HG3	1.91	0.52
1:c:560:MET:HE1	1:c:796:THR:HG23	1.90	0.52
1:c:898:ASN:ND2	1:c:1275:PRO:O	2.42	0.52
2:H:515:PHE:HB2	2:H:576:SER:HA	1.92	0.52
2:J:570:ASP:OD1	2:K:852:ARG:NH1	2.43	0.52
3:R:1077:LEU:HD11	3:R:1097:PRO:HG3	1.92	0.52
1:c:186:CYS:SG	1:c:199:HIS:NE2	2.71	0.52
1:C:399:ALA:HA	1:C:402:TRP:HD1	1.74	0.52
1:C:638:LEU:HD11	1:C:886:LEU:HD21	1.92	0.52
1:E:290:TYR:HE2	1:d:1121:TYR:HD1	1.57	0.52
2:H:578:VAL:CG2	6:H:1301:SAM:C8	2.84	0.52
2:J:578:VAL:HG23	6:J:1302:SAM:C8	2.40	0.52
2:L:872:TYR:CE1	6:L:1301:SAM:C6	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:892:PRO:HD2	1:d:895:LEU:HD12	1.91	0.52
2:I:44:ARG:NH2	2:I:58:GLN:OE1	2.44	0.52
1:b:333:HIS:HA	1:b:336:LYS:HG2	1.91	0.52
1:C:1119:THR:O	1:C:1123:ASN:ND2	2.42	0.51
1:D:385:PHE:HE1	1:c:1117:MET:HA	1.75	0.51
2:K:44:ARG:NH2	2:K:58:GLN:OE1	2.44	0.51
3:R:1222:LEU:HD13	3:R:1225:LEU:HD23	1.91	0.51
1:b:949:LEU:HD13	1:b:952:ILE:HD12	1.91	0.51
1:C:1036:ASN:HD21	1:C:1205:ASN:HD22	1.59	0.51
1:D:336:LYS:HA	1:D:340:ASN:HD22	1.74	0.51
3:R:197:ILE:HD12	3:R:221:ARG:HG3	1.92	0.51
3:R:418:THR:HG22	3:R:420:SER:H	1.75	0.51
1:a:227:TRP:NE1	1:a:903:ASP:OD1	2.43	0.51
1:a:336:LYS:HA	1:a:340:ASN:HD22	1.75	0.51
1:b:336:LYS:NZ	1:b:346:VAL:O	2.36	0.51
1:c:920:ARG:NH2	1:c:982:MET:O	2.36	0.51
1:B:399:ALA:HA	1:B:402:TRP:HD1	1.75	0.51
1:c:264:THR:HB	1:c:454:SER:HA	1.93	0.51
1:2:89:GLY:HA3	1:2:137:GLY:HA3	1.92	0.51
2:H:44:ARG:NH2	2:H:58:GLN:OE1	2.43	0.51
2:H:278:ARG:HD2	2:H:281:GLN:HG3	1.93	0.51
2:L:278:ARG:HD2	2:L:281:GLN:HG3	1.93	0.51
4:U:443:VAL:HB	4:U:526:THR:HA	1.92	0.51
1:A:970:ASN:ND2	1:A:985:GLU:OE2	2.44	0.51
1:B:1082:ARG:H	1:B:1095:ARG:HB3	1.75	0.51
1:E:552:ASP:HB2	1:E:890:LYS:HB3	1.93	0.51
2:L:44:ARG:NH2	2:L:58:GLN:OE1	2.44	0.51
1:2:78:GLU:HG3	1:2:89:GLY:HA2	1.93	0.51
1:B:278:GLN:HE21	1:B:281:LEU:HB3	1.74	0.51
1:C:711:ARG:HH21	2:J:242:VAL:HG12	1.76	0.51
2:J:515:PHE:HB2	2:J:576:SER:HA	1.92	0.51
3:R:83:ARG:HD3	3:R:92:VAL:HA	1.93	0.51
1:a:599:LEU:HA	1:a:832:GLN:HE21	1.75	0.51
1:b:1095:ARG:HE	1:b:1099:GLY:HA2	1.76	0.51
1:d:260:ALA:HB3	1:d:313:ASN:HB3	1.91	0.51
1:d:339:LEU:HD23	1:d:353:MET:HG2	1.92	0.51
1:e:852:GLN:HG3	1:e:858:THR:HG21	1.92	0.51
1:e:1045:ILE:HG12	1:e:1141:MET:HE1	1.93	0.51
1:D:333:HIS:HA	1:D:336:LYS:HG2	1.92	0.51
1:E:278:GLN:HE21	1:E:281:LEU:HB3	1.76	0.51
2:H:13:LEU:HD22	2:H:379:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:44:ARG:NH2	2:J:58:GLN:OE1	2.44	0.51
4:U:11:ASP:HA	4:U:39:ASP:HA	1.93	0.51
1:a:920:ARG:NH2	1:a:982:MET:O	2.39	0.51
1:b:478:GLU:HB3	1:b:726:VAL:HG11	1.93	0.51
1:b:931:LEU:HD22	1:b:984:LEU:HD23	1.93	0.51
1:c:1055:LEU:HB2	1:c:1183:PRO:HG3	1.92	0.51
1:B:664:MET:HE1	1:B:685:PRO:HG3	1.93	0.51
1:C:970:ASN:ND2	1:C:985:GLU:OE2	2.44	0.51
1:E:704:GLN:HE22	1:E:774:ASN:HD22	1.58	0.51
4:U:451:GLN:HE22	4:U:514:PHE:HB2	1.75	0.51
1:c:262:LEU:HD21	1:c:406:MET:HG2	1.93	0.51
1:d:543:LEU:O	1:d:547:SER:HB3	2.11	0.51
1:e:303:ARG:HD2	1:e:327:PRO:HG2	1.92	0.51
1:D:1272:MET:HB3	1:D:1274:VAL:HG13	1.93	0.51
1:E:692:GLN:HE22	2:H:95:TYR:HD2	1.59	0.51
1:E:892:PRO:HD2	1:E:895:LEU:HD13	1.93	0.51
4:U:327:ILE:HG13	4:U:357:LEU:HD21	1.92	0.51
1:a:504:LEU:HD23	1:a:506:PRO:HD3	1.93	0.51
1:b:606:THR:HG22	1:b:875:LEU:HD23	1.91	0.51
1:d:508:ARG:HH12	1:d:726:VAL:HG12	1.76	0.51
1:2:128:ASN:ND2	1:C:494:THR:O	2.44	0.51
1:B:466:MET:HG2	1:B:1260:TYR:HE2	1.75	0.51
2:L:13:LEU:HD22	2:L:379:MET:HG3	1.93	0.51
1:d:601:ASN:ND2	1:d:833:VAL:O	2.43	0.51
1:d:898:ASN:ND2	1:d:1275:PRO:O	2.44	0.51
1:e:1241:PRO:HG2	1:e:1244:GLN:HB2	1.93	0.51
1:2:63:GLN:HA	1:2:66:THR:HG22	1.92	0.50
1:C:578:LEU:O	1:C:582:ARG:NH1	2.38	0.50
1:D:732:LEU:HD23	1:D:999:ILE:HG21	1.91	0.50
1:D:842:ARG:HA	1:D:1003:GLN:HE21	1.77	0.50
2:L:512:VAL:HG12	2:L:573:PHE:HB3	1.93	0.50
1:a:258:TRP:HB3	1:a:374:ARG:HD3	1.92	0.50
1:1:2:LYS:HZ3	1:a:374:ARG:HH22	1.59	0.50
1:C:332:ILE:HG21	1:C:347:ARG:HA	1.93	0.50
1:E:692:GLN:HB2	2:L:245:PRO:HB3	1.93	0.50
1:E:1007:ARG:NH2	2:L:290:GLN:O	2.44	0.50
2:H:851:ILE:CG2	6:H:1302:SAM:N1	2.73	0.50
2:I:515:PHE:HB2	2:I:576:SER:HA	1.92	0.50
2:J:512:VAL:HG12	2:J:573:PHE:HB3	1.93	0.50
2:L:578:VAL:HA	6:L:1302:SAM:HE1	1.93	0.50
1:d:335:PHE:O	1:d:357:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:500:SER:OG	1:e:502:ASN:OD1	2.26	0.50
1:B:851:ARG:NH1	1:B:986:PRO:O	2.44	0.50
3:R:1217:TRP:HE3	3:R:1221:ILE:HD13	1.75	0.50
1:b:987:LEU:HD13	1:b:994:MET:HE1	1.93	0.50
1:c:234:GLN:HE21	1:c:911:ASP:HA	1.75	0.50
1:c:306:VAL:HG21	1:c:1038:PHE:HD1	1.76	0.50
1:d:466:MET:HG3	1:d:1260:TYR:HE2	1.77	0.50
1:4:4:ILE:HG21	1:d:254:ARG:HH22	1.76	0.50
1:A:416:VAL:HG21	1:e:1084:SER:HB2	1.93	0.50
1:D:416:VAL:HG21	1:c:1084:SER:HB3	1.93	0.50
2:J:13:LEU:HD22	2:J:379:MET:HG3	1.93	0.50
2:J:278:ARG:HD2	2:J:281:GLN:HG3	1.93	0.50
3:R:470:LEU:HD21	3:R:508:ALA:HB2	1.92	0.50
4:U:462:GLU:OE1	4:U:465:LYS:NZ	2.44	0.50
1:C:618:GLY:O	1:C:625:ASN:ND2	2.45	0.50
1:C:759:ASN:O	1:C:763:ASN:ND2	2.45	0.50
1:2:63:GLN:OE1	1:b:246:GLN:NE2	2.43	0.50
1:A:614:PRO:HB2	1:A:625:ASN:HD22	1.76	0.50
2:H:512:VAL:HG12	2:H:573:PHE:HB3	1.93	0.50
2:K:13:LEU:HD22	2:K:379:MET:HG3	1.93	0.50
2:K:552:TYR:HE2	6:K:1301:SAM:N3	2.07	0.50
2:K:872:TYR:CE1	6:K:1302:SAM:C6	2.95	0.50
1:B:700:PRO:HG2	1:B:701:ILE:HD12	1.93	0.50
1:D:731:ASN:ND2	1:D:735:PRO:O	2.44	0.50
1:E:731:ASN:ND2	1:E:735:PRO:O	2.45	0.50
2:L:741:ILE:HG22	2:L:754:ILE:HG12	1.94	0.50
3:R:295:PRO:HG3	3:R:1075:LEU:HD21	1.93	0.50
1:c:1203:GLU:OE2	1:c:1205:ASN:ND2	2.44	0.50
1:2:131:ASN:HD22	1:C:498:ALA:HB3	1.77	0.50
1:3:128:ASN:ND2	1:D:494:THR:O	2.43	0.50
1:A:620:VAL:HG11	1:A:656:MET:HE2	1.93	0.50
1:E:246:GLN:HE21	1:E:982:MET:HB3	1.76	0.50
2:I:278:ARG:HD2	2:I:281:GLN:HG3	1.93	0.50
1:b:504:LEU:HD23	1:b:506:PRO:HD3	1.94	0.50
1:B:689:MET:HE1	1:B:840:ARG:HH11	1.77	0.50
1:C:576:SER:OG	1:C:627:TRP:NE1	2.45	0.50
2:H:872:TYR:H	6:H:1302:SAM:H2	1.77	0.50
1:b:690:ASN:HB3	1:b:693:LEU:HD13	1.94	0.50
1:d:706:ALA:O	1:d:710:HIS:ND1	2.35	0.50
1:B:1068:ASP:OD1	1:B:1071:THR:OG1	2.30	0.49
1:C:731:ASN:ND2	1:C:735:PRO:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:HIS:HA	1:E:336:LYS:HG2	1.94	0.49
2:K:278:ARG:HD2	2:K:281:GLN:HG3	1.93	0.49
2:L:851:ILE:HG23	6:L:1301:SAM:C2	2.42	0.49
1:c:268:ILE:HG12	1:c:304:ILE:HG12	1.94	0.49
1:c:1065:LEU:O	1:c:1136:ARG:NH2	2.45	0.49
2:I:13:LEU:HD22	2:I:379:MET:HG3	1.93	0.49
1:e:694:ILE:O	1:e:703:ARG:NH1	2.44	0.49
1:4:145:SER:O	1:4:153:ARG:NH2	2.40	0.49
1:5:160:ALA:O	1:A:293:GLN:NE2	2.45	0.49
1:A:1034:GLU:HG2	1:A:1207:ARG:HE	1.77	0.49
1:B:272:VAL:HG23	1:B:300:ALA:HB3	1.94	0.49
2:H:741:ILE:HG22	2:H:754:ILE:HG12	1.94	0.49
3:R:709:GLU:OE2	1:e:582:ARG:NH2	2.45	0.49
1:1:71:LEU:HD12	1:1:72:PRO:HD2	1.95	0.49
1:E:309:ARG:NH2	1:E:320:SER:O	2.45	0.49
2:I:733:ASN:O	2:I:762:SER:OG	2.31	0.49
1:a:523:MET:HE3	1:a:986:PRO:HB2	1.94	0.49
1:c:588:PHE:HE1	1:c:884:VAL:HG13	1.77	0.49
1:e:392:ARG:HH12	1:e:1259:ARG:HE	1.60	0.49
3:R:1142:THR:HG22	3:R:1156:ASP:HA	1.94	0.49
4:U:431:VAL:HG12	4:U:432:LEU:HG	1.94	0.49
1:a:303:ARG:HA	1:a:1210:PHE:H	1.78	0.49
1:B:362:LEU:HD22	1:B:1027:THR:HG22	1.94	0.49
1:D:761:LEU:HB2	1:D:808:PRO:HB3	1.95	0.49
2:H:577:ASP:OD2	6:H:1301:SAM:CB	2.60	0.49
2:K:96:GLU:OE2	2:K:99:ARG:NH2	2.45	0.49
2:K:512:VAL:HG12	2:K:573:PHE:HB3	1.93	0.49
3:R:28:GLU:HA	3:R:864:GLN:HE22	1.78	0.49
4:U:57:GLY:HA2	4:U:237:ARG:HH12	1.78	0.49
1:a:392:ARG:NE	1:a:452:GLU:OE1	2.42	0.49
1:d:186:CYS:SG	1:d:203:HIS:NE2	2.63	0.49
1:4:6:ARG:NH2	1:d:975:THR:O	2.40	0.49
1:C:776:VAL:HG23	1:C:785:TRP:HZ3	1.77	0.49
1:D:601:ASN:ND2	1:D:833:VAL:O	2.34	0.49
2:I:512:VAL:HG12	2:I:573:PHE:HB3	1.93	0.49
2:K:861:TRP:CD1	2:K:865:THR:HG1	2.30	0.49
3:R:83:ARG:NH1	3:R:91:ASP:O	2.46	0.49
1:4:11:LYS:NZ	1:d:321:SER:O	2.36	0.49
2:H:861:TRP:CD1	2:H:865:THR:HG1	2.30	0.49
2:I:552:TYR:HB2	6:I:1302:SAM:C2'	2.40	0.49
2:I:578:VAL:CG2	6:I:1302:SAM:C4	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:872:TYR:CE1	6:L:1301:SAM:C2	2.96	0.49
1:a:280:VAL:H	1:a:415:ASN:HB3	1.76	0.49
1:a:600:TYR:OH	1:a:828:PHE:O	2.27	0.49
1:A:480:GLU:HG3	1:A:493:VAL:HG23	1.94	0.49
1:B:353:MET:O	1:B:357:ASN:ND2	2.46	0.49
1:D:719:ILE:HG22	1:D:739:LEU:HB3	1.94	0.49
2:I:96:GLU:OE2	2:I:99:ARG:NH2	2.45	0.49
3:R:840:ARG:HA	3:R:843:TRP:HD1	1.77	0.49
1:a:1171:THR:HG23	1:a:1174:SER:H	1.78	0.49
1:e:987:LEU:HB3	1:e:994:MET:HE1	1.95	0.49
1:1:148:LYS:O	1:1:153:ARG:NH2	2.46	0.49
1:3:87:THR:HG21	1:3:140:ASP:HA	1.94	0.49
1:5:87:THR:HG21	1:5:140:ASP:HA	1.95	0.49
1:A:719:ILE:HG22	1:A:739:LEU:HB3	1.95	0.49
1:B:509:ILE:HG12	1:B:918:LEU:HD23	1.94	0.49
1:E:261:GLY:HA3	1:E:312:SER:HA	1.95	0.49
4:U:76:LEU:HD21	4:U:168:LEU:HD13	1.94	0.49
4:U:531:ASP:OD2	4:U:545:ARG:NE	2.37	0.49
1:b:713:TRP:HB3	1:b:837:ARG:HH21	1.77	0.49
1:e:430:ARG:O	1:e:1254:TYR:OH	2.29	0.49
1:e:984:LEU:HD12	1:e:987:LEU:HD12	1.95	0.49
1:5:140:ASP:OD1	1:5:144:GLY:N	2.41	0.48
2:I:508:ALA:HB2	2:I:542:PRO:HB2	1.95	0.48
2:J:733:ASN:O	2:J:762:SER:OG	2.31	0.48
1:c:599:LEU:HA	1:c:832:GLN:HE21	1.78	0.48
1:c:1120:ARG:HH22	1:c:1168:GLU:HA	1.78	0.48
1:A:466:MET:HG2	1:A:1260:TYR:HE2	1.77	0.48
1:D:529:ALA:HA	1:D:532:ILE:HB	1.95	0.48
1:E:353:MET:O	1:E:357:ASN:ND2	2.46	0.48
1:E:790:VAL:O	1:E:794:ARG:HD3	2.12	0.48
2:H:733:ASN:O	2:H:762:SER:OG	2.31	0.48
2:H:832:PRO:HA	2:H:854:THR:HA	1.95	0.48
2:H:851:ILE:HG22	2:H:871:ASP:HA	1.95	0.48
2:I:851:ILE:HG22	2:I:871:ASP:HA	1.95	0.48
2:K:741:ILE:HG22	2:K:754:ILE:HG12	1.94	0.48
2:K:832:PRO:HA	2:K:854:THR:HA	1.95	0.48
2:K:851:ILE:HG22	2:K:871:ASP:HA	1.95	0.48
3:R:430:TYR:HE1	3:R:608:GLU:HG3	1.78	0.48
1:a:417:SER:H	1:a:420:CYS:HB2	1.76	0.48
1:c:761:LEU:HB2	1:c:808:PRO:HB3	1.93	0.48
1:A:455:ASP:HB3	1:A:458:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:GLU:OE2	1:A:792:SER:OG	2.30	0.48
1:C:1186:SER:HB3	1:C:1221:ALA:HB3	1.95	0.48
1:D:290:TYR:HE2	1:c:1121:TYR:HD1	1.61	0.48
1:D:465:TRP:HZ3	1:D:1020:ILE:HD11	1.78	0.48
2:J:741:ILE:HG22	2:J:754:ILE:HG12	1.94	0.48
2:K:733:ASN:O	2:K:762:SER:OG	2.31	0.48
2:K:831:GLY:HA2	6:K:1302:SAM:O3'	2.12	0.48
2:K:938:GLY:O	2:K:953:LYS:NZ	2.47	0.48
1:e:1067:PHE:O	1:e:1138:ARG:NH1	2.46	0.48
1:D:1233:ASN:ND2	1:D:1244:GLN:OE1	2.46	0.48
1:E:631:ILE:HG23	1:E:883:THR:HG21	1.96	0.48
2:H:508:ALA:HB2	2:H:542:PRO:HB2	1.95	0.48
2:H:776:ASP:HB2	2:L:564:ARG:HH21	1.78	0.48
3:R:4:MET:O	3:R:7:THR:OG1	2.31	0.48
3:R:162:GLU:OE1	3:R:837:ARG:NE	2.46	0.48
4:U:681:VAL:O	4:U:711:MET:N	2.46	0.48
1:c:970:ASN:ND2	1:c:985:GLU:OE2	2.46	0.48
1:e:355:ARG:NH2	1:e:952:ILE:O	2.46	0.48
1:C:355:ARG:NH2	1:C:952:ILE:O	2.46	0.48
1:D:970:ASN:ND2	1:D:985:GLU:OE2	2.47	0.48
2:I:741:ILE:HG22	2:I:754:ILE:HG12	1.94	0.48
2:I:885:ILE:HG13	2:I:922:LEU:HA	1.96	0.48
2:J:938:GLY:O	2:J:953:LYS:NZ	2.47	0.48
2:K:498:ASP:OD2	2:K:501:THR:OG1	2.31	0.48
1:c:455:ASP:OD1	1:c:458:THR:OG1	2.26	0.48
1:d:507:TYR:HE2	1:d:1267:ILE:HD11	1.78	0.48
1:5:98:ALA:HB2	1:5:134:SER:H	1.78	0.48
1:A:660:GLU:OE2	1:A:781:TYR:OH	2.27	0.48
1:D:455:ASP:HB3	1:D:458:THR:HG22	1.96	0.48
2:H:938:GLY:O	2:H:953:LYS:NZ	2.47	0.48
2:K:757:ARG:NH2	2:K:793:VAL:O	2.45	0.48
1:a:546:ILE:HG13	1:a:904:ALA:HB1	1.95	0.48
1:b:1166:TRP:CD1	1:b:1176:PRO:HG2	2.49	0.48
1:d:285:PHE:HB3	1:d:288:SER:HB2	1.96	0.48
2:H:399:GLN:HE21	2:L:566:PHE:HB3	1.78	0.48
2:J:885:ILE:HG13	2:J:922:LEU:HA	1.96	0.48
2:K:552:TYR:CE1	6:K:1301:SAM:N7	2.82	0.48
2:L:885:ILE:HG13	2:L:922:LEU:HA	1.96	0.48
3:R:16:ILE:HA	3:R:22:GLN:HE21	1.78	0.48
3:R:1208:ASN:HB3	3:R:1245:ILE:HG12	1.94	0.48
1:a:373:ASN:HB3	1:a:1259:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:369:ASN:HD21	1:e:458:THR:HA	1.77	0.48
1:e:1115:TRP:HE1	1:e:1170:ILE:HG21	1.79	0.48
1:1:74:LYS:HB3	1:a:531:VAL:HG12	1.96	0.48
1:B:406:MET:HA	1:B:453:THR:HG22	1.95	0.48
1:D:493:VAL:HA	1:D:1273:GLY:HA2	1.96	0.48
2:I:907:PHE:HE1	2:I:924:ILE:HD11	1.79	0.48
2:J:96:GLU:OE2	2:J:99:ARG:NH2	2.45	0.48
4:U:485:LEU:HD13	4:U:557:MET:HE1	1.96	0.48
1:c:483:LEU:HB2	1:c:493:VAL:HG21	1.96	0.48
1:1:77:ASP:OD1	1:1:80:THR:OG1	2.28	0.48
1:B:416:VAL:HG23	1:B:1217:PRO:HB3	1.94	0.48
2:H:907:PHE:HE1	2:H:924:ILE:HD11	1.79	0.48
2:K:560:VAL:HG12	2:L:397:LEU:HB2	1.94	0.48
3:R:286:TYR:O	3:R:288:SER:N	2.41	0.48
3:R:1067:ARG:NH1	3:R:1094:SER:O	2.46	0.48
1:b:614:PRO:HB3	1:b:625:ASN:HD22	1.78	0.48
1:C:755:LEU:HB2	1:C:806:MET:HE2	1.96	0.48
2:I:938:GLY:O	2:I:953:LYS:NZ	2.47	0.48
2:J:508:ALA:HB2	2:J:542:PRO:HB2	1.95	0.48
2:J:832:PRO:HA	2:J:854:THR:HA	1.95	0.48
2:K:508:ALA:HB2	2:K:542:PRO:HB2	1.95	0.48
2:L:872:TYR:CE1	6:L:1301:SAM:C4	2.91	0.48
3:R:632:VAL:HB	3:R:635:VAL:HG12	1.94	0.48
3:R:1008:SER:HB3	3:R:1147:MET:HE2	1.96	0.48
1:d:234:GLN:HE21	1:d:911:ASP:HA	1.79	0.48
1:d:430:ARG:O	1:d:1254:TYR:OH	2.32	0.48
1:3:125:THR:HG22	1:c:876:ALA:HB2	1.95	0.47
1:5:12:SER:O	1:5:12:SER:OG	2.23	0.47
1:A:1163:THR:HG21	1:A:1198:TYR:HB2	1.96	0.47
1:B:603:VAL:HG23	1:B:604:VAL:HG23	1.94	0.47
1:C:586:SER:OG	1:C:587:ASP:N	2.47	0.47
1:C:1166:TRP:HD1	1:C:1176:PRO:HG2	1.79	0.47
1:D:1241:PRO:HG2	1:D:1244:GLN:HB2	1.95	0.47
1:E:242:ARG:HE	3:R:639:ARG:HH12	1.62	0.47
2:I:552:TYR:CD2	6:I:1302:SAM:C8	2.97	0.47
2:I:602:CYS:O	2:I:606:THR:OG1	2.32	0.47
2:K:552:TYR:CZ	6:K:1301:SAM:N7	2.80	0.47
2:L:832:PRO:HA	2:L:854:THR:HA	1.95	0.47
1:a:352:LEU:HD23	1:a:955:LEU:HD13	1.96	0.47
1:b:600:TYR:OH	1:b:828:PHE:O	2.28	0.47
1:c:1166:TRP:CD1	1:c:1176:PRO:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:MET:HE1	1:B:499:PRO:HB2	1.97	0.47
1:E:335:PHE:O	1:E:357:ASN:ND2	2.47	0.47
2:I:559:ILE:HG13	2:J:396:TRP:HD1	1.79	0.47
2:I:566:PHE:HB3	2:J:399:GLN:HE21	1.79	0.47
2:I:578:VAL:CG2	6:I:1302:SAM:C5	2.92	0.47
2:I:851:ILE:HG22	6:I:1301:SAM:N1	2.22	0.47
2:K:61:ARG:O	2:K:117:ASN:ND2	2.39	0.47
3:R:1081:ILE:HB	3:R:1089:PHE:HB2	1.95	0.47
4:U:621:HIS:NE2	4:U:637:ASP:OD2	2.47	0.47
1:C:180:GLY:HA2	1:C:191:PHE:HA	1.95	0.47
1:D:257:THR:OG1	1:D:318:ARG:NH2	2.48	0.47
1:D:1034:GLU:HG3	1:D:1207:ARG:HE	1.78	0.47
1:E:353:MET:HE2	1:E:955:LEU:HD22	1.95	0.47
2:H:552:TYR:CE2	6:H:1301:SAM:N7	2.80	0.47
2:J:757:ARG:NH2	2:J:793:VAL:O	2.45	0.47
2:K:602:CYS:O	2:K:606:THR:OG1	2.32	0.47
2:L:733:ASN:O	2:L:762:SER:OG	2.30	0.47
3:R:147:ILE:O	3:R:805:ARG:NH1	2.38	0.47
3:R:876:PRO:HG3	3:R:890:TRP:HA	1.95	0.47
1:e:599:LEU:HA	1:e:832:GLN:HE21	1.79	0.47
1:e:761:LEU:HB2	1:e:808:PRO:HB3	1.94	0.47
1:1:10:GLY:HA3	1:a:319:ASP:HB3	1.96	0.47
1:A:813:GLN:HG3	1:A:814:LEU:HD12	1.96	0.47
1:B:290:TYR:HE2	1:a:1121:TYR:HD1	1.61	0.47
1:B:411:MET:HG2	1:B:423:VAL:HG11	1.95	0.47
2:J:907:PHE:HE1	2:J:924:ILE:HD11	1.79	0.47
2:J:987:ASP:OD1	2:J:987:ASP:N	2.48	0.47
2:K:907:PHE:HE1	2:K:924:ILE:HD11	1.79	0.47
2:L:907:PHE:HE1	2:L:924:ILE:HD11	1.79	0.47
3:R:470:LEU:HA	3:R:473:ILE:HG12	1.97	0.47
1:c:433:ARG:HA	1:c:450:VAL:HG12	1.97	0.47
1:2:141:ASN:HD22	1:b:990:GLY:H	1.61	0.47
1:A:189:VAL:O	1:B:550:GLN:NE2	2.47	0.47
1:A:478:GLU:OE1	1:A:508:ARG:NH2	2.41	0.47
2:H:871:ASP:HA	6:H:1302:SAM:N1	2.30	0.47
2:L:96:GLU:OE2	2:L:99:ARG:NH2	2.45	0.47
1:e:466:MET:HE1	1:e:1262:TYR:HE2	1.80	0.47
1:2:81:PRO:HG3	1:b:963:ALA:HB1	1.96	0.47
1:B:1170:ILE:HG23	1:B:1175:ILE:HG22	1.97	0.47
1:D:272:VAL:HG23	1:D:300:ALA:HB3	1.96	0.47
1:E:412:GLY:HA2	1:d:1079:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:602:CYS:O	2:H:606:THR:OG1	2.32	0.47
3:R:35:SER:OG	3:R:851:ARG:NH1	2.47	0.47
1:d:483:LEU:HB2	1:d:493:VAL:HG21	1.96	0.47
1:e:660:GLU:OE2	1:e:781:TYR:OH	2.22	0.47
1:A:426:CYS:HB3	1:A:1235:LEU:HD12	1.96	0.47
1:A:773:LYS:HA	1:A:776:VAL:HG12	1.97	0.47
1:B:313:ASN:HD22	1:B:395:PRO:HG2	1.78	0.47
1:B:480:GLU:HG3	1:B:493:VAL:HG23	1.95	0.47
1:D:934:LEU:HD21	1:D:1024:VAL:HG11	1.96	0.47
1:E:224:ILE:HD11	4:U:554:VAL:HG21	1.95	0.47
1:E:525:ILE:HD11	1:E:532:ILE:HB	1.96	0.47
2:H:570:ASP:HB3	2:H:607:ALA:HB2	1.97	0.47
2:H:885:ILE:HG13	2:H:922:LEU:HA	1.96	0.47
2:H:987:ASP:N	2:H:987:ASP:OD1	2.47	0.47
2:I:832:PRO:HA	2:I:854:THR:HA	1.95	0.47
2:K:885:ILE:HG13	2:K:922:LEU:HA	1.96	0.47
2:L:938:GLY:O	2:L:953:LYS:NZ	2.47	0.47
3:R:145:ARG:NH2	3:R:809:SER:O	2.41	0.47
3:R:346:GLU:OE2	3:R:349:ARG:NH2	2.48	0.47
4:U:415:LYS:NZ	4:U:569:GLN:OE1	2.40	0.47
1:a:363:LEU:HG	1:a:367:LEU:HD23	1.97	0.47
1:a:741:LEU:HD21	1:a:816:PRO:HB3	1.96	0.47
1:a:892:PRO:HA	1:a:893:PRO:HD3	1.80	0.47
1:b:398:ASP:OD2	1:b:401:LYS:NZ	2.43	0.47
1:c:707:GLU:OE1	1:c:711:ARG:NH1	2.47	0.47
1:c:1228:PRO:HB2	1:c:1231:ARG:HD3	1.94	0.47
1:d:527:ASN:ND2	1:d:864:LEU:O	2.47	0.47
1:e:263:CYS:SG	1:e:462:ARG:NH1	2.88	0.47
1:A:438:GLN:NE2	1:A:440:MET:O	2.43	0.47
1:A:1166:TRP:CD1	1:A:1176:PRO:HG2	2.49	0.47
1:B:969:VAL:HG12	1:B:973:MET:HE2	1.97	0.47
1:C:1034:GLU:OE2	1:C:1207:ARG:NH2	2.45	0.47
1:E:719:ILE:HG22	1:E:739:LEU:HB3	1.97	0.47
2:H:811:TYR:OH	2:H:1016:MET:O	2.33	0.47
2:H:824:VAL:HG12	2:H:845:PRO:HG2	1.97	0.47
2:L:552:TYR:CD2	6:L:1302:SAM:H2'	2.45	0.47
4:U:304:VAL:HB	4:U:316:ARG:HB2	1.97	0.47
1:a:1166:TRP:CD1	1:a:1176:PRO:HG2	2.50	0.47
1:d:1181:MET:O	1:d:1197:GLN:NE2	2.48	0.47
1:e:652:LEU:O	1:e:656:MET:HB2	2.15	0.47
1:A:440:MET:HE1	1:A:499:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:TRP:HE3	1:A:771:LEU:HD13	1.80	0.47
1:A:1188:HIS:HA	1:A:1220:ILE:HD12	1.97	0.47
1:B:1096:ASP:HB3	1:B:1100:MET:H	1.80	0.47
1:E:654:ASN:ND2	1:E:673:ARG:O	2.42	0.47
2:I:552:TYR:CE2	6:I:1302:SAM:C8	2.98	0.47
2:I:811:TYR:OH	2:I:1016:MET:O	2.33	0.47
2:I:824:VAL:HG12	2:I:845:PRO:HG2	1.97	0.47
2:J:811:TYR:OH	2:J:1016:MET:O	2.33	0.47
2:L:508:ALA:HB2	2:L:542:PRO:HB2	1.95	0.47
1:A:1079:ARG:HG3	1:A:1080:ASP:H	1.80	0.47
1:D:514:ARG:HH12	1:D:727:PHE:HD2	1.63	0.47
1:E:276:VAL:HG13	1:E:286:PHE:HD2	1.80	0.47
1:E:399:ALA:HA	1:E:402:TRP:HD1	1.79	0.47
2:H:757:ARG:NH2	2:H:793:VAL:O	2.45	0.47
2:I:570:ASP:HB3	2:I:607:ALA:HB2	1.97	0.47
2:K:824:VAL:HG12	2:K:845:PRO:HG2	1.97	0.47
3:R:607:HIS:HB2	3:R:648:ILE:HG21	1.97	0.47
1:b:272:VAL:HG23	1:b:300:ALA:HB3	1.97	0.47
1:1:97:GLU:O	1:1:101:GLU:HB2	2.16	0.46
1:5:6:ARG:NH1	1:5:6:ARG:CB	2.75	0.46
1:A:430:ARG:HH12	1:A:1242:PRO:HG3	1.78	0.46
1:D:1166:TRP:CD1	1:D:1176:PRO:HG2	2.50	0.46
1:E:1166:TRP:CD1	1:E:1176:PRO:HG2	2.49	0.46
2:H:96:GLU:OE2	2:H:99:ARG:NH2	2.45	0.46
2:K:489:VAL:HG23	2:K:641:ILE:HD11	1.98	0.46
4:U:674:VAL:HG12	4:U:680:ARG:HH12	1.80	0.46
1:e:262:LEU:HD21	1:e:406:MET:HG2	1.97	0.46
1:e:448:VAL:HG12	1:e:1259:ARG:HB2	1.97	0.46
1:e:713:TRP:HD1	1:e:837:ARG:HG3	1.80	0.46
1:D:836:VAL:HG11	1:D:842:ARG:HB3	1.96	0.46
2:J:564:ARG:HH21	2:K:776:ASP:HB2	1.79	0.46
3:R:21:ASP:HA	3:R:879:LYS:HB2	1.97	0.46
1:b:892:PRO:HA	1:b:893:PRO:HD3	1.81	0.46
1:d:1067:PHE:O	1:d:1138:ARG:NH1	2.41	0.46
1:d:1181:MET:HB3	1:d:1197:GLN:HE22	1.80	0.46
1:A:313:ASN:HD22	1:A:395:PRO:HG2	1.79	0.46
1:B:253:PRO:HB3	1:B:979:LEU:HD11	1.97	0.46
1:D:287:THR:OG1	1:D:298:GLU:OE2	2.33	0.46
1:E:695:SER:HB3	1:E:698:ASP:HB2	1.98	0.46
1:E:732:LEU:HD22	1:E:831:PHE:HE1	1.80	0.46
2:H:489:VAL:HG23	2:H:641:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:497:ILE:HA	2:I:504:GLU:HA	1.98	0.46
2:K:811:TYR:OH	2:K:1016:MET:O	2.33	0.46
3:R:654:LEU:HG	3:R:659:PHE:HE1	1.80	0.46
1:c:810:TYR:OH	1:c:818:GLU:OE1	2.26	0.46
1:B:413:THR:HG21	1:B:424:ALA:HB2	1.96	0.46
1:D:232:ILE:HG13	1:D:233:VAL:HG23	1.96	0.46
2:H:564:ARG:HH21	2:I:776:ASP:HB2	1.79	0.46
2:H:578:VAL:HA	6:H:1301:SAM:HE1	1.97	0.46
2:L:49:GLN:HB2	2:L:183:ASP:HB3	1.97	0.46
2:L:194:ASP:OD1	2:L:194:ASP:N	2.48	0.46
3:R:299:TRP:NE1	3:R:303:ARG:HG2	2.31	0.46
1:c:691:ILE:HD11	1:c:710:HIS:CE1	2.51	0.46
1:d:1166:TRP:CD1	1:d:1176:PRO:HG2	2.51	0.46
1:B:666:ASN:HD21	1:B:669:TYR:HD2	1.64	0.46
2:H:49:GLN:HB2	2:H:183:ASP:HB3	1.97	0.46
2:L:497:ILE:HA	2:L:504:GLU:HA	1.98	0.46
3:R:451:MET:HE1	3:R:544:LEU:HD11	1.98	0.46
1:b:221:THR:HG22	1:b:1267:ILE:HB	1.98	0.46
1:b:737:GLU:HG2	1:b:738:VAL:HG13	1.96	0.46
1:b:761:LEU:HB2	1:b:808:PRO:HB3	1.97	0.46
1:b:870:THR:OG1	1:b:872:GLY:O	2.34	0.46
1:c:223:PHE:HD2	1:c:910:ALA:HA	1.80	0.46
1:c:1171:THR:HG23	1:c:1174:SER:H	1.80	0.46
1:d:621:THR:HA	1:d:782:GLN:HG3	1.97	0.46
1:A:406:MET:HA	1:A:453:THR:HG22	1.97	0.46
2:H:102:PRO:HB2	2:H:105:THR:HG22	1.98	0.46
2:H:552:TYR:CD2	6:H:1301:SAM:N9	2.84	0.46
2:J:49:GLN:HB2	2:J:183:ASP:HB3	1.97	0.46
2:J:872:TYR:CE1	6:J:1301:SAM:C4	2.89	0.46
1:c:260:ALA:HB3	1:c:313:ASN:HB3	1.97	0.46
1:c:493:VAL:HG12	1:c:1271:VAL:HG22	1.97	0.46
1:c:892:PRO:HA	1:c:893:PRO:HD3	1.84	0.46
1:d:943:TYR:HB2	1:d:995:THR:HG22	1.98	0.46
1:e:961:THR:O	1:e:964:THR:OG1	2.33	0.46
1:3:73:MET:HE1	1:c:828:PHE:HB2	1.97	0.46
1:A:272:VAL:HG23	1:A:300:ALA:HB3	1.97	0.46
1:C:478:GLU:OE1	1:C:508:ARG:NH2	2.42	0.46
2:H:497:ILE:HA	2:H:504:GLU:HA	1.98	0.46
2:J:824:VAL:HG12	2:J:845:PRO:HG2	1.97	0.46
2:J:889:MET:HB2	6:J:1301:SAM:C	2.46	0.46
2:L:757:ARG:NH2	2:L:793:VAL:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:466:LEU:HD11	3:R:508:ALA:HB1	1.96	0.46
1:b:378:PHE:HE2	1:b:433:ARG:HD3	1.81	0.46
1:4:109:GLN:OE1	1:d:537:GLN:NE2	2.49	0.46
1:C:278:GLN:HE21	1:C:281:LEU:HB3	1.81	0.46
1:D:551:ILE:HD11	1:D:885:ALA:HA	1.98	0.46
2:H:566:PHE:HB3	2:I:399:GLN:HE21	1.81	0.46
2:L:489:VAL:HG23	2:L:641:ILE:HD11	1.97	0.46
1:b:472:MET:HG2	1:b:508:ARG:H	1.80	0.46
1:c:606:THR:HG22	1:c:875:LEU:HD23	1.97	0.46
1:B:268:ILE:HG12	1:B:304:ILE:HG22	1.98	0.46
1:D:1058:PRO:HD2	1:D:1182:VAL:HG12	1.97	0.46
1:E:452:GLU:OE2	1:E:1259:ARG:NH2	2.41	0.46
1:E:745:HIS:ND1	1:E:812:GLN:O	2.47	0.46
2:J:602:CYS:O	2:J:606:THR:OG1	2.32	0.46
2:K:567:PRO:HA	2:L:832:PRO:HB2	1.96	0.46
2:L:36:ALA:HB3	2:L:87:LYS:HG2	1.98	0.46
2:L:824:VAL:HG12	2:L:845:PRO:HG2	1.97	0.46
1:A:1166:TRP:HD1	1:A:1176:PRO:HG2	1.81	0.46
1:D:1207:ARG:HH22	1:D:1250:VAL:HG12	1.81	0.46
2:I:489:VAL:HG23	2:I:641:ILE:HD11	1.98	0.46
2:J:570:ASP:HB3	2:J:607:ALA:HB2	1.97	0.46
2:K:49:GLN:HB2	2:K:183:ASP:HB3	1.97	0.46
2:K:102:PRO:HB2	2:K:105:THR:HG22	1.98	0.46
2:L:552:TYR:CZ	6:L:1302:SAM:N7	2.83	0.46
2:L:602:CYS:O	2:L:606:THR:OG1	2.32	0.46
3:R:146:GLN:NE2	3:R:805:ARG:O	2.40	0.46
3:R:256:ILE:HD11	3:R:343:VAL:HG11	1.97	0.46
3:R:987:ARG:NH2	3:R:1151:GLN:OE1	2.49	0.46
1:b:383:THR:HG22	1:b:385:PHE:H	1.80	0.46
1:E:580:LYS:O	1:E:582:ARG:NH1	2.49	0.45
2:H:194:ASP:N	2:H:194:ASP:OD1	2.48	0.45
2:H:514:TYR:OH	6:H:1301:SAM:O	2.34	0.45
2:J:489:VAL:HG23	2:J:641:ILE:HD11	1.97	0.45
2:J:497:ILE:HA	2:J:504:GLU:HA	1.98	0.45
4:U:4:ILE:HB	4:U:204:VAL:HG23	1.99	0.45
4:U:136:SER:OG	4:U:138:THR:N	2.48	0.45
4:U:359:ASP:HB2	4:U:587:TRP:CD1	2.51	0.45
1:C:220:ILE:HD12	1:C:557:SER:HB2	1.97	0.45
1:D:478:GLU:OE1	1:D:508:ARG:NH2	2.49	0.45
2:I:102:PRO:HB2	2:I:105:THR:HG22	1.98	0.45
2:I:194:ASP:OD1	2:I:194:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:36:ALA:HB3	2:K:87:LYS:HG2	1.98	0.45
2:L:61:ARG:O	2:L:117:ASN:ND2	2.39	0.45
4:U:99:ASP:OD1	1:d:575:SER:OG	2.26	0.45
4:U:299:ASN:OD1	4:U:322:THR:N	2.45	0.45
1:b:352:LEU:HD23	1:b:955:LEU:HD13	1.97	0.45
1:c:355:ARG:NH2	1:c:950:ASP:O	2.49	0.45
1:e:237:ALA:HA	1:e:247:LEU:HD11	1.97	0.45
1:1:53:TYR:OH	1:a:903:ASP:OD2	2.33	0.45
1:C:1170:ILE:HG23	1:C:1175:ILE:HG22	1.99	0.45
1:D:351:PRO:HG3	1:D:1175:ILE:HG12	1.97	0.45
2:J:498:ASP:OD2	2:J:501:THR:OG1	2.31	0.45
2:L:570:ASP:HB3	2:L:607:ALA:HB2	1.97	0.45
2:L:811:TYR:OH	2:L:1016:MET:O	2.33	0.45
3:R:776:ASP:OD1	3:R:776:ASP:N	2.48	0.45
1:a:192:SER:HB3	1:a:195:ASP:HB2	1.98	0.45
1:e:417:SER:H	1:e:420:CYS:HB2	1.81	0.45
1:e:851:ARG:NH1	1:e:991:ASP:O	2.49	0.45
1:2:97:GLU:HG2	1:2:136:SER:HB2	1.98	0.45
1:A:543:LEU:HD22	1:A:592:ARG:HG3	1.98	0.45
1:C:732:LEU:HD23	1:C:999:ILE:HG21	1.97	0.45
2:J:102:PRO:HB2	2:J:105:THR:HG22	1.98	0.45
2:J:566:PHE:HB3	2:K:399:GLN:HE21	1.81	0.45
2:K:570:ASP:HB3	2:K:607:ALA:HB2	1.97	0.45
2:L:821:ASP:OD1	2:L:843:THR:OG1	2.35	0.45
2:L:829:GLY:HA2	2:L:850:ASP:HB3	1.98	0.45
3:R:627:VAL:HG22	3:R:641:ILE:HG13	1.99	0.45
4:U:353:LEU:O	4:U:357:LEU:HB2	2.17	0.45
1:e:375:HIS:HB3	1:e:1261:ALA:HB2	1.99	0.45
1:1:130:ALA:HB3	1:B:496:PRO:HG3	1.99	0.45
1:4:54:LYS:HG2	1:D:344:LEU:HD22	1.99	0.45
1:5:6:ARG:NH1	1:e:316:PHE:CE1	2.84	0.45
1:A:926:GLU:HB3	1:A:1020:ILE:HD12	1.98	0.45
1:B:543:LEU:HD21	1:B:595:LEU:HD23	1.97	0.45
1:E:362:LEU:HD22	1:E:1027:THR:HG22	1.97	0.45
1:E:787:GLN:O	1:E:791:SER:HB3	2.17	0.45
2:I:5:TRP:NE1	2:I:338:GLY:O	2.50	0.45
1:B:954:SER:OG	1:B:955:LEU:N	2.49	0.45
1:D:1207:ARG:NH2	1:D:1249:GLU:O	2.49	0.45
2:H:36:ALA:HB3	2:H:87:LYS:HG2	1.98	0.45
2:I:47:ARG:NH1	2:I:52:ASN:OD1	2.47	0.45
2:L:5:TRP:NE1	2:L:338:GLY:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:693:PRO:HG2	4:U:696:LEU:HB2	1.99	0.45
1:d:259:ASP:N	1:d:372:LEU:O	2.49	0.45
1:A:892:PRO:HD2	1:A:895:LEU:HD13	1.98	0.45
1:B:411:MET:O	1:a:1079:ARG:NH2	2.50	0.45
1:C:378:PHE:HE2	1:C:433:ARG:HD3	1.80	0.45
1:C:670:THR:HG23	1:C:672:SER:H	1.80	0.45
1:C:1166:TRP:CD1	1:C:1176:PRO:HG2	2.51	0.45
2:J:36:ALA:HB3	2:J:87:LYS:HG2	1.98	0.45
2:J:194:ASP:OD1	2:J:194:ASP:N	2.48	0.45
2:J:821:ASP:OD1	2:J:843:THR:OG1	2.35	0.45
2:L:533:TRP:HD1	2:L:541:VAL:HG21	1.82	0.45
3:R:519:ASN:HB2	3:R:804:GLU:HG2	1.98	0.45
3:R:778:THR:OG1	3:R:786:PHE:O	2.31	0.45
4:U:299:ASN:HB2	4:U:391:ILE:HG22	1.99	0.45
1:c:457:LEU:HD12	1:c:1030:VAL:HG11	1.98	0.45
1:e:457:LEU:HD13	1:e:1030:VAL:HG21	1.98	0.45
1:e:1166:TRP:CD1	1:e:1176:PRO:HG2	2.51	0.45
1:5:9:LYS:C	1:e:319:ASP:OD2	2.53	0.45
1:B:926:GLU:HB3	1:B:1020:ILE:HD12	1.98	0.45
1:C:746:GLN:OE1	1:C:812:GLN:NE2	2.50	0.45
1:D:946:ASP:OD1	1:D:1025:GLN:NE2	2.50	0.45
2:L:552:TYR:CE1	6:L:1302:SAM:N7	2.85	0.45
1:e:306:VAL:HG21	1:e:1038:PHE:HD1	1.82	0.45
1:e:729:SER:OG	1:e:731:ASN:OD1	2.35	0.45
1:3:142:GLU:OE2	1:D:433:ARG:NH2	2.49	0.45
1:5:6:ARG:NH1	1:5:6:ARG:CG	2.73	0.45
1:C:1047:ILE:HD13	1:C:1167:LEU:HD11	1.99	0.45
2:I:61:ARG:O	2:I:117:ASN:ND2	2.39	0.45
2:I:872:TYR:CE1	6:I:1301:SAM:N1	2.84	0.45
2:K:497:ILE:HA	2:K:504:GLU:HA	1.98	0.45
3:R:1128:LEU:HD11	3:R:1145:LEU:HD21	1.99	0.45
4:U:50:MET:HE3	4:U:59:VAL:HG22	1.98	0.45
1:b:483:LEU:HB2	1:b:493:VAL:HG21	1.98	0.45
1:b:773:LYS:HG3	1:b:794:ARG:HG2	1.99	0.45
1:3:141:ASN:OD1	1:c:990:GLY:N	2.49	0.45
1:A:372:LEU:HA	1:A:372:LEU:HD13	1.85	0.45
1:B:620:VAL:HG12	1:B:655:MET:HE3	1.99	0.45
1:B:1007:ARG:HH12	2:I:293:GLY:HA3	1.82	0.45
1:D:926:GLU:HG2	1:D:1020:ILE:HD13	1.99	0.45
2:H:5:TRP:NE1	2:H:338:GLY:O	2.50	0.45
2:H:61:ARG:O	2:H:117:ASN:ND2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:183:ASP:OD1	2:H:325:ARG:NH2	2.50	0.45
2:I:49:GLN:HB2	2:I:183:ASP:HB3	1.97	0.45
2:J:47:ARG:NH1	2:J:52:ASN:OD1	2.47	0.45
2:J:183:ASP:OD1	2:J:325:ARG:NH2	2.50	0.45
2:J:533:TRP:HD1	2:J:541:VAL:HG21	1.82	0.45
2:K:566:PHE:HB3	2:L:399:GLN:HE21	1.81	0.45
2:L:102:PRO:HB2	2:L:105:THR:HG22	1.98	0.45
1:a:588:PHE:HE1	1:a:884:VAL:HG13	1.82	0.45
1:c:660:GLU:OE2	1:c:781:TYR:OH	2.24	0.45
1:d:220:ILE:HD13	1:d:248:LEU:HD22	1.99	0.45
1:d:984:LEU:HG	1:d:987:LEU:HD12	1.98	0.45
1:C:252:THR:HB	1:C:916:SER:HB3	1.98	0.44
1:E:232:ILE:HG22	1:E:233:VAL:HG23	1.97	0.44
1:E:626:LEU:HD11	1:E:782:GLN:HE22	1.82	0.44
1:E:934:LEU:HD21	1:E:1024:VAL:HG11	1.99	0.44
2:J:5:TRP:NE1	2:J:338:GLY:O	2.50	0.44
2:J:559:ILE:HG13	2:K:396:TRP:HD1	1.83	0.44
2:J:560:VAL:HG12	2:K:397:LEU:HB2	1.99	0.44
2:K:564:ARG:HH22	2:L:401:THR:HG22	1.81	0.44
2:K:821:ASP:OD1	2:K:843:THR:OG1	2.35	0.44
1:a:261:GLY:O	1:a:1259:ARG:NH2	2.51	0.44
1:d:336:LYS:HA	1:d:340:ASN:HD22	1.81	0.44
1:B:1166:TRP:CD1	1:B:1176:PRO:HG2	2.52	0.44
1:C:546:ILE:HD11	1:C:905:ILE:HG12	1.98	0.44
1:E:836:VAL:HG23	1:E:842:ARG:HH21	1.82	0.44
2:I:183:ASP:OD1	2:I:325:ARG:NH2	2.50	0.44
2:J:567:PRO:HB3	2:K:833:GLU:HB3	2.00	0.44
2:K:47:ARG:NH1	2:K:52:ASN:OD1	2.47	0.44
2:K:183:ASP:OD1	2:K:325:ARG:NH2	2.50	0.44
2:L:47:ARG:NH1	2:L:52:ASN:OD1	2.47	0.44
3:R:1019:GLY:HA2	3:R:1022:GLU:HG2	1.99	0.44
3:R:1192:MET:HE3	3:R:1227:ALA:HB1	2.00	0.44
1:c:713:TRP:HD1	1:c:837:ARG:HG3	1.82	0.44
1:B:1207:ARG:HH22	1:B:1250:VAL:HG12	1.82	0.44
1:C:1207:ARG:HH22	1:C:1250:VAL:HG12	1.83	0.44
2:H:533:TRP:HD1	2:H:541:VAL:HG21	1.82	0.44
2:H:578:VAL:CG2	6:H:1301:SAM:N7	2.80	0.44
2:H:821:ASP:OD1	2:H:843:THR:OG1	2.35	0.44
2:I:201:SER:OG	2:I:202:ASP:N	2.51	0.44
2:I:564:ARG:HH21	2:J:776:ASP:HB2	1.82	0.44
2:L:331:VAL:HA	2:L:334:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:34:ASP:O	4:U:200:SER:OG	2.33	0.44
1:b:266:PHE:HE2	1:b:1251:VAL:HG11	1.83	0.44
1:e:892:PRO:HA	1:e:893:PRO:HD3	1.84	0.44
1:e:1170:ILE:HG13	1:e:1175:ILE:HG22	2.00	0.44
1:B:514:ARG:HB3	1:B:730:ALA:HB2	1.98	0.44
1:B:934:LEU:HD21	1:B:1024:VAL:HG11	2.00	0.44
2:I:36:ALA:HB3	2:I:87:LYS:HG2	1.98	0.44
2:K:5:TRP:NE1	2:K:338:GLY:O	2.50	0.44
2:K:331:VAL:HA	2:K:334:VAL:HG12	2.00	0.44
2:K:533:TRP:HD1	2:K:541:VAL:HG21	1.82	0.44
2:L:183:ASP:OD1	2:L:325:ARG:NH2	2.50	0.44
1:a:237:ALA:HA	1:a:247:LEU:HD22	1.99	0.44
1:b:436:ARG:HA	1:b:448:VAL:HA	2.00	0.44
1:b:732:LEU:HD13	1:b:999:ILE:HG21	1.99	0.44
1:b:1209:LEU:HD21	1:b:1212:THR:HG23	2.00	0.44
1:e:336:LYS:NZ	1:e:346:VAL:O	2.46	0.44
1:A:372:LEU:HD11	1:A:466:MET:HB2	1.99	0.44
1:B:193:PRO:HA	1:B:196:LEU:HB3	2.00	0.44
1:B:433:ARG:HD2	1:B:436:ARG:HB3	1.98	0.44
1:B:436:ARG:NH1	1:B:438:GLN:OE1	2.49	0.44
1:C:669:TYR:HE2	1:c:780:ARG:HA	1.83	0.44
1:C:777:ASP:OD1	1:C:794:ARG:NH1	2.51	0.44
1:D:842:ARG:HD2	1:D:1003:GLN:NE2	2.33	0.44
2:I:567:PRO:HB3	2:J:833:GLU:HB3	2.00	0.44
2:J:583:ASP:HB3	2:J:594:LEU:HD11	2.00	0.44
2:K:562:LEU:H	6:K:1301:SAM:HN61	1.65	0.44
3:R:394:GLU:HB2	4:U:500:LEU:HD21	1.98	0.44
3:R:786:PHE:HE1	3:R:791:ARG:HG3	1.82	0.44
3:R:921:THR:HG22	3:R:923:LYS:H	1.81	0.44
1:d:931:LEU:HD22	1:d:984:LEU:HD23	1.98	0.44
1:d:1057:SER:HB3	1:d:1223:PRO:HG3	2.00	0.44
1:e:1082:ARG:HH21	1:e:1095:ARG:HH11	1.64	0.44
1:2:131:ASN:OD1	1:C:503:ARG:NH2	2.51	0.44
1:C:341:THR:HG23	1:C:342:GLU:HG2	1.98	0.44
1:C:517:SER:OG	1:C:521:ARG:NH1	2.51	0.44
1:E:363:LEU:HD13	1:E:934:LEU:HD11	1.99	0.44
1:E:1166:TRP:HD1	1:E:1176:PRO:HG2	1.82	0.44
2:H:201:SER:OG	2:H:202:ASP:N	2.51	0.44
2:I:533:TRP:HD1	2:I:541:VAL:HG21	1.82	0.44
2:J:514:TYR:HB3	2:J:549:GLN:HA	2.00	0.44
4:U:592:LEU:HD23	4:U:595:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:258:TRP:HB3	1:c:374:ARG:HD3	1.99	0.44
1:d:1027:THR:HA	1:d:1030:VAL:HG12	1.99	0.44
1:e:503:ARG:HD2	1:e:505:MET:HE3	1.98	0.44
1:5:6:ARG:HG2	1:e:316:PHE:CE1	2.53	0.44
2:H:331:VAL:HA	2:H:334:VAL:HG12	2.00	0.44
2:I:564:ARG:HH22	2:J:401:THR:HG22	1.82	0.44
1:a:406:MET:HA	1:a:453:THR:HG22	2.00	0.44
1:c:1062:PRO:HG2	1:c:1065:LEU:HD13	1.99	0.44
1:B:567:THR:HA	3:R:1205:ARG:HH11	1.82	0.44
1:C:629:PHE:HB2	1:C:655:MET:SD	2.58	0.44
1:E:327:PRO:HB2	1:E:1148:LEU:HD12	2.00	0.44
2:I:514:TYR:HB3	2:I:549:GLN:HA	2.00	0.44
2:K:486:ASP:HA	2:K:489:VAL:HG12	2.00	0.44
3:R:232:ASP:OD2	3:R:266:TYR:OH	2.34	0.44
1:a:1057:SER:HB2	1:a:1223:PRO:HG3	1.99	0.44
1:d:364:GLU:OE2	1:d:972:SER:OG	2.33	0.44
1:A:1044:ASP:OD2	1:A:1138:ARG:NE	2.45	0.44
1:B:383:THR:OG1	1:B:410:ARG:NH2	2.49	0.44
1:E:773:LYS:HB2	1:E:797:LEU:HD21	2.00	0.44
2:I:418:THR:HB	2:I:420:LEU:HB2	2.00	0.44
2:J:486:ASP:HA	2:J:489:VAL:HG12	2.00	0.44
1:c:514:ARG:NH1	1:c:727:PHE:O	2.51	0.44
1:c:1095:ARG:HE	1:c:1099:GLY:HA2	1.83	0.44
1:d:699:ALA:HB1	1:d:702:LEU:HB3	2.00	0.44
1:A:362:LEU:HD22	1:A:1027:THR:HG22	2.00	0.43
1:B:1077:PHE:HD2	1:B:1110:PHE:HE1	1.66	0.43
1:B:1213:ASN:O	1:B:1215:SER:N	2.50	0.43
1:D:1116:GLN:HG2	1:D:1172:PRO:HA	1.99	0.43
1:E:575:SER:HB2	3:R:1164:LEU:HB3	1.99	0.43
2:J:182:ASP:OD2	2:K:91:ARG:NH2	2.51	0.43
2:J:418:THR:HB	2:J:420:LEU:HB2	2.00	0.43
3:R:868:TRP:CE3	3:R:942:LEU:HD13	2.53	0.43
1:a:486:CYS:HG	1:a:723:THR:HG1	1.64	0.43
1:b:1118:ASN:OD1	1:b:1118:ASN:N	2.51	0.43
1:c:543:LEU:O	1:c:547:SER:HB3	2.17	0.43
1:1:141:ASN:HD22	1:a:990:GLY:H	1.65	0.43
1:1:144:GLY:HA3	1:B:377:GLY:HA2	2.00	0.43
1:A:532:ILE:HG12	1:A:604:VAL:HB	2.00	0.43
1:C:543:LEU:HA	1:C:546:ILE:HG22	2.01	0.43
1:D:758:THR:HG22	2:K:72:LEU:HD11	1.99	0.43
1:D:1166:TRP:HD1	1:D:1176:PRO:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:331:VAL:HA	2:I:334:VAL:HG12	2.00	0.43
2:I:486:ASP:HA	2:I:489:VAL:HG12	2.00	0.43
2:J:20:THR:O	2:J:226:LYS:NZ	2.51	0.43
2:K:20:THR:O	2:K:226:LYS:NZ	2.51	0.43
2:L:20:THR:O	2:L:226:LYS:NZ	2.51	0.43
3:R:1117:SER:OG	3:R:1119:LEU:O	2.32	0.43
4:U:490:ASP:OD1	4:U:490:ASP:N	2.50	0.43
1:a:318:ARG:O	1:a:320:SER:N	2.51	0.43
1:b:1044:ASP:OD2	1:b:1138:ARG:NE	2.40	0.43
1:c:225:SER:OG	1:c:226:SER:N	2.50	0.43
1:4:130:ALA:HB3	1:E:496:PRO:HG3	1.99	0.43
1:A:571:LEU:HB2	1:A:789:LEU:HD11	2.01	0.43
1:C:493:VAL:HA	1:C:1273:GLY:HA2	1.99	0.43
1:E:704:GLN:HE22	1:E:774:ASN:ND2	2.16	0.43
2:L:929:PRO:HB3	2:L:933:ILE:HD11	2.01	0.43
3:R:700:GLU:HB2	3:R:725:ILE:HD13	1.99	0.43
1:c:699:ALA:HB1	1:c:702:LEU:HB3	2.01	0.43
1:B:382:HIS:HD2	1:a:353:MET:HE3	1.83	0.43
1:C:362:LEU:HD22	1:C:1027:THR:HG22	2.00	0.43
1:C:468:ARG:HB2	1:C:1019:VAL:HG11	2.00	0.43
1:D:262:LEU:HA	1:D:1259:ARG:HH22	1.83	0.43
1:D:543:LEU:HA	1:D:546:ILE:HG22	2.01	0.43
2:H:559:ILE:HG13	2:I:396:TRP:HD1	1.84	0.43
2:H:583:ASP:HB3	2:H:594:LEU:HD11	2.00	0.43
4:U:300:VAL:HG22	4:U:320:MET:HB3	2.00	0.43
4:U:405:PHE:HB2	4:U:407:LYS:HE3	2.00	0.43
1:c:472:MET:HE3	1:c:506:PRO:HB2	2.00	0.43
1:d:1047:ILE:HD11	1:d:1166:TRP:HZ3	1.83	0.43
1:e:306:VAL:HG21	1:e:1038:PHE:CD1	2.53	0.43
1:A:646:VAL:HG21	1:A:684:TRP:CG	2.54	0.43
1:B:180:GLY:HA3	1:B:193:PRO:HG3	2.00	0.43
1:D:1160:TRP:HB2	1:D:1198:TYR:HE2	1.83	0.43
1:E:251:ASP:OD1	4:U:240:SER:OG	2.33	0.43
2:H:560:VAL:HG12	2:I:397:LEU:HB2	2.01	0.43
2:I:821:ASP:OD1	2:I:843:THR:OG1	2.35	0.43
2:K:257:LEU:HD21	2:K:327:LEU:HD11	2.01	0.43
2:K:514:TYR:HB3	2:K:549:GLN:HA	2.00	0.43
3:R:667:PHE:HE1	3:R:808:SER:HB2	1.84	0.43
1:c:892:PRO:HD2	1:c:895:LEU:HD12	2.00	0.43
1:e:326:PRO:HA	1:e:327:PRO:HD3	1.88	0.43
1:e:638:LEU:HD11	1:e:886:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:VAL:HA	1:A:525:ILE:HG22	1.99	0.43
1:B:1083:ILE:HD13	1:B:1121:TYR:HE2	1.83	0.43
1:B:1119:THR:HG21	1:B:1172:PRO:HD3	2.01	0.43
1:C:1077:PHE:HD2	1:C:1110:PHE:HE1	1.67	0.43
1:E:759:ASN:O	1:E:763:ASN:ND2	2.51	0.43
2:I:20:THR:O	2:I:226:LYS:NZ	2.51	0.43
2:I:929:PRO:HB3	2:I:933:ILE:HD11	2.01	0.43
2:J:201:SER:OG	2:J:202:ASP:N	2.51	0.43
2:J:564:ARG:HH22	2:K:401:THR:HG22	1.84	0.43
2:L:486:ASP:HA	2:L:489:VAL:HG12	2.00	0.43
3:R:243:ALA:O	3:R:366:ARG:NH1	2.47	0.43
1:a:1000:GLN:HG3	1:a:1010:ASN:HA	2.00	0.43
1:b:507:TYR:CE1	1:b:915:PHE:HB3	2.53	0.43
1:c:1209:LEU:HD21	1:c:1212:THR:HG23	2.00	0.43
1:d:192:SER:HB3	1:d:195:ASP:HB2	2.01	0.43
1:d:504:LEU:HD23	1:d:506:PRO:HD3	2.01	0.43
1:e:631:ILE:HG23	1:e:883:THR:HG21	2.00	0.43
1:A:278:GLN:HE21	1:A:281:LEU:HB3	1.84	0.43
1:B:298:GLU:HG3	1:B:1215:SER:HB3	2.00	0.43
1:B:398:ASP:OD2	1:B:401:LYS:NZ	2.49	0.43
1:D:552:ASP:OD2	1:D:554:THR:OG1	2.31	0.43
1:D:709:ILE:HD13	1:D:764:TRP:HH2	1.84	0.43
2:H:929:PRO:HB3	2:H:933:ILE:HD11	2.01	0.43
2:K:194:ASP:N	2:K:194:ASP:OD1	2.48	0.43
3:R:662:ARG:HA	3:R:674:THR:HG22	1.99	0.43
3:R:900:TYR:HE1	3:R:1057:LEU:HA	1.84	0.43
1:a:690:ASN:HB3	1:a:693:LEU:HD23	2.00	0.43
1:c:819:LEU:HA	1:c:822:ILE:HG22	2.01	0.43
1:c:926:GLU:HB3	1:c:1020:ILE:HD12	2.01	0.43
1:c:937:GLN:HE22	1:c:947:ARG:HA	1.84	0.43
1:A:390:ASN:OD1	1:A:433:ARG:NH2	2.52	0.43
1:A:600:TYR:OH	1:A:828:PHE:O	2.34	0.43
1:A:1049:ARG:HG3	1:A:1198:TYR:HE1	1.83	0.43
1:E:705:TRP:HH2	1:E:768:VAL:HG22	1.84	0.43
2:H:514:TYR:HB3	2:H:549:GLN:HA	2.00	0.43
2:H:564:ARG:HH22	2:I:401:THR:HG22	1.83	0.43
2:J:61:ARG:O	2:J:117:ASN:ND2	2.39	0.43
2:K:201:SER:OG	2:K:202:ASP:N	2.51	0.43
1:a:352:LEU:HB3	1:a:955:LEU:HD22	2.00	0.43
1:d:690:ASN:HB3	1:d:693:LEU:HD13	2.01	0.43
1:E:799:LYS:HE3	1:E:799:LYS:HB3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:THR:O	2:H:226:LYS:NZ	2.51	0.43
2:H:257:LEU:HD21	2:H:327:LEU:HD11	2.01	0.43
2:H:486:ASP:HA	2:H:489:VAL:HG12	2.00	0.43
2:J:578:VAL:CG2	6:J:1302:SAM:C5	2.97	0.43
1:a:448:VAL:HG12	1:a:1259:ARG:HB2	2.01	0.43
1:e:630:PHE:HB2	1:e:772:MET:HE1	2.00	0.43
1:A:551:ILE:HG22	1:A:553:PRO:HD3	2.01	0.43
1:A:1170:ILE:HG23	1:A:1175:ILE:HG22	2.01	0.43
2:H:418:THR:HB	2:H:420:LEU:HB2	2.00	0.43
2:I:498:ASP:OD2	2:I:501:THR:OG1	2.31	0.43
2:I:987:ASP:OD1	2:I:987:ASP:N	2.48	0.43
2:J:331:VAL:HA	2:J:334:VAL:HG12	2.00	0.43
2:K:583:ASP:HB3	2:K:594:LEU:HD11	2.00	0.43
2:L:514:TYR:HB3	2:L:549:GLN:HA	2.00	0.43
2:L:583:ASP:HB3	2:L:594:LEU:HD11	2.00	0.43
3:R:1199:LEU:HG	3:R:1242:LEU:HD13	2.01	0.43
1:c:650:MET:HE3	1:c:678:PHE:HE2	1.84	0.43
1:A:840:ARG:NH2	1:A:1004:TYR:OH	2.52	0.42
1:C:709:ILE:HD13	1:C:764:TRP:HH2	1.84	0.42
1:C:786:THR:HG23	1:C:789:LEU:H	1.84	0.42
1:D:1031:PHE:HZ	1:D:1040:ILE:HD12	1.83	0.42
2:H:567:PRO:HB3	2:I:833:GLU:HB3	2.01	0.42
2:H:628:GLU:HB2	2:H:666:TRP:HE1	1.84	0.42
3:R:234:VAL:HG13	3:R:801:VAL:HG21	2.00	0.42
1:b:731:ASN:HD22	1:b:736:PRO:HA	1.84	0.42
1:b:819:LEU:HA	1:b:822:ILE:HG22	2.01	0.42
1:b:1233:ASN:ND2	1:b:1244:GLN:OE1	2.52	0.42
1:e:488:GLN:HE22	1:e:820:ALA:HB1	1.84	0.42
1:B:300:ALA:HA	1:B:1213:ASN:HA	2.00	0.42
1:D:378:PHE:HE2	1:D:448:VAL:HG11	1.84	0.42
1:D:851:ARG:NH1	1:D:989:SER:OG	2.52	0.42
2:I:628:GLU:HB2	2:I:666:TRP:HE1	1.84	0.42
2:J:257:LEU:HD21	2:J:327:LEU:HD11	2.01	0.42
2:J:832:PRO:HG3	2:J:852:ARG:HD3	2.00	0.42
2:J:929:PRO:HB3	2:J:933:ILE:HD11	2.01	0.42
1:a:1110:PHE:HD1	1:a:1114:LEU:HD22	1.84	0.42
1:b:770:GLU:OE2	1:b:801:LYS:NZ	2.43	0.42
1:c:478:GLU:HB2	1:c:726:VAL:HG11	2.01	0.42
1:e:656:MET:HG3	1:e:660:GLU:HB2	2.02	0.42
1:A:776:VAL:HG21	1:A:793:MET:HG2	2.00	0.42
1:B:305:VAL:HG11	1:B:326:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:981:ASP:HB2	1:D:982:MET:HG2	2.00	0.42
2:I:583:ASP:HB3	2:I:594:LEU:HD11	2.00	0.42
2:K:850:ASP:OD1	6:K:1302:SAM:N3	2.52	0.42
3:R:43:TYR:HE2	3:R:205:ALA:HA	1.84	0.42
3:R:408:ILE:HG12	3:R:629:ASP:HB2	2.01	0.42
1:c:1083:ILE:HD12	1:c:1121:TYR:HE2	1.84	0.42
1:e:433:ARG:HA	1:e:450:VAL:HG12	2.01	0.42
1:4:133:LEU:HD11	1:E:501:VAL:HB	2.00	0.42
1:A:355:ARG:NH2	1:A:952:ILE:O	2.52	0.42
1:A:577:ILE:HG23	1:A:581:LEU:HD13	2.01	0.42
1:B:709:ILE:HD13	1:B:764:TRP:HH2	1.84	0.42
1:E:355:ARG:NH2	1:E:952:ILE:O	2.48	0.42
2:I:974:TRP:HB2	2:I:977:CYS:HB3	2.02	0.42
2:J:552:TYR:CE2	6:J:1302:SAM:N9	2.78	0.42
4:U:692:LEU:HD11	4:U:696:LEU:HD22	2.01	0.42
1:a:521:ARG:HB3	1:a:828:PHE:HE1	1.84	0.42
1:a:1083:ILE:HD12	1:a:1121:TYR:HE2	1.84	0.42
1:b:656:MET:HG3	1:b:660:GLU:HB3	2.01	0.42
1:d:1229:VAL:HG13	1:d:1236:THR:HG21	2.00	0.42
1:2:144:GLY:HA3	1:C:377:GLY:HA2	2.02	0.42
1:4:11:LYS:N	1:d:319:ASP:OD2	2.50	0.42
1:B:175:ALA:HB2	1:B:194:LEU:HD22	2.01	0.42
1:D:620:VAL:HG21	1:D:656:MET:HE2	2.01	0.42
1:E:336:LYS:HA	1:E:340:ASN:HD22	1.84	0.42
2:I:509:GLY:HA2	2:I:545:SER:HB3	2.02	0.42
2:J:578:VAL:HG21	6:J:1302:SAM:C5	2.49	0.42
2:K:509:GLY:HA2	2:K:545:SER:HB3	2.02	0.42
2:K:929:PRO:HB3	2:K:933:ILE:HD11	2.01	0.42
2:L:515:PHE:HB2	2:L:576:SER:HA	2.01	0.42
3:R:168:TYR:OH	3:R:173:GLN:OE1	2.30	0.42
4:U:346:MET:HE2	4:U:421:THR:HG21	2.01	0.42
1:B:386:THR:HG21	1:B:431:VAL:HG11	2.02	0.42
1:D:939:SER:OG	1:D:940:GLU:N	2.53	0.42
1:E:632:LEU:HD13	1:E:632:LEU:HA	1.86	0.42
2:I:182:ASP:OD2	2:J:91:ARG:NH2	2.52	0.42
2:I:554:VAL:O	2:J:785:ARG:NH1	2.45	0.42
2:J:613:VAL:HG13	2:J:654:VAL:HG22	2.02	0.42
2:K:628:GLU:HB2	2:K:666:TRP:HE1	1.84	0.42
2:K:974:TRP:HB2	2:K:977:CYS:HB3	2.02	0.42
3:R:17:SER:HB2	3:R:167:LEU:HD21	2.01	0.42
1:d:253:PRO:HB3	1:d:979:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ASN:ND2	1:a:851:ARG:HH12	2.18	0.42
1:E:304:ILE:HG23	1:E:1210:PHE:HB2	2.02	0.42
1:E:680:THR:HG22	1:E:682:HIS:H	1.84	0.42
2:I:560:VAL:HG12	2:J:397:LEU:HB2	2.01	0.42
2:I:872:TYR:CE1	6:I:1301:SAM:C5	3.03	0.42
2:L:257:LEU:HD21	2:L:327:LEU:HD11	2.01	0.42
3:R:141:GLU:OE2	3:R:216:TRP:NE1	2.43	0.42
1:a:1049:ARG:HG3	1:a:1198:TYR:HE1	1.84	0.42
1:e:1062:PRO:HG2	1:e:1065:LEU:HD13	2.01	0.42
1:C:257:THR:HG21	1:C:318:ARG:HH12	1.84	0.42
1:E:351:PRO:HG3	1:E:1175:ILE:HG12	2.01	0.42
2:H:851:ILE:HG21	6:H:1302:SAM:C5	2.50	0.42
2:J:509:GLY:HA2	2:J:545:SER:HB3	2.02	0.42
2:K:418:THR:HB	2:K:420:LEU:HB2	2.00	0.42
1:a:480:GLU:OE1	1:a:495:SER:N	2.41	0.42
1:a:870:THR:OG1	1:a:872:GLY:O	2.38	0.42
1:b:1117:MET:HB2	1:b:1117:MET:HE3	1.76	0.42
1:c:285:PHE:HD2	1:c:288:SER:H	1.67	0.42
1:2:11:LYS:N	1:b:319:ASP:OD2	2.53	0.42
1:B:326:PRO:HA	1:B:327:PRO:HD3	1.92	0.42
1:C:669:TYR:OH	1:c:779:GLN:O	2.33	0.42
1:E:1077:PHE:HD2	1:E:1110:PHE:HE1	1.68	0.42
2:J:628:GLU:HB2	2:J:666:TRP:HE1	1.85	0.42
2:K:570:ASP:OD2	6:L:1301:SAM:H3'	2.20	0.42
2:K:987:ASP:OD1	2:K:987:ASP:N	2.48	0.42
2:L:201:SER:OG	2:L:202:ASP:N	2.51	0.42
2:L:498:ASP:OD2	2:L:501:THR:OG1	2.31	0.42
2:L:552:TYR:HE2	6:L:1302:SAM:C2	2.32	0.42
3:R:737:LEU:HD23	3:R:781:TYR:HB2	2.01	0.42
3:R:1067:ARG:HE	3:R:1196:HIS:CG	2.38	0.42
1:a:810:TYR:OH	1:a:818:GLU:OE1	2.27	0.42
1:b:338:LEU:HD23	1:b:339:LEU:HB2	2.00	0.42
1:c:1079:ARG:HA	1:c:1114:LEU:HD21	2.02	0.42
1:e:507:TYR:CE1	1:e:915:PHE:HB3	2.54	0.42
1:A:786:THR:OG1	1:A:787:GLN:N	2.53	0.42
1:A:865:SER:HA	1:A:1000:GLN:HE22	1.85	0.42
1:B:492:THR:HG21	1:a:673:ARG:HA	2.02	0.42
1:C:616:ASP:OD1	1:C:674:ARG:NH1	2.52	0.42
1:C:1171:THR:HG22	1:C:1173:THR:H	1.85	0.42
2:H:141:THR:HG23	2:H:144:SER:H	1.85	0.42
2:H:974:TRP:HB2	2:H:977:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:418:THR:HB	2:L:420:LEU:HB2	2.00	0.42
2:L:851:ILE:HG23	6:L:1301:SAM:H2	2.02	0.42
1:a:954:SER:OG	1:a:955:LEU:N	2.51	0.42
1:c:776:VAL:HG12	1:c:790:VAL:HG23	2.02	0.42
1:c:1056:TRP:CZ3	1:c:1058:PRO:HA	2.55	0.42
1:A:1233:ASN:OD1	1:A:1237:ASN:ND2	2.38	0.41
1:E:272:VAL:HG23	1:E:300:ALA:HB3	2.02	0.41
1:E:1232:TYR:HB3	1:E:1235:LEU:HD13	2.02	0.41
2:I:141:THR:HG23	2:I:144:SER:H	1.86	0.41
2:I:757:ARG:NH2	2:I:793:VAL:O	2.45	0.41
2:J:578:VAL:CG2	6:J:1302:SAM:C4	2.98	0.41
2:J:712:GLU:HA	2:J:751:VAL:HA	2.01	0.41
2:L:141:THR:HG23	2:L:144:SER:H	1.85	0.41
1:a:452:GLU:OE2	1:a:1259:ARG:NH2	2.50	0.41
1:e:578:LEU:HD23	1:e:578:LEU:HA	1.77	0.41
1:A:692:GLN:HE21	2:I:92:VAL:HG22	1.85	0.41
1:B:692:GLN:NE2	1:B:703:ARG:HH22	2.19	0.41
1:C:416:VAL:HG21	1:b:1084:SER:HB2	2.02	0.41
1:E:501:VAL:HG13	1:E:502:ASN:H	1.85	0.41
2:L:628:GLU:HB2	2:L:666:TRP:HE1	1.84	0.41
3:R:299:TRP:HZ2	3:R:303:ARG:HA	1.84	0.41
3:R:455:TYR:HH	3:R:977:TYR:HH	1.52	0.41
3:R:535:GLN:NE2	3:R:654:LEU:HD21	2.36	0.41
3:R:628:ASN:ND2	4:U:224:GLU:OE2	2.52	0.41
1:b:705:TRP:HE3	1:b:771:LEU:HD13	1.85	0.41
1:b:1083:ILE:HD12	1:b:1121:TYR:HE2	1.85	0.41
1:c:494:THR:O	1:c:1270:VAL:N	2.49	0.41
1:c:504:LEU:HD23	1:c:506:PRO:HD3	2.01	0.41
1:e:896:VAL:HB	1:e:899:VAL:HG12	2.01	0.41
1:3:57:PRO:HG2	1:c:904:ALA:HB2	2.01	0.41
1:D:472:MET:HE3	1:D:922:VAL:HG21	2.03	0.41
1:D:691:ILE:HD11	1:D:710:HIS:CE1	2.56	0.41
1:D:1044:ASP:CG	1:D:1138:ARG:HE	2.29	0.41
1:E:247:LEU:HD11	1:E:525:ILE:HD12	2.03	0.41
2:H:498:ASP:OD2	2:H:501:THR:OG1	2.31	0.41
2:I:712:GLU:HA	2:I:751:VAL:HA	2.01	0.41
2:K:712:GLU:HA	2:K:751:VAL:HA	2.01	0.41
2:L:974:TRP:HB2	2:L:977:CYS:HB3	2.02	0.41
3:R:990:ARG:HE	3:R:994:GLU:HG3	1.85	0.41
3:R:992:ARG:HH22	3:R:1010:PHE:HB2	1.84	0.41
1:a:221:THR:HG22	1:a:1267:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:638:LEU:HD11	1:a:886:LEU:HD21	2.01	0.41
1:a:646:VAL:HG21	1:a:684:TRP:CD1	2.55	0.41
1:a:941:THR:HG22	1:a:943:TYR:H	1.84	0.41
1:c:314:VAL:HG22	1:c:316:PHE:H	1.85	0.41
1:d:456:ALA:HA	1:d:459:VAL:HG22	2.03	0.41
1:d:475:ASN:HB3	1:d:478:GLU:OE1	2.20	0.41
1:A:363:LEU:HD13	1:A:934:LEU:HD11	2.02	0.41
1:A:452:GLU:OE2	1:A:1259:ARG:NH2	2.39	0.41
1:B:266:PHE:HE2	1:B:1251:VAL:HG21	1.85	0.41
1:C:385:PHE:O	1:b:1079:ARG:NH2	2.53	0.41
1:D:1049:ARG:HG3	1:D:1198:TYR:HE1	1.86	0.41
2:I:257:LEU:HD21	2:I:327:LEU:HD11	2.01	0.41
2:L:509:GLY:HA2	2:L:545:SER:HB3	2.02	0.41
3:R:466:LEU:HD23	3:R:493:GLN:HE21	1.86	0.41
1:a:699:ALA:HB1	1:a:702:LEU:HB3	2.02	0.41
1:a:1245:ILE:HD12	1:a:1247:LEU:HB2	2.03	0.41
1:e:1095:ARG:HE	1:e:1099:GLY:HA2	1.86	0.41
1:A:355:ARG:HB3	1:A:954:SER:HB2	2.02	0.41
1:B:1058:PRO:HD2	1:B:1182:VAL:HB	2.01	0.41
1:D:755:LEU:HB2	1:D:806:MET:HE2	2.02	0.41
1:E:457:LEU:HD13	1:E:1030:VAL:HG21	2.01	0.41
1:E:826:LEU:HD12	1:E:827:PRO:HD2	2.02	0.41
2:I:743:ILE:O	2:I:787:ILE:N	2.54	0.41
2:J:45:PRO:HB2	2:J:54:ILE:HD12	2.03	0.41
2:K:45:PRO:HB2	2:K:54:ILE:HD12	2.03	0.41
3:R:197:ILE:HD11	3:R:222:MET:HA	2.02	0.41
1:a:223:PHE:HD2	1:a:910:ALA:HA	1.86	0.41
1:a:805:SER:OG	1:a:886:LEU:O	2.28	0.41
1:c:1034:GLU:CD	1:c:1207:ARG:HH12	2.28	0.41
1:d:649:PHE:HA	1:d:705:TRP:HE1	1.84	0.41
1:5:7:LYS:HB2	1:e:978:ASP:OD1	2.20	0.41
1:5:131:ASN:ND2	1:A:503:ARG:HH12	2.18	0.41
1:B:571:LEU:HD21	1:B:623:LEU:HD22	2.02	0.41
1:B:599:LEU:HD12	1:B:830:PRO:HB3	2.02	0.41
1:C:1186:SER:O	1:C:1213:ASN:ND2	2.53	0.41
2:H:45:PRO:HB2	2:H:54:ILE:HD12	2.03	0.41
2:K:613:VAL:HG13	2:K:654:VAL:HG22	2.02	0.41
1:a:507:TYR:HE2	1:a:1267:ILE:HD11	1.85	0.41
1:b:456:ALA:HA	1:b:459:VAL:HG12	2.02	0.41
1:d:242:ARG:HH11	1:d:247:LEU:HD21	1.85	0.41
1:d:272:VAL:HG23	1:d:300:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:306:VAL:HG21	1:d:1038:PHE:CD1	2.55	0.41
1:d:326:PRO:HA	1:d:327:PRO:HD3	1.87	0.41
1:e:392:ARG:HH11	1:e:450:VAL:HG21	1.84	0.41
1:D:438:GLN:NE2	1:D:440:MET:O	2.43	0.41
1:E:294:SER:HA	1:E:411:MET:HE1	2.01	0.41
1:E:438:GLN:H	1:d:859:GLN:NE2	2.16	0.41
2:H:712:GLU:HA	2:H:751:VAL:HA	2.01	0.41
2:I:310:ASN:HD21	2:I:353:ILE:HA	1.86	0.41
2:J:743:ILE:O	2:J:787:ILE:N	2.54	0.41
3:R:279:GLN:HA	3:R:283:HIS:HB2	2.03	0.41
3:R:556:SER:OG	3:R:557:THR:N	2.53	0.41
4:U:488:HIS:HB2	4:U:491:ARG:HD3	2.03	0.41
1:c:255:LEU:HD21	1:c:923:ILE:HD11	2.02	0.41
1:e:336:LYS:HA	1:e:340:ASN:HD22	1.86	0.41
1:A:318:ARG:HH12	1:A:370:LEU:HB2	1.86	0.41
1:D:220:ILE:HG13	1:D:578:LEU:HD21	2.03	0.41
2:J:974:TRP:HB2	2:J:977:CYS:HB3	2.02	0.41
2:L:712:GLU:HA	2:L:751:VAL:HA	2.02	0.41
3:R:1134:LEU:HD11	3:R:1260:MET:HB3	2.03	0.41
3:R:1219:ARG:O	3:R:1223:ARG:HG2	2.20	0.41
1:a:491:VAL:HG23	1:a:1273:GLY:HA2	2.02	0.41
1:c:825:MET:SD	1:c:912:THR:OG1	2.68	0.41
1:A:337:GLN:H	1:A:357:ASN:HD21	1.69	0.41
1:A:569:GLN:NE2	1:A:788:SER:OG	2.54	0.41
1:B:373:ASN:OD1	1:B:462:ARG:NH1	2.53	0.41
1:B:378:PHE:CE2	1:B:433:ARG:HD3	2.56	0.41
1:B:1120:ARG:NH1	1:b:187:SER:HG	2.17	0.41
1:D:406:MET:HA	1:D:453:THR:HG22	2.03	0.41
1:D:630:PHE:HB2	1:D:772:MET:HE1	2.03	0.41
1:E:272:VAL:HA	1:E:273:PRO:HD3	1.94	0.41
1:E:385:PHE:HE1	1:d:1117:MET:HA	1.86	0.41
1:E:851:ARG:HH12	1:E:990:GLY:H	1.69	0.41
2:H:310:ASN:HD21	2:H:353:ILE:HA	1.86	0.41
2:I:476:ARG:NH1	2:I:477:LYS:O	2.54	0.41
2:J:476:ARG:NH1	2:J:477:LYS:O	2.54	0.41
2:K:141:THR:HG23	2:K:144:SER:H	1.85	0.41
2:K:476:ARG:NH1	2:K:477:LYS:O	2.54	0.41
2:K:577:ASP:OD2	6:K:1301:SAM:C	2.69	0.41
2:L:310:ASN:HD21	2:L:353:ILE:HA	1.86	0.41
3:R:139:ILE:HD12	3:R:139:ILE:HA	1.96	0.41
3:R:284:SER:HG	3:R:327:ASN:HD22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:286:TYR:C	3:R:288:SER:H	2.27	0.41
3:R:303:ARG:HD2	3:R:727:ARG:HG2	2.02	0.41
3:R:639:ARG:HA	3:R:640:PRO:HD3	1.97	0.41
3:R:716:VAL:HG12	3:R:720:MET:HE2	2.03	0.41
4:U:208:PRO:HD2	4:U:234:PHE:HE2	1.86	0.41
1:c:352:LEU:HD23	1:c:955:LEU:HD13	2.02	0.41
1:c:505:MET:HE3	1:c:505:MET:HB2	1.86	0.41
1:c:1059:LEU:HB2	1:c:1206:ASP:HB2	2.03	0.41
1:d:453:THR:HA	1:d:1254:TYR:HA	2.02	0.41
1:d:566:SER:OG	1:d:567:THR:N	2.54	0.41
1:A:553:PRO:HD2	3:R:309:MET:HE3	2.03	0.41
1:E:353:MET:HE1	1:e:894:ASP:HB2	2.03	0.41
1:E:669:TYR:OH	1:e:779:GLN:O	2.33	0.41
2:H:476:ARG:NH1	2:H:477:LYS:O	2.54	0.41
2:H:509:GLY:HA2	2:H:545:SER:HB3	2.02	0.41
2:H:743:ILE:O	2:H:787:ILE:N	2.54	0.41
3:R:1172:LEU:HD23	3:R:1172:LEU:HA	1.88	0.41
4:U:67:ASN:H	4:U:149:ASN:HD21	1.68	0.41
1:a:457:LEU:HD12	1:a:1030:VAL:HG11	2.03	0.41
1:b:821:VAL:HG11	1:b:905:ILE:HG12	2.02	0.41
1:c:690:ASN:HB3	1:c:693:LEU:HD13	2.03	0.41
1:c:853:SER:OG	1:c:854:ARG:N	2.54	0.41
1:e:819:LEU:HA	1:e:822:ILE:HG22	2.02	0.41
1:5:12:SER:N	1:e:319:ASP:OD1	2.52	0.40
1:A:852:GLN:O	1:A:996:GLN:NE2	2.54	0.40
1:B:915:PHE:HE2	1:B:1267:ILE:HG21	1.86	0.40
1:E:620:VAL:HB	1:E:659:PHE:HE2	1.84	0.40
2:H:47:ARG:NH1	2:H:52:ASN:OD1	2.47	0.40
2:H:613:VAL:HG13	2:H:654:VAL:HG22	2.02	0.40
2:I:613:VAL:HG13	2:I:654:VAL:HG22	2.02	0.40
2:L:476:ARG:NH1	2:L:477:LYS:O	2.54	0.40
1:a:339:LEU:HD23	1:a:339:LEU:HA	1.85	0.40
1:a:958:SER:OG	1:a:959:ALA:N	2.54	0.40
1:b:200:VAL:HB	1:b:205:LEU:HB2	2.03	0.40
1:c:303:ARG:NH2	1:c:1150:TYR:OH	2.54	0.40
1:c:577:ILE:HG21	1:c:577:ILE:HD13	1.81	0.40
1:e:836:VAL:HG21	1:e:843:VAL:HG22	2.03	0.40
1:3:166:PRO:HG3	1:D:290:TYR:HE1	1.86	0.40
1:B:842:ARG:HA	1:B:1003:GLN:HE21	1.86	0.40
1:C:253:PRO:HG3	1:C:923:ILE:HG13	2.04	0.40
1:C:836:VAL:HG21	1:C:842:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:ASN:HD22	1:b:657:VAL:HG13	1.86	0.40
2:K:743:ILE:O	2:K:787:ILE:N	2.54	0.40
2:L:613:VAL:HG13	2:L:654:VAL:HG22	2.02	0.40
3:R:937:PHE:CG	3:R:942:LEU:HD23	2.56	0.40
3:R:1049:PHE:CD1	3:R:1053:LEU:HD23	2.57	0.40
1:e:259:ASP:OD1	1:e:312:SER:OG	2.34	0.40
1:e:472:MET:HE3	1:e:506:PRO:HB2	2.03	0.40
1:e:839:ASP:OD2	1:e:842:ARG:NH1	2.54	0.40
1:e:952:ILE:HD11	1:e:1031:PHE:HE2	1.87	0.40
1:e:954:SER:OG	1:e:955:LEU:N	2.53	0.40
1:2:69:ALA:HA	1:b:538:ASP:HB3	2.04	0.40
1:5:135:ARG:HH11	1:e:989:SER:HB3	1.86	0.40
1:A:318:ARG:NH1	1:A:370:LEU:O	2.54	0.40
1:A:646:VAL:HG21	1:A:684:TRP:CD2	2.56	0.40
2:H:569:GLY:O	2:I:852:ARG:NH1	2.41	0.40
2:I:419:GLN:HE21	2:J:108:HIS:HE1	1.68	0.40
2:J:310:ASN:HD21	2:J:353:ILE:HA	1.86	0.40
2:L:743:ILE:O	2:L:787:ILE:N	2.54	0.40
3:R:1130:ARG:HG2	3:R:1260:MET:HE3	2.03	0.40
4:U:563:GLU:O	4:U:569:GLN:NE2	2.43	0.40
1:c:186:CYS:HB3	1:c:203:HIS:CE1	2.56	0.40
1:c:306:VAL:HG21	1:c:1038:PHE:CD1	2.56	0.40
1:c:448:VAL:HG12	1:c:1259:ARG:HB2	2.04	0.40
1:c:507:TYR:CE1	1:c:915:PHE:HB3	2.55	0.40
1:d:939:SER:HB3	1:d:957:ALA:HB3	2.03	0.40
1:e:333:HIS:HA	1:e:336:LYS:HG2	2.04	0.40
1:3:59:ILE:O	1:3:63:GLN:HG2	2.22	0.40
1:5:65:ALA:HB2	1:e:545:ARG:HG3	2.03	0.40
1:A:598:TRP:O	1:A:835:TYR:OH	2.38	0.40
1:B:1104:PHE:HE1	1:B:1126:PHE:HE1	1.69	0.40
1:C:351:PRO:HG3	1:C:1116:GLN:HE22	1.87	0.40
1:D:386:THR:HG21	1:D:431:VAL:HG11	2.03	0.40
1:D:669:TYR:HE2	1:d:780:ARG:HA	1.87	0.40
1:D:670:THR:HG23	1:D:672:SER:H	1.86	0.40
2:I:850:ASP:CG	6:I:1301:SAM:H1'	2.18	0.40
2:J:141:THR:HG23	2:J:144:SER:H	1.85	0.40
2:K:310:ASN:HD21	2:K:353:ILE:HA	1.86	0.40
3:R:376:PHE:HE1	3:R:521:VAL:HG22	1.86	0.40
3:R:450:ILE:HD12	3:R:450:ILE:HA	1.94	0.40
1:d:524:ASN:ND2	1:d:982:MET:SD	2.94	0.40
1:e:554:THR:OG1	1:e:558:ASN:OD1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:63:GLN:O	1:4:67:GLU:HG2	2.22	0.40
1:5:77:ASP:OD1	1:5:80:THR:OG1	2.40	0.40
1:C:501:VAL:HG13	1:C:502:ASN:H	1.87	0.40
1:E:339:LEU:HD22	1:E:353:MET:SD	2.62	0.40
1:E:860:PRO:HB2	1:E:1012:ILE:HD13	2.04	0.40
2:H:397:LEU:HB2	2:L:560:VAL:HG12	2.04	0.40
2:K:344:LEU:HD23	2:K:375:LEU:HD11	2.03	0.40
2:L:45:PRO:HB2	2:L:54:ILE:HD12	2.03	0.40
1:a:621:THR:HA	1:a:782:GLN:HG3	2.03	0.40
1:b:520:ILE:HG22	1:b:982:MET:HE1	2.03	0.40
1:b:525:ILE:HD13	1:b:603:VAL:HG11	2.03	0.40
1:e:565:GLU:HA	1:e:572:SER:HB2	2.04	0.40
1:e:936:ALA:O	1:e:947:ARG:NH1	2.55	0.40
1:e:958:SER:OG	1:e:959:ALA:N	2.55	0.40
1:e:1056:TRP:CZ3	1:e:1058:PRO:HA	2.56	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	1	136/1275 (11%)	123 (90%)	13 (10%)	0	100	100
1	2	135/1275 (11%)	125 (93%)	10 (7%)	0	100	100
1	3	134/1275 (10%)	124 (92%)	10 (8%)	0	100	100
1	4	125/1275 (10%)	115 (92%)	10 (8%)	0	100	100
1	5	136/1275 (11%)	126 (93%)	10 (7%)	0	100	100
1	A	1126/1275 (88%)	1045 (93%)	80 (7%)	1 (0%)	48	79
1	B	1069/1275 (84%)	991 (93%)	76 (7%)	2 (0%)	43	72
1	C	1084/1275 (85%)	1016 (94%)	67 (6%)	1 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1046/1275 (82%)	974 (93%)	72 (7%)	0	100	100
1	E	1059/1275 (83%)	992 (94%)	66 (6%)	1 (0%)	48	79
1	a	1083/1275 (85%)	1002 (92%)	79 (7%)	2 (0%)	43	72
1	b	1083/1275 (85%)	1015 (94%)	68 (6%)	0	100	100
1	c	1076/1275 (84%)	1016 (94%)	59 (6%)	1 (0%)	48	79
1	d	1083/1275 (85%)	1017 (94%)	66 (6%)	0	100	100
1	e	1083/1275 (85%)	1002 (92%)	80 (7%)	1 (0%)	48	79
2	H	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	I	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	J	1022/1289 (79%)	949 (93%)	73 (7%)	0	100	100
2	K	1022/1289 (79%)	950 (93%)	72 (7%)	0	100	100
2	L	1022/1289 (79%)	946 (93%)	76 (7%)	0	100	100
3	R	1249/1267 (99%)	1166 (93%)	82 (7%)	1 (0%)	48	79
4	U	658/736 (89%)	591 (90%)	60 (9%)	7 (1%)	11	43
All	All	18475/27573 (67%)	17185 (93%)	1273 (7%)	17 (0%)	49	79

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	TRP
1	B	310	TRP
3	R	287	GLU
1	a	310	TRP
1	B	1214	SER
4	U	585	PRO
4	U	136	SER
4	U	471	ASP
1	e	1058	PRO
4	U	456	PHE
4	U	531	ASP
1	C	586	SER
4	U	133	PRO
4	U	135	ILE
1	E	583	PRO
1	a	346	VAL
1	c	1058	PRO

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	1	112/1113 (10%)	112 (100%)	0	100	100
1	2	111/1113 (10%)	111 (100%)	0	100	100
1	3	111/1113 (10%)	111 (100%)	0	100	100
1	4	104/1113 (9%)	104 (100%)	0	100	100
1	5	112/1113 (10%)	109 (97%)	3 (3%)	39	61
1	A	994/1113 (89%)	993 (100%)	1 (0%)	88	87
1	B	945/1113 (85%)	942 (100%)	3 (0%)	86	83
1	C	963/1113 (86%)	962 (100%)	1 (0%)	88	87
1	D	931/1113 (84%)	930 (100%)	1 (0%)	88	87
1	E	940/1113 (84%)	939 (100%)	1 (0%)	88	87
1	a	960/1113 (86%)	959 (100%)	1 (0%)	88	87
1	b	960/1113 (86%)	960 (100%)	0	100	100
1	c	955/1113 (86%)	954 (100%)	1 (0%)	88	87
1	d	960/1113 (86%)	959 (100%)	1 (0%)	88	87
1	e	960/1113 (86%)	958 (100%)	2 (0%)	87	85
2	H	884/1118 (79%)	883 (100%)	1 (0%)	88	87
2	I	884/1118 (79%)	883 (100%)	1 (0%)	88	87
2	J	884/1118 (79%)	882 (100%)	2 (0%)	87	85
2	K	884/1118 (79%)	883 (100%)	1 (0%)	88	87
2	L	884/1118 (79%)	879 (99%)	5 (1%)	78	79
3	R	1074/1084 (99%)	1071 (100%)	3 (0%)	86	83
4	U	592/650 (91%)	591 (100%)	1 (0%)	87	85
All	All	16204/24019 (68%)	16175 (100%)	29 (0%)	85	85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	6	ARG
1	5	9	LYS
1	5	13	SER
1	A	154	ILE
1	B	567	THR
1	B	701	ILE
1	B	752	THR
1	C	416	VAL
1	D	416	VAL
1	E	794	ARG
2	H	969	ILE
2	I	969	ILE
2	J	849	VAL
2	J	969	ILE
2	K	969	ILE
2	L	574	VAL
2	L	578	VAL
2	L	849	VAL
2	L	851	ILE
2	L	969	ILE
3	R	880	VAL
3	R	1018	GLN
3	R	1221	ILE
4	U	212	THR
1	a	338	LEU
1	c	1182	VAL
1	d	870	THR
1	e	480	GLU
1	e	945	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (261) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	52	HIS
1	1	119	GLN
1	1	141	ASN
1	1	146	ASN
1	2	76	ASN
1	2	86	ASN
1	2	141	ASN
1	3	146	ASN
1	4	76	ASN
1	4	109	GLN

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Mol	Chain	Res	Type
1	4	131	ASN
1	5	52	HIS
1	5	76	ASN
1	5	131	ASN
1	5	146	ASN
1	5	165	HIS
1	A	184	HIS
1	A	228	GLN
1	A	278	GLN
1	A	293	GLN
1	A	313	ASN
1	A	357	ASN
1	A	441	ASN
1	A	511	ASN
1	A	527	ASN
1	A	569	GLN
1	A	682	HIS
1	A	692	GLN
1	A	731	ASN
1	A	812	GLN
1	A	1000	GLN
1	A	1003	GLN
1	A	1075	HIS
1	A	1123	ASN
1	B	278	GLN
1	B	307	HIS
1	B	313	ASN
1	B	357	ASN
1	B	375	HIS
1	B	382	HIS
1	B	421	ASN
1	B	441	ASN
1	B	527	ASN
1	B	528	ASN
1	B	569	GLN
1	B	692	GLN
1	B	763	ASN
1	B	779	GLN
1	B	1000	GLN
1	B	1003	GLN
1	B	1025	GLN
1	B	1075	HIS

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Mol	Chain	Res	Type
1	B	1116	GLN
1	B	1123	ASN
1	B	1213	ASN
1	B	1233	ASN
1	C	340	ASN
1	C	357	ASN
1	C	375	HIS
1	C	438	GLN
1	C	527	ASN
1	C	692	GLN
1	C	718	GLN
1	C	749	ASN
1	C	787	GLN
1	C	812	GLN
1	C	970	ASN
1	C	1036	ASN
1	C	1116	GLN
1	C	1123	ASN
1	C	1149	HIS
1	D	217	GLN
1	D	278	GLN
1	D	340	ASN
1	D	357	ASN
1	D	524	ASN
1	D	682	HIS
1	D	692	GLN
1	D	704	GLN
1	D	787	GLN
1	D	812	GLN
1	D	970	ASN
1	D	1025	GLN
1	D	1033	HIS
1	D	1036	ASN
1	D	1123	ASN
1	D	1149	HIS
1	D	1233	ASN
1	D	1244	GLN
1	E	217	GLN
1	E	246	GLN
1	E	249	HIS
1	E	278	GLN
1	E	340	ASN

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Mol	Chain	Res	Type
1	E	357	ASN
1	E	382	HIS
1	E	585	ASN
1	E	690	ASN
1	E	692	GLN
1	E	774	ASN
1	E	782	GLN
1	E	929	GLN
1	E	996	GLN
1	E	1000	GLN
1	E	1075	HIS
1	E	1149	HIS
1	E	1246	GLN
2	H	108	HIS
2	H	127	GLN
2	H	310	ASN
2	H	313	GLN
2	H	321	GLN
2	H	352	GLN
2	H	549	GLN
2	H	572	GLN
2	H	634	ASN
2	H	677	HIS
2	H	804	HIS
2	I	108	HIS
2	I	127	GLN
2	I	310	ASN
2	I	313	GLN
2	I	321	GLN
2	I	352	GLN
2	I	549	GLN
2	I	572	GLN
2	I	634	ASN
2	I	804	HIS
2	J	28	HIS
2	J	108	HIS
2	J	127	GLN
2	J	310	ASN
2	J	321	GLN
2	J	352	GLN
2	J	549	GLN
2	J	572	GLN

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Mol	Chain	Res	Type
2	J	634	ASN
2	J	677	HIS
2	J	804	HIS
2	K	108	HIS
2	K	223	HIS
2	K	310	ASN
2	K	313	GLN
2	K	321	GLN
2	K	352	GLN
2	K	549	GLN
2	K	572	GLN
2	K	634	ASN
2	K	677	HIS
2	K	804	HIS
2	K	944	GLN
2	L	108	HIS
2	L	127	GLN
2	L	310	ASN
2	L	313	GLN
2	L	321	GLN
2	L	352	GLN
2	L	549	GLN
2	L	572	GLN
2	L	604	HIS
2	L	634	ASN
2	L	677	HIS
2	L	804	HIS
3	R	22	GLN
3	R	29	ASN
3	R	143	GLN
3	R	183	HIS
3	R	454	GLN
3	R	493	GLN
3	R	535	GLN
3	R	536	GLN
3	R	646	ASN
3	R	732	GLN
3	R	754	GLN
3	R	836	GLN
3	R	864	GLN
3	R	938	ASN
3	R	950	GLN

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Mol	Chain	Res	Type
3	R	1018	GLN
3	R	1085	ASN
3	R	1108	GLN
3	R	1144	GLN
3	R	1195	HIS
3	R	1206	HIS
4	U	119	ASN
4	U	146	GLN
4	U	147	ASN
4	U	149	ASN
4	U	203	ASN
4	U	247	ASN
4	U	451	GLN
4	U	488	HIS
4	U	536	ASN
4	U	538	ASN
1	a	184	HIS
1	a	241	ASN
1	a	357	ASN
1	a	360	HIS
1	a	382	HIS
1	a	438	GLN
1	a	524	ASN
1	a	667	GLN
1	a	692	GLN
1	a	774	ASN
1	a	787	GLN
1	a	859	GLN
1	a	937	GLN
1	a	1033	HIS
1	a	1036	ASN
1	b	246	GLN
1	b	275	GLN
1	b	357	ASN
1	b	415	ASN
1	b	518	GLN
1	b	731	ASN
1	b	746	GLN
1	b	929	GLN
1	b	1213	ASN
1	b	1233	ASN
1	c	184	HIS

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Mol	Chain	Res	Type
1	c	206	HIS
1	c	219	HIS
1	c	234	GLN
1	c	275	GLN
1	c	331	ASN
1	c	337	GLN
1	c	524	ASN
1	c	731	ASN
1	c	937	GLN
1	c	970	ASN
1	c	1003	GLN
1	c	1033	HIS
1	c	1255	ASN
1	d	230	HIS
1	d	340	ASN
1	d	357	ASN
1	d	518	GLN
1	d	524	ASN
1	d	537	GLN
1	d	558	ASN
1	d	569	GLN
1	d	782	GLN
1	d	859	GLN
1	d	868	ASN
1	d	898	ASN
1	d	1036	ASN
1	d	1075	HIS
1	d	1197	GLN
1	d	1205	ASN
1	d	1233	ASN
1	e	246	GLN
1	e	488	GLN
1	e	518	GLN
1	e	524	ASN
1	e	745	HIS
1	e	868	ASN
1	e	942	GLN
1	e	1036	ASN
1	e	1125	GLN
1	e	1205	ASN
1	e	1213	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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$
6	SAM	K	1301	-	27,29,29	1.47	6 (22%)	34,42,42	2.16	8 (23%)
6	SAM	I	1301	-	27,29,29	1.44	5 (18%)	34,42,42	2.16	12 (35%)
6	SAM	J	1302	-	27,29,29	1.45	6 (22%)	34,42,42	2.14	10 (29%)
6	SAM	H	1302	-	27,29,29	1.45	6 (22%)	34,42,42	2.06	11 (32%)
6	SAM	L	1302	-	27,29,29	1.47	5 (18%)	34,42,42	1.95	10 (29%)
6	SAM	J	1301	-	27,29,29	1.45	6 (22%)	34,42,42	2.16	10 (29%)
6	SAM	K	1302	-	27,29,29	1.42	5 (18%)	34,42,42	2.17	10 (29%)
6	SAM	H	1301	-	27,29,29	1.44	6 (22%)	34,42,42	2.10	12 (35%)
6	SAM	L	1301	-	27,29,29	1.45	6 (22%)	34,42,42	2.15	13 (38%)
6	SAM	I	1302	-	27,29,29	1.46	6 (22%)	34,42,42	2.07	12 (35%)

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
6	SAM	K	1301	-	-	8/17/33/33	0/3/3/3
6	SAM	I	1301	-	-	0/17/33/33	0/3/3/3
6	SAM	J	1302	-	-	8/17/33/33	0/3/3/3
6	SAM	H	1302	-	-	6/17/33/33	0/3/3/3
6	SAM	L	1302	-	-	4/17/33/33	0/3/3/3
6	SAM	J	1301	-	-	6/17/33/33	0/3/3/3
6	SAM	K	1302	-	-	2/17/33/33	0/3/3/3
6	SAM	H	1301	-	-	4/17/33/33	0/3/3/3
6	SAM	L	1301	-	-	6/17/33/33	0/3/3/3
6	SAM	I	1302	-	-	8/17/33/33	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1301	SAM	C5-C4	4.44	1.47	1.39
6	L	1302	SAM	C5-C4	4.36	1.46	1.39
6	J	1301	SAM	C5-C4	4.30	1.46	1.39
6	I	1301	SAM	C5-C4	4.23	1.46	1.39
6	L	1301	SAM	C5-C4	4.22	1.46	1.39
6	I	1302	SAM	C5-C4	4.17	1.46	1.39
6	H	1302	SAM	C5-C4	4.12	1.46	1.39
6	K	1302	SAM	C5-C4	4.12	1.46	1.39
6	J	1302	SAM	C5-C4	4.11	1.46	1.39
6	H	1301	SAM	C5-C4	4.11	1.46	1.39
6	K	1301	SAM	C5-N7	-2.86	1.33	1.39
6	L	1302	SAM	C5-N7	-2.73	1.34	1.39
6	J	1302	SAM	C5-N7	-2.71	1.34	1.39
6	H	1302	SAM	C5-N7	-2.61	1.34	1.39
6	L	1301	SAM	C5-C6	2.61	1.48	1.41
6	I	1302	SAM	C5-N7	-2.57	1.34	1.39
6	H	1301	SAM	C5-N7	-2.57	1.34	1.39
6	I	1301	SAM	C5-N7	-2.53	1.34	1.39
6	H	1302	SAM	C5-C6	2.52	1.48	1.41
6	J	1301	SAM	C5-C6	2.52	1.48	1.41
6	J	1301	SAM	C5-N7	-2.52	1.34	1.39
6	I	1301	SAM	C5-C6	2.51	1.48	1.41
6	K	1302	SAM	C5-C6	2.47	1.47	1.41
6	I	1302	SAM	C5-C6	2.47	1.47	1.41
6	J	1302	SAM	C5-C6	2.47	1.47	1.41
6	K	1302	SAM	C5-N7	-2.40	1.34	1.39
6	H	1301	SAM	C5-C6	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1302	SAM	OXT-C	-2.39	1.23	1.30
6	L	1301	SAM	C5-N7	-2.38	1.34	1.39
6	L	1302	SAM	C4-N9	-2.36	1.32	1.37
6	K	1301	SAM	C5-C6	2.32	1.47	1.41
6	L	1302	SAM	C8-N7	2.31	1.36	1.31
6	H	1302	SAM	C4-N9	-2.28	1.32	1.37
6	L	1302	SAM	C5-C6	2.28	1.47	1.41
6	L	1301	SAM	C8-N7	2.27	1.36	1.31
6	K	1302	SAM	C8-N7	2.23	1.36	1.31
6	H	1301	SAM	C8-N7	2.23	1.36	1.31
6	I	1301	SAM	C4-N9	-2.22	1.33	1.37
6	H	1301	SAM	C4-N9	-2.19	1.33	1.37
6	J	1302	SAM	C8-N7	2.17	1.35	1.31
6	H	1302	SAM	C8-N7	2.17	1.35	1.31
6	L	1301	SAM	C4-N9	-2.16	1.33	1.37
6	I	1302	SAM	C4-N9	-2.16	1.33	1.37
6	J	1301	SAM	C8-N7	2.14	1.35	1.31
6	I	1301	SAM	C8-N7	2.12	1.35	1.31
6	I	1302	SAM	C8-N7	2.11	1.35	1.31
6	J	1302	SAM	C4-N9	-2.07	1.33	1.37
6	L	1301	SAM	OXT-C	-2.06	1.24	1.30
6	K	1302	SAM	C4-N9	-2.06	1.33	1.37
6	H	1301	SAM	OXT-C	-2.05	1.24	1.30
6	K	1301	SAM	C8-N7	2.03	1.35	1.31
6	J	1301	SAM	C4-N9	-2.03	1.33	1.37
6	J	1302	SAM	OXT-C	-2.02	1.24	1.30
6	K	1301	SAM	CE-SD	-2.02	1.66	1.78
6	H	1302	SAM	CE-SD	-2.02	1.66	1.78
6	K	1301	SAM	OXT-C	-2.01	1.24	1.30
6	J	1301	SAM	CE-SD	-2.00	1.66	1.78

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1301	SAM	C5-C4-N3	-6.57	117.66	126.72
6	J	1302	SAM	C5-C4-N3	-6.05	118.39	126.72
6	J	1301	SAM	C5-C4-N3	-6.03	118.42	126.72
6	I	1302	SAM	C5-C4-N3	-5.87	118.63	126.72
6	K	1302	SAM	C5-C4-N3	-5.78	118.75	126.72
6	H	1301	SAM	C5-C4-N3	-5.69	118.88	126.72
6	I	1301	SAM	C5-C4-N3	-5.67	118.91	126.72
6	H	1302	SAM	C5-C4-N3	-5.57	119.05	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1301	SAM	C5-C4-N3	-5.54	119.09	126.72
6	L	1302	SAM	C5-C4-N3	-5.29	119.43	126.72
6	K	1301	SAM	N3-C4-N9	5.25	136.09	127.17
6	J	1301	SAM	N3-C4-N9	4.81	135.34	127.17
6	K	1302	SAM	N3-C4-N9	4.66	135.10	127.17
6	I	1302	SAM	N3-C4-N9	4.61	135.00	127.17
6	I	1301	SAM	N3-C4-N9	4.55	134.91	127.17
6	H	1301	SAM	N3-C4-N9	4.53	134.88	127.17
6	H	1302	SAM	N3-C4-N9	4.51	134.84	127.17
6	J	1302	SAM	N3-C4-N9	4.46	134.74	127.17
6	L	1301	SAM	N3-C4-N9	4.41	134.67	127.17
6	L	1302	SAM	N3-C4-N9	4.23	134.37	127.17
6	K	1302	SAM	CG-SD-C5'	4.13	113.53	103.43
6	K	1301	SAM	C2-N3-C4	4.11	121.87	111.83
6	J	1302	SAM	C2-N3-C4	3.99	121.56	111.83
6	J	1301	SAM	C2-N3-C4	3.98	121.54	111.83
6	K	1302	SAM	C2-N3-C4	3.92	121.40	111.83
6	H	1301	SAM	N3-C2-N1	-3.89	122.69	128.58
6	I	1302	SAM	C2-N3-C4	3.89	121.33	111.83
6	H	1301	SAM	C2-N3-C4	3.88	121.31	111.83
6	L	1301	SAM	C2-N3-C4	3.87	121.28	111.83
6	I	1301	SAM	C2-N3-C4	3.85	121.24	111.83
6	I	1301	SAM	CG-SD-C5'	3.84	112.81	103.43
6	L	1301	SAM	N3-C2-N1	-3.83	122.79	128.58
6	H	1302	SAM	C2-N3-C4	3.82	121.15	111.83
6	I	1301	SAM	N3-C2-N1	-3.80	122.84	128.58
6	L	1302	SAM	N3-C2-N1	-3.78	122.86	128.58
6	K	1302	SAM	N3-C2-N1	-3.76	122.89	128.58
6	J	1301	SAM	N3-C2-N1	-3.74	122.91	128.58
6	J	1302	SAM	CG-SD-C5'	3.74	112.58	103.43
6	H	1302	SAM	N3-C2-N1	-3.73	122.94	128.58
6	J	1302	SAM	N3-C2-N1	-3.72	122.95	128.58
6	I	1302	SAM	N3-C2-N1	-3.66	123.03	128.58
6	L	1302	SAM	C2-N3-C4	3.66	120.77	111.83
6	K	1301	SAM	N3-C2-N1	-3.64	123.07	128.58
6	J	1301	SAM	C4-C5-N7	-3.64	106.42	110.58
6	J	1302	SAM	C4-C5-N7	-3.59	106.47	110.58
6	L	1301	SAM	C4-C5-N7	-3.50	106.58	110.58
6	I	1301	SAM	C4-C5-N7	-3.50	106.58	110.58
6	I	1302	SAM	C4-C5-N7	-3.45	106.64	110.58
6	K	1302	SAM	C4-C5-N7	-3.45	106.64	110.58
6	H	1302	SAM	C4-C5-N7	-3.43	106.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1301	SAM	C4-C5-N7	-3.33	106.77	110.58
6	H	1302	SAM	C4-N9-C8	3.28	109.18	105.74
6	K	1302	SAM	C4-N9-C8	3.21	109.11	105.74
6	L	1301	SAM	C4-N9-C8	3.20	109.09	105.74
6	I	1301	SAM	C4-N9-C8	3.17	109.07	105.74
6	L	1302	SAM	C4-C5-N7	-3.03	107.11	110.58
6	J	1301	SAM	C4-N9-C8	3.02	108.91	105.74
6	H	1301	SAM	C4-N9-C8	3.01	108.89	105.74
6	L	1301	SAM	CG-SD-C5'	2.98	110.72	103.43
6	K	1301	SAM	C4-C5-N7	-2.90	107.27	110.58
6	J	1301	SAM	C5-N7-C8	2.86	107.94	103.45
6	I	1302	SAM	C4-N9-C8	2.79	108.67	105.74
6	I	1301	SAM	C5-N7-C8	2.79	107.83	103.45
6	L	1302	SAM	C4-N9-C8	2.78	108.65	105.74
6	H	1302	SAM	C5-N7-C8	2.74	107.76	103.45
6	J	1302	SAM	C5-N7-C8	2.74	107.75	103.45
6	K	1302	SAM	C5-N7-C8	2.74	107.75	103.45
6	L	1301	SAM	C5-N7-C8	2.73	107.73	103.45
6	K	1301	SAM	CG-SD-C5'	2.69	110.01	103.43
6	I	1302	SAM	C5-N7-C8	2.68	107.66	103.45
6	H	1301	SAM	C5-N7-C8	2.62	107.56	103.45
6	H	1302	SAM	N9-C8-N7	-2.58	110.27	113.94
6	L	1301	SAM	O4'-C1'-N9	2.54	112.97	108.09
6	I	1301	SAM	N9-C8-N7	-2.53	110.35	113.94
6	K	1302	SAM	N9-C8-N7	-2.53	110.35	113.94
6	L	1301	SAM	N9-C8-N7	-2.52	110.36	113.94
6	J	1301	SAM	CG-SD-C5'	2.51	109.57	103.43
6	H	1302	SAM	CG-SD-C5'	2.45	109.43	103.43
6	J	1301	SAM	N9-C8-N7	-2.44	110.47	113.94
6	H	1301	SAM	N9-C8-N7	-2.40	110.53	113.94
6	K	1301	SAM	C1'-N9-C8	-2.40	121.78	127.09
6	L	1301	SAM	C6-C5-N7	2.34	136.60	132.09
6	I	1302	SAM	C3'-C2'-C1'	2.32	105.85	101.46
6	L	1302	SAM	C2-N1-C6	2.31	122.52	118.73
6	I	1302	SAM	N9-C8-N7	-2.30	110.67	113.94
6	L	1302	SAM	C5-N7-C8	2.30	107.06	103.45
6	H	1301	SAM	O4'-C1'-N9	2.26	112.42	108.09
6	L	1302	SAM	CG-SD-C5'	2.21	108.84	103.43
6	J	1302	SAM	C4-N9-C8	2.20	108.05	105.74
6	K	1302	SAM	C6-C5-N7	2.20	136.33	132.09
6	K	1301	SAM	C5-N7-C8	2.19	106.90	103.45
6	I	1302	SAM	CG-SD-C5'	2.19	108.78	103.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1302	SAM	C6-C5-N7	2.18	136.30	132.09
6	J	1302	SAM	N9-C8-N7	-2.17	110.85	113.94
6	H	1301	SAM	C2-N1-C6	2.17	122.30	118.73
6	I	1301	SAM	C6-C5-N7	2.17	136.28	132.09
6	J	1301	SAM	C6-C5-N7	2.17	136.27	132.09
6	I	1302	SAM	C6-C5-N7	2.13	136.20	132.09
6	I	1301	SAM	C2-N1-C6	2.12	122.21	118.73
6	L	1301	SAM	C2-N1-C6	2.11	122.19	118.73
6	J	1302	SAM	C6-C5-N7	2.10	136.13	132.09
6	H	1301	SAM	C6-C5-N7	2.09	136.12	132.09
6	L	1302	SAM	N9-C8-N7	-2.09	110.97	113.94
6	I	1302	SAM	C2-N1-C6	2.07	122.13	118.73
6	H	1301	SAM	CG-SD-C5'	2.07	108.48	103.43
6	I	1301	SAM	C3'-C2'-C1'	2.04	105.33	101.46
6	H	1302	SAM	C2-N1-C6	2.02	122.04	118.73
6	L	1301	SAM	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1301	SAM	C4'-C5'-SD-CE
6	H	1302	SAM	C-CA-CB-CG
6	H	1302	SAM	CB-CG-SD-CE
6	H	1302	SAM	CB-CG-SD-C5'
6	H	1302	SAM	O4'-C4'-C5'-SD
6	H	1302	SAM	C3'-C4'-C5'-SD
6	I	1302	SAM	N-CA-CB-CG
6	I	1302	SAM	C-CA-CB-CG
6	I	1302	SAM	CA-CB-CG-SD
6	I	1302	SAM	C4'-C5'-SD-CE
6	I	1302	SAM	C3'-C4'-C5'-SD
6	J	1301	SAM	CB-CG-SD-CE
6	J	1302	SAM	N-CA-CB-CG
6	J	1302	SAM	C-CA-CB-CG
6	J	1302	SAM	C4'-C5'-SD-CE
6	K	1301	SAM	N-CA-CB-CG
6	K	1301	SAM	C-CA-CB-CG
6	L	1301	SAM	N-CA-CB-CG
6	L	1301	SAM	C-CA-CB-CG
6	L	1301	SAM	CB-CG-SD-CE
6	L	1301	SAM	CB-CG-SD-C5'

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Mol	Chain	Res	Type	Atoms
6	L	1301	SAM	O4'-C4'-C5'-SD
6	L	1301	SAM	C3'-C4'-C5'-SD
6	L	1302	SAM	CB-CG-SD-CE
6	L	1302	SAM	CB-CG-SD-C5'
6	L	1302	SAM	C4'-C5'-SD-CE
6	H	1301	SAM	OXT-C-CA-N
6	J	1302	SAM	CB-CG-SD-CE
6	H	1301	SAM	O-C-CA-N
6	J	1302	SAM	OXT-C-CA-CB
6	H	1302	SAM	CA-CB-CG-SD
6	K	1301	SAM	CA-CB-CG-SD
6	K	1302	SAM	CA-CB-CG-SD
6	I	1302	SAM	O4'-C4'-C5'-SD
6	J	1301	SAM	O4'-C4'-C5'-SD
6	J	1301	SAM	CB-CG-SD-C5'
6	J	1302	SAM	CB-CG-SD-C5'
6	K	1301	SAM	C2'-C1'-N9-C4
6	J	1301	SAM	C3'-C4'-C5'-SD
6	J	1302	SAM	O-C-CA-CB
6	K	1301	SAM	C2'-C1'-N9-C8
6	J	1301	SAM	O-C-CA-N
6	L	1302	SAM	O-C-CA-N
6	K	1302	SAM	OXT-C-CA-N
6	K	1301	SAM	CB-CG-SD-CE
6	J	1301	SAM	OXT-C-CA-N
6	K	1301	SAM	O4'-C1'-N9-C8
6	I	1302	SAM	OXT-C-CA-CB
6	J	1302	SAM	C2'-C1'-N9-C8
6	I	1302	SAM	O-C-CA-CB
6	H	1301	SAM	O4'-C4'-C5'-SD
6	K	1301	SAM	CB-CG-SD-C5'

There are no ring outliers.

10 monomers are involved in 266 short contacts:

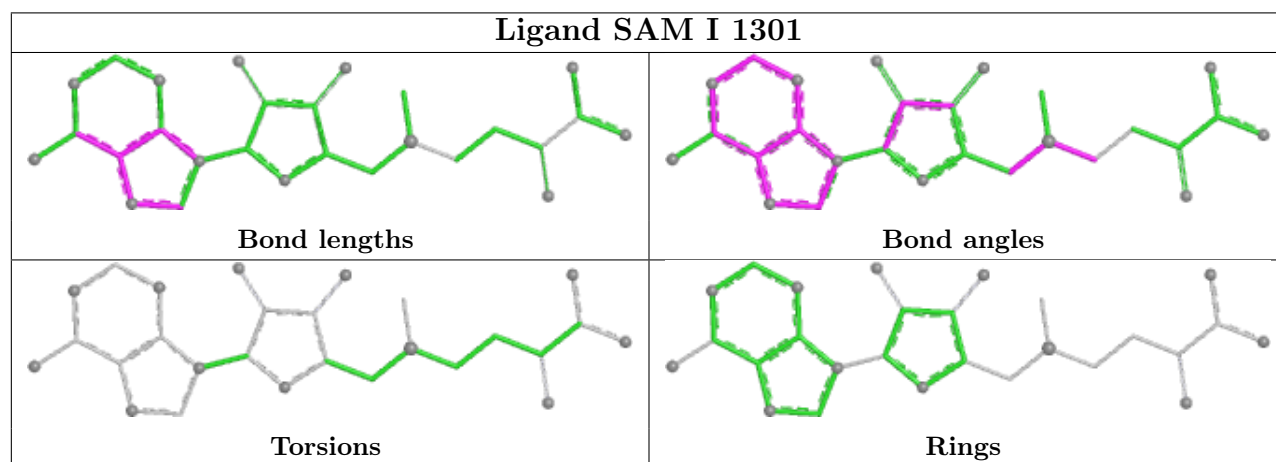
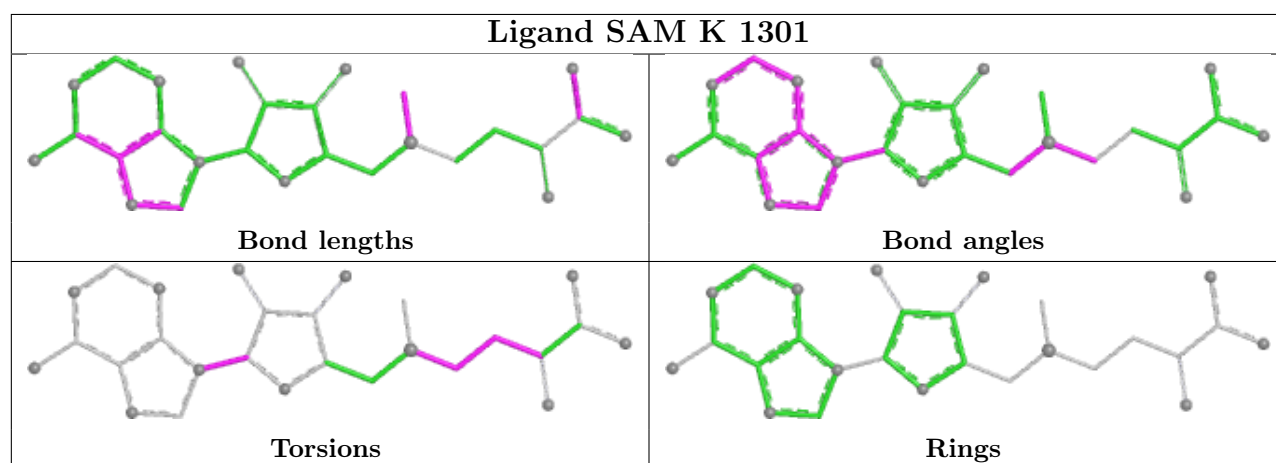
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1301	SAM	33	0
6	I	1301	SAM	23	0
6	J	1302	SAM	30	0
6	H	1302	SAM	29	0
6	L	1302	SAM	25	0
6	J	1301	SAM	13	0

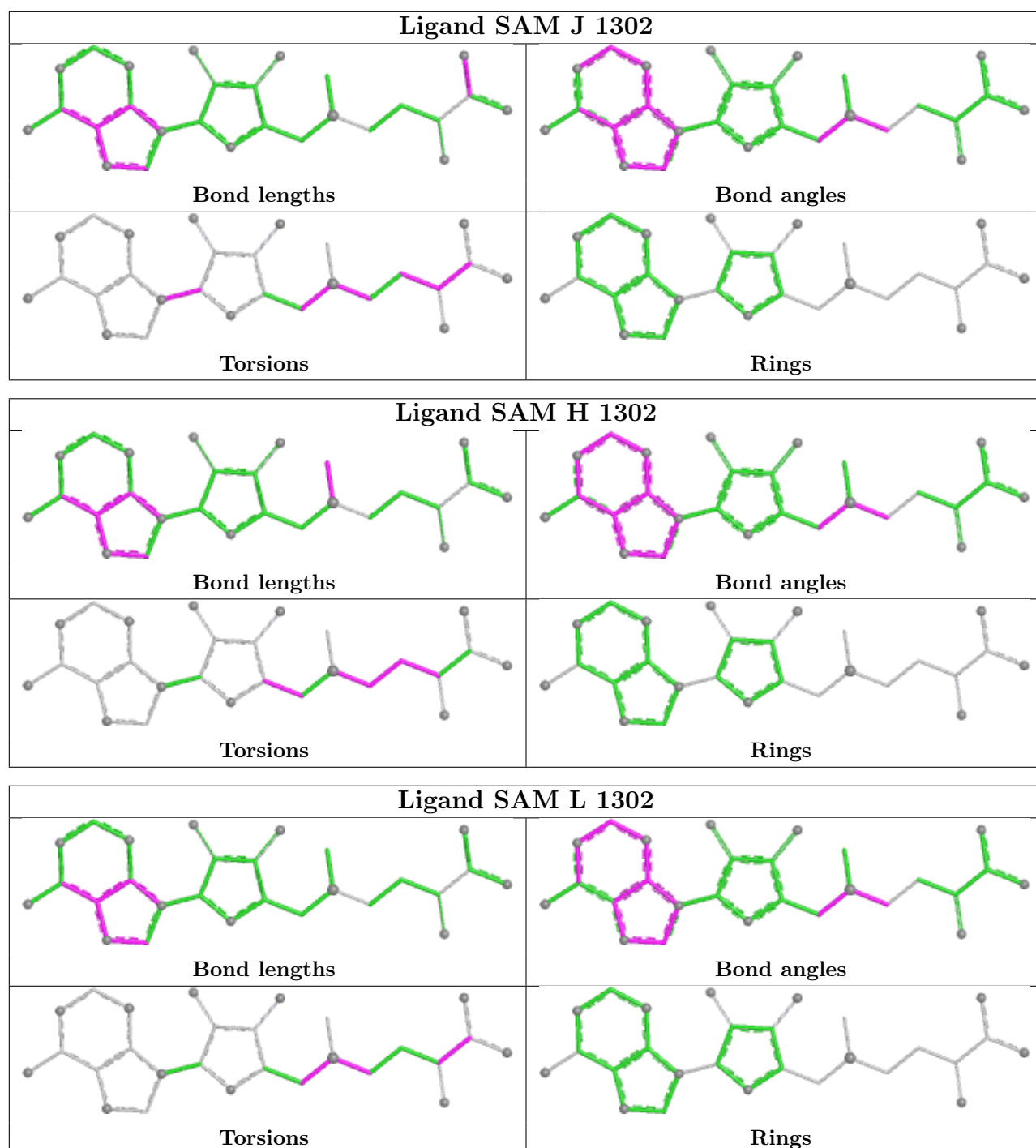
Continued on next page...

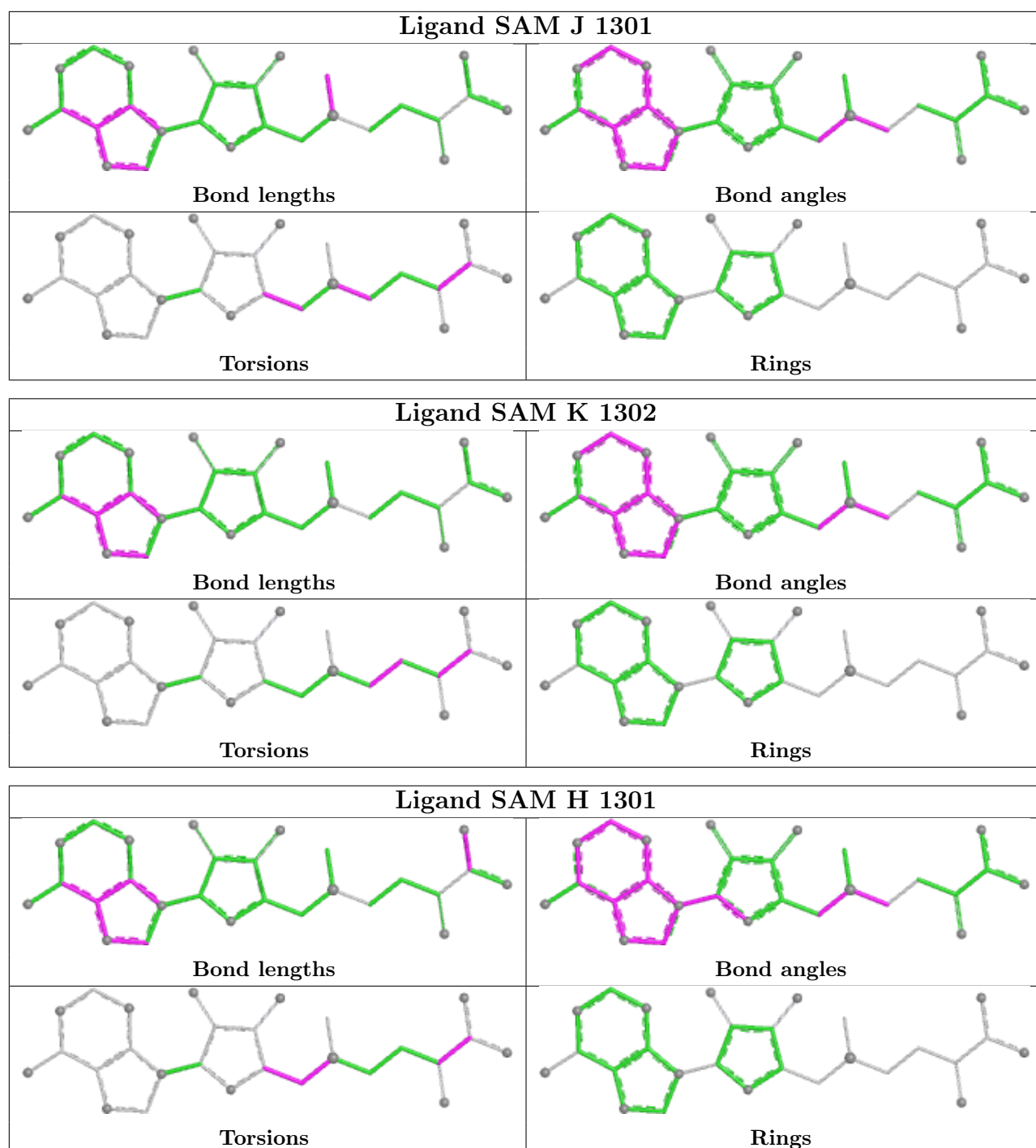
Continued from previous page...

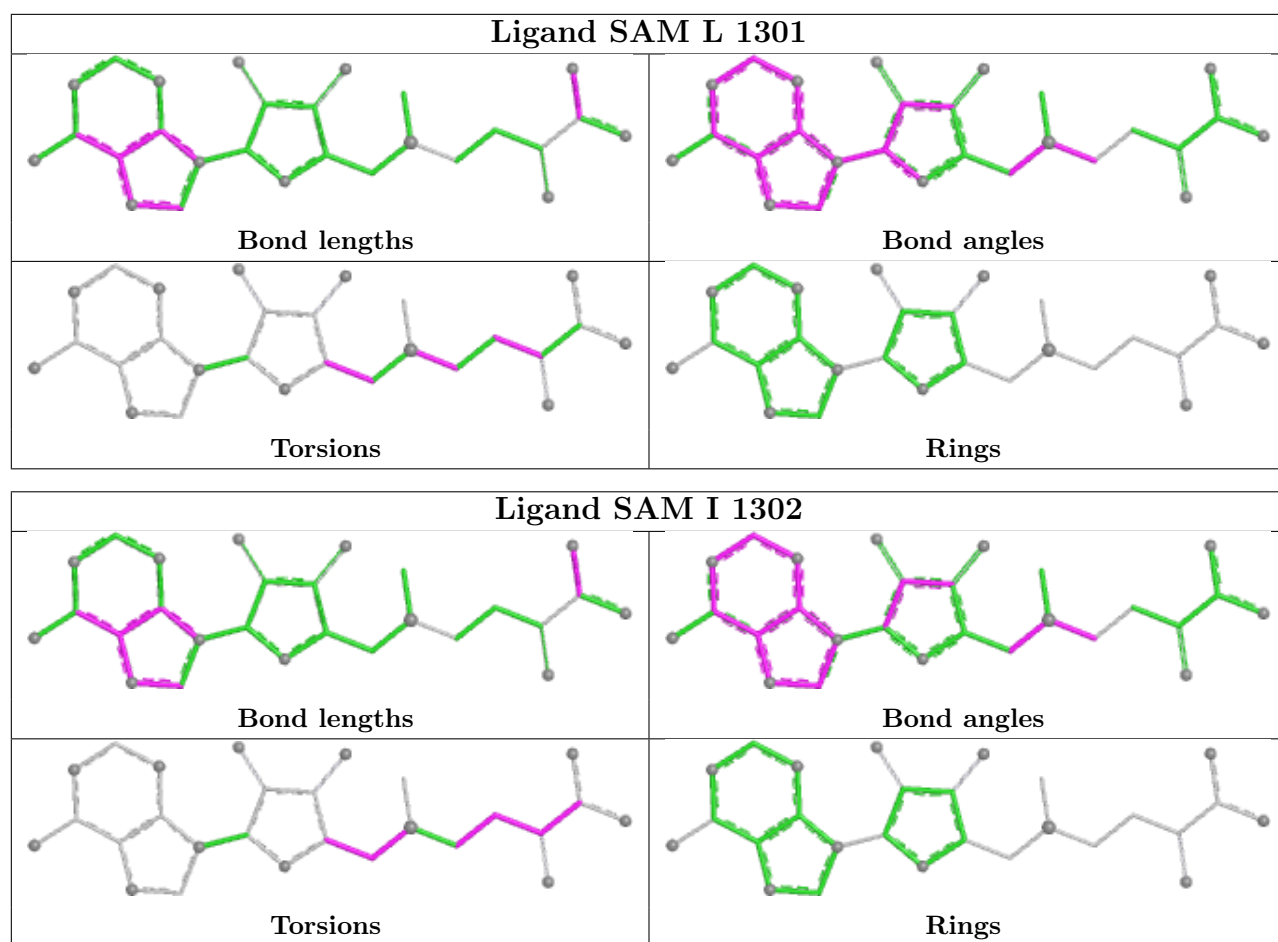
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1302	SAM	32	0
6	H	1301	SAM	37	0
6	L	1301	SAM	12	0
6	I	1302	SAM	32	0

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.









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.

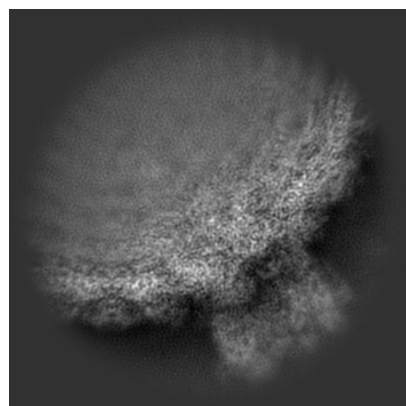
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33778. These allow visual inspection of the internal detail of the map and identification of artifacts.

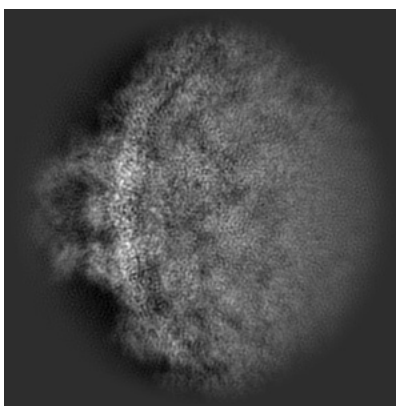
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

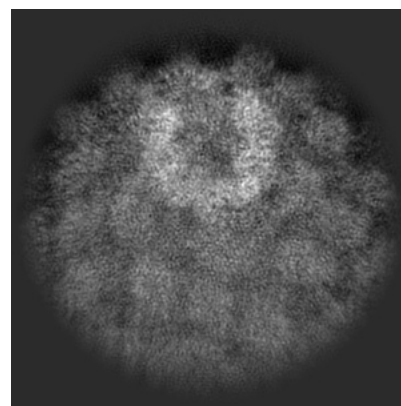
6.1.1 Primary map



X

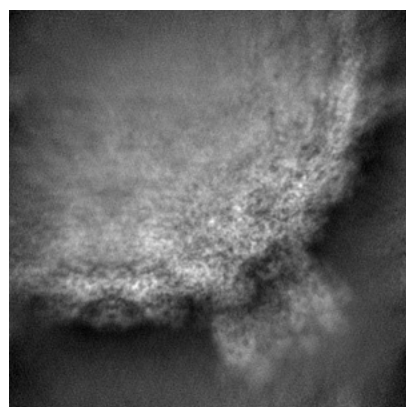


Y

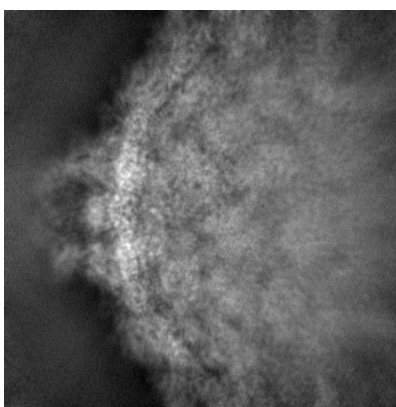


Z

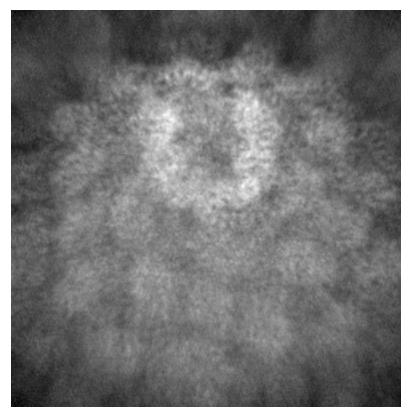
6.1.2 Raw map



X



Y

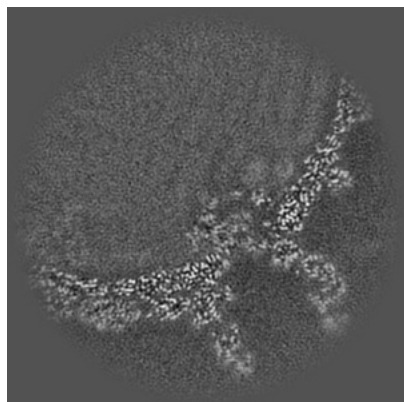


Z

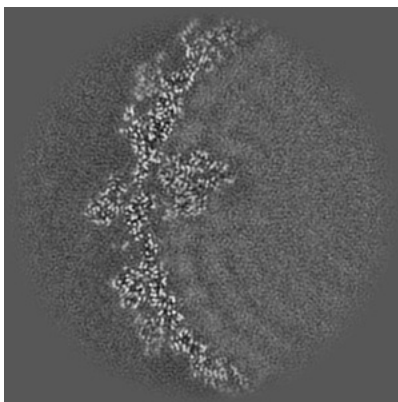
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

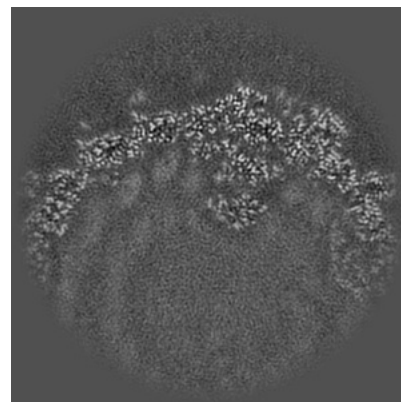
6.2.1 Primary map



X Index: 160

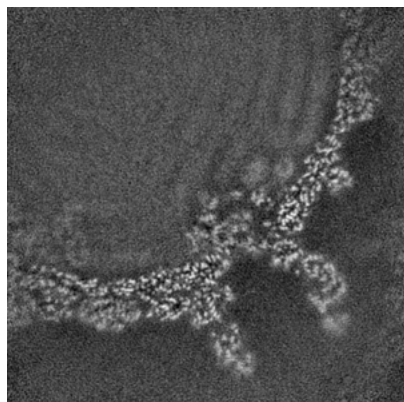


Y Index: 160

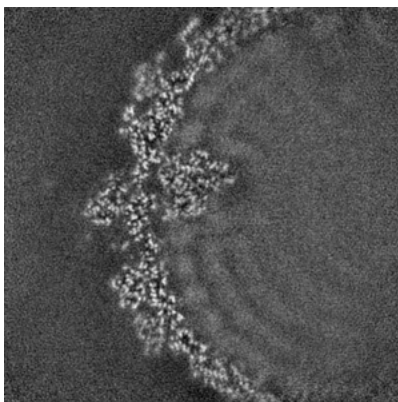


Z Index: 160

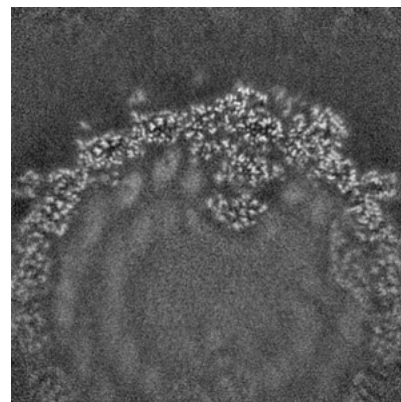
6.2.2 Raw map



X Index: 160



Y Index: 160

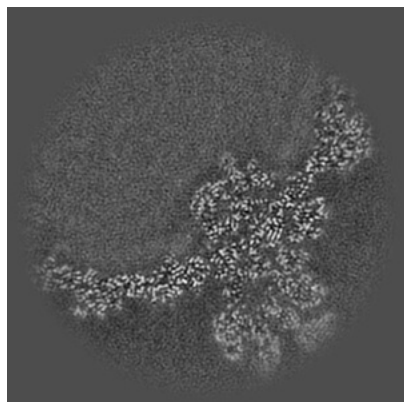


Z Index: 160

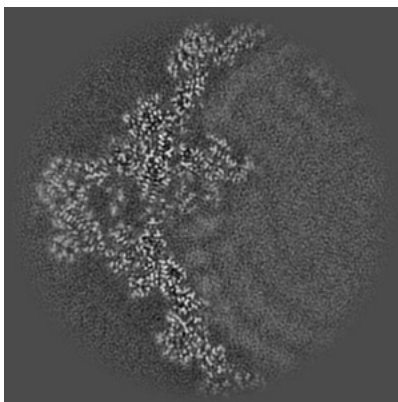
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

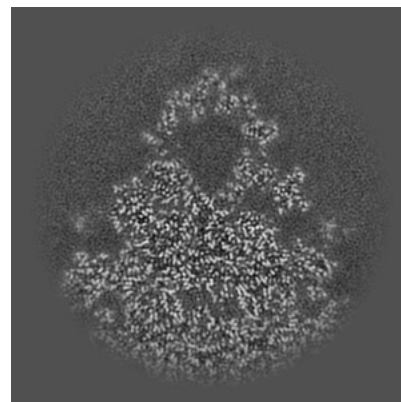
6.3.1 Primary map



X Index: 193

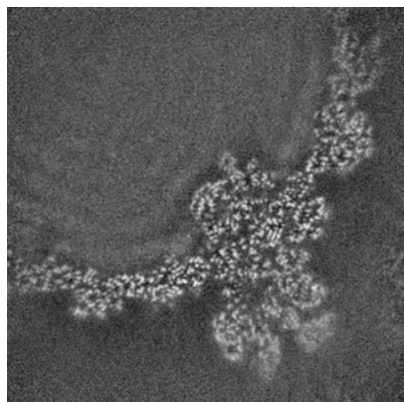


Y Index: 180

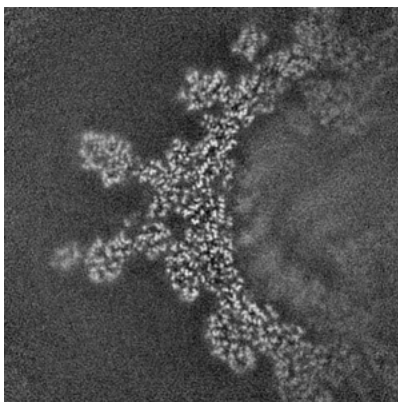


Z Index: 100

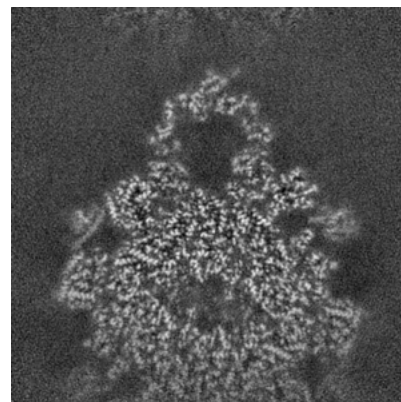
6.3.2 Raw map



X Index: 193



Y Index: 228

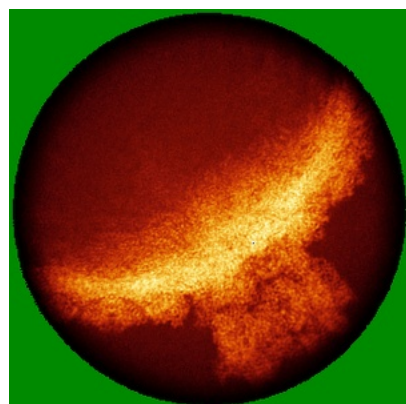


Z Index: 103

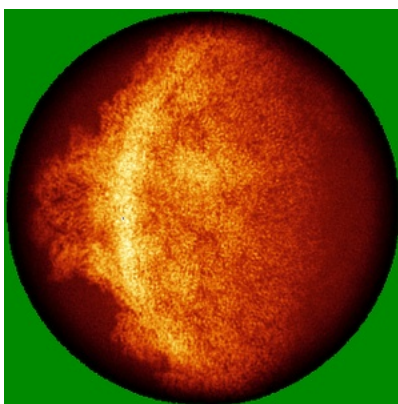
The images above show the largest variance slices of the map in three orthogonal directions.

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

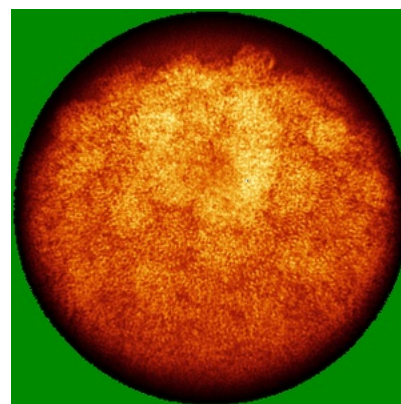
6.4.1 Primary map



X

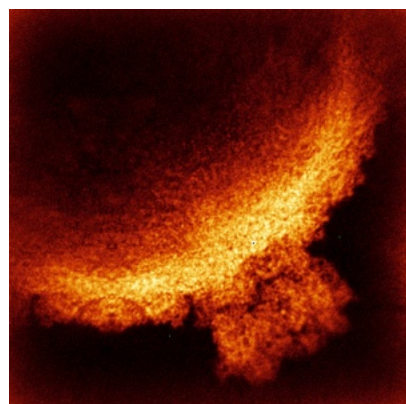


Y

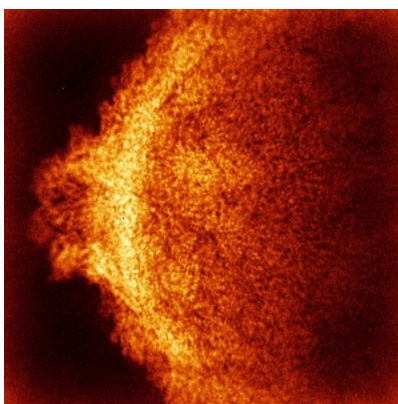


Z

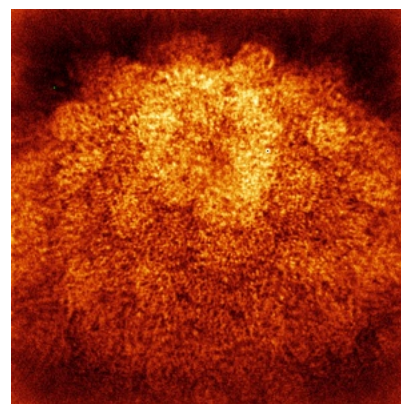
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

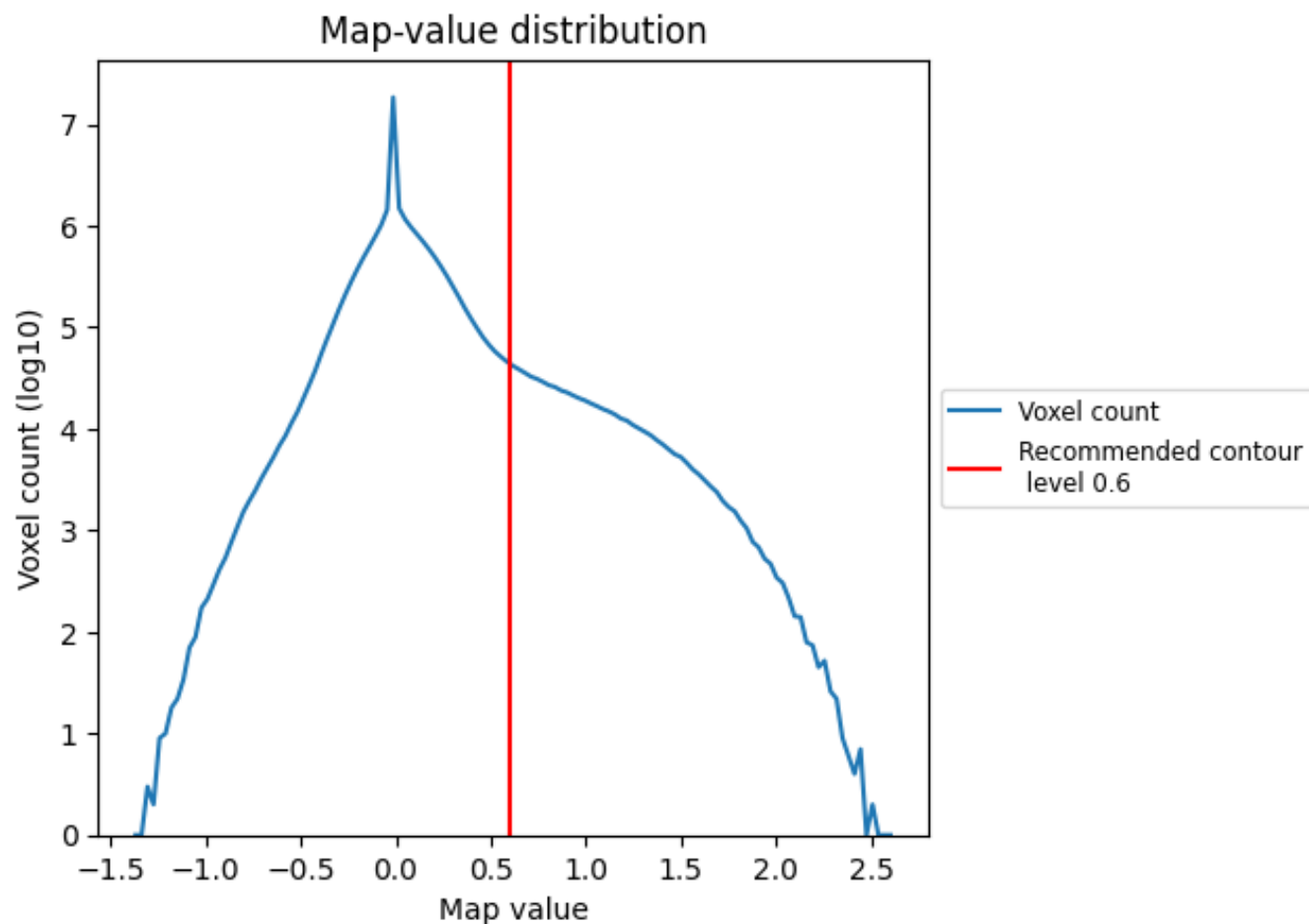
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

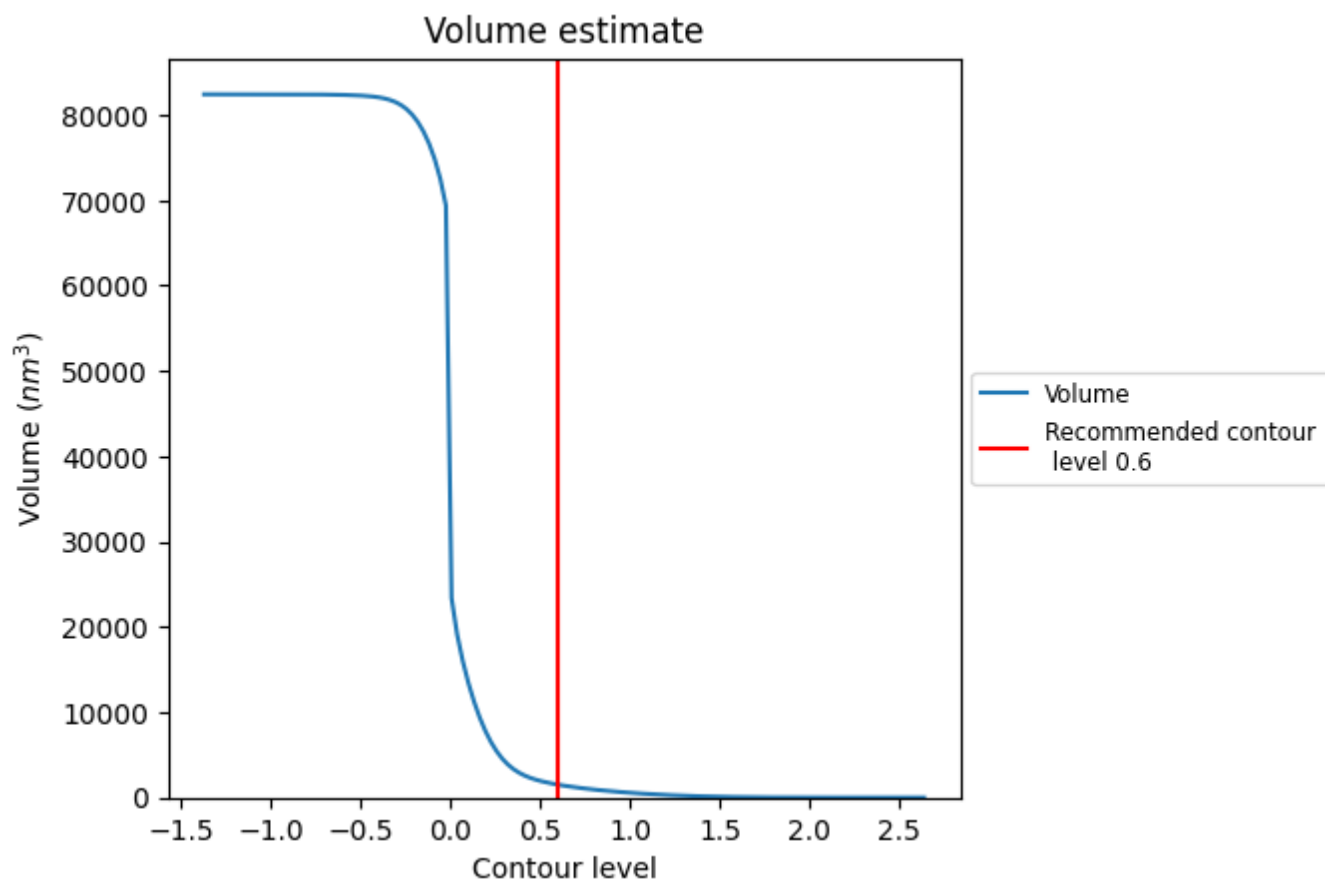
This section contains the results of statistical analysis of the map.

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.

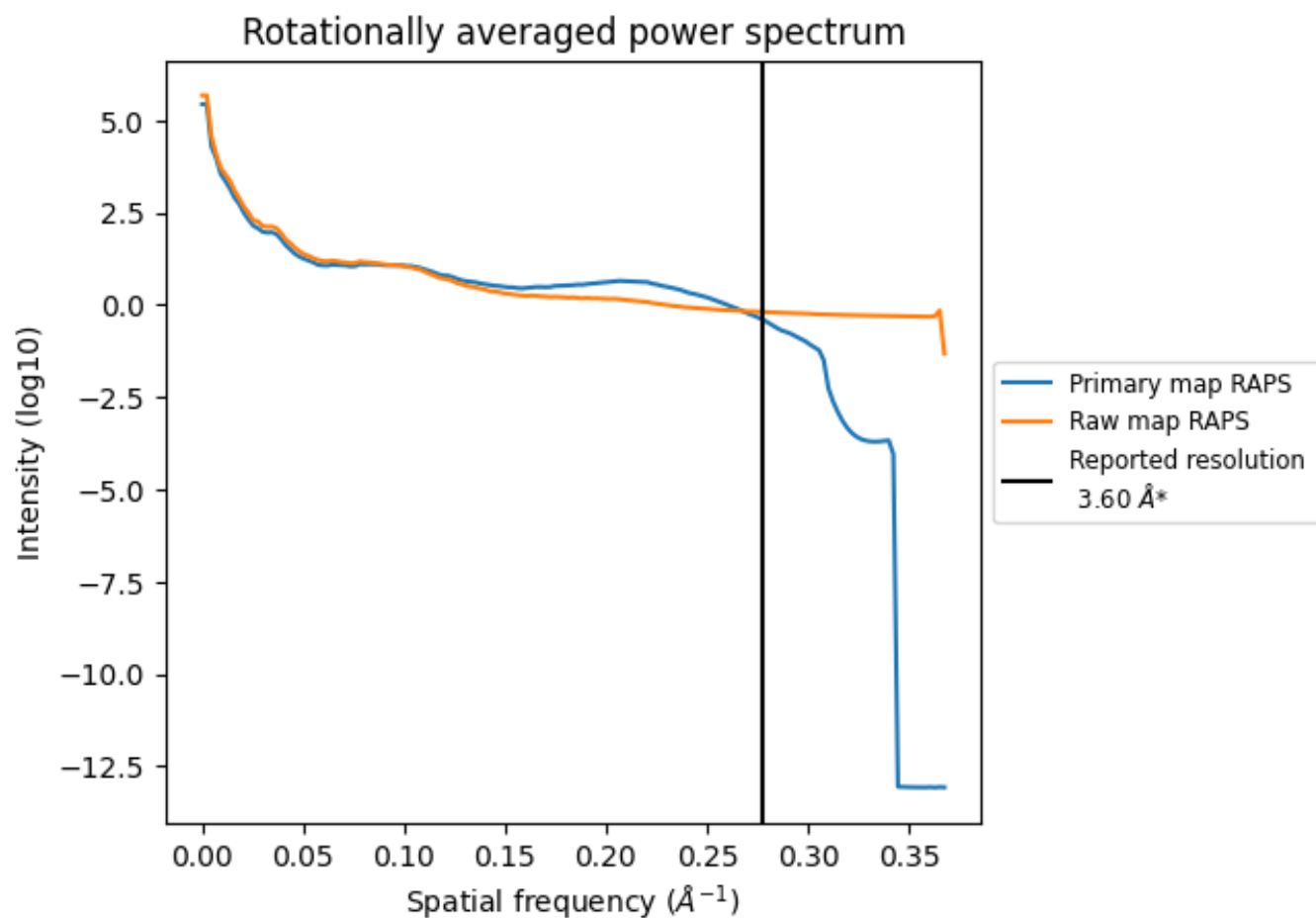
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1507 nm³; this corresponds to an approximate mass of 1361 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 ⓘ

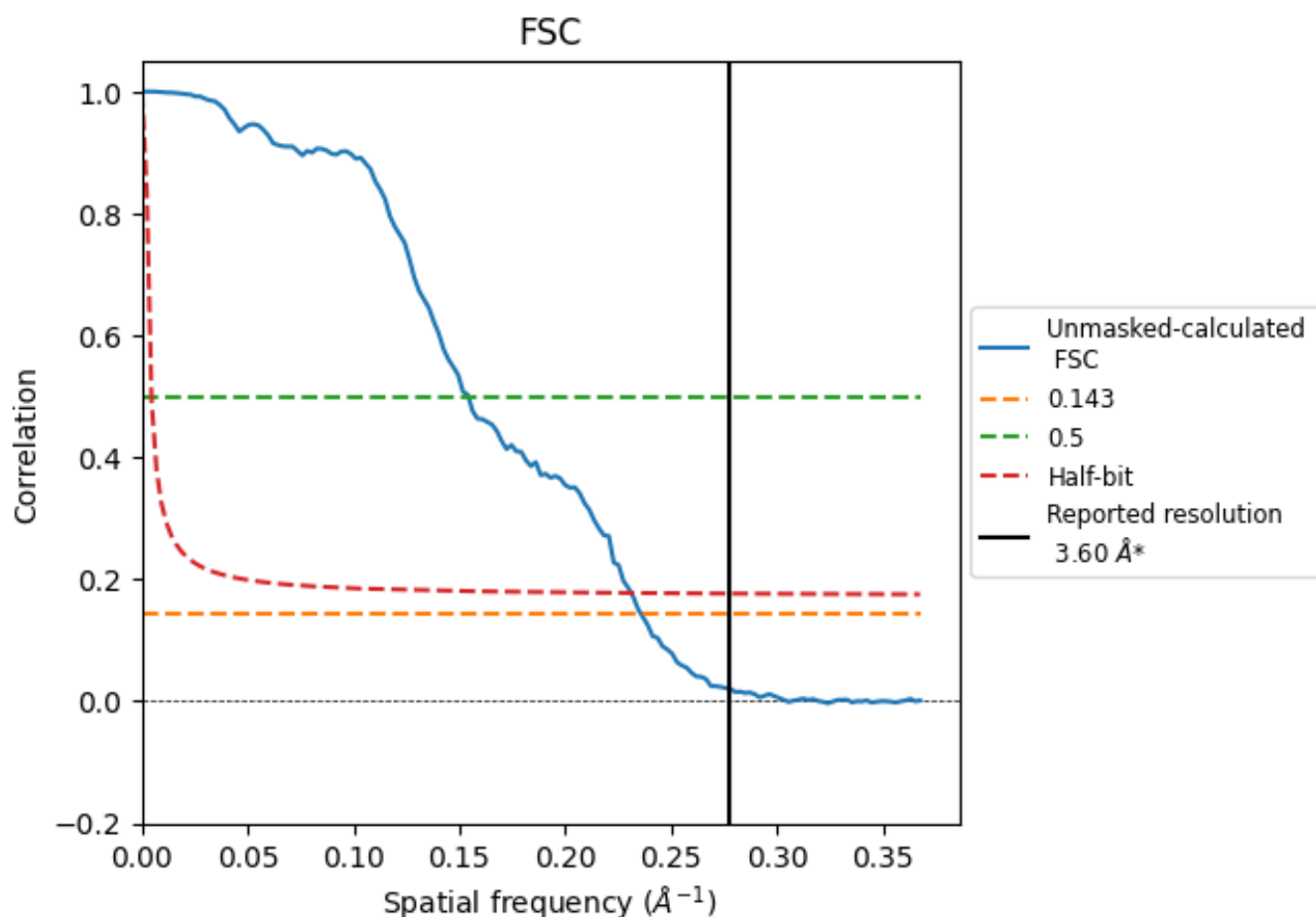


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	6.49	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.6 by more than 10 %

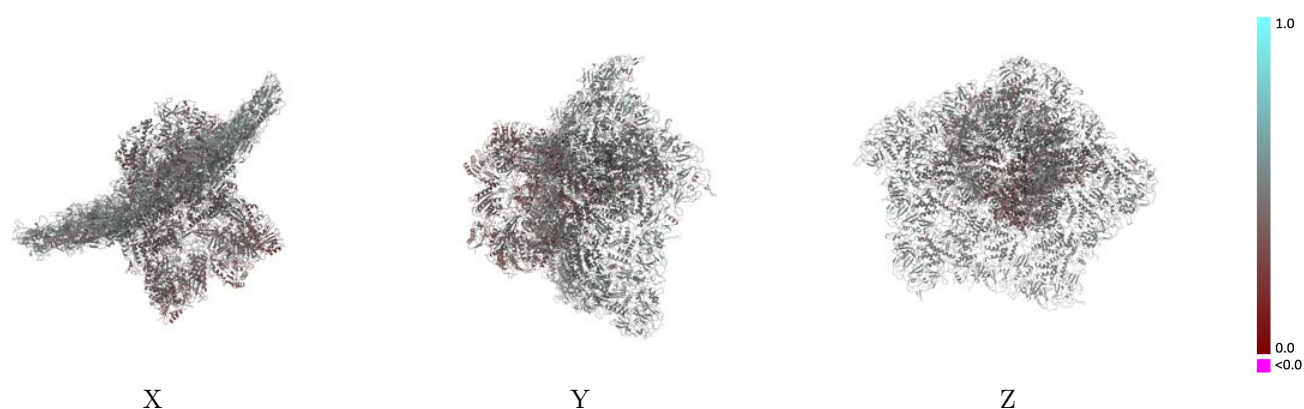
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33778 and PDB model 7YEV. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

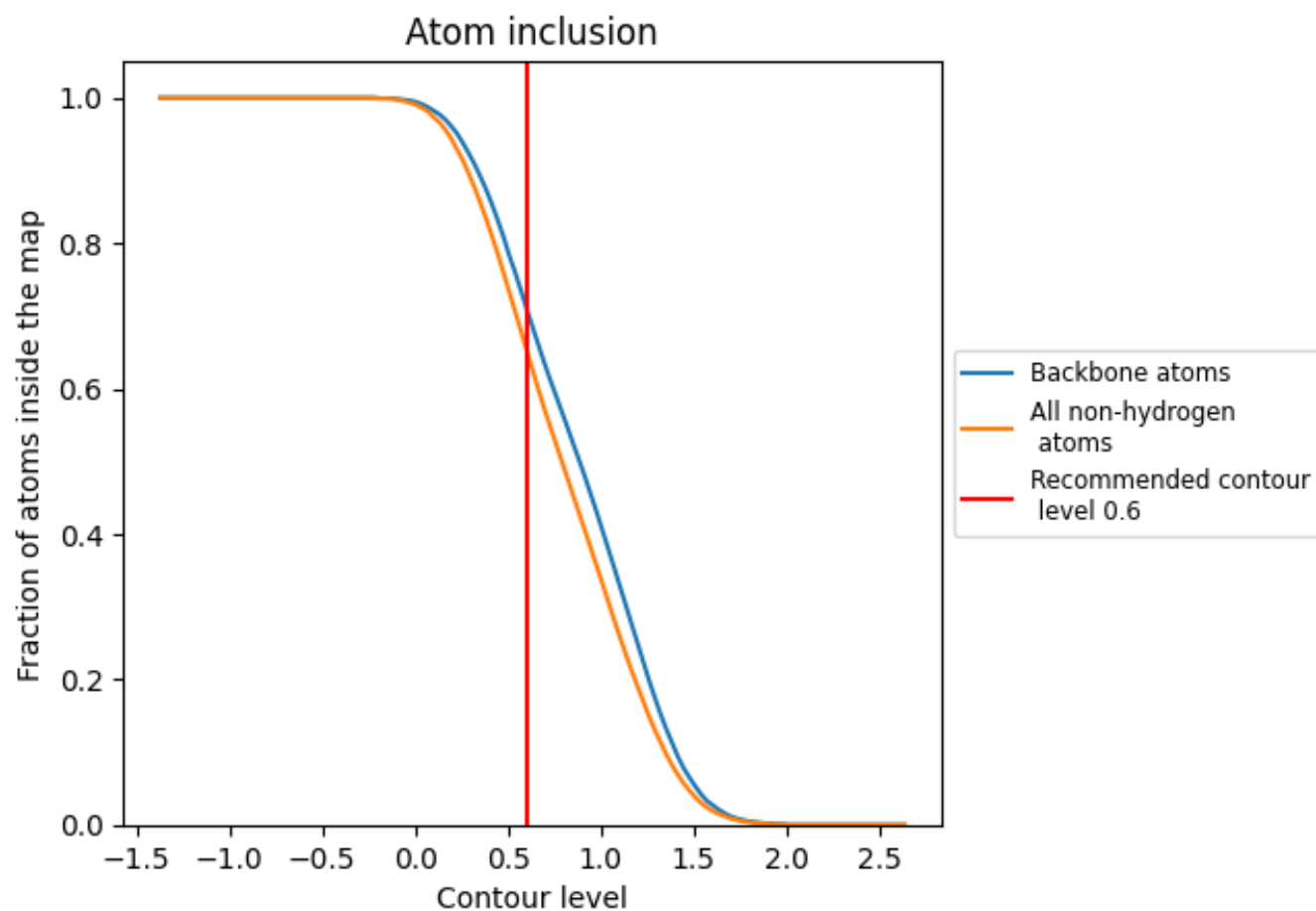


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6530	 0.4570
1	 0.5300	 0.4540
2	 0.5980	 0.4660
3	 0.6020	 0.4560
4	 0.4770	 0.4560
5	 0.3040	 0.4250
A	 0.6740	 0.4720
B	 0.6850	 0.4730
C	 0.6880	 0.4730
D	 0.7050	 0.4810
E	 0.6890	 0.4790
H	 0.6450	 0.4230
I	 0.6430	 0.4230
J	 0.6500	 0.4270
K	 0.6550	 0.4260
L	 0.6500	 0.4310
R	 0.5440	 0.4260
U	 0.5810	 0.4500
a	 0.6960	 0.4780
b	 0.7050	 0.4790
c	 0.7030	 0.4800
d	 0.7030	 0.4780
e	 0.6900	 0.4760

