



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 7YEZ / pdb_00007yez
EMDB ID : EMD-33779
Title : In situ structure of polymerase complex of mammalian reovirus in the reloaded state
Authors : Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.
Deposited on : 2022-07-06
Resolution : 3.40 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:

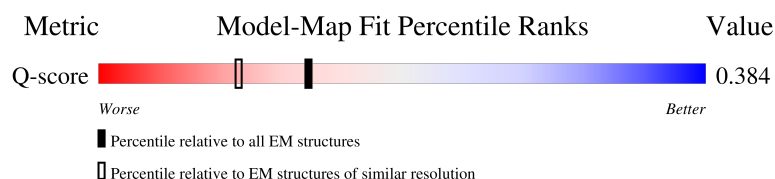
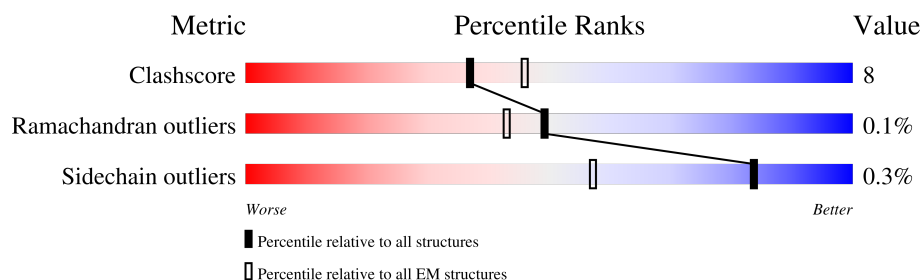
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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.



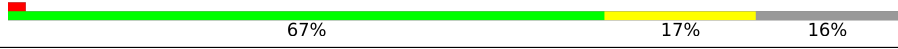
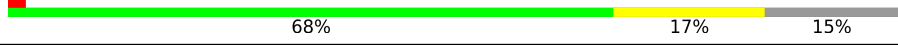
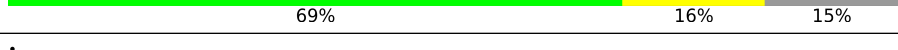
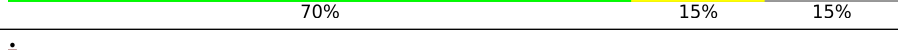
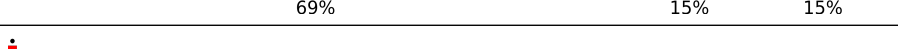
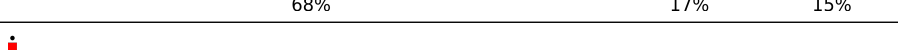
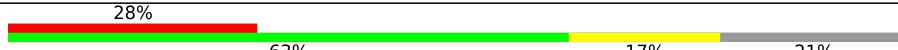
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	9% . 89%
1	3	1275	9% . 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
5	SAM	H	1301	-	-	X	-
5	SAM	I	1301	-	-	X	-
5	SAM	J	1301	-	-	X	-
5	SAM	K	1301	-	-	X	-
5	SAM	L	1301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 146162 atoms, of which 110 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	138	Total	C	N	O	S	0	0
			1026	610	195	218	3		
1	3	137	Total	C	N	O	S	0	0
			1023	608	195	217	3		
1	4	128	Total	C	N	O	S	0	0
			950	565	180	202	3		
1	5	139	Total	C	N	O	S	0	0
			1036	616	197	220	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	1082	Total	C	N	O	S	0	0
			8535	5453	1444	1587	51		
1	D	1050	Total	C	N	O	S	0	0
			8300	5306	1403	1542	49		
1	E	1060	Total	C	N	O	S	0	0
			8376	5351	1419	1557	49		
1	a	1088	Total	C	N	O	S	0	0
			8580	5478	1457	1594	51		
1	b	1087	Total	C	N	O	S	0	0
			8571	5473	1455	1592	51		
1	c	1080	Total	C	N	O	S	0	0
			8517	5444	1444	1578	51		
1	d	1085	Total	C	N	O	S	0	0
			8559	5467	1452	1589	51		
1	e	1075	Total	C	N	O	S	0	0
			8492	5422	1442	1578	50		

- 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		

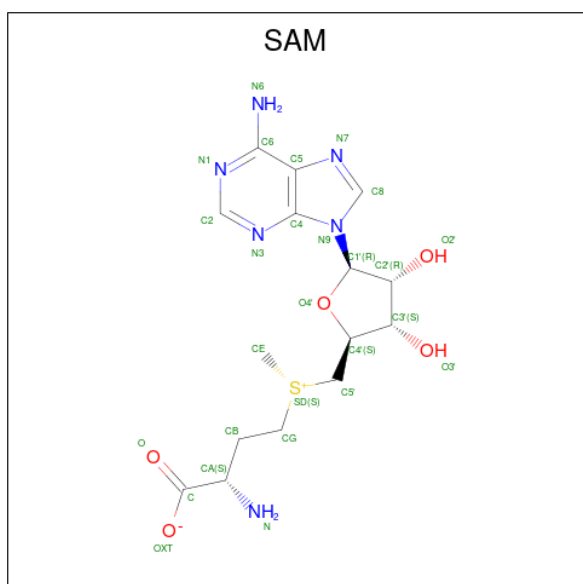
- Molecule 3 is a protein called RNA-directed RNA polymerase.

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		

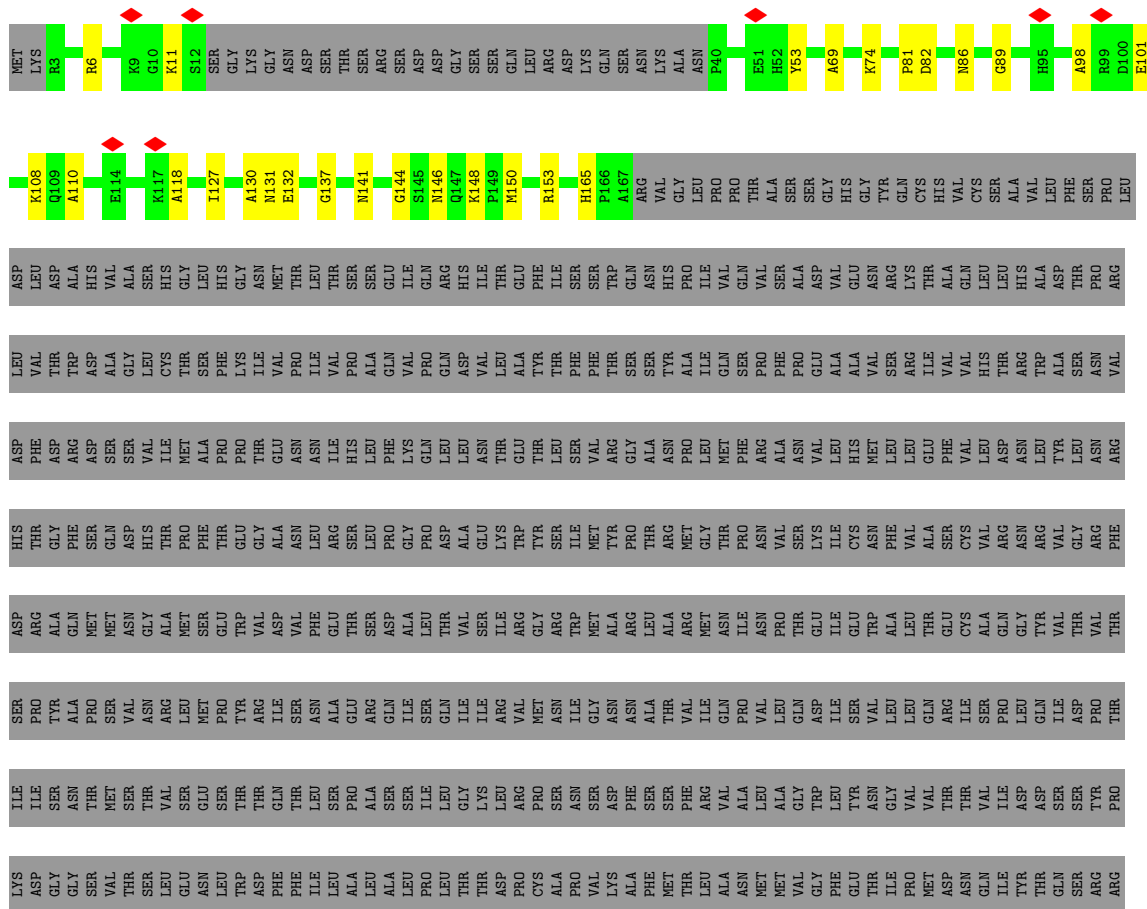
- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

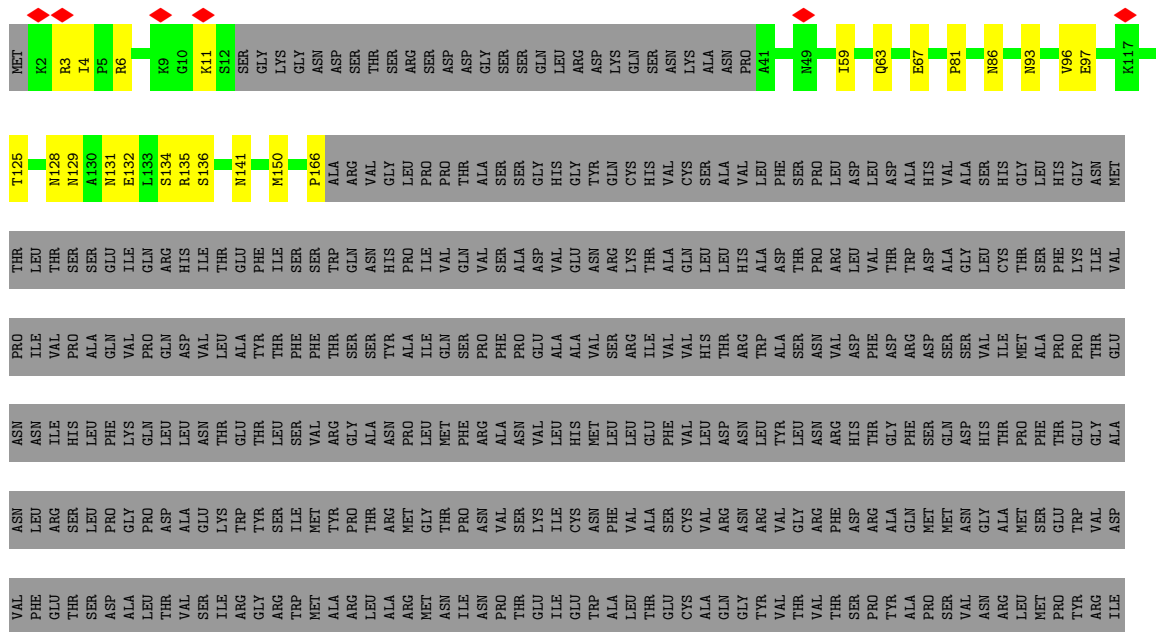


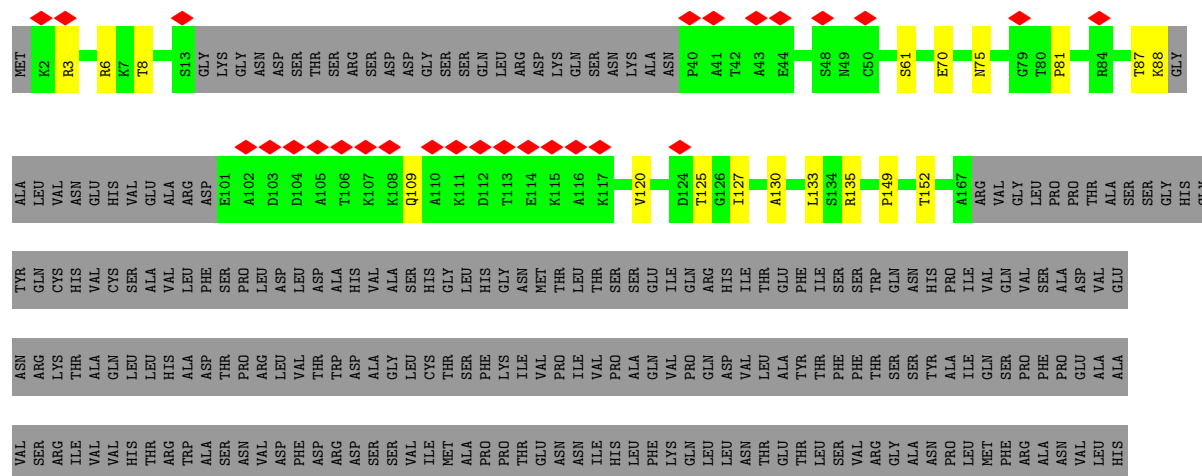
Mol	Chain	Residues	Atoms						AltConf
5	H	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
5	I	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
5	J	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
5	K	1	Total 49	C 15	H 22	N 6	O 5	S 1	0
5	L	1	Total 49	C 15	H 22	N 6	O 5	S 1	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

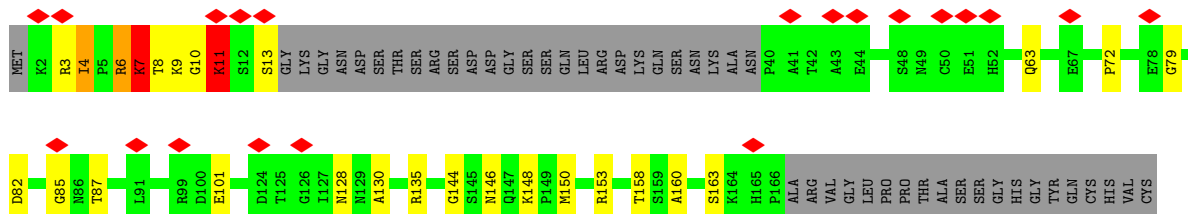
Mol	Chain	Residues	Atoms		AltConf
6	b	1	Total 1	Zn 1	0





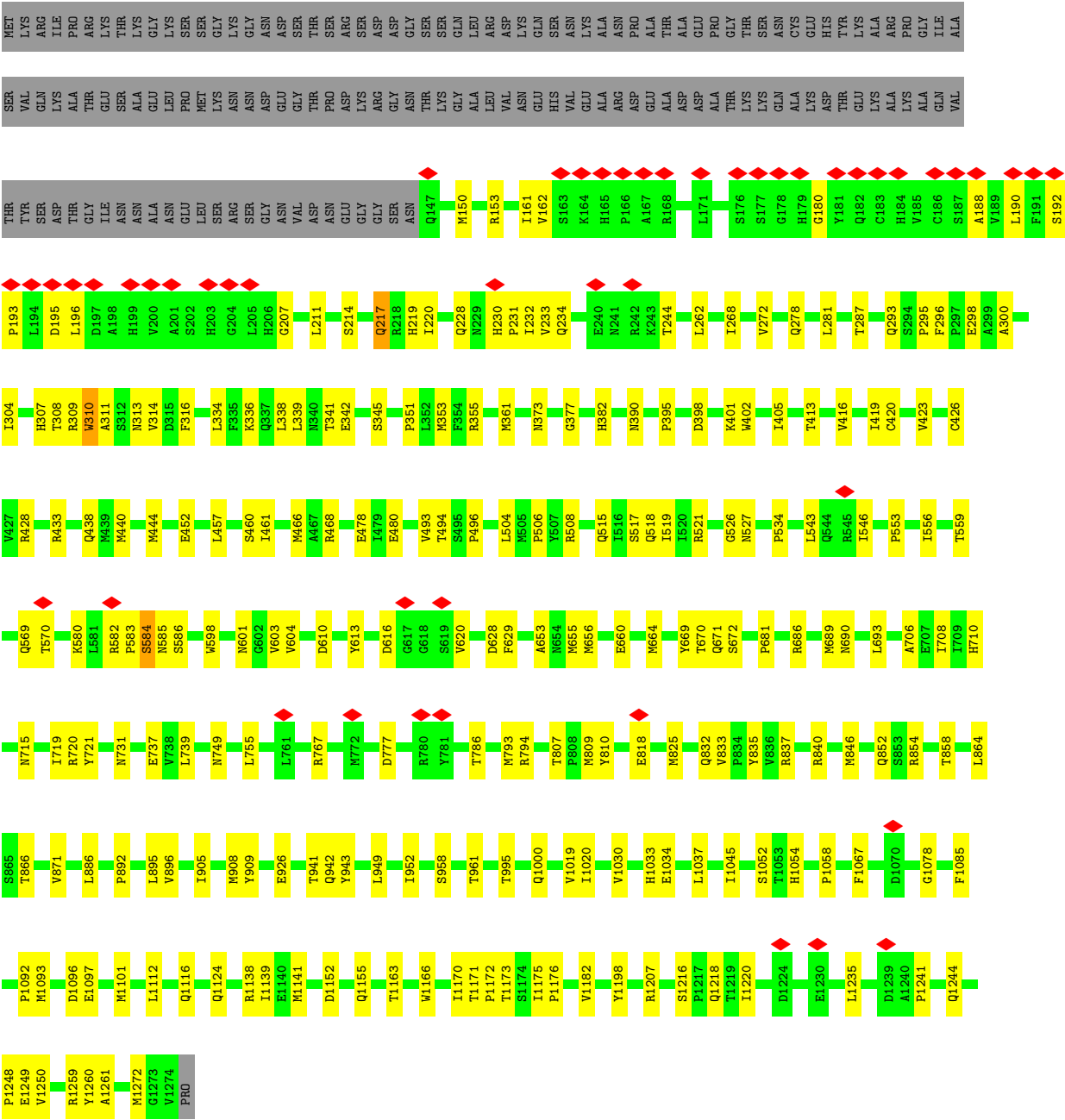


- Molecule 1: RNA helicase

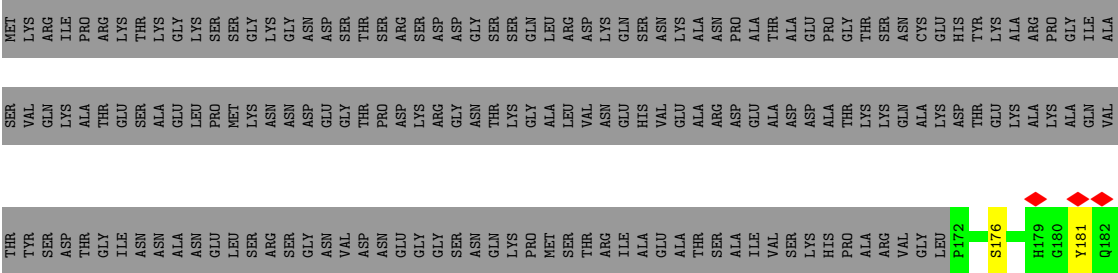


- Molecule 1: RNA helicase

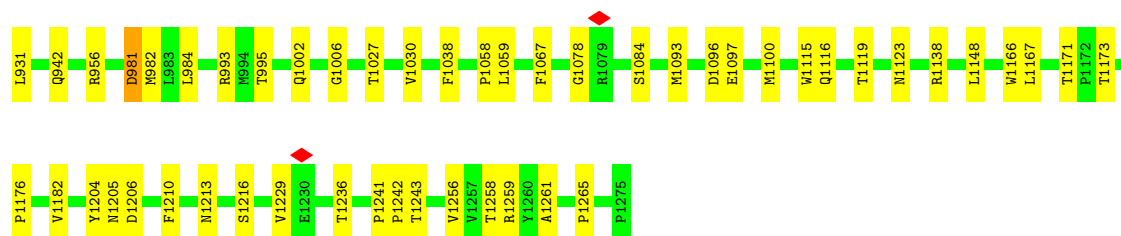
Frequency	Percentage
Daily	70%
Weekly	18%
Monthly	12%



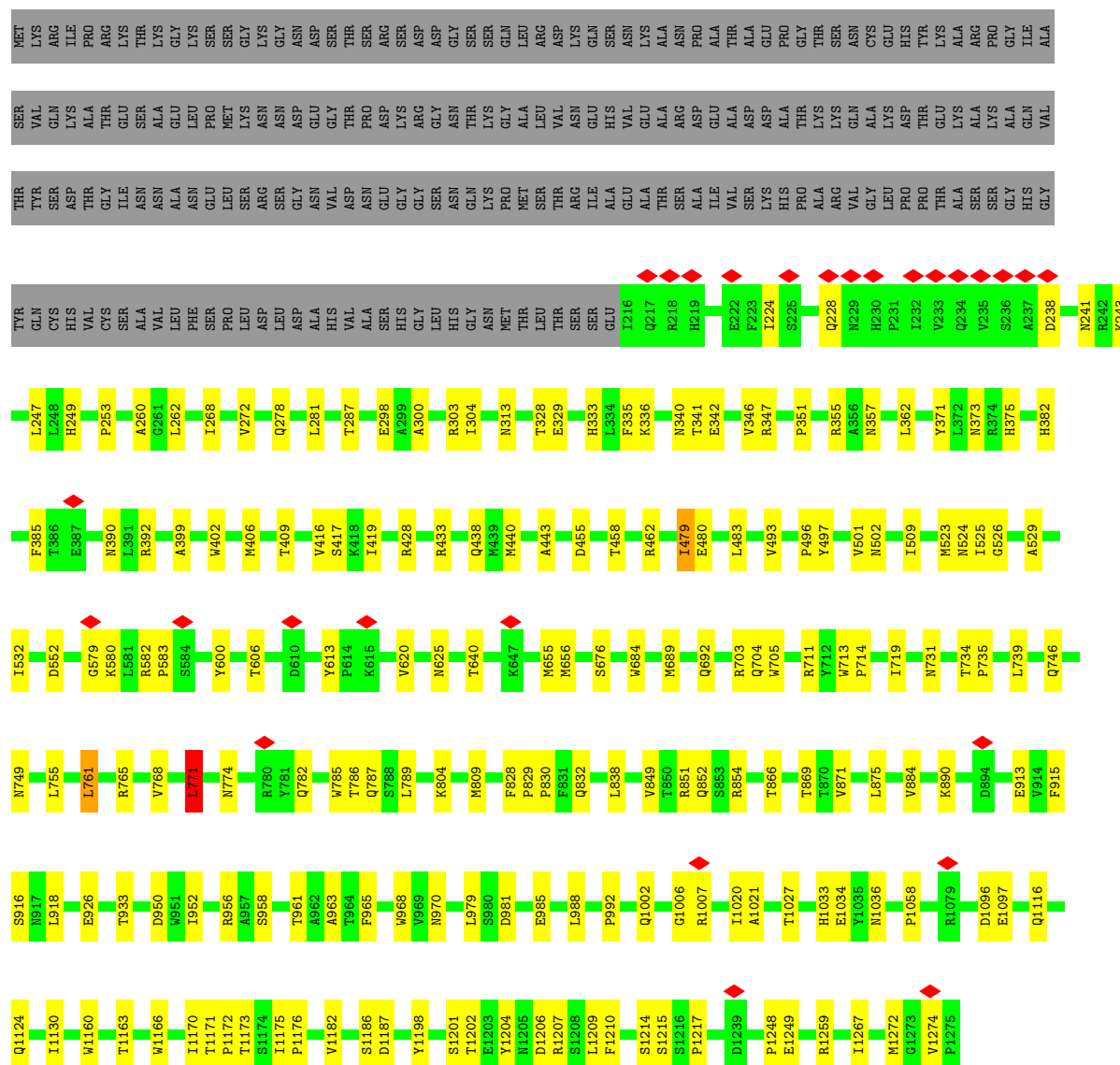
● Molecule 1: RNA helicase





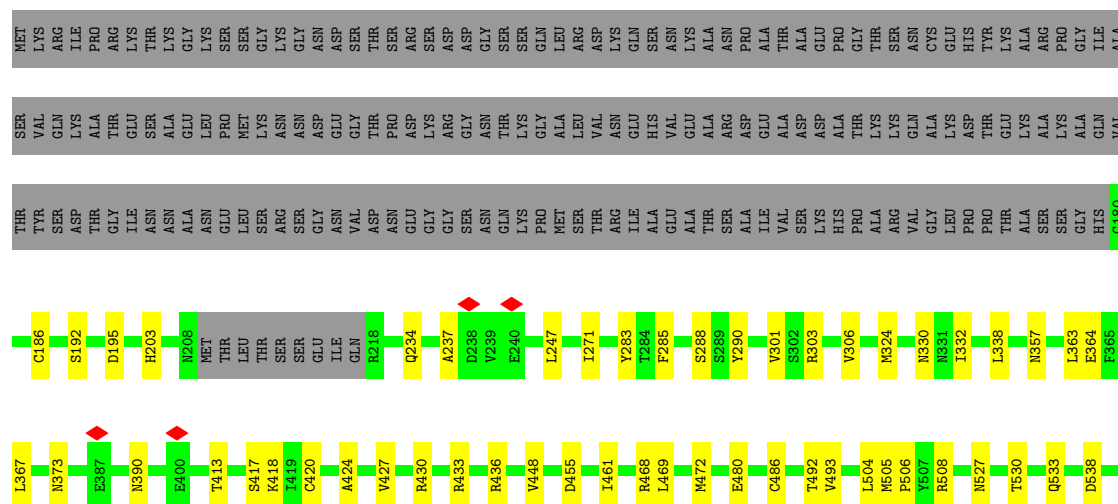


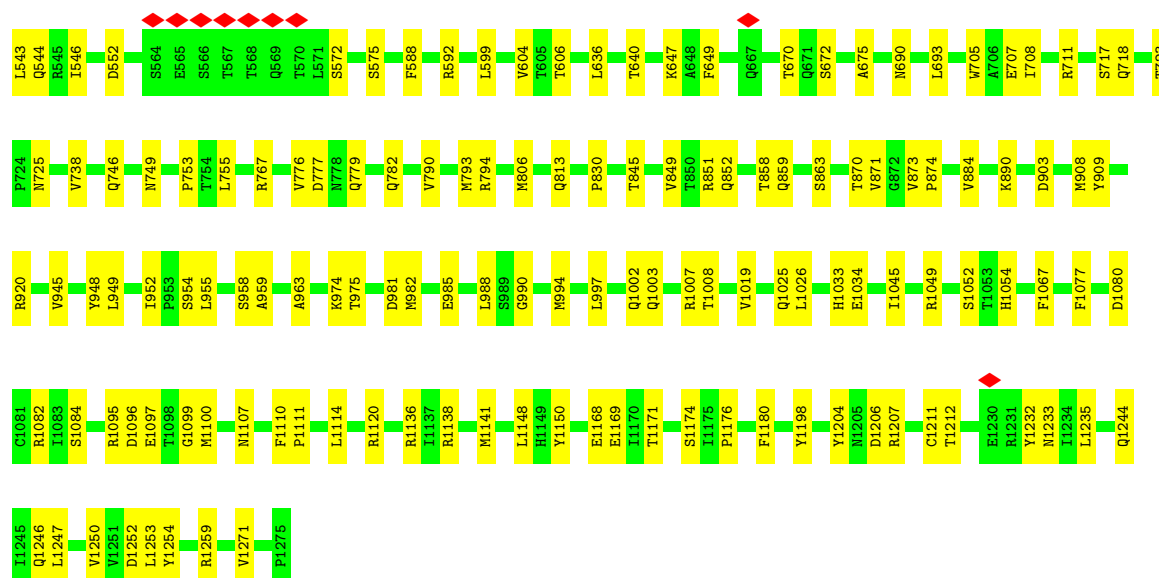
• Molecule 1: RNA helicase



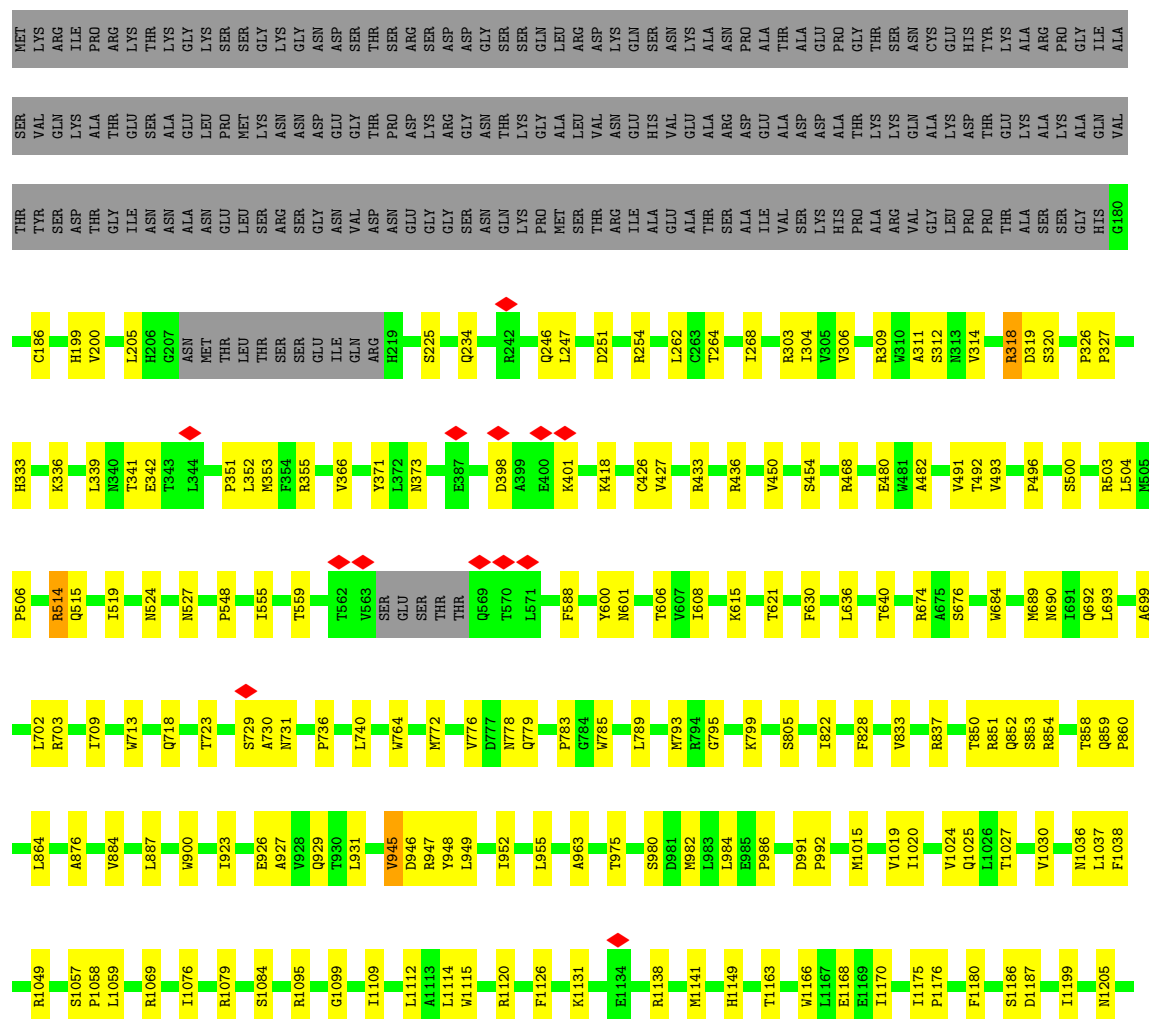
• Molecule 1: RNA helicase





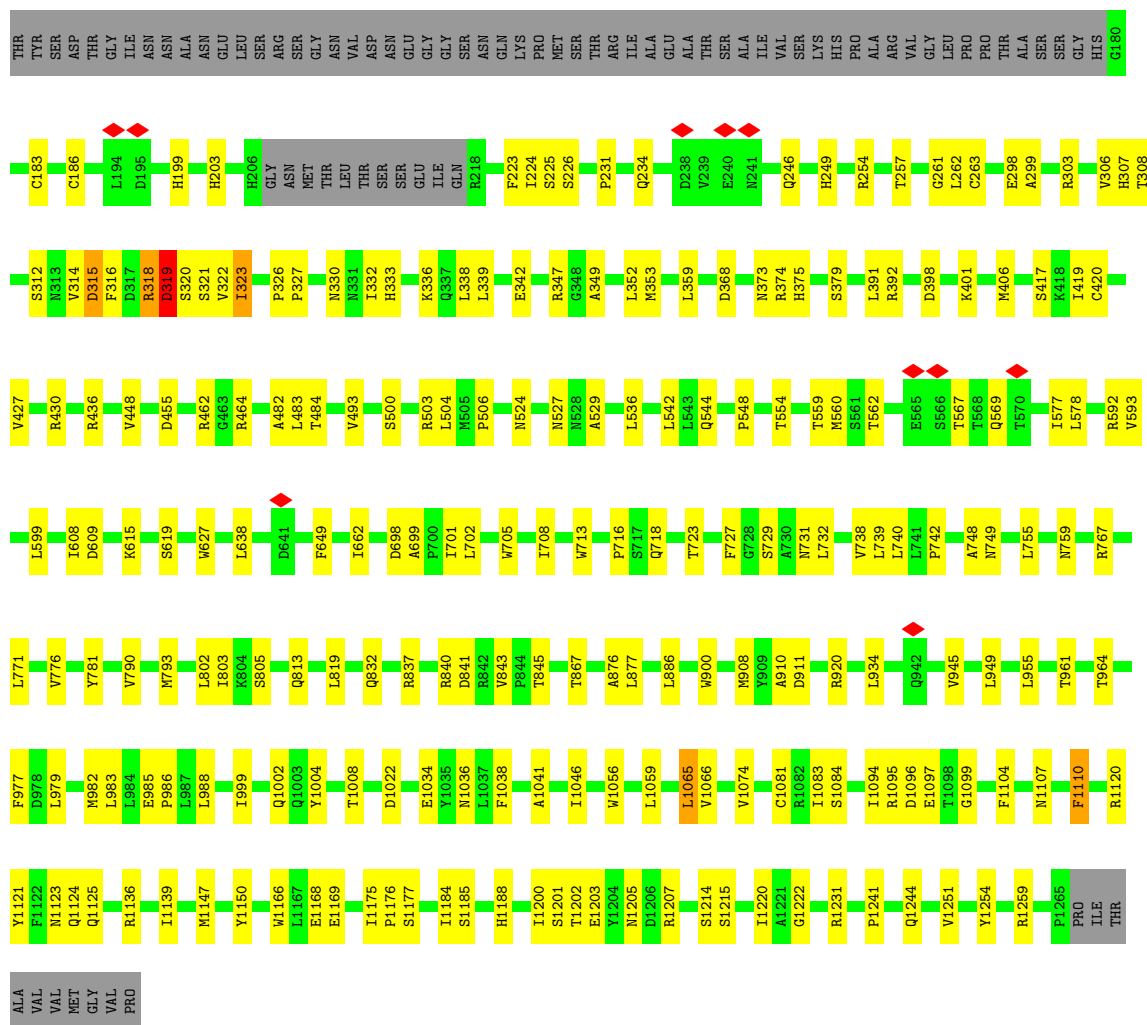


• Molecule 1: RNA helicase

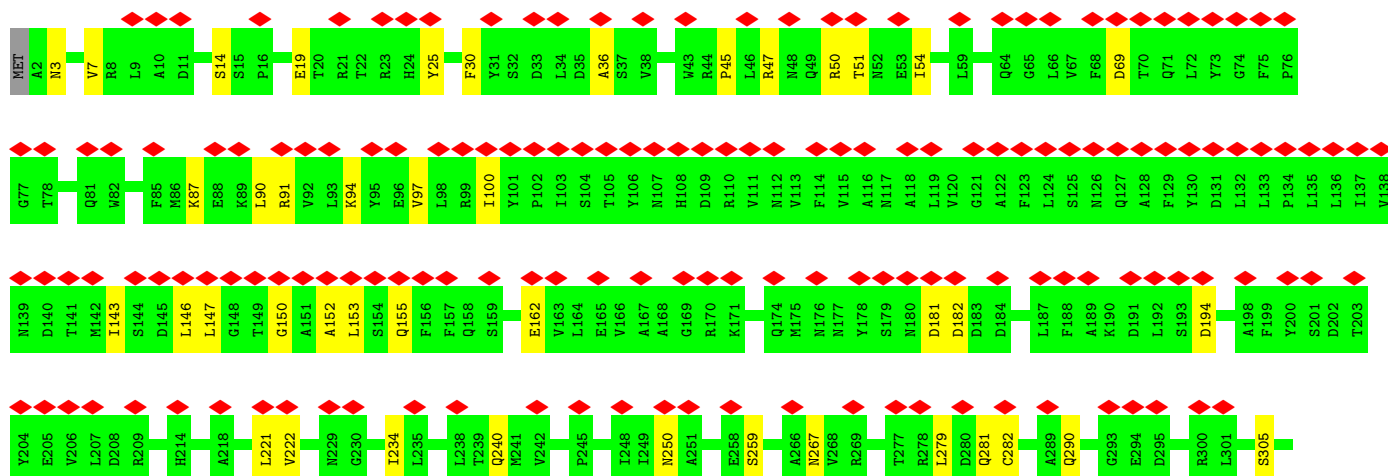


Chain d: 68% 17% 15%

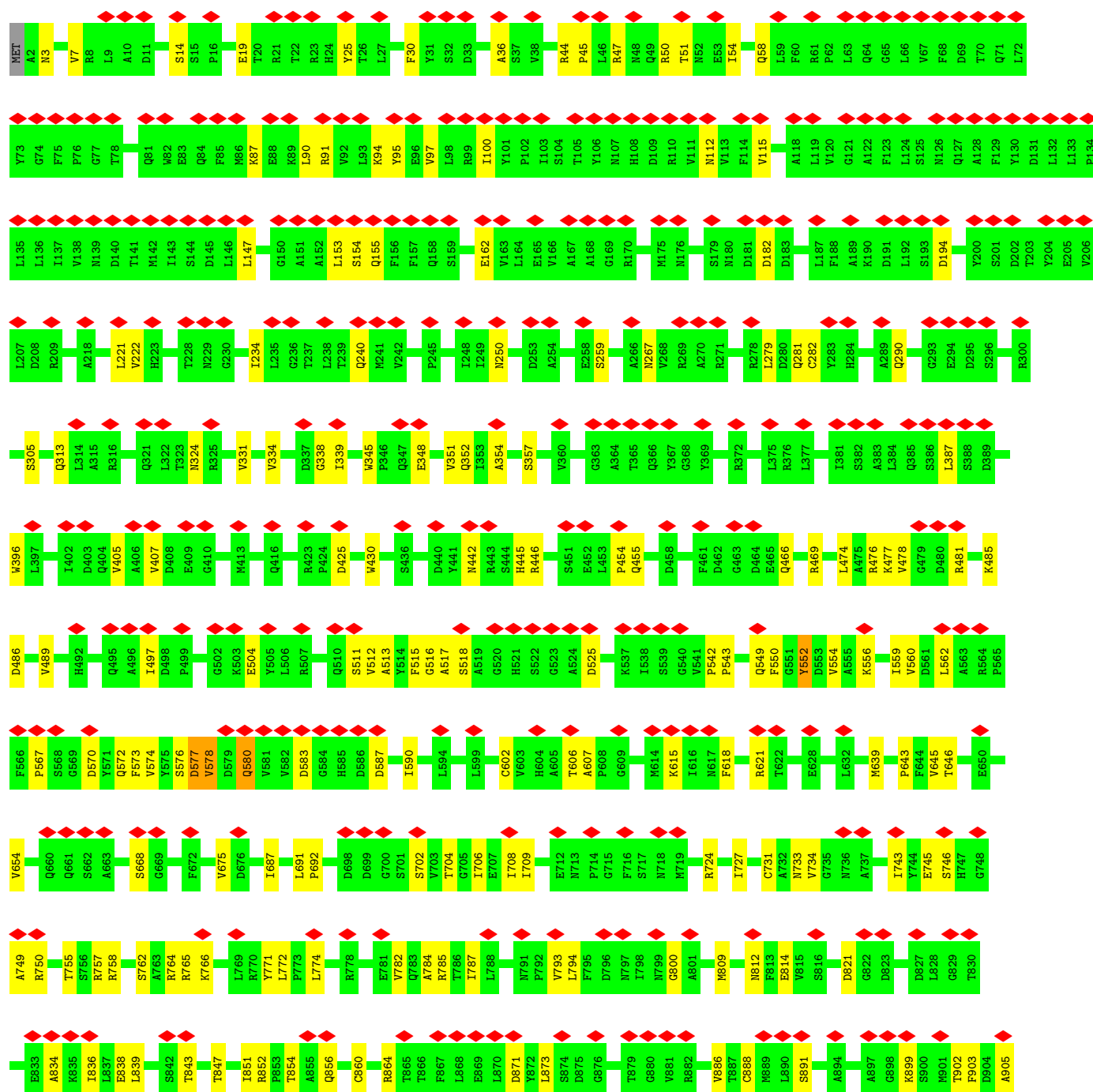


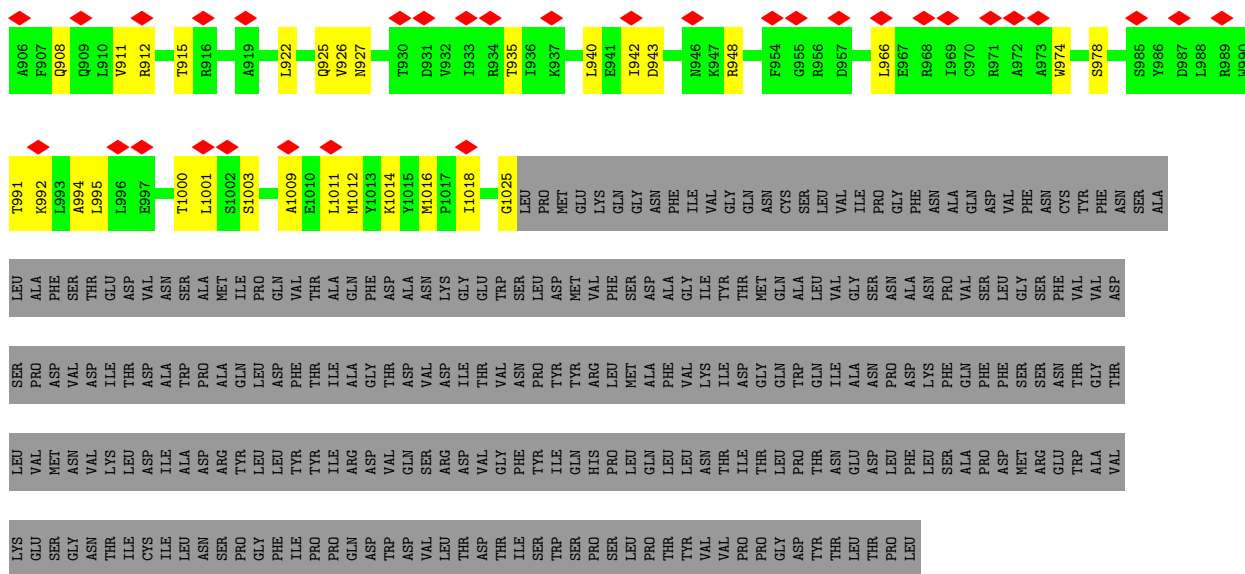


• Molecule 2: Lambda-2 protein

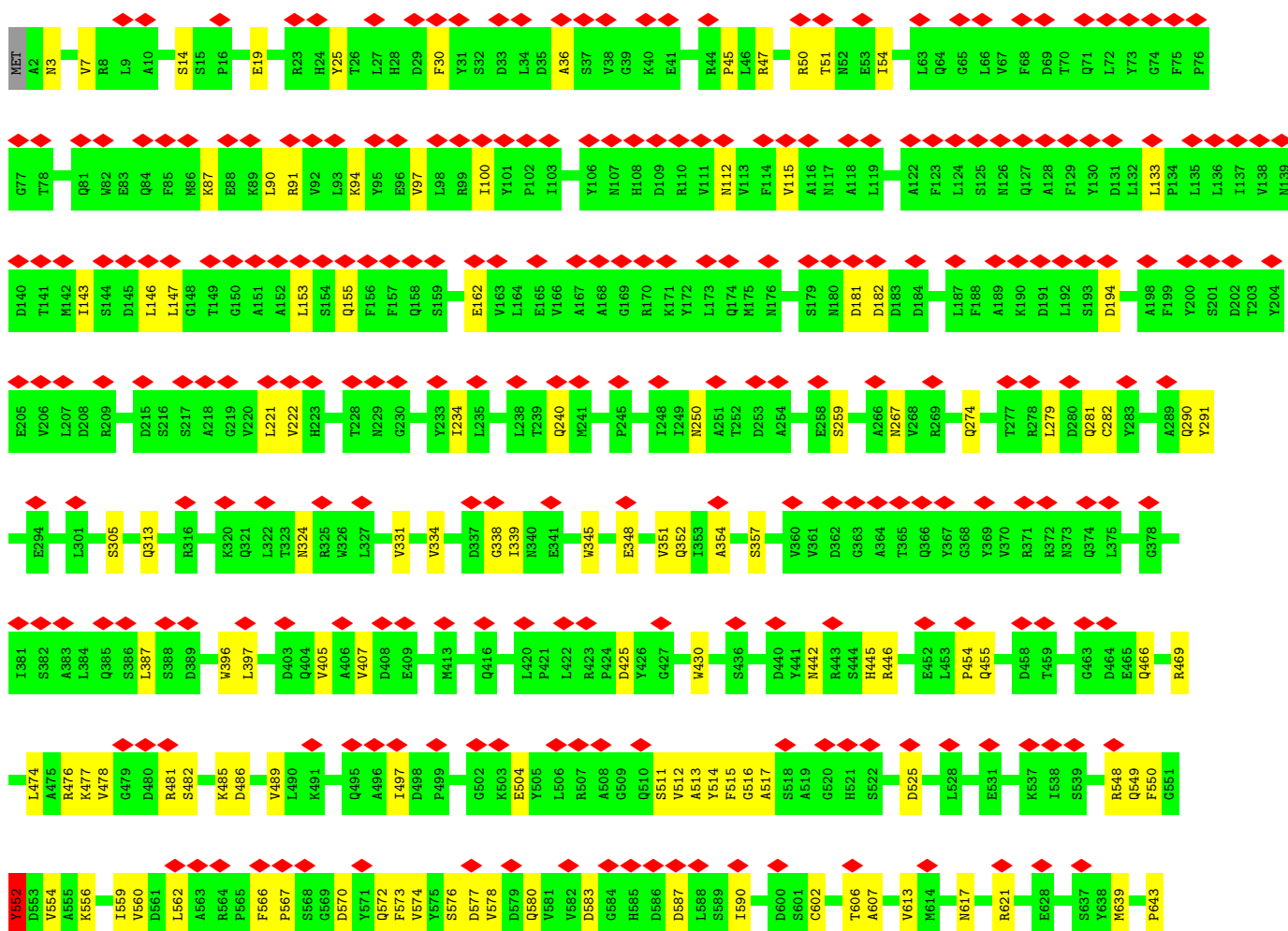


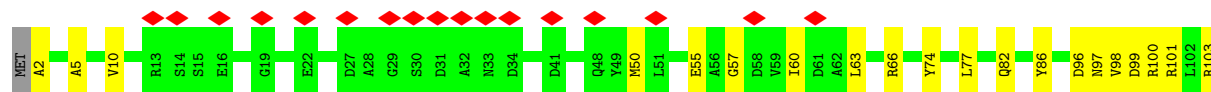


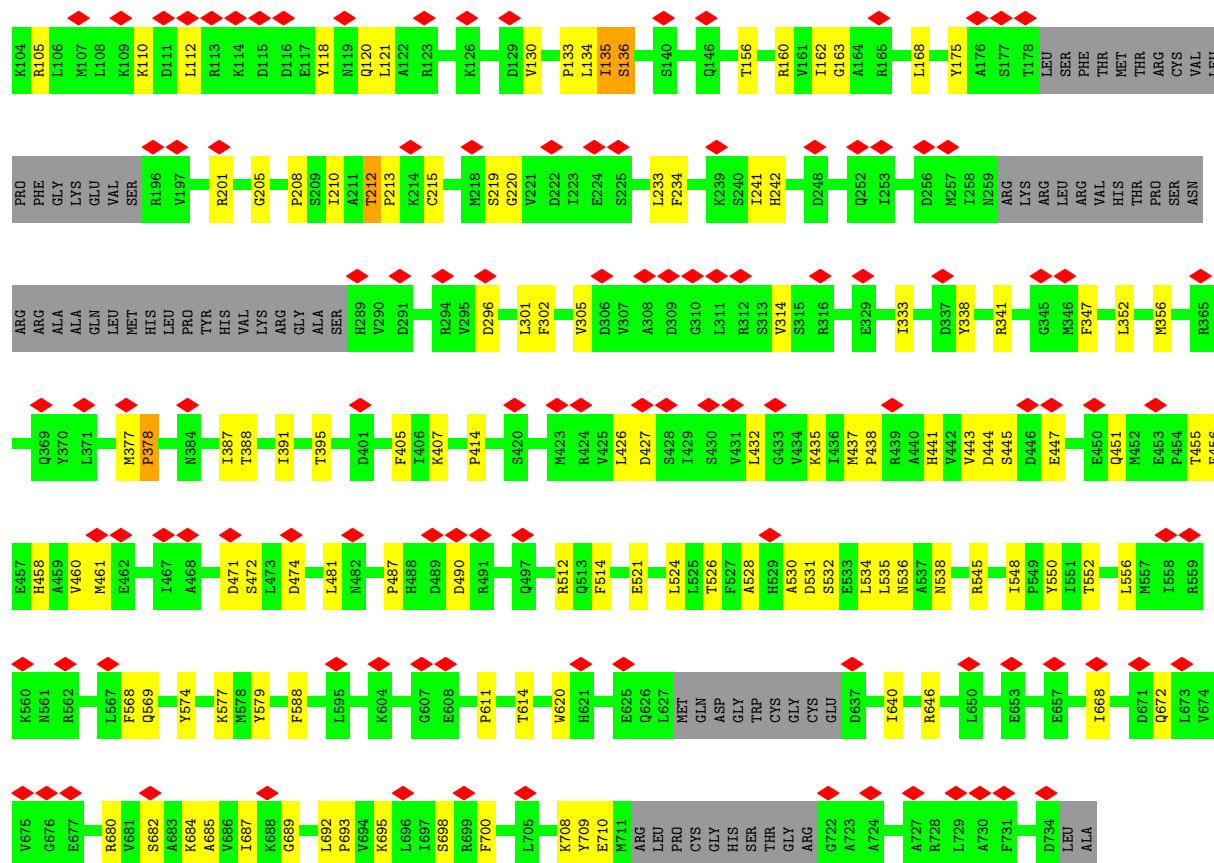




- Molecule 2: Lambda-2 protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50491	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	2.244	Depositor
Minimum map value	-1.209	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.4	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.29	0/1052	0.57	0/1413
1	2	0.31	0/1037	0.58	0/1394
1	3	0.29	0/1033	0.54	0/1387
1	4	0.29	0/959	0.59	0/1285
1	5	0.32	0/1047	0.68	2/1406 (0.1%)
1	A	0.36	0/9107	0.62	3/12474 (0.0%)
1	B	0.37	0/8671	0.63	3/11878 (0.0%)
1	C	0.36	0/8765	0.63	2/12006 (0.0%)
1	D	0.37	0/8526	0.63	2/11680 (0.0%)
1	E	0.39	0/8603	0.67	8/11786 (0.1%)
1	a	0.35	0/8813	0.64	5/12073 (0.0%)
1	b	0.34	0/8804	0.60	0/12061
1	c	0.35	0/8749	0.60	8/11985 (0.1%)
1	d	0.35	0/8792	0.62	3/12045 (0.0%)
1	e	0.38	0/8723	0.66	9/11948 (0.1%)
2	H	0.25	0/8275	0.57	1/11284 (0.0%)
2	I	0.25	1/8275 (0.0%)	0.57	3/11284 (0.0%)
2	J	0.26	1/8275 (0.0%)	0.58	3/11284 (0.0%)
2	K	0.25	1/8275 (0.0%)	0.57	3/11284 (0.0%)
2	L	0.25	1/8275 (0.0%)	0.58	2/11284 (0.0%)
3	R	0.34	0/10166	0.68	5/13806 (0.0%)
4	U	0.35	0/5439	0.70	2/7385 (0.0%)
All	All	0.33	4/149661 (0.0%)	0.62	64/204432 (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	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	a	0	2
1	b	0	1
1	c	0	1
1	d	0	4
1	e	0	2
4	U	0	1
All	All	0	17

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	552	TYR	C-N	6.13	1.44	1.34
2	K	552	TYR	C-N	6.05	1.44	1.34
2	L	552	TYR	C-N	6.04	1.44	1.34
2	J	552	TYR	C-N	5.91	1.43	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	713	TRP	N-CA-C	-17.82	92.19	108.22
1	e	318	ARG	N-CA-C	-10.76	91.09	108.41
2	L	71	GLN	N-CA-C	-9.66	100.71	111.14
1	c	514	ARG	NE-CZ-NH2	8.32	126.69	119.20
1	e	314	VAL	N-CA-C	7.25	118.31	108.17
2	L	339	ILE	N-CA-C	6.92	117.62	110.36
2	H	339	ILE	N-CA-C	6.90	117.61	110.36
2	I	339	ILE	N-CA-C	6.87	117.58	110.36
2	J	339	ILE	N-CA-C	6.86	117.56	110.36
2	K	339	ILE	N-CA-C	6.82	117.52	110.36
1	E	771	LEU	N-CA-C	-6.79	103.88	111.28
1	a	308	THR	CA-C-N	6.70	134.33	121.54
1	a	308	THR	C-N-CA	6.70	134.33	121.54
3	R	1151	GLN	CA-C-N	6.64	134.22	121.54
3	R	1151	GLN	C-N-CA	6.64	134.22	121.54
1	c	514	ARG	NH1-CZ-NH2	-6.51	110.84	119.30
1	E	713	TRP	CA-C-N	-6.41	112.93	120.11
1	E	713	TRP	C-N-CA	-6.41	112.93	120.11
1	A	308	THR	CA-C-N	6.29	133.55	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	THR	C-N-CA	6.29	133.55	121.54
1	B	416	VAL	N-CA-C	-6.24	106.36	111.91
1	5	7	LYS	N-CA-C	6.12	117.95	111.28
1	D	686	ARG	CB-CG-CD	6.11	125.36	111.30
1	D	686	ARG	CG-CD-NE	-6.09	98.59	112.00
3	R	1176	VAL	N-CA-C	-5.86	106.78	112.29
3	R	1215	MET	CA-CB-CG	5.86	125.83	114.10
1	A	720	ARG	CA-CB-CG	5.80	125.71	114.10
1	c	318	ARG	CA-C-N	5.69	132.41	121.54
1	c	318	ARG	C-N-CA	5.69	132.41	121.54
1	c	945	VAL	CA-C-N	5.61	131.36	122.61
1	c	945	VAL	C-N-CA	5.61	131.36	122.61
1	d	1229	VAL	N-CA-C	-5.61	108.38	113.71
1	e	319	ASP	N-CA-C	5.58	119.35	110.70
1	E	714	PRO	N-CA-C	5.44	119.10	111.33
4	U	378	PRO	N-CA-C	5.35	117.23	110.70
1	B	528	ASN	CA-C-N	5.31	131.67	121.54
1	B	528	ASN	C-N-CA	5.31	131.67	121.54
1	d	1065	LEU	CA-C-N	5.25	131.41	121.97
1	d	1065	LEU	C-N-CA	5.25	131.41	121.97
1	e	759	ASN	CA-C-N	5.24	131.54	121.54
1	e	759	ASN	C-N-CA	5.24	131.54	121.54
1	E	711	ARG	N-CA-C	5.22	116.78	111.14
1	e	1065	LEU	CA-C-N	5.22	131.36	121.97
1	e	1065	LEU	C-N-CA	5.22	131.36	121.97
1	a	560	MET	CA-C-N	5.21	131.49	121.54
1	a	560	MET	C-N-CA	5.21	131.49	121.54
1	E	786	THR	CA-C-N	5.17	131.41	121.54
1	E	786	THR	C-N-CA	5.17	131.41	121.54
3	R	1065	GLU	CA-CB-CG	5.15	124.39	114.10
1	e	615	LYS	CA-C-N	5.12	131.33	121.54
1	e	615	LYS	C-N-CA	5.12	131.33	121.54
1	a	339	LEU	N-CA-C	5.12	121.72	110.80
4	U	213	PRO	N-CA-C	-5.07	106.49	113.53
1	5	11	LYS	CB-CA-C	-5.06	110.76	116.63
2	K	338	GLY	CA-C-N	5.06	127.12	120.60
2	K	338	GLY	C-N-CA	5.06	127.12	120.60
1	c	615	LYS	CA-C-N	5.03	131.15	121.54
1	c	615	LYS	C-N-CA	5.03	131.15	121.54
2	J	338	GLY	CA-C-N	5.03	127.09	120.60
2	J	338	GLY	C-N-CA	5.03	127.09	120.60
2	I	338	GLY	CA-C-N	5.02	127.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	338	GLY	C-N-CA	5.02	127.08	120.60
1	C	428	ARG	CA-C-N	5.02	131.13	121.54
1	C	428	ARG	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	PRO	Peptide
1	B	308	THR	Peptide
1	B	782	GLN	Peptide
1	C	317	ASP	Peptide
1	D	981	ASP	Peptide
1	E	238	ASP	Peptide
4	U	135	ILE	Peptide
1	a	1110	PHE	Peptide
1	a	1220	ILE	Peptide
1	b	945	VAL	Peptide
1	c	946	ASP	Peptide
1	d	1055	LEU	Peptide
1	d	1065	LEU	Peptide
1	d	342	GLU	Peptide
1	d	838	LEU	Peptide
1	e	1065	LEU	Peptide
1	e	1110	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1041	0	1024	24	0
1	2	1026	0	1006	22	0
1	3	1023	0	1006	18	0
1	4	950	0	939	18	0
1	5	1036	0	1019	59	0
1	A	8868	0	8763	142	0
1	B	8442	0	8330	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8535	0	8427	131	0
1	D	8300	0	8200	116	0
1	E	8376	0	8280	116	0
1	a	8580	0	8463	128	0
1	b	8571	0	8454	116	0
1	c	8517	0	8405	120	0
1	d	8559	0	8446	135	0
1	e	8492	0	8370	156	0
2	H	8073	0	7924	147	0
2	I	8073	0	7924	142	0
2	J	8073	0	7925	132	0
2	K	8073	0	7925	159	0
2	L	8073	0	7925	145	0
3	R	9913	0	9836	166	0
4	U	5322	0	5341	79	0
5	H	27	22	22	27	0
5	I	27	22	21	22	0
5	J	27	22	22	11	0
5	K	27	22	22	37	0
5	L	27	22	22	19	0
6	b	1	0	0	0	0
All	All	146052	110	144041	2203	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 8.

All (2203) 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:K:578:VAL:HG21	5:K:1301:SAM:N9	1.25	1.44
1:5:11:LYS:CD	1:e:320:SER:HA	1.51	1.40
2:H:578:VAL:CG2	5:H:1301:SAM:C8	1.97	1.39
2:K:578:VAL:CG2	5:K:1301:SAM:N9	1.86	1.35
2:K:578:VAL:HG23	5:K:1301:SAM:O4'	1.24	1.30
2:K:578:VAL:HG21	5:K:1301:SAM:C4	1.62	1.27
2:K:578:VAL:CG2	5:K:1301:SAM:O4'	1.82	1.25
2:K:578:VAL:HG23	5:K:1301:SAM:C1'	1.66	1.25
2:K:578:VAL:CG2	5:K:1301:SAM:C8	2.16	1.21
2:K:578:VAL:HA	5:K:1301:SAM:C5'	1.72	1.20
2:H:578:VAL:HG21	5:H:1301:SAM:C4	1.72	1.19
2:K:514:TYR:OH	5:K:1301:SAM:N	1.77	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:578:VAL:CG2	5:K:1301:SAM:C1'	2.23	1.17
2:H:578:VAL:HG23	5:H:1301:SAM:C8	1.76	1.16
2:H:578:VAL:CG2	5:H:1301:SAM:N9	2.08	1.15
2:H:578:VAL:HG21	5:H:1301:SAM:N9	1.62	1.14
2:K:577:ASP:OD2	5:K:1301:SAM:N	1.82	1.12
1:5:10:GLY:HA3	1:e:319:ASP:HB2	1.23	1.10
1:5:11:LYS:HD3	1:e:320:SER:CA	1.79	1.09
1:e:308:THR:OG1	1:e:321:SER:HB3	1.54	1.08
2:K:578:VAL:HA	5:K:1301:SAM:H5'2	1.06	1.06
1:5:4:ILE:CD1	1:e:315:ASP:OD1	2.05	1.05
2:H:578:VAL:HG21	5:H:1301:SAM:C8	1.77	1.04
2:L:578:VAL:HG21	5:L:1301:SAM:C5	1.88	1.03
2:H:578:VAL:HA	5:H:1301:SAM:H5'2	1.41	1.02
1:5:4:ILE:HD11	1:e:315:ASP:OD1	1.60	1.02
2:I:577:ASP:OD2	5:I:1301:SAM:N	1.92	1.01
1:5:10:GLY:HA3	1:e:319:ASP:CB	1.90	1.00
2:H:577:ASP:OD2	5:H:1301:SAM:N	1.94	1.00
1:5:11:LYS:HD2	1:e:320:SER:HA	1.44	0.99
2:K:578:VAL:HG21	5:K:1301:SAM:C8	1.86	0.98
1:5:11:LYS:HD3	1:e:320:SER:HA	0.99	0.98
2:K:578:VAL:CA	5:K:1301:SAM:H5'2	1.93	0.98
2:K:578:VAL:CB	5:K:1301:SAM:O4'	2.12	0.97
2:H:578:VAL:HG21	5:H:1301:SAM:C5	1.96	0.95
2:I:578:VAL:HA	5:I:1301:SAM:H5'2	1.47	0.94
2:I:578:VAL:HG21	5:I:1301:SAM:C4	1.98	0.94
2:I:578:VAL:HG23	5:I:1301:SAM:O4'	1.67	0.93
2:I:578:VAL:HG21	5:I:1301:SAM:N9	1.83	0.93
1:5:7:LYS:H	1:5:7:LYS:HD2	1.33	0.91
2:I:578:VAL:CG2	5:I:1301:SAM:C8	2.50	0.89
1:5:11:LYS:HA	1:5:11:LYS:HZ3	1.38	0.88
1:5:10:GLY:CA	1:e:319:ASP:HB2	2.03	0.88
1:e:323:ILE:H	1:e:323:ILE:HD12	1.38	0.86
2:I:518:SER:HB3	5:I:1301:SAM:HB1	1.57	0.85
2:K:578:VAL:HG22	5:K:1301:SAM:C8	2.06	0.85
1:5:4:ILE:HG21	1:e:254:ARG:HH22	1.41	0.84
1:5:6:ARG:HD2	1:5:6:ARG:H	1.42	0.84
2:I:578:VAL:CG2	5:I:1301:SAM:N9	2.41	0.84
1:5:4:ILE:H	1:5:4:ILE:HD12	1.43	0.81
2:H:518:SER:HB3	5:H:1301:SAM:HB1	1.63	0.81
2:H:578:VAL:HG23	5:H:1301:SAM:N9	1.82	0.81
2:J:562:LEU:HG	5:J:1301:SAM:H2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:577:ASP:OD2	5:K:1301:SAM:OXT	1.99	0.80
1:5:4:ILE:HD13	1:e:315:ASP:OD1	1.81	0.80
2:I:578:VAL:HG21	5:I:1301:SAM:C8	2.13	0.79
4:U:352:LEU:O	4:U:356:MET:HB2	1.83	0.78
2:K:578:VAL:HB	5:K:1301:SAM:O4'	1.82	0.78
2:L:578:VAL:HG21	5:L:1301:SAM:C4	2.13	0.78
2:H:527:PRO:HG3	5:H:1301:SAM:OXT	1.84	0.78
1:5:7:LYS:NZ	1:5:7:LYS:HB3	1.98	0.78
1:e:308:THR:OG1	1:e:321:SER:CB	2.33	0.77
1:5:11:LYS:HA	1:5:11:LYS:NZ	1.98	0.77
2:K:562:LEU:HG	5:K:1301:SAM:H2	1.64	0.77
1:5:7:LYS:HD2	1:5:7:LYS:N	2.00	0.77
2:H:578:VAL:HG22	5:H:1301:SAM:C8	2.12	0.76
2:H:578:VAL:HG21	5:H:1301:SAM:N7	2.00	0.76
1:a:723:THR:O	1:a:727:PHE:HB2	1.84	0.76
1:E:579:GLY:HA3	3:R:1161:LYS:HD3	1.68	0.76
2:K:583:ASP:OD2	5:K:1301:SAM:N6	2.18	0.76
1:e:723:THR:O	1:e:727:PHE:HB2	1.86	0.75
2:J:518:SER:OG	5:J:1301:SAM:O	2.05	0.75
2:H:578:VAL:CG2	5:H:1301:SAM:N7	2.49	0.74
2:J:578:VAL:HA	5:J:1301:SAM:H5'2	1.69	0.74
1:d:940:GLU:H	1:d:956:ARG:HH22	1.35	0.73
2:H:578:VAL:HG23	5:H:1301:SAM:O4'	1.88	0.73
2:I:578:VAL:CG2	5:I:1301:SAM:O4'	2.37	0.72
2:K:482:SER:OG	5:K:1301:SAM:C	2.38	0.72
2:H:578:VAL:HG23	5:H:1301:SAM:C1'	2.20	0.71
1:A:351:PRO:HG3	1:A:1116:GLN:HE22	1.56	0.71
1:D:268:ILE:HG12	1:D:304:ILE:HG22	1.73	0.71
1:B:380:GLN:HE21	1:a:958:SER:HB2	1.57	0.70
1:e:186:CYS:HG	1:e:199:HIS:HE2	1.24	0.70
1:5:7:LYS:HB3	1:5:7:LYS:HZ2	1.54	0.70
1:C:336:LYS:HA	1:C:340:ASN:HD22	1.55	0.70
2:J:562:LEU:HG	5:J:1301:SAM:C2	2.22	0.70
1:C:612:SER:HB3	1:C:632:LEU:HD21	1.74	0.69
1:D:761:LEU:HB2	1:D:808:PRO:HB3	1.73	0.69
1:e:323:ILE:HD12	1:e:323:ILE:N	2.07	0.69
2:J:516:GLY:O	5:J:1301:SAM:HA	1.92	0.69
1:a:309:ARG:NH2	1:a:368:ASP:O	2.25	0.69
1:C:480:GLU:HG2	1:C:493:VAL:HG23	1.75	0.68
2:H:559:ILE:HG13	2:I:396:TRP:HD1	1.58	0.68
4:U:82:GLN:HE22	4:U:86:TYR:HB2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:482:SER:CB	5:K:1301:SAM:O	2.42	0.68
1:B:351:PRO:HG3	1:B:1116:GLN:HE22	1.58	0.67
1:D:1058:PRO:HD2	1:D:1182:VAL:HG12	1.75	0.67
1:d:336:LYS:HA	1:d:340:ASN:HD22	1.59	0.67
1:b:1111:PRO:HD2	1:b:1114:LEU:HD12	1.77	0.67
1:5:6:ARG:H	1:5:6:ARG:CD	2.08	0.66
1:A:161:ILE:HG23	1:A:162:VAL:HG23	1.77	0.66
1:A:268:ILE:HG12	1:A:304:ILE:HG22	1.78	0.66
2:I:552:TYR:CE1	2:J:782:VAL:HG11	2.30	0.66
4:U:110:LYS:HD3	4:U:112:LEU:H	1.59	0.66
1:d:1033:HIS:HB3	1:d:1207:ARG:HH12	1.61	0.66
1:c:433:ARG:HH12	1:c:436:ARG:HD2	1.60	0.66
1:A:1207:ARG:HH22	1:A:1250:VAL:HG12	1.60	0.66
1:e:708:ILE:HD11	1:e:767:ARG:HB3	1.77	0.65
1:5:150:MET:HA	1:5:153:ARG:HG2	1.78	0.65
1:C:373:ASN:HB3	1:C:1259:ARG:HD3	1.78	0.65
1:D:399:ALA:HA	1:D:402:TRP:HD1	1.61	0.65
1:2:130:ALA:HB3	1:C:496:PRO:HG3	1.78	0.65
1:E:224:ILE:HG22	1:E:228:GLN:HE22	1.62	0.65
2:I:513:ALA:HB3	2:I:574:VAL:HG12	1.79	0.65
4:U:556:LEU:HD12	4:U:569:GLN:HB3	1.77	0.65
1:5:6:ARG:HD2	1:5:6:ARG:N	2.11	0.65
1:d:616:ASP:HA	1:d:674:ARG:HH22	1.62	0.65
1:c:1036:ASN:ND2	1:c:1205:ASN:OD1	2.30	0.64
1:A:150:MET:SD	1:A:153:ARG:NH1	2.71	0.64
1:D:503:ARG:HD2	1:D:1265:PRO:HG3	1.79	0.64
1:D:776:VAL:HA	1:D:782:GLN:HE22	1.61	0.64
2:I:577:ASP:CG	5:I:1301:SAM:HN2	2.06	0.64
1:a:544:GLN:OE1	1:a:545:ARG:NH1	2.29	0.64
1:d:1093:MET:HB3	1:d:1101:MET:HB3	1.79	0.64
2:L:513:ALA:HB3	2:L:574:VAL:HG12	1.79	0.64
1:B:749:ASN:HD21	2:I:154:SER:H	1.45	0.64
2:K:513:ALA:HB3	2:K:574:VAL:HG12	1.79	0.64
2:H:513:ALA:HB3	2:H:574:VAL:HG12	1.79	0.64
1:2:144:GLY:HA3	1:C:377:GLY:HA2	1.79	0.64
3:R:987:ARG:NH1	3:R:1150:LEU:O	2.29	0.64
1:b:746:GLN:HG2	1:b:813:GLN:HE21	1.63	0.64
1:E:692:GLN:HA	1:E:703:ARG:HH12	1.63	0.63
3:R:158:LEU:HD12	3:R:238:ILE:HD13	1.79	0.63
4:U:208:PRO:HD2	4:U:234:PHE:HE2	1.63	0.63
2:J:518:SER:CB	5:J:1301:SAM:O	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:14:GLU:HB2	3:R:19:ILE:HB	1.80	0.63
1:a:569:GLN:HG3	1:a:570:THR:HG22	1.79	0.63
1:5:4:ILE:CD1	1:e:315:ASP:O	2.46	0.63
1:d:373:ASN:HB3	1:d:1259:ARG:HD3	1.79	0.63
1:D:413:THR:HG23	1:D:420:CYS:HB3	1.80	0.63
2:K:578:VAL:HG21	5:K:1301:SAM:C1'	2.07	0.63
2:H:578:VAL:HA	5:H:1301:SAM:C5'	2.25	0.63
3:R:240:GLN:HE21	3:R:250:VAL:HG11	1.63	0.63
3:R:569:PRO:HG2	3:R:1099:LEU:HA	1.79	0.63
1:A:629:PHE:HB2	1:A:655:MET:HE3	1.81	0.63
1:C:518:GLN:OE1	1:C:521:ARG:NH2	2.31	0.63
1:E:336:LYS:HA	1:E:340:ASN:HD22	1.63	0.63
2:L:515:PHE:HB2	2:L:576:SER:HA	1.81	0.63
3:R:145:ARG:NH2	3:R:809:SER:O	2.31	0.63
1:b:851:ARG:NH1	1:b:990:GLY:O	2.32	0.63
1:B:181:TYR:HB2	1:B:189:VAL:HB	1.79	0.63
2:I:150:GLY:HA2	1:a:698:ASP:HB3	1.79	0.63
1:a:352:LEU:HD12	1:a:955:LEU:HB3	1.81	0.63
1:a:524:ASN:ND2	1:a:982:MET:SD	2.72	0.63
2:I:583:ASP:OD2	5:I:1301:SAM:N6	2.30	0.63
2:J:513:ALA:HB3	2:J:574:VAL:HG12	1.79	0.63
1:2:6:ARG:NH2	1:b:975:THR:O	2.32	0.63
1:A:1116:GLN:HB3	1:A:1172:PRO:HA	1.81	0.63
2:H:515:PHE:HB2	2:H:576:SER:HA	1.81	0.63
4:U:50:MET:HG2	4:U:160:ARG:HB2	1.80	0.63
2:J:515:PHE:HB2	2:J:576:SER:HA	1.81	0.62
3:R:35:SER:OG	3:R:851:ARG:NH1	2.32	0.62
1:e:262:LEU:HD21	1:e:406:MET:HE2	1.81	0.62
1:e:1120:ARG:NH1	1:e:1168:GLU:OE2	2.32	0.62
1:C:189:VAL:O	3:R:930:ASN:ND2	2.31	0.62
2:K:182:ASP:OD1	2:L:91:ARG:NH2	2.31	0.62
2:H:567:PRO:HG3	2:I:854:THR:HA	1.81	0.62
2:K:515:PHE:HB2	2:K:576:SER:HA	1.81	0.62
1:3:6:ARG:NH1	1:c:319:ASP:OD1	2.32	0.62
1:C:985:GLU:HA	1:C:988:LEU:HD13	1.81	0.62
2:I:527:PRO:HG3	5:I:1301:SAM:OXT	2.00	0.62
1:C:438:GLN:HB3	1:b:859:GLN:HG3	1.82	0.62
2:I:518:SER:HB3	5:I:1301:SAM:CB	2.29	0.62
2:I:639:MET:HB3	2:I:654:VAL:HB	1.82	0.62
2:K:514:TYR:HH	5:K:1301:SAM:HN1	1.38	0.62
1:E:1124:GLN:NE2	1:e:183:CYS:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:ILE:HD11	1:C:879:ALA:HB2	1.81	0.62
1:E:1116:GLN:HB3	1:E:1172:PRO:HA	1.81	0.62
2:L:706:ILE:HG22	2:L:757:ARG:HG2	1.82	0.62
1:b:777:ASP:OD1	1:b:794:ARG:NH2	2.32	0.62
1:A:1163:THR:HG21	1:A:1198:TYR:HB2	1.82	0.62
1:D:603:VAL:HG23	1:D:604:VAL:HG23	1.82	0.62
2:H:639:MET:HB3	2:H:654:VAL:HB	1.82	0.62
1:E:373:ASN:HB3	1:E:1259:ARG:HG2	1.82	0.61
4:U:66:ARG:HH12	4:U:163:GLY:HA2	1.65	0.61
1:d:351:PRO:HD3	1:d:1175:ILE:HG13	1.82	0.61
1:A:504:LEU:HD23	1:A:506:PRO:HD3	1.82	0.61
2:J:706:ILE:HG22	2:J:757:ARG:HG2	1.82	0.61
1:A:1045:ILE:HG12	1:A:1141:MET:HE1	1.82	0.61
1:B:600:TYR:OH	1:B:828:PHE:O	2.18	0.61
1:E:480:GLU:HG2	1:E:493:VAL:HG23	1.81	0.61
2:I:515:PHE:HB2	2:I:576:SER:HA	1.81	0.61
2:J:639:MET:HB3	2:J:654:VAL:HB	1.82	0.61
1:e:920:ARG:NH2	1:e:982:MET:O	2.34	0.61
1:B:412:GLY:HA2	1:a:1079:ARG:HH22	1.65	0.61
2:H:181:ASP:OD1	2:I:91:ARG:NH2	2.33	0.61
1:e:359:LEU:HB3	1:e:934:LEU:HD11	1.81	0.61
1:A:706:ALA:O	1:A:710:HIS:ND1	2.31	0.61
1:B:1067:PHE:O	1:B:1138:ARG:NH1	2.33	0.61
1:E:390:ASN:OD1	1:E:433:ARG:NH2	2.33	0.61
2:L:578:VAL:CG2	5:L:1301:SAM:C8	2.79	0.61
1:b:572:SER:HG	1:b:575:SER:HG	1.48	0.61
1:c:186:CYS:HG	1:c:199:HIS:HE2	1.47	0.61
1:A:339:LEU:HB2	1:A:353:MET:HG2	1.82	0.61
1:C:601:ASN:ND2	1:C:833:VAL:O	2.32	0.61
2:I:1011:LEU:HD23	2:I:1014:LYS:HZ3	1.66	0.61
2:K:639:MET:HB3	2:K:654:VAL:HB	1.82	0.61
1:a:278:GLN:OE1	1:a:415:ASN:ND2	2.34	0.61
1:c:482:ALA:HA	1:c:723:THR:HG21	1.82	0.61
1:B:559:THR:O	1:B:799:LYS:NZ	2.33	0.61
1:C:600:TYR:OH	1:C:828:PHE:O	2.18	0.61
1:D:600:TYR:OH	1:D:828:PHE:O	2.18	0.61
3:R:418:THR:HG22	3:R:420:SER:H	1.66	0.61
1:d:314:VAL:HG22	1:d:316:PHE:H	1.66	0.61
1:E:523:MET:HE1	1:E:851:ARG:HB3	1.83	0.61
1:E:782:GLN:HB3	1:E:785:TRP:HZ3	1.65	0.61
1:A:1067:PHE:O	1:A:1138:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1120:ARG:NH2	1:c:225:SER:O	2.34	0.61
1:D:601:ASN:ND2	1:D:833:VAL:O	2.34	0.61
1:D:616:ASP:O	1:E:804:LYS:NZ	2.33	0.61
1:c:268:ILE:HG12	1:c:304:ILE:HG12	1.83	0.61
1:2:81:PRO:HG3	1:b:963:ALA:HB1	1.83	0.60
1:E:351:PRO:HG3	1:E:1116:GLN:HE22	1.64	0.60
2:L:639:MET:HB3	2:L:654:VAL:HB	1.82	0.60
3:R:307:LYS:HG2	3:R:1100:GLN:HE22	1.66	0.60
3:R:1199:LEU:HD22	3:R:1242:LEU:HD22	1.83	0.60
1:a:707:GLU:OE2	1:a:711:ARG:NH1	2.34	0.60
1:d:1034:GLU:OE2	1:d:1207:ARG:NH2	2.34	0.60
1:D:341:THR:HG23	1:D:342:GLU:HG2	1.83	0.60
2:H:706:ILE:HG22	2:H:757:ARG:HG2	1.82	0.60
2:I:405:VAL:HG22	2:I:774:LEU:HD11	1.83	0.60
2:I:562:LEU:HG	5:I:1301:SAM:H2	1.82	0.60
2:J:1011:LEU:HD23	2:J:1014:LYS:HZ3	1.65	0.60
2:K:706:ILE:HG22	2:K:757:ARG:HG2	1.82	0.60
1:3:135:ARG:HH22	1:c:986:PRO:HB3	1.66	0.60
1:5:6:ARG:O	1:5:6:ARG:HD3	2.00	0.60
1:D:1119:THR:O	1:D:1123:ASN:ND2	2.35	0.60
1:e:542:LEU:HD11	1:e:908:MET:HE1	1.84	0.60
1:A:1058:PRO:HD2	1:A:1182:VAL:HG12	1.82	0.60
1:D:438:GLN:O	1:c:859:GLN:NE2	2.34	0.60
1:b:1095:ARG:HE	1:b:1099:GLY:HA2	1.65	0.60
1:d:469:LEU:HD21	1:d:504:LEU:HD13	1.83	0.60
2:L:405:VAL:HG22	2:L:774:LEU:HD11	1.84	0.60
1:c:373:ASN:HB3	1:c:1259:ARG:HD3	1.83	0.60
1:c:524:ASN:ND2	1:c:982:MET:SD	2.75	0.60
1:A:517:SER:OG	1:A:521:ARG:NH1	2.35	0.60
1:C:761:LEU:HB2	1:C:808:PRO:HB3	1.84	0.60
2:H:405:VAL:HG22	2:H:774:LEU:HD11	1.84	0.60
2:L:345:TRP:O	2:L:352:GLN:NE2	2.35	0.60
1:b:373:ASN:HB3	1:b:1259:ARG:HG2	1.83	0.60
1:B:419:ILE:HD13	1:B:1227:ILE:HD11	1.83	0.60
1:E:600:TYR:OH	1:E:828:PHE:O	2.20	0.60
3:R:83:ARG:HH22	3:R:95:PRO:HG3	1.67	0.60
4:U:443:VAL:HB	4:U:526:THR:HA	1.82	0.60
1:3:81:PRO:HD3	1:3:141:ASN:HD21	1.67	0.59
1:4:81:PRO:O	1:4:88:LYS:NZ	2.35	0.59
2:I:706:ILE:HG22	2:I:757:ARG:HG2	1.82	0.59
2:K:405:VAL:HG22	2:K:774:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ARG:NH1	1:A:866:THR:OG1	2.35	0.59
1:B:956:ARG:NH2	1:b:749:ASN:OD1	2.34	0.59
2:H:743:ILE:H	2:H:787:ILE:HB	1.67	0.59
2:J:559:ILE:HG13	2:K:396:TRP:HD1	1.68	0.59
2:L:1011:LEU:HD23	2:L:1014:LYS:HZ3	1.67	0.59
1:A:670:THR:HG23	1:A:672:SER:H	1.67	0.59
2:K:345:TRP:O	2:K:352:GLN:NE2	2.35	0.59
2:L:578:VAL:HG21	5:L:1301:SAM:N7	2.17	0.59
1:d:753:PRO:HB2	1:d:756:ASP:HB2	1.84	0.59
1:D:336:LYS:HA	1:D:340:ASN:HD22	1.66	0.59
2:H:345:TRP:O	2:H:352:GLN:NE2	2.35	0.59
2:H:517:ALA:HB3	2:H:554:VAL:HG12	1.85	0.59
2:I:559:ILE:HG13	2:J:396:TRP:HD1	1.67	0.59
1:A:616:ASP:O	1:B:804:LYS:NZ	2.35	0.59
1:E:247:LEU:HD22	1:E:525:ILE:HG21	1.84	0.59
2:I:345:TRP:O	2:I:352:GLN:NE2	2.35	0.59
2:K:517:ALA:HB3	2:K:554:VAL:HG12	1.85	0.59
1:e:1041:ALA:HB1	1:e:1205:ASN:HD21	1.66	0.59
2:J:345:TRP:O	2:J:352:GLN:NE2	2.35	0.59
1:a:601:ASN:ND2	1:a:833:VAL:O	2.35	0.59
1:5:11:LYS:CD	1:e:320:SER:CA	2.47	0.59
1:5:160:ALA:O	1:A:293:GLN:NE2	2.35	0.59
1:E:613:TYR:HE2	1:E:676:SER:HB3	1.66	0.59
2:H:583:ASP:OD2	5:H:1301:SAM:N6	2.36	0.59
2:J:405:VAL:HG22	2:J:774:LEU:HD11	1.84	0.59
1:a:598:TRP:O	1:a:832:GLN:NE2	2.36	0.59
1:b:974:LYS:NZ	1:b:981:ASP:O	2.27	0.59
1:1:6:ARG:NH2	1:a:975:THR:O	2.35	0.59
1:C:1163:THR:HG21	1:C:1198:TYR:HB2	1.85	0.59
2:I:517:ALA:HB3	2:I:554:VAL:HG12	1.85	0.59
3:R:106:HIS:HB3	3:R:109:LEU:HB2	1.85	0.59
3:R:321:ALA:O	3:R:747:LYS:NZ	2.36	0.59
1:a:506:PRO:O	1:a:919:GLN:NE2	2.35	0.59
1:A:846:MET:SD	1:A:1000:GLN:NE2	2.68	0.59
1:B:705:TRP:HE3	1:B:771:LEU:HD13	1.68	0.59
1:C:625:ASN:HB3	1:C:655:MET:HE1	1.85	0.59
2:J:517:ALA:HB3	2:J:554:VAL:HG12	1.85	0.59
2:J:743:ILE:H	2:J:787:ILE:HB	1.68	0.59
1:b:237:ALA:HA	1:b:247:LEU:HD12	1.84	0.59
4:U:521:GLU:HB2	4:U:708:LYS:HE2	1.83	0.58
1:a:263:CYS:SG	1:a:462:ARG:NH1	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:743:ILE:H	2:K:787:ILE:HB	1.68	0.58
3:R:241:GLN:HB3	3:R:837:ARG:HH21	1.66	0.58
1:a:259:ASP:OD1	1:a:312:SER:OG	2.21	0.58
1:A:426:CYS:HB3	1:A:1235:LEU:HD12	1.84	0.58
2:L:743:ILE:H	2:L:787:ILE:HB	1.68	0.58
1:e:338:LEU:HG	1:e:339:LEU:HG	1.84	0.58
1:B:599:LEU:HD12	1:B:830:PRO:HB3	1.85	0.58
1:D:215:GLU:O	1:D:219:HIS:ND1	2.37	0.58
1:c:398:ASP:OD1	1:c:401:LYS:NZ	2.35	0.58
1:c:601:ASN:ND2	1:c:833:VAL:O	2.36	0.58
1:A:1112:LEU:HA	1:A:1139:ILE:HD11	1.86	0.58
2:L:517:ALA:HB3	2:L:554:VAL:HG12	1.85	0.58
2:L:578:VAL:CG2	5:L:1301:SAM:N7	2.66	0.58
1:b:1120:ARG:NH2	1:b:1168:GLU:O	2.36	0.58
1:d:621:THR:HG22	1:d:783:PRO:HD2	1.83	0.58
1:d:836:VAL:HB	1:d:839:ASP:HB3	1.84	0.58
1:B:268:ILE:HG12	1:B:304:ILE:HG22	1.85	0.58
1:B:272:VAL:HG23	1:B:300:ALA:HB3	1.85	0.58
1:B:426:CYS:HB3	1:B:1235:LEU:HD12	1.84	0.58
1:C:438:GLN:NE2	1:C:440:MET:O	2.37	0.58
1:D:1078:GLY:H	1:D:1097:GLU:HB2	1.69	0.58
2:K:387:LEU:HD12	2:K:784:ALA:H	1.69	0.58
3:R:1132:ARG:NE	3:R:1162:ILE:O	2.36	0.58
1:a:261:GLY:O	1:a:1259:ARG:NH2	2.37	0.58
1:a:378:PHE:HA	1:a:392:ARG:HA	1.84	0.58
1:c:491:VAL:HG23	1:c:1273:GLY:HA2	1.85	0.58
2:H:91:ARG:NH2	2:L:181:ASP:OD1	2.37	0.58
2:I:182:ASP:OD1	2:J:91:ARG:NH2	2.35	0.58
2:K:482:SER:OG	5:K:1301:SAM:OXT	2.20	0.58
3:R:499:ASN:ND2	3:R:976:ASP:OD2	2.37	0.58
1:c:1030:VAL:HG12	1:c:1248:PRO:HA	1.86	0.58
1:e:347:ARG:HH21	1:e:1169:GLU:HG3	1.68	0.58
1:a:970:ASN:HD22	1:a:988:LEU:HD11	1.68	0.58
1:A:231:PRO:HG2	1:A:232:ILE:HD12	1.85	0.58
1:b:285:PHE:HD2	1:b:288:SER:H	1.51	0.58
1:c:699:ALA:HB1	1:c:702:LEU:HB2	1.85	0.58
2:I:764:ARG:NH2	2:I:838:GLU:O	2.37	0.58
4:U:490:ASP:N	4:U:490:ASP:OD1	2.37	0.58
1:a:306:VAL:H	1:a:324:MET:HE2	1.69	0.58
1:C:1067:PHE:O	1:C:1138:ARG:NH1	2.37	0.57
1:D:224:ILE:O	1:D:228:GLN:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:743:ILE:H	2:I:787:ILE:HB	1.68	0.57
2:I:771:TYR:HB2	2:I:860:CYS:HB2	1.86	0.57
3:R:626:ILE:HB	4:U:233:LEU:HD12	1.86	0.57
1:b:649:PHE:HA	1:b:705:TRP:HE1	1.69	0.57
1:2:148:LYS:O	1:2:153:ARG:NH1	2.37	0.57
1:C:720:ARG:NH2	1:C:737:GLU:OE2	2.37	0.57
2:L:771:TYR:HB2	2:L:860:CYS:HB2	1.86	0.57
1:c:186:CYS:SG	1:c:199:HIS:NE2	2.70	0.57
1:c:1115:TRP:HE1	1:c:1170:ILE:HG21	1.69	0.57
1:e:352:LEU:HD12	1:e:955:LEU:HB3	1.86	0.57
1:e:716:PRO:HA	1:e:742:PRO:HA	1.85	0.57
1:C:1116:GLN:HB3	1:C:1172:PRO:HA	1.86	0.57
1:E:606:THR:HG22	1:E:640:THR:HG22	1.85	0.57
1:E:1033:HIS:HD1	1:E:1249:GLU:HA	1.69	0.57
2:H:578:VAL:CG2	5:H:1301:SAM:O4'	2.52	0.57
2:J:771:TYR:HB2	2:J:860:CYS:HB2	1.86	0.57
1:a:359:LEU:HD21	1:a:934:LEU:HG	1.86	0.57
2:K:764:ARG:NH2	2:K:838:GLU:O	2.37	0.57
1:5:4:ILE:HD12	1:e:315:ASP:O	2.05	0.57
1:A:749:ASN:ND2	2:H:152:ALA:O	2.38	0.57
1:E:371:TYR:HB2	1:E:462:ARG:HH12	1.70	0.57
1:E:746:GLN:NE2	2:L:154:SER:O	2.36	0.57
2:L:387:LEU:HD12	2:L:784:ALA:H	1.69	0.57
1:c:859:GLN:NE2	1:c:860:PRO:O	2.37	0.57
1:e:263:CYS:SG	1:e:462:ARG:NH1	2.77	0.57
1:D:759:ASN:O	1:D:763:ASN:HB2	2.04	0.57
1:E:1272:MET:HB3	1:E:1274:VAL:HG13	1.86	0.57
2:H:396:TRP:HD1	2:L:559:ILE:HG13	1.69	0.57
2:H:764:ARG:NH2	2:H:838:GLU:O	2.37	0.57
2:H:771:TYR:HB2	2:H:860:CYS:HB2	1.86	0.57
2:J:387:LEU:HD12	2:J:784:ALA:H	1.69	0.57
1:c:514:ARG:CZ	1:c:730:ALA:H	2.18	0.57
1:d:1163:THR:HG21	1:d:1198:TYR:HB2	1.86	0.57
1:a:468:ARG:HB2	1:a:1019:VAL:HG21	1.87	0.57
1:d:278:GLN:OE1	1:d:415:ASN:ND2	2.37	0.57
1:4:81:PRO:HA	1:4:87:THR:HA	1.87	0.57
1:5:79:GLY:HA3	1:5:135:ARG:HG2	1.87	0.57
1:A:653:ALA:O	1:A:671:GLN:NE2	2.38	0.57
2:I:387:LEU:HD12	2:I:784:ALA:H	1.69	0.57
2:L:764:ARG:NH2	2:L:838:GLU:O	2.37	0.57
1:c:805:SER:OG	1:c:887:LEU:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:598:TRP:O	1:d:832:GLN:NE2	2.38	0.57
1:B:330:ASN:HA	1:B:1147:MET:HE1	1.87	0.57
1:B:413:THR:HG23	1:B:420:CYS:HB3	1.85	0.57
1:B:825:MET:HE3	1:B:909:TYR:HE1	1.70	0.57
2:K:1011:LEU:HD23	2:K:1014:LYS:HZ3	1.70	0.57
4:U:302:PHE:HB3	4:U:387:ILE:HG13	1.87	0.57
4:U:432:LEU:O	4:U:646:ARG:NH1	2.38	0.57
1:c:949:LEU:HD13	1:c:952:ILE:HD12	1.85	0.57
1:1:6:ARG:NH1	1:a:317:ASP:O	2.38	0.57
1:1:7:LYS:NZ	1:a:251:ASP:OD1	2.38	0.57
1:5:11:LYS:HZ2	1:5:11:LYS:HB3	1.69	0.57
1:A:336:LYS:NZ	1:A:345:SER:O	2.38	0.57
1:A:480:GLU:HG3	1:A:493:VAL:HG23	1.87	0.57
1:B:765:ARG:NH1	1:B:800:LEU:O	2.37	0.57
1:E:268:ILE:HG12	1:E:304:ILE:HG22	1.86	0.57
1:E:749:ASN:ND2	2:L:152:ALA:O	2.38	0.57
2:J:764:ARG:NH2	2:J:838:GLU:O	2.37	0.57
3:R:1167:VAL:HB	3:R:1171:GLN:HG3	1.85	0.57
1:A:262:LEU:HA	1:A:1259:ARG:HH22	1.69	0.56
1:D:392:ARG:NH1	1:D:452:GLU:OE2	2.38	0.56
2:I:943:ASP:HB3	2:I:948:ARG:H	1.71	0.56
1:3:128:ASN:ND2	1:D:494:THR:O	2.39	0.56
1:5:4:ILE:HD12	1:5:4:ILE:N	2.19	0.56
1:A:211:LEU:HD22	3:R:887:ILE:HG13	1.88	0.56
1:A:526:GLY:HA2	1:A:871:VAL:HG13	1.85	0.56
1:A:1093:MET:HE1	1:A:1101:MET:HB2	1.85	0.56
1:E:260:ALA:HB3	1:E:313:ASN:HB2	1.86	0.56
1:E:1002:GLN:HE21	1:E:1006:GLY:HA2	1.69	0.56
2:H:387:LEU:HD12	2:H:784:ALA:H	1.69	0.56
2:I:578:VAL:HG23	5:I:1301:SAM:C1'	2.34	0.56
1:b:845:THR:OG1	1:b:1002:GLN:NE2	2.37	0.56
1:1:148:LYS:O	1:1:153:ARG:NH1	2.38	0.56
1:5:3:ARG:O	1:5:3:ARG:HG3	2.04	0.56
1:5:148:LYS:O	1:5:153:ARG:NH2	2.37	0.56
1:B:398:ASP:OD2	1:B:401:LYS:NZ	2.38	0.56
1:D:731:ASN:ND2	1:D:735:PRO:O	2.38	0.56
1:E:1163:THR:HG21	1:E:1198:TYR:HB2	1.87	0.56
2:J:182:ASP:HA	2:J:324:ASN:HB2	1.87	0.56
1:A:309:ARG:O	1:A:311:ALA:N	2.39	0.56
1:B:701:ILE:HD12	1:B:704:GLN:HE21	1.70	0.56
1:C:668:ILE:O	1:C:673:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:842:ARG:NH2	2:K:291:TYR:OH	2.38	0.56
1:E:526:GLY:HA2	1:E:871:VAL:HG23	1.86	0.56
2:H:182:ASP:OD1	2:I:91:ARG:NH2	2.38	0.56
3:R:96:ASN:ND2	3:R:261:ALA:O	2.38	0.56
1:d:453:THR:HA	1:d:1254:TYR:HA	1.86	0.56
1:e:261:GLY:HA3	1:e:312:SER:HA	1.86	0.56
1:e:1036:ASN:ND2	1:e:1205:ASN:OD1	2.38	0.56
1:C:858:THR:HG23	1:C:942:GLN:HB2	1.87	0.56
2:K:645:VAL:HG23	2:K:646:THR:HG23	1.87	0.56
3:R:610:VAL:HG21	3:R:644:MET:HG3	1.86	0.56
1:A:1124:GLN:NE2	1:a:182:GLN:OE1	2.38	0.56
1:D:1213:ASN:HB3	1:D:1216:SER:HB3	1.88	0.56
2:H:645:VAL:HG23	2:H:646:THR:HG23	1.87	0.56
2:H:943:ASP:HB3	2:H:948:ARG:H	1.71	0.56
2:I:182:ASP:HA	2:I:324:ASN:HB2	1.87	0.56
2:J:943:ASP:HB3	2:J:948:ARG:H	1.71	0.56
2:K:771:TYR:HB2	2:K:860:CYS:HB2	1.86	0.56
1:A:313:ASN:HD22	1:A:395:PRO:HG2	1.70	0.56
1:B:599:LEU:HA	1:B:832:GLN:HE21	1.69	0.56
2:L:645:VAL:HG23	2:L:646:THR:HG23	1.87	0.56
4:U:10:VAL:HG11	4:U:205:GLY:HA2	1.86	0.56
1:a:355:ARG:NH2	1:a:950:ASP:O	2.39	0.56
1:A:580:LYS:NZ	1:A:628:ASP:OD1	2.39	0.56
1:A:656:MET:O	1:A:671:GLN:NE2	2.38	0.56
1:B:1119:THR:O	1:B:1123:ASN:ND2	2.39	0.56
1:C:669:TYR:OH	1:c:779:GLN:O	2.24	0.56
1:E:838:LEU:HD23	2:L:240:GLN:HE22	1.71	0.56
2:L:518:SER:HB3	5:L:1301:SAM:CB	2.36	0.56
3:R:328:ASP:OD1	3:R:348:ARG:NH2	2.37	0.56
3:R:897:LEU:HD11	3:R:1178:LEU:HG	1.87	0.56
1:c:352:LEU:HD23	1:c:955:LEU:HD13	1.87	0.56
1:e:482:ALA:HA	1:e:723:THR:HG21	1.87	0.56
1:A:373:ASN:HB3	1:A:1259:ARG:HG2	1.87	0.56
1:D:1067:PHE:O	1:D:1138:ARG:NH1	2.37	0.56
2:L:14:SER:OG	2:L:313:GLN:NE2	2.39	0.56
2:L:182:ASP:HA	2:L:324:ASN:HB2	1.87	0.56
3:R:840:ARG:HA	3:R:843:TRP:HD1	1.69	0.56
1:a:670:THR:HG23	1:a:672:SER:H	1.71	0.56
1:b:303:ARG:NH2	1:b:1150:TYR:OH	2.39	0.56
1:b:708:ILE:HD11	1:b:767:ARG:HB3	1.88	0.56
1:b:949:LEU:HD13	1:b:952:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:336:LYS:HE3	1:d:343:THR:HB	1.88	0.56
1:A:518:GLN:OE1	1:A:521:ARG:NH2	2.38	0.56
1:B:280:VAL:HG11	1:B:1188:HIS:HB3	1.88	0.56
1:D:619:SER:OG	1:D:625:ASN:ND2	2.36	0.56
2:H:14:SER:OG	2:H:313:GLN:NE2	2.39	0.55
2:K:14:SER:OG	2:K:313:GLN:NE2	2.39	0.55
3:R:285:MET:HG2	3:R:365:ILE:HD11	1.88	0.55
1:c:264:THR:HB	1:c:454:SER:HA	1.89	0.55
1:c:527:ASN:ND2	1:c:864:LEU:O	2.39	0.55
1:d:601:ASN:ND2	1:d:833:VAL:O	2.39	0.55
1:1:86:ASN:HD21	1:1:151:SER:H	1.53	0.55
1:5:128:ASN:ND2	1:A:494:THR:O	2.38	0.55
1:A:708:ILE:HD11	1:A:767:ARG:HB3	1.86	0.55
2:L:943:ASP:HB3	2:L:948:ARG:H	1.70	0.55
1:e:699:ALA:HB1	1:e:702:LEU:HB2	1.88	0.55
1:2:150:MET:HE1	1:C:379:SER:HA	1.89	0.55
1:3:67:GLU:OE2	1:c:246:GLN:NE2	2.39	0.55
2:J:14:SER:OG	2:J:313:GLN:NE2	2.39	0.55
1:a:694:ILE:O	1:a:703:ARG:NH1	2.39	0.55
1:d:352:LEU:HD12	1:d:955:LEU:HB3	1.87	0.55
1:B:278:GLN:HE21	1:B:281:LEU:HB3	1.72	0.55
1:C:622:SER:OG	1:C:623:LEU:N	2.39	0.55
1:D:776:VAL:HG21	1:D:793:MET:HG2	1.88	0.55
2:L:578:VAL:HG23	5:L:1301:SAM:C8	2.36	0.55
1:b:1080:ASP:OD1	1:b:1082:ARG:NH1	2.40	0.55
1:d:1057:SER:HB3	1:d:1223:PRO:HB3	1.88	0.55
2:H:90:LEU:O	2:H:94:LYS:HB2	2.07	0.55
2:J:552:TYR:CE1	2:K:782:VAL:HG11	2.41	0.55
1:1:161:ILE:HD11	1:B:410:ARG:HH22	1.72	0.55
1:C:603:VAL:HG23	1:C:604:VAL:HG23	1.89	0.55
1:D:607:VAL:HG11	1:d:787:GLN:HE22	1.71	0.55
2:H:182:ASP:HA	2:H:324:ASN:HB2	1.87	0.55
2:J:90:LEU:O	2:J:94:LYS:HB2	2.07	0.55
3:R:90:ASP:HB3	3:R:268:TRP:HE1	1.72	0.55
1:a:723:THR:OG1	1:a:725:ASN:OD1	2.20	0.55
1:a:1228:PRO:HB2	1:a:1231:ARG:HD3	1.87	0.55
1:d:634:LEU:HD21	1:d:886:LEU:HD22	1.87	0.55
1:e:186:CYS:SG	1:e:199:HIS:NE2	2.65	0.55
1:e:544:GLN:HG2	1:e:592:ARG:HG3	1.88	0.55
1:1:76:ASN:HD22	1:a:528:ASN:HD22	1.55	0.55
1:A:438:GLN:NE2	1:A:440:MET:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ASN:ND2	3:R:608:GLU:OE1	2.40	0.55
1:E:262:LEU:HA	1:E:1259:ARG:HH22	1.72	0.55
2:H:147:LEU:HD21	2:H:162:GLU:HA	1.89	0.55
2:H:290:GLN:NE2	2:H:348:GLU:OE2	2.40	0.55
2:J:147:LEU:HD21	2:J:162:GLU:HA	1.89	0.55
2:K:90:LEU:O	2:K:94:LYS:HB2	2.07	0.55
2:K:559:ILE:HG13	2:L:396:TRP:HD1	1.70	0.55
2:K:943:ASP:HB3	2:K:948:ARG:H	1.71	0.55
3:R:900:TYR:OH	3:R:1059:VAL:O	2.25	0.55
1:4:109:GLN:OE1	1:d:537:GLN:NE2	2.40	0.55
1:B:309:ARG:NH1	1:B:368:ASP:OD1	2.40	0.55
1:B:852:GLN:HE21	1:b:755:LEU:HD11	1.71	0.55
1:C:1096:ASP:HB3	1:C:1100:MET:H	1.72	0.55
2:H:578:VAL:HG23	5:H:1301:SAM:H8	1.83	0.55
2:I:645:VAL:HG23	2:I:646:THR:HG23	1.87	0.55
2:J:290:GLN:NE2	2:J:348:GLU:OE2	2.40	0.55
4:U:60:ILE:HD12	4:U:234:PHE:HD1	1.70	0.55
1:a:1049:ARG:NH2	1:a:1132:THR:O	2.40	0.55
1:c:1079:ARG:HA	1:c:1114:LEU:HD21	1.89	0.55
1:d:262:LEU:HD21	1:d:406:MET:HG2	1.89	0.55
1:d:473:ASN:HA	1:d:506:PRO:HA	1.89	0.55
2:I:290:GLN:NE2	2:I:348:GLU:OE2	2.40	0.55
2:I:578:VAL:HG23	5:I:1301:SAM:N9	2.21	0.55
2:K:182:ASP:HA	2:K:324:ASN:HB2	1.87	0.55
2:K:290:GLN:NE2	2:K:348:GLU:OE2	2.40	0.55
4:U:305:VAL:HG12	4:U:314:VAL:HA	1.88	0.55
1:b:1232:TYR:HE1	1:b:1253:LEU:HB2	1.71	0.55
1:4:61:SER:O	1:d:545:ARG:NH1	2.38	0.55
1:D:373:ASN:ND2	1:D:1258:THR:O	2.40	0.55
2:L:602:CYS:O	2:L:606:THR:OG1	2.25	0.55
1:d:629:PHE:HB2	1:d:655:MET:HE1	1.89	0.55
1:e:316:PHE:C	1:e:316:PHE:CD1	2.85	0.55
1:5:7:LYS:H	1:5:7:LYS:CD	2.14	0.54
1:C:791:SER:HA	1:C:794:ARG:HE	1.72	0.54
2:J:562:LEU:N	5:J:1301:SAM:N1	2.39	0.54
2:K:578:VAL:HA	5:K:1301:SAM:H5'1	1.83	0.54
1:e:427:VAL:HG21	1:e:430:ARG:HE	1.72	0.54
1:B:656:MET:O	1:B:671:GLN:NE2	2.40	0.54
1:B:841:ASP:OD2	1:B:1003:GLN:NE2	2.41	0.54
1:a:259:ASP:OD2	1:a:462:ARG:NH1	2.40	0.54
1:4:130:ALA:HB3	1:E:496:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:87:THR:OG1	1:5:146:ASN:OD1	2.25	0.54
1:A:1033:HIS:HD1	1:A:1249:GLU:HA	1.72	0.54
1:A:1112:LEU:HD22	1:A:1141:MET:HG3	1.90	0.54
1:C:731:ASN:ND2	1:C:735:PRO:O	2.40	0.54
2:J:645:VAL:HG23	2:J:646:THR:HG23	1.87	0.54
2:L:90:LEU:O	2:L:94:LYS:HB2	2.07	0.54
2:L:290:GLN:NE2	2:L:348:GLU:OE2	2.40	0.54
2:L:724:ARG:HG2	2:L:774:LEU:HD23	1.90	0.54
1:c:776:VAL:HG21	1:c:793:MET:HG2	1.90	0.54
1:d:841:ASP:HA	1:d:1004:TYR:HB3	1.88	0.54
2:H:577:ASP:CG	5:H:1301:SAM:HN2	2.11	0.54
1:d:1036:ASN:ND2	1:d:1205:ASN:O	2.40	0.54
1:e:321:SER:OG	1:e:368:ASP:CG	2.51	0.54
1:e:1231:ARG:NH1	1:e:1251:VAL:O	2.40	0.54
1:A:296:PHE:HB2	1:A:419:ILE:HD12	1.89	0.54
1:A:398:ASP:OD2	1:A:401:LYS:NZ	2.39	0.54
1:E:1033:HIS:O	1:E:1207:ARG:NH1	2.41	0.54
1:a:732:LEU:HD13	1:a:999:ILE:HG21	1.90	0.54
1:d:681:PRO:HG2	1:d:845:THR:HG22	1.90	0.54
1:e:308:THR:HG1	1:e:321:SER:HB3	1.66	0.54
1:e:500:SER:O	1:e:503:ARG:NH1	2.40	0.54
1:2:146:ASN:ND2	1:2:148:LYS:O	2.41	0.54
1:D:711:ARG:HH22	1:D:767:ARG:HG2	1.73	0.54
1:E:970:ASN:HD22	1:E:988:LEU:HD11	1.73	0.54
2:K:147:LEU:HD21	2:K:162:GLU:HA	1.89	0.54
2:L:497:ILE:HG22	2:L:504:GLU:HA	1.90	0.54
3:R:876:PRO:HG3	3:R:890:TRP:HB3	1.90	0.54
1:c:851:ARG:NH1	1:c:991:ASP:O	2.40	0.54
1:d:234:GLN:HE21	1:d:911:ASP:HA	1.73	0.54
1:d:350:ASN:HD22	1:d:353:MET:HG2	1.71	0.54
1:2:82:ASP:OD1	1:2:86:ASN:N	2.38	0.54
1:4:133:LEU:HD11	1:E:443:ALA:HB2	1.89	0.54
1:D:278:GLN:HE21	1:D:281:LEU:HB3	1.72	0.54
1:E:620:VAL:HG21	1:E:656:MET:HE2	1.90	0.54
1:E:1034:GLU:OE2	1:E:1207:ARG:NH2	2.41	0.54
2:I:14:SER:OG	2:I:313:GLN:NE2	2.39	0.54
2:I:90:LEU:O	2:I:94:LYS:HB2	2.07	0.54
1:d:186:CYS:SG	1:d:199:HIS:NE2	2.78	0.54
1:E:479:ILE:HG21	1:E:1267:ILE:HD11	1.90	0.54
1:a:449:ASP:HA	1:a:1258:THR:HA	1.89	0.54
1:d:1018:SER:HB2	1:d:1021:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:234:GLN:HE21	1:e:911:ASP:HA	1.72	0.54
1:A:478:GLU:OE1	1:A:508:ARG:NH2	2.41	0.54
1:A:543:LEU:HA	1:A:546:ILE:HG22	1.89	0.54
2:H:497:ILE:HG22	2:H:504:GLU:HA	1.90	0.54
2:I:147:LEU:HD21	2:I:162:GLU:HA	1.89	0.54
2:J:476:ARG:NH1	2:J:477:LYS:O	2.41	0.54
2:J:602:CYS:O	2:J:606:THR:OG1	2.25	0.54
1:c:200:VAL:HG22	1:c:205:LEU:HB2	1.89	0.54
1:e:417:SER:HG	1:e:420:CYS:HG	1.55	0.54
1:B:526:GLY:HA2	1:B:871:VAL:HG13	1.91	0.53
2:H:476:ARG:NH1	2:H:477:LYS:O	2.41	0.53
2:I:45:PRO:HB2	2:I:54:ILE:HD12	1.90	0.53
2:I:578:VAL:HG23	5:I:1301:SAM:C8	2.36	0.53
2:K:45:PRO:HB2	2:K:54:ILE:HD12	1.90	0.53
2:L:147:LEU:HD21	2:L:162:GLU:HA	1.89	0.53
3:R:54:ASP:O	3:R:251:ARG:NH1	2.42	0.53
4:U:444:ASP:HB3	4:U:447:GLU:HG3	1.90	0.53
1:e:1056:TRP:HE1	1:e:1200:ILE:HD11	1.73	0.53
1:B:1033:HIS:O	1:B:1207:ARG:NH1	2.41	0.53
2:H:45:PRO:HB2	2:H:54:ILE:HD12	1.90	0.53
2:K:724:ARG:HG2	2:K:774:LEU:HD23	1.90	0.53
2:L:267:ASN:O	2:L:313:GLN:NE2	2.42	0.53
3:R:461:GLY:O	3:R:493:GLN:NE2	2.38	0.53
1:l:130:ALA:HB3	1:B:496:PRO:HG3	1.91	0.53
1:B:520:ILE:HA	1:B:523:MET:HE2	1.91	0.53
2:I:580:GLN:HE22	2:I:617:ASN:H	1.57	0.53
2:I:602:CYS:O	2:I:606:THR:OG1	2.26	0.53
2:L:45:PRO:HB2	2:L:54:ILE:HD12	1.90	0.53
1:a:309:ARG:O	1:a:311:ALA:N	2.42	0.53
1:d:260:ALA:HB3	1:d:313:ASN:HB2	1.90	0.53
1:B:983:LEU:N	1:B:985:GLU:OE1	2.41	0.53
1:C:682:HIS:ND1	1:c:778:ASN:OD1	2.41	0.53
2:H:580:GLN:HE22	2:H:617:ASN:H	1.56	0.53
2:H:1011:LEU:HD23	2:H:1014:LYS:HZ3	1.71	0.53
2:J:497:ILE:HG22	2:J:504:GLU:HA	1.90	0.53
2:K:267:ASN:O	2:K:313:GLN:NE2	2.42	0.53
4:U:611:PRO:HA	4:U:614:THR:HG22	1.90	0.53
1:e:1241:PRO:HD2	1:e:1244:GLN:HG2	1.91	0.53
1:B:300:ALA:HA	1:B:1213:ASN:HA	1.89	0.53
1:B:546:ILE:HD11	1:B:908:MET:HE1	1.90	0.53
1:C:1078:GLY:H	1:C:1097:GLU:HB2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:ASN:O	2:H:313:GLN:NE2	2.42	0.53
2:H:602:CYS:O	2:H:606:THR:OG1	2.25	0.53
2:I:578:VAL:HG21	5:I:1301:SAM:C5	2.39	0.53
2:K:580:GLN:HE22	2:K:617:ASN:H	1.57	0.53
2:K:602:CYS:O	2:K:606:THR:OG1	2.25	0.53
3:R:117:GLU:OE1	3:R:121:ASN:ND2	2.41	0.53
1:d:534:PRO:O	1:d:538:ASP:HB2	2.08	0.53
1:C:527:ASN:HD21	1:c:795:GLY:HA3	1.74	0.53
1:E:438:GLN:NE2	1:E:440:MET:O	2.40	0.53
2:H:724:ARG:HG2	2:H:774:LEU:HD23	1.90	0.53
2:I:476:ARG:NH1	2:I:477:LYS:O	2.41	0.53
2:K:476:ARG:NH1	2:K:477:LYS:O	2.41	0.53
2:L:476:ARG:NH1	2:L:477:LYS:O	2.41	0.53
4:U:98:VAL:HG23	4:U:99:ASP:H	1.72	0.53
1:a:426:CYS:HB2	1:a:1235:LEU:HB3	1.90	0.53
1:a:508:ARG:HH12	1:a:726:VAL:HG12	1.73	0.53
1:e:333:HIS:HA	1:e:336:LYS:HG2	1.90	0.53
1:2:141:ASN:HD22	1:b:963:ALA:HB2	1.74	0.53
1:B:946:ASP:OD1	1:B:946:ASP:N	2.42	0.53
1:C:268:ILE:HG13	1:C:304:ILE:HG22	1.91	0.53
1:C:838:LEU:HD23	2:J:240:GLN:HE22	1.74	0.53
1:E:583:PRO:HA	1:E:884:VAL:HG11	1.89	0.53
1:E:765:ARG:O	1:E:768:VAL:HG12	2.09	0.53
1:2:127:ILE:HD11	1:b:874:PRO:HB3	1.91	0.53
1:5:9:LYS:HD3	1:5:9:LYS:N	2.23	0.53
1:A:287:THR:OG1	1:A:298:GLU:OE2	2.27	0.53
1:A:355:ARG:NH2	1:A:952:ILE:O	2.40	0.53
1:C:521:ARG:HH12	1:C:829:PRO:HD2	1.73	0.53
1:C:649:PHE:HD1	1:C:705:TRP:HD1	1.55	0.53
2:J:45:PRO:HB2	2:J:54:ILE:HD12	1.90	0.53
3:R:478:PRO:O	3:R:496:GLN:NE2	2.41	0.53
3:R:936:CYS:SG	3:R:937:PHE:N	2.81	0.53
1:e:1110:PHE:HB2	1:e:1139:ILE:HG12	1.91	0.53
1:C:413:THR:HG23	1:C:420:CYS:HB3	1.90	0.53
2:I:724:ARG:HG2	2:I:774:LEU:HD23	1.90	0.53
1:a:338:LEU:HD23	1:a:339:LEU:H	1.74	0.53
1:c:514:ARG:HH21	1:c:729:SER:HA	1.73	0.53
1:A:582:ARG:HD3	1:A:583:PRO:HD2	1.89	0.52
1:A:715:ASN:OD1	1:A:837:ARG:NH1	2.40	0.52
2:H:888:CYS:SG	2:H:891:SER:OG	2.67	0.52
2:J:580:GLN:NE2	2:J:618:PHE:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:851:ILE:HG13	2:L:852:ARG:HD3	1.91	0.52
4:U:672:GLN:NE2	4:U:682:SER:OG	2.42	0.52
1:c:433:ARG:HA	1:c:450:VAL:HG12	1.91	0.52
1:e:979:LEU:HD22	1:e:983:LEU:HD22	1.89	0.52
1:A:892:PRO:HD2	1:A:895:LEU:HD13	1.90	0.52
1:B:493:VAL:HA	1:B:1273:GLY:HA2	1.90	0.52
2:J:724:ARG:HG2	2:J:774:LEU:HD23	1.90	0.52
2:K:497:ILE:HG22	2:K:504:GLU:HA	1.90	0.52
2:K:578:VAL:HG23	5:K:1301:SAM:C8	2.22	0.52
2:K:851:ILE:HG13	2:K:852:ARG:HD3	1.91	0.52
3:R:535:GLN:HA	3:R:538:VAL:HG12	1.90	0.52
4:U:472:SER:OG	4:U:474:ASP:OD1	2.26	0.52
1:C:505:MET:HE1	1:C:1270:VAL:HG21	1.90	0.52
1:D:455:ASP:HB3	1:D:458:THR:HG22	1.91	0.52
1:D:673:ARG:HH12	1:d:783:PRO:HB2	1.74	0.52
3:R:614:SER:HA	3:R:617:LYS:HE3	1.91	0.52
1:c:426:CYS:SG	1:c:427:VAL:N	2.82	0.52
1:4:125:THR:HG22	1:d:876:ALA:HB2	1.90	0.52
2:I:497:ILE:HG22	2:I:504:GLU:HA	1.90	0.52
3:R:373:SER:O	3:R:522:GLN:NE2	2.41	0.52
3:R:687:THR:O	3:R:691:HIS:ND1	2.35	0.52
1:b:690:ASN:HB3	1:b:693:LEU:HD13	1.90	0.52
1:d:699:ALA:HB1	1:d:702:LEU:HB2	1.91	0.52
1:4:75:ASN:ND2	1:d:981:ASP:O	2.42	0.52
2:J:182:ASP:OD1	2:K:91:ARG:NH2	2.42	0.52
4:U:481:LEU:HA	4:U:487:PRO:HA	1.90	0.52
1:a:254:ARG:O	1:a:318:ARG:NH2	2.40	0.52
1:c:333:HIS:HA	1:c:336:LYS:HG2	1.90	0.52
1:e:1185:SER:HA	1:e:1222:GLY:HA3	1.91	0.52
1:A:527:ASN:HD21	1:a:795:GLY:HA3	1.75	0.52
2:H:153:LEU:HD22	2:H:155:GLN:HE22	1.75	0.52
2:K:482:SER:HB2	5:K:1301:SAM:O	2.09	0.52
3:R:1132:ARG:NH2	3:R:1163:MET:O	2.42	0.52
1:c:500:SER:O	1:c:503:ARG:NH1	2.42	0.52
1:3:6:ARG:NH2	1:c:975:THR:O	2.42	0.52
1:B:704:GLN:HE22	1:B:774:ASN:HD22	1.57	0.52
1:E:335:PHE:O	1:E:357:ASN:ND2	2.43	0.52
2:J:888:CYS:SG	2:J:891:SER:OG	2.67	0.52
2:L:821:ASP:OD1	2:L:843:THR:OG1	2.28	0.52
1:b:954:SER:OG	1:b:955:LEU:N	2.42	0.52
1:c:480:GLU:HG2	1:c:493:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:1232:TYR:HE1	1:c:1253:LEU:HB2	1.75	0.52
1:d:1036:ASN:ND2	1:d:1205:ASN:OD1	2.42	0.52
1:e:845:THR:OG1	1:e:1002:GLN:NE2	2.43	0.52
1:2:132:GLU:HG2	1:b:527:ASN:HD21	1.75	0.52
1:D:480:GLU:HG3	1:D:493:VAL:HG23	1.92	0.52
1:D:1204:TYR:CZ	1:D:1206:ASP:HB2	2.45	0.52
2:K:888:CYS:SG	2:K:891:SER:OG	2.67	0.52
2:L:580:GLN:HE22	2:L:617:ASN:H	1.57	0.52
4:U:530:ALA:HB1	4:U:579:TYR:HD2	1.75	0.52
1:b:417:SER:H	1:b:420:CYS:HB2	1.75	0.52
1:b:718:GLN:HB2	1:b:738:VAL:HB	1.90	0.52
1:c:351:PRO:HD3	1:c:1175:ILE:HG12	1.91	0.52
1:d:492:THR:HG23	1:d:1272:MET:HB3	1.91	0.52
1:5:11:LYS:NZ	1:5:11:LYS:CB	2.73	0.52
2:J:851:ILE:HG13	2:J:852:ARG:HD3	1.91	0.52
2:K:153:LEU:HD22	2:K:155:GLN:HE22	1.75	0.52
2:K:583:ASP:HB2	5:K:1301:SAM:N7	2.25	0.52
2:L:153:LEU:HD22	2:L:155:GLN:HE22	1.75	0.52
2:L:888:CYS:SG	2:L:891:SER:OG	2.67	0.52
3:R:491:ILE:HD12	3:R:1020:ALA:HB2	1.90	0.52
1:c:418:LYS:NZ	1:c:1212:THR:O	2.40	0.52
1:B:190:LEU:HD12	1:B:196:LEU:HD23	1.92	0.52
1:B:418:LYS:NZ	1:B:1212:THR:OG1	2.43	0.52
2:I:267:ASN:O	2:I:313:GLN:NE2	2.42	0.52
3:R:659:PHE:HE2	3:R:681:PRO:HD3	1.75	0.52
4:U:427:ASP:O	4:U:435:LYS:NZ	2.38	0.52
4:U:692:LEU:HD12	4:U:693:PRO:HD2	1.91	0.52
1:a:1078:GLY:H	1:a:1097:GLU:HB3	1.73	0.52
1:e:732:LEU:HD13	1:e:999:ILE:HG21	1.91	0.52
1:D:1059:LEU:HD12	1:D:1205:ASN:HB2	1.92	0.51
1:E:963:ALA:HA	1:E:992:PRO:HG2	1.91	0.51
2:I:153:LEU:HD22	2:I:155:GLN:HE22	1.75	0.51
2:J:821:ASP:OD1	2:J:843:THR:OG1	2.28	0.51
2:L:552:TYR:CE1	5:L:1301:SAM:C4	2.93	0.51
3:R:279:GLN:O	3:R:327:ASN:ND2	2.42	0.51
4:U:548:ILE:HG23	4:U:550:TYR:H	1.76	0.51
1:a:351:PRO:HD3	1:a:1175:ILE:HG12	1.91	0.51
1:a:471:ARG:NH1	1:a:508:ARG:O	2.42	0.51
1:c:1059:LEU:HB3	1:c:1205:ASN:HB3	1.92	0.51
1:d:383:THR:HG22	1:d:385:PHE:H	1.76	0.51
1:A:852:GLN:HA	1:A:995:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:HIS:ND1	1:A:1248:PRO:O	2.41	0.51
1:B:993:ARG:HH22	1:b:753:PRO:HA	1.75	0.51
1:C:392:ARG:NH2	1:C:452:GLU:OE1	2.44	0.51
2:H:821:ASP:OD1	2:H:843:THR:OG1	2.28	0.51
2:H:851:ILE:HG13	2:H:852:ARG:HD3	1.91	0.51
3:R:295:PRO:HB3	3:R:310:TYR:HE1	1.75	0.51
1:d:493:VAL:HG12	1:d:1271:VAL:HA	1.92	0.51
1:e:1124:GLN:OE1	1:e:1125:GLN:NE2	2.43	0.51
1:1:95:HIS:NE2	1:1:130:ALA:O	2.44	0.51
1:D:1229:VAL:HB	1:D:1236:THR:HG21	1.93	0.51
1:E:455:ASP:HB3	1:E:458:THR:HG22	1.93	0.51
2:I:821:ASP:OD1	2:I:843:THR:OG1	2.28	0.51
2:K:482:SER:OG	5:K:1301:SAM:O	2.27	0.51
2:K:821:ASP:OD1	2:K:843:THR:OG1	2.28	0.51
2:L:552:TYR:CZ	5:L:1301:SAM:C5	2.93	0.51
2:L:834:ALA:HB1	2:L:836:ILE:HG22	1.93	0.51
3:R:96:ASN:HB3	3:R:225:ALA:HB3	1.91	0.51
1:c:850:THR:HG22	1:c:852:GLN:H	1.74	0.51
1:c:1237:ASN:HB3	1:c:1240:ALA:HB2	1.91	0.51
1:d:544:GLN:HA	1:d:592:ARG:HE	1.75	0.51
1:5:11:LYS:NZ	1:5:11:LYS:CA	2.73	0.51
1:A:755:LEU:HA	1:A:809:MET:HE1	1.92	0.51
2:K:182:ASP:OD2	2:L:95:TYR:OH	2.28	0.51
2:K:834:ALA:HB1	2:K:836:ILE:HG22	1.93	0.51
4:U:620:TRP:HB2	4:U:640:ILE:HB	1.91	0.51
1:a:341:THR:OG1	1:a:342:GLU:OE1	2.29	0.51
1:a:453:THR:HA	1:a:1254:TYR:HA	1.92	0.51
1:3:4:ILE:HG21	1:c:254:ARG:HH22	1.76	0.51
2:H:514:TYR:OH	5:H:1301:SAM:N	2.44	0.51
2:J:267:ASN:O	2:J:313:GLN:NE2	2.42	0.51
3:R:71:SER:O	3:R:86:TYR:OH	2.29	0.51
4:U:74:TYR:OH	4:U:162:ILE:O	2.27	0.51
4:U:441:HIS:HB2	4:U:524:LEU:HG	1.92	0.51
1:b:192:SER:HB3	1:b:195:ASP:HB2	1.93	0.51
1:B:469:LEU:HD21	1:B:504:LEU:HD21	1.93	0.51
1:C:974:LYS:NZ	1:C:985:GLU:OE2	2.36	0.51
1:E:970:ASN:ND2	1:E:985:GLU:OE2	2.44	0.51
2:K:482:SER:HG	5:K:1301:SAM:C	2.16	0.51
2:K:560:VAL:HG22	2:L:397:LEU:HB2	1.92	0.51
4:U:101:ARG:HE	4:U:121:LEU:HD21	1.76	0.51
1:a:1109:ILE:HG22	1:a:1138:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:929:GLN:HB2	1:c:1015:MET:HE2	1.92	0.51
1:A:188:ALA:HB2	1:B:544:GLN:HE22	1.75	0.51
1:A:570:THR:OG1	1:B:565:GLU:OE2	2.21	0.51
1:B:1171:THR:HG22	1:B:1173:THR:H	1.76	0.51
2:H:854:THR:HA	2:L:567:PRO:HG3	1.92	0.51
3:R:184:ASN:HB2	3:R:186:PRO:HD2	1.93	0.51
3:R:595:TRP:HA	3:R:599:LEU:HB2	1.91	0.51
1:e:1002:GLN:HB3	1:e:1008:THR:HG22	1.93	0.51
1:A:468:ARG:HB2	1:A:1019:VAL:HG11	1.93	0.51
1:A:569:GLN:NE2	1:A:786:THR:OG1	2.43	0.51
1:A:584:SER:O	1:A:586:SER:N	2.38	0.51
1:B:963:ALA:HA	1:B:992:PRO:HG2	1.92	0.51
1:C:821:VAL:O	1:C:909:TYR:OH	2.29	0.51
2:I:518:SER:H	5:I:1301:SAM:C	2.23	0.51
2:I:851:ILE:HG13	2:I:852:ARG:HD3	1.91	0.51
2:J:702:SER:OG	2:J:758:ARG:NH2	2.44	0.51
3:R:941:LYS:HB2	3:R:944:GLN:HB2	1.92	0.51
1:c:718:GLN:HB3	1:c:740:LEU:HD23	1.91	0.51
1:d:422:PHE:HB2	1:d:1227:ILE:HG21	1.93	0.51
1:d:1033:HIS:O	1:d:1207:ARG:NH1	2.43	0.51
1:B:416:VAL:HG21	1:a:1084:SER:HB3	1.92	0.51
2:I:442:ASN:HB3	2:I:445:HIS:HB2	1.93	0.51
2:J:153:LEU:HD22	2:J:155:GLN:HE22	1.75	0.51
2:J:834:ALA:HB1	2:J:836:ILE:HG22	1.93	0.51
2:K:562:LEU:HG	5:K:1301:SAM:C2	2.36	0.51
2:K:902:THR:HG23	2:K:905:ALA:H	1.76	0.51
3:R:162:GLU:OE1	3:R:837:ARG:NH2	2.44	0.51
3:R:692:THR:HG22	3:R:732:GLN:HA	1.93	0.51
1:d:941:THR:HG22	1:d:943:TYR:H	1.75	0.51
2:H:702:SER:OG	2:H:758:ARG:NH2	2.44	0.51
2:K:474:LEU:HD21	2:L:274:GLN:HE21	1.76	0.51
3:R:900:TYR:HE1	3:R:1057:LEU:HA	1.75	0.51
1:A:896:VAL:HG11	1:e:619:SER:HB3	1.93	0.50
1:B:480:GLU:HG3	1:B:493:VAL:HG23	1.93	0.50
1:B:1147:MET:HB3	1:B:1179:PRO:HA	1.92	0.50
1:C:715:ASN:OD1	1:C:837:ARG:NH1	2.44	0.50
1:D:1002:GLN:HE21	1:D:1006:GLY:HA2	1.76	0.50
2:J:570:ASP:HB3	2:J:607:ALA:HB2	1.93	0.50
3:R:707:GLY:HA3	3:R:720:MET:HE3	1.93	0.50
4:U:296:ASP:HA	4:U:395:THR:HG22	1.93	0.50
1:b:468:ARG:HB2	1:b:1019:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:606:THR:HG1	1:c:640:THR:H	1.59	0.50
1:d:363:LEU:O	1:d:367:LEU:HB2	2.12	0.50
1:4:3:ARG:NH1	1:d:314:VAL:O	2.44	0.50
1:A:466:MET:HG2	1:A:1260:TYR:HE2	1.74	0.50
1:D:336:LYS:NZ	1:D:345:SER:O	2.44	0.50
1:E:328:THR:OG1	1:E:329:GLU:OE1	2.28	0.50
1:a:369:ASN:HD21	1:a:458:THR:HA	1.76	0.50
1:d:870:THR:OG1	1:d:871:VAL:N	2.44	0.50
1:A:681:PRO:O	1:A:840:ARG:NH1	2.44	0.50
1:A:719:ILE:HG22	1:A:739:LEU:HB3	1.93	0.50
1:A:1166:TRP:CD1	1:A:1176:PRO:HG2	2.46	0.50
1:D:333:HIS:HA	1:D:336:LYS:HG2	1.92	0.50
1:D:476:PRO:HG2	1:D:503:ARG:HH21	1.77	0.50
1:D:1171:THR:HG22	1:D:1173:THR:H	1.76	0.50
2:J:902:THR:HG23	2:J:905:ALA:H	1.76	0.50
3:R:646:ASN:O	3:R:650:HIS:ND1	2.35	0.50
3:R:680:PHE:HE2	3:R:687:THR:HA	1.76	0.50
1:e:1074:VAL:HG22	1:e:1107:ASN:HB2	1.93	0.50
1:2:86:ASN:OD1	1:2:150:MET:N	2.44	0.50
1:C:351:PRO:HG3	1:C:1116:GLN:HE22	1.76	0.50
1:E:552:ASP:HB2	1:E:890:LYS:HB3	1.93	0.50
2:I:570:ASP:HB3	2:I:607:ALA:HB2	1.93	0.50
2:I:902:THR:HG23	2:I:905:ALA:H	1.76	0.50
2:K:570:ASP:HB3	2:K:607:ALA:HB2	1.93	0.50
2:L:702:SER:OG	2:L:758:ARG:NH2	2.44	0.50
3:R:322:ARG:NH1	3:R:776:ASP:O	2.44	0.50
1:d:929:GLN:HG3	1:d:1015:MET:HE2	1.93	0.50
1:A:1216:SER:OG	1:A:1218:GLN:O	2.29	0.50
1:B:860:PRO:O	1:B:864:LEU:HB2	2.12	0.50
1:D:399:ALA:HA	1:D:402:TRP:CD1	2.44	0.50
1:E:341:THR:HG23	1:E:342:GLU:HG2	1.94	0.50
2:H:150:GLY:HA2	1:e:698:ASP:HB3	1.93	0.50
2:I:702:SER:OG	2:I:758:ARG:NH2	2.44	0.50
2:L:570:ASP:HB3	2:L:607:ALA:HB2	1.93	0.50
3:R:1081:ILE:HB	3:R:1089:PHE:HB2	1.93	0.50
1:b:1233:ASN:ND2	1:b:1244:GLN:OE1	2.44	0.50
1:C:746:GLN:OE1	1:C:812:GLN:NE2	2.45	0.50
2:I:834:ALA:HB1	2:I:836:ILE:HG22	1.93	0.50
3:R:198:SER:OG	3:R:204:ARG:NH1	2.44	0.50
4:U:63:LEU:HD13	4:U:162:ILE:HD12	1.93	0.50
1:d:863:SER:OG	1:d:864:LEU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ILE:HA	1:A:908:MET:HE3	1.94	0.50
1:C:807:THR:HG21	1:C:886:LEU:HA	1.94	0.50
2:I:908:GLN:OE1	2:I:912:ARG:NH2	2.45	0.50
1:b:469:LEU:HD21	1:b:504:LEU:HD21	1.92	0.50
1:c:355:ARG:NH2	1:c:952:ILE:O	2.44	0.50
1:e:225:SER:OG	1:e:226:SER:N	2.43	0.50
1:e:776:VAL:HG12	1:e:790:VAL:HG23	1.93	0.50
1:B:507:TYR:HE2	1:B:1267:ILE:HD11	1.77	0.50
1:B:1163:THR:HG21	1:B:1198:TYR:HB2	1.94	0.50
1:D:441:ASN:HD21	1:c:851:ARG:HH21	1.60	0.50
2:K:430:TRP:HZ3	2:K:1001:LEU:HD22	1.77	0.50
2:K:908:GLN:OE1	2:K:912:ARG:NH2	2.45	0.50
2:L:902:THR:HG23	2:L:905:ALA:H	1.76	0.50
3:R:1109:THR:O	3:R:1171:GLN:NE2	2.34	0.50
1:b:948:TYR:HE2	1:b:1025:GLN:HB3	1.76	0.50
1:d:920:ARG:NH2	1:d:982:MET:O	2.45	0.50
1:5:11:LYS:HD3	1:e:320:SER:C	2.34	0.50
1:B:731:ASN:ND2	1:B:735:PRO:O	2.43	0.50
1:E:375:HIS:HA	1:E:392:ARG:HH21	1.77	0.50
1:E:580:LYS:O	1:E:582:ARG:NH1	2.45	0.50
2:H:578:VAL:CG2	5:H:1301:SAM:C1'	2.83	0.50
2:L:442:ASN:HB3	2:L:445:HIS:HB2	1.93	0.50
2:L:908:GLN:OE1	2:L:912:ARG:NH2	2.45	0.50
1:c:1141:MET:N	1:c:1141:MET:SD	2.85	0.50
1:3:59:ILE:O	1:3:63:GLN:HB2	2.11	0.49
1:B:745:HIS:ND1	1:B:812:GLN:O	2.44	0.49
1:E:731:ASN:ND2	1:E:734:THR:OG1	2.44	0.49
1:E:1166:TRP:CD1	1:E:1176:PRO:HG2	2.47	0.49
2:J:442:ASN:HB3	2:J:445:HIS:HB2	1.93	0.49
1:a:373:ASN:HB3	1:a:1259:ARG:HD3	1.93	0.49
1:a:430:ARG:NH1	1:a:1234:ILE:O	2.44	0.49
1:e:483:LEU:HB2	1:e:493:VAL:HG11	1.94	0.49
1:e:1081:CYS:HB2	1:e:1094:ILE:HD11	1.93	0.49
1:1:122:TYR:HE2	1:a:533:GLN:HB3	1.76	0.49
1:C:420:CYS:HA	1:C:423:VAL:HG12	1.93	0.49
1:C:610:ASP:OD1	1:C:674:ARG:NH2	2.46	0.49
2:H:902:THR:HG23	2:H:905:ALA:H	1.76	0.49
2:K:587:ASP:HB3	2:K:590:ILE:HG22	1.94	0.49
3:R:509:ILE:HG22	3:R:534:PRO:HB2	1.92	0.49
3:R:943:TYR:HB3	3:R:1046:TYR:HD2	1.77	0.49
1:d:430:ARG:NH1	1:d:1234:ILE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:SER:OG	1:D:215:GLU:N	2.42	0.49
2:H:834:ALA:HB1	2:H:836:ILE:HG22	1.93	0.49
2:I:888:CYS:SG	2:I:891:SER:OG	2.67	0.49
2:K:847:THR:HG22	2:K:864:ARG:HH12	1.78	0.49
1:a:349:ALA:N	1:a:1174:SER:OG	2.44	0.49
1:a:1107:ASN:HA	1:a:1136:ARG:HB2	1.92	0.49
1:c:493:VAL:HG12	1:c:1271:VAL:HG22	1.93	0.49
1:B:1166:TRP:CD1	1:B:1176:PRO:HG2	2.46	0.49
1:B:1187:ASP:OD1	1:B:1213:ASN:ND2	2.45	0.49
2:H:587:ASP:HB3	2:H:590:ILE:HG22	1.94	0.49
2:J:485:LYS:HE2	2:J:645:VAL:HG22	1.94	0.49
3:R:1132:ARG:HD2	3:R:1162:ILE:HG13	1.94	0.49
1:d:776:VAL:HG21	1:d:793:MET:HG2	1.94	0.49
1:e:373:ASN:HB3	1:e:1259:ARG:HG2	1.93	0.49
1:l:63:GLN:NE2	1:a:911:ASP:OD2	2.44	0.49
1:B:308:THR:OG1	1:B:321:SER:OG	2.30	0.49
1:B:777:ASP:OD1	1:B:794:ARG:NH2	2.46	0.49
2:H:570:ASP:HB3	2:H:607:ALA:HB2	1.93	0.49
2:K:485:LYS:HE2	2:K:645:VAL:HG22	1.94	0.49
2:L:587:ASP:HB3	2:L:590:ILE:HG22	1.95	0.49
3:R:863:LEU:HD22	3:R:1038:LEU:HD22	1.93	0.49
1:5:63:GLN:NE2	1:e:246:GLN:OE1	2.46	0.49
1:C:755:LEU:HA	1:C:809:MET:HE1	1.94	0.49
1:D:504:LEU:HD23	1:D:506:PRO:HD3	1.94	0.49
2:K:702:SER:OG	2:K:758:ARG:NH2	2.44	0.49
3:R:167:LEU:HB3	3:R:836:GLN:HE21	1.77	0.49
3:R:757:LEU:HB2	3:R:773:ILE:HG21	1.95	0.49
1:b:390:ASN:OD1	1:b:433:ARG:NH2	2.45	0.49
1:d:898:ASN:ND2	1:d:1275:PRO:O	2.46	0.49
1:C:336:LYS:NZ	1:C:345:SER:O	2.46	0.49
2:H:746:SER:N	2:H:749:ALA:O	2.45	0.49
2:I:430:TRP:HZ3	2:I:1001:LEU:HD22	1.77	0.49
2:L:847:THR:HG22	2:L:864:ARG:HH12	1.78	0.49
4:U:426:LEU:HD13	4:U:437:MET:HG3	1.93	0.49
1:a:892:PRO:HD2	1:a:895:LEU:HD12	1.94	0.49
1:c:1036:ASN:ND2	1:c:1205:ASN:O	2.46	0.49
1:d:349:ALA:O	1:d:1175:ILE:N	2.42	0.49
1:B:193:PRO:HA	1:B:196:LEU:HB2	1.94	0.49
1:C:599:LEU:HA	1:C:832:GLN:HE21	1.78	0.49
1:C:1082:ARG:HH22	1:c:492:THR:HG21	1.77	0.49
1:E:333:HIS:HA	1:E:336:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:442:ASN:HB3	2:H:445:HIS:HB2	1.93	0.49
2:H:485:LYS:HE2	2:H:645:VAL:HG22	1.94	0.49
2:I:485:LYS:HE2	2:I:645:VAL:HG22	1.94	0.49
2:I:702:SER:OG	2:I:704:THR:O	2.28	0.49
2:J:587:ASP:HB3	2:J:590:ILE:HG22	1.94	0.49
2:J:800:GLY:HA2	2:J:1000:THR:HG23	1.95	0.49
2:K:442:ASN:HB3	2:K:445:HIS:HB2	1.93	0.49
2:L:430:TRP:HZ3	2:L:1001:LEU:HD22	1.77	0.49
3:R:676:MET:O	4:U:538:ASN:ND2	2.45	0.49
1:c:630:PHE:HB2	1:c:772:MET:HE1	1.95	0.49
1:c:1209:LEU:HD21	1:c:1212:THR:HG23	1.95	0.49
1:e:1202:THR:OG1	1:e:1203:GLU:OE1	2.31	0.49
1:B:577:ILE:O	1:B:581:LEU:HB2	2.13	0.49
1:C:755:LEU:HB2	1:C:806:MET:HE1	1.94	0.49
3:R:541:PRO:HA	3:R:544:LEU:HB2	1.93	0.49
3:R:764:GLY:HA2	3:R:769:TRP:HB2	1.95	0.49
4:U:347:PHE:HD2	4:U:352:LEU:HD12	1.77	0.49
4:U:512:ARG:NH2	4:U:536:ASN:O	2.42	0.49
4:U:687:ILE:HG22	4:U:689:GLY:H	1.78	0.49
1:b:920:ARG:NH2	1:b:982:MET:O	2.46	0.49
1:b:1067:PHE:O	1:b:1138:ARG:NH1	2.46	0.49
1:d:1115:TRP:HE1	1:d:1170:ILE:HG21	1.78	0.49
1:A:858:THR:HG23	1:A:942:GLN:HB2	1.94	0.49
1:C:892:PRO:HG2	1:C:895:LEU:HB3	1.95	0.49
1:E:272:VAL:HG23	1:E:300:ALA:HB3	1.94	0.49
1:E:956:ARG:NH2	1:e:749:ASN:OD1	2.39	0.49
1:E:1166:TRP:HD1	1:E:1176:PRO:HG2	1.78	0.49
2:H:873:LEU:HD23	2:H:899:LYS:HZ2	1.76	0.49
1:b:1169:GLU:HG3	1:b:1176:PRO:HG3	1.94	0.49
1:5:11:LYS:HD3	1:e:321:SER:N	2.26	0.48
1:B:1082:ARG:NH2	1:b:492:THR:OG1	2.46	0.48
1:D:222:GLU:OE1	1:D:582:ARG:NH2	2.46	0.48
2:I:873:LEU:HD23	2:I:899:LYS:HZ2	1.78	0.48
3:R:240:GLN:HG2	3:R:250:VAL:HG21	1.95	0.48
1:b:306:VAL:H	1:b:324:MET:HB2	1.78	0.48
1:e:504:LEU:HD23	1:e:506:PRO:HD3	1.94	0.48
1:e:1046:ILE:HD12	1:e:1136:ARG:HH21	1.77	0.48
1:1:154:ILE:HD12	1:1:157:ALA:HB3	1.95	0.48
1:A:228:GLN:O	1:A:234:GLN:NE2	2.36	0.48
1:A:553:PRO:HD2	3:R:309:MET:HG3	1.95	0.48
1:A:941:THR:HG23	1:A:943:TYR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:SER:OG	1:C:627:TRP:NE1	2.46	0.48
1:D:858:THR:HG23	1:D:942:GLN:HB2	1.95	0.48
1:E:1007:ARG:HH12	2:L:293:GLY:H	1.61	0.48
2:H:430:TRP:HZ3	2:H:1001:LEU:HD22	1.77	0.48
2:H:702:SER:OG	2:H:704:THR:O	2.28	0.48
2:H:800:GLY:HA2	2:H:1000:THR:HG23	1.95	0.48
2:H:908:GLN:OE1	2:H:912:ARG:NH2	2.45	0.48
3:R:1171:GLN:HA	3:R:1174:ARG:HH21	1.78	0.48
1:a:690:ASN:HB3	1:a:693:LEU:HD13	1.93	0.48
1:b:1171:THR:HG23	1:b:1174:SER:H	1.78	0.48
1:c:690:ASN:HB3	1:c:693:LEU:HD13	1.95	0.48
1:5:130:ALA:HB3	1:A:496:PRO:HG3	1.96	0.48
1:D:610:ASP:OD1	1:D:674:ARG:NH2	2.43	0.48
3:R:1182:ASP:HA	3:R:1185:MET:HE1	1.96	0.48
4:U:120:GLN:NE2	1:d:567:THR:O	2.35	0.48
4:U:438:PRO:HD2	4:U:441:HIS:HE1	1.78	0.48
1:b:427:VAL:HG22	1:b:1235:LEU:HA	1.96	0.48
1:b:1211:CYS:SG	1:b:1212:THR:N	2.87	0.48
1:d:335:PHE:HZ	1:d:1040:ILE:HD11	1.78	0.48
1:e:224:ILE:HG22	1:e:231:PRO:HB3	1.94	0.48
1:1:131:ASN:HD22	1:B:500:SER:HA	1.78	0.48
1:A:416:VAL:HG21	1:e:1084:SER:HB2	1.95	0.48
1:A:444:MET:HE3	1:A:1261:ALA:HB1	1.96	0.48
1:B:713:TRP:HB3	1:B:837:ARG:HH21	1.79	0.48
1:C:468:ARG:HB2	1:C:1019:VAL:HG11	1.95	0.48
1:C:613:TYR:HB2	1:C:674:ARG:HH21	1.78	0.48
1:D:232:ILE:HG13	1:D:233:VAL:HG23	1.94	0.48
1:E:1033:HIS:ND1	1:E:1248:PRO:O	2.45	0.48
2:H:91:ARG:NH2	2:L:182:ASP:OD1	2.45	0.48
2:I:587:ASP:HB3	2:I:590:ILE:HG22	1.95	0.48
2:I:800:GLY:HA2	2:I:1000:THR:HG23	1.95	0.48
3:R:667:PHE:HE1	3:R:808:SER:HB3	1.78	0.48
1:c:234:GLN:NE2	1:c:247:LEU:O	2.42	0.48
1:c:555:ILE:O	1:c:559:THR:OG1	2.26	0.48
1:B:413:THR:HG21	1:B:424:ALA:HB2	1.96	0.48
1:B:731:ASN:ND2	1:B:734:THR:OG1	2.46	0.48
2:J:757:ARG:NE	2:J:794:LEU:O	2.45	0.48
2:L:527:PRO:HG3	5:L:1301:SAM:O	2.13	0.48
2:L:578:VAL:CG2	5:L:1301:SAM:C4	2.89	0.48
1:b:455:ASP:N	1:b:455:ASP:OD1	2.46	0.48
1:c:692:GLN:OE1	1:c:703:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:93:ASN:HB3	1:3:96:VAL:HG22	1.96	0.48
1:A:180:GLY:HA2	1:A:196:LEU:HD13	1.94	0.48
2:I:746:SER:N	2:I:749:ALA:O	2.45	0.48
2:L:578:VAL:CG2	5:L:1301:SAM:C5	2.75	0.48
2:L:746:SER:N	2:L:749:ALA:O	2.45	0.48
3:R:153:LYS:HD2	3:R:848:ALA:HB1	1.96	0.48
1:a:313:ASN:HD22	1:a:395:PRO:HG2	1.79	0.48
1:d:809:MET:SD	1:d:813:GLN:NE2	2.77	0.48
1:e:803:ILE:HG23	1:e:805:SER:H	1.79	0.48
1:A:426:CYS:O	1:A:428:ARG:NH1	2.47	0.48
1:B:1062:PRO:HG2	1:B:1065:LEU:HD13	1.96	0.48
1:D:1166:TRP:CD1	1:D:1176:PRO:HG2	2.49	0.48
2:L:485:LYS:HE2	2:L:645:VAL:HG22	1.94	0.48
2:L:733:ASN:HA	2:L:766:LYS:HD3	1.96	0.48
1:a:309:ARG:HD3	1:a:312:SER:HB3	1.96	0.48
1:b:849:VAL:O	1:b:863:SER:OG	2.31	0.48
1:c:262:LEU:HB2	1:c:311:ALA:HB3	1.95	0.48
1:c:309:ARG:HB3	1:c:312:SER:HB2	1.94	0.48
1:c:731:ASN:HB2	1:c:736:PRO:HA	1.96	0.48
1:e:257:THR:HG21	1:e:318:ARG:NH2	2.29	0.48
1:e:718:GLN:HB2	1:e:738:VAL:HB	1.96	0.48
1:A:767:ARG:NH2	2:H:69:ASP:OD2	2.45	0.48
1:B:1051:GLN:HG2	1:B:1196:VAL:HG22	1.96	0.48
1:C:705:TRP:HE3	1:C:771:LEU:HD13	1.77	0.48
1:C:949:LEU:HD12	1:C:952:ILE:HD12	1.96	0.48
1:D:492:THR:HG21	1:c:674:ARG:H	1.78	0.48
2:H:847:THR:HG22	2:H:864:ARG:HH12	1.78	0.48
2:J:50:ARG:HE	2:J:51:THR:HG23	1.79	0.48
2:J:430:TRP:HZ3	2:J:1001:LEU:HD22	1.77	0.48
2:K:733:ASN:HA	2:K:766:LYS:HD3	1.96	0.48
3:R:480:PHE:HE1	3:R:969:GLN:HG3	1.77	0.48
4:U:105:ARG:HE	4:U:118:TYR:HB2	1.79	0.48
1:A:690:ASN:HB3	1:A:693:LEU:HD23	1.95	0.48
1:B:689:MET:HE3	1:B:840:ARG:HD3	1.94	0.48
1:D:259:ASP:O	1:D:1259:ARG:NH2	2.35	0.48
1:D:351:PRO:HG3	1:D:1116:GLN:HE22	1.79	0.48
1:E:852:GLN:HE21	1:e:802:LEU:HD12	1.78	0.48
2:I:733:ASN:HA	2:I:766:LYS:HD3	1.96	0.48
2:L:518:SER:H	5:L:1301:SAM:C	2.27	0.48
1:e:318:ARG:NH1	1:e:977:PHE:CD1	2.81	0.48
1:A:1170:ILE:HG13	1:A:1175:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:TYR:CE1	1:C:915:PHE:HB3	2.49	0.48
1:C:552:ASP:OD2	1:C:554:THR:OG1	2.31	0.48
1:D:981:ASP:HB2	1:D:982:MET:HG2	1.96	0.48
2:J:908:GLN:OE1	2:J:912:ARG:NH2	2.45	0.48
3:R:83:ARG:HD3	3:R:92:VAL:HA	1.96	0.48
1:a:521:ARG:HB3	1:a:828:PHE:HE1	1.79	0.48
1:d:376:THR:HG21	1:d:392:ARG:HH11	1.78	0.48
1:e:303:ARG:HD2	1:e:327:PRO:HG2	1.95	0.48
1:B:259:ASP:OD1	1:B:312:SER:OG	2.29	0.47
1:B:686:ARG:HA	1:B:689:MET:HE2	1.96	0.47
1:D:304:ILE:HG23	1:D:1210:PHE:HB2	1.96	0.47
1:E:385:PHE:HE1	1:d:1117:MET:HA	1.79	0.47
1:E:1036:ASN:HD22	1:E:1207:ARG:HB2	1.77	0.47
2:I:425:ASP:HB3	2:I:793:VAL:HG12	1.96	0.47
2:L:800:GLY:HA2	2:L:1000:THR:HG23	1.95	0.47
3:R:41:ASP:HA	3:R:44:LYS:HG2	1.96	0.47
4:U:100:ARG:HD3	1:d:578:LEU:HD13	1.95	0.47
1:e:1166:TRP:CD1	1:e:1176:PRO:HG2	2.49	0.47
1:E:965:PHE:HA	1:E:968:TRP:HD1	1.78	0.47
1:E:981:ASP:N	1:E:981:ASP:OD1	2.47	0.47
2:L:702:SER:OG	2:L:704:THR:O	2.28	0.47
1:b:493:VAL:HG12	1:b:1271:VAL:HG22	1.95	0.47
1:e:298:GLU:OE2	1:e:1214:SER:OG	2.27	0.47
1:e:1083:ILE:HD13	1:e:1121:TYR:HE2	1.79	0.47
1:C:324:MET:HB3	1:C:334:LEU:HD11	1.96	0.47
1:C:409:THR:OG1	1:C:428:ARG:NH2	2.47	0.47
1:C:641:ASP:HB3	1:C:644:ALA:HB2	1.95	0.47
1:D:715:ASN:HA	1:D:837:ARG:HD2	1.96	0.47
2:I:847:THR:HG22	2:I:864:ARG:HH12	1.78	0.47
2:K:425:ASP:HB3	2:K:793:VAL:HG12	1.96	0.47
3:R:197:ILE:HA	3:R:221:ARG:HD2	1.96	0.47
3:R:582:ILE:HD12	3:R:738:MET:HG3	1.96	0.47
1:c:1112:LEU:HD21	1:c:1175:ILE:HD11	1.95	0.47
1:5:4:ILE:HD13	1:e:315:ASP:O	2.14	0.47
1:A:272:VAL:HG23	1:A:300:ALA:HB3	1.97	0.47
1:A:721:TYR:HD1	1:A:739:LEU:HB2	1.77	0.47
1:A:810:TYR:OH	1:A:818:GLU:OE2	2.25	0.47
1:C:478:GLU:OE1	1:C:508:ARG:NH2	2.48	0.47
1:D:931:LEU:HD22	1:D:984:LEU:HD23	1.97	0.47
2:H:19:GLU:HB2	2:H:279:LEU:HD21	1.97	0.47
2:J:733:ASN:HA	2:J:766:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:800:GLY:HA2	2:K:1000:THR:HG23	1.95	0.47
2:L:687:ILE:HG12	2:L:992:LYS:HB3	1.97	0.47
3:R:662:ARG:HA	3:R:674:THR:HG22	1.96	0.47
1:a:839:ASP:OD1	1:a:839:ASP:N	2.45	0.47
1:b:413:THR:HG21	1:b:424:ALA:HB2	1.96	0.47
1:2:108:LYS:HD2	1:b:533:GLN:HE22	1.80	0.47
1:A:926:GLU:HB3	1:A:1020:ILE:HD12	1.97	0.47
1:C:231:PRO:HA	1:C:234:GLN:HB3	1.95	0.47
1:C:304:ILE:HG23	1:C:1210:PHE:HB2	1.96	0.47
1:D:446:GLU:HA	1:D:1261:ALA:HB3	1.97	0.47
1:D:682:HIS:CE1	1:d:779:GLN:H	2.32	0.47
2:H:425:ASP:HB3	2:H:793:VAL:HG12	1.96	0.47
2:H:733:ASN:HA	2:H:766:LYS:HD3	1.96	0.47
2:I:50:ARG:HE	2:I:51:THR:HG23	1.79	0.47
2:I:708:ILE:HG22	2:I:755:THR:HA	1.96	0.47
2:I:991:THR:HG22	2:I:995:LEU:HD23	1.96	0.47
2:J:425:ASP:HB3	2:J:793:VAL:HG12	1.96	0.47
2:J:733:ASN:O	2:J:762:SER:OG	2.33	0.47
2:J:888:CYS:HG	2:J:891:SER:HG	1.62	0.47
3:R:497:LEU:HA	3:R:500:LEU:HD23	1.95	0.47
1:a:746:GLN:HB3	1:a:813:GLN:HG2	1.96	0.47
1:b:234:GLN:NE2	1:b:247:LEU:O	2.39	0.47
1:b:985:GLU:HA	1:b:988:LEU:HB2	1.96	0.47
1:d:1045:ILE:HG12	1:d:1141:MET:HE1	1.95	0.47
1:A:656:MET:HE1	1:A:660:GLU:H	1.80	0.47
1:E:298:GLU:HB3	1:E:1215:SER:HB3	1.96	0.47
2:H:991:THR:HG22	2:H:995:LEU:HD23	1.96	0.47
2:I:567:PRO:HG3	2:J:854:THR:HA	1.97	0.47
2:J:36:ALA:HB3	2:J:87:LYS:HD3	1.97	0.47
2:K:578:VAL:HG23	5:K:1301:SAM:C4'	2.33	0.47
2:K:708:ILE:HG22	2:K:755:THR:HA	1.97	0.47
2:L:50:ARG:HE	2:L:51:THR:HG23	1.79	0.47
2:L:991:THR:HG22	2:L:995:LEU:HD23	1.96	0.47
1:b:271:ILE:HB	1:b:301:VAL:HG23	1.97	0.47
1:b:1096:ASP:HB3	1:b:1100:MET:H	1.80	0.47
1:e:740:LEU:HB2	1:e:832:GLN:HG3	1.97	0.47
1:A:825:MET:HG3	1:A:909:TYR:HE1	1.80	0.47
1:C:278:GLN:HE21	1:C:281:LEU:HB3	1.79	0.47
1:C:381:ASP:HB2	1:C:391:LEU:HD13	1.96	0.47
1:C:1082:ARG:H	1:C:1095:ARG:HB3	1.80	0.47
1:D:276:VAL:HG13	1:D:286:PHE:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:ILE:HG22	1:D:739:LEU:HB3	1.96	0.47
1:D:870:THR:HG21	1:d:794:ARG:HE	1.80	0.47
1:E:419:ILE:HD11	1:E:1214:SER:HB2	1.95	0.47
2:I:687:ILE:HG12	2:I:992:LYS:HB3	1.97	0.47
2:J:562:LEU:CG	5:J:1301:SAM:C2	2.91	0.47
2:J:708:ILE:HG22	2:J:755:THR:HA	1.97	0.47
2:J:746:SER:N	2:J:749:ALA:O	2.45	0.47
2:K:549:GLN:HE21	2:K:556:LYS:HB2	1.80	0.47
2:K:812:ASN:HB3	2:K:839:LEU:HD21	1.97	0.47
2:L:425:ASP:HB3	2:L:793:VAL:HG12	1.96	0.47
3:R:1008:SER:HA	3:R:1147:MET:HB3	1.97	0.47
3:R:1201:PRO:HB3	3:R:1241:TYR:HB3	1.96	0.47
4:U:2:ALA:N	4:U:201:ARG:O	2.48	0.47
1:a:776:VAL:HG12	1:a:790:VAL:HG23	1.95	0.47
1:a:1083:ILE:HD12	1:a:1121:TYR:HE2	1.79	0.47
1:a:1124:GLN:OE1	1:a:1125:GLN:NE2	2.48	0.47
1:b:776:VAL:HG21	1:b:793:MET:HG2	1.97	0.47
1:b:779:GLN:NE2	1:b:782:GLN:O	2.48	0.47
1:d:418:LYS:NZ	1:d:1224:ASP:OD1	2.47	0.47
1:e:527:ASN:ND2	1:e:867:THR:OG1	2.48	0.47
1:e:559:THR:HG21	1:e:803:ILE:HG13	1.95	0.47
1:D:763:ASN:O	1:D:767:ARG:NE	2.42	0.47
1:E:416:VAL:HG11	1:d:1084:SER:HB2	1.97	0.47
1:E:739:LEU:HG	1:E:832:GLN:HE22	1.80	0.47
1:E:1170:ILE:HG13	1:E:1175:ILE:HG22	1.96	0.47
2:H:549:GLN:HE21	2:H:556:LYS:HB2	1.80	0.47
2:I:19:GLU:HB2	2:I:279:LEU:HD21	1.97	0.47
2:I:182:ASP:OD2	2:J:95:TYR:OH	2.32	0.47
2:I:812:ASN:HB3	2:I:839:LEU:HD21	1.97	0.47
2:J:847:THR:HG22	2:J:864:ARG:HH12	1.78	0.47
2:K:19:GLU:HB2	2:K:279:LEU:HD21	1.97	0.47
2:K:746:SER:N	2:K:749:ALA:O	2.45	0.47
2:L:708:ILE:HG22	2:L:755:THR:HA	1.97	0.47
2:L:873:LEU:HB3	2:L:899:LYS:HZ1	1.79	0.47
3:R:1168:ASN:HB3	3:R:1171:GLN:HG2	1.96	0.47
1:d:839:ASP:OD1	1:d:842:ARG:NE	2.46	0.47
1:e:776:VAL:HG21	1:e:793:MET:HG2	1.96	0.47
1:A:556:ILE:HA	1:A:559:THR:HG22	1.97	0.47
1:C:266:PHE:O	1:C:310:TRP:NE1	2.48	0.47
1:C:634:LEU:HD23	1:C:883:THR:HG23	1.96	0.47
2:H:733:ASN:O	2:H:762:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:36:ALA:HB3	2:I:87:LYS:HD3	1.97	0.47
2:J:549:GLN:HE21	2:J:556:LYS:HB2	1.80	0.47
2:K:486:ASP:HA	2:K:489:VAL:HG12	1.97	0.47
3:R:410:GLU:OE1	3:R:652:SER:OG	2.30	0.47
3:R:1067:ARG:HE	3:R:1196:HIS:CD2	2.33	0.47
1:d:741:LEU:HD23	1:d:743:ILE:H	1.80	0.47
1:d:915:PHE:HE2	1:d:1267:ILE:HG21	1.79	0.47
1:e:374:ARG:NH1	1:e:375:HIS:O	2.48	0.47
1:3:134:SER:OG	1:3:135:ARG:N	2.49	0.47
2:I:757:ARG:NE	2:I:794:LEU:O	2.45	0.47
2:J:978:SER:HB2	2:J:1025:GLY:HA3	1.97	0.47
2:K:765:ARG:HH22	2:K:856:GLN:HE22	1.63	0.47
2:L:19:GLU:HB2	2:L:279:LEU:HD21	1.97	0.47
3:R:51:PHE:HE2	3:R:191:ARG:HE	1.62	0.47
3:R:881:PHE:HE2	3:R:910:MET:HE3	1.80	0.47
4:U:680:ARG:HB3	4:U:710:GLU:HB3	1.96	0.47
4:U:698:SER:HB2	4:U:700:PHE:H	1.80	0.47
1:a:983:LEU:HD23	1:a:984:LEU:HG	1.97	0.47
1:b:486:CYS:O	1:b:909:TYR:OH	2.33	0.47
1:b:670:THR:HG22	1:b:672:SER:H	1.79	0.47
1:c:318:ARG:H	1:c:371:TYR:HH	1.61	0.47
1:c:1069:ARG:HE	1:c:1076:ILE:HD13	1.79	0.47
1:e:608:ILE:HD13	1:e:877:LEU:HB2	1.97	0.47
1:1:94:GLU:OE2	1:1:134:SER:N	2.37	0.46
1:E:926:GLU:HB3	1:E:1020:ILE:HD12	1.97	0.46
1:E:1186:SER:OG	1:E:1187:ASP:N	2.48	0.46
2:H:36:ALA:HB3	2:H:87:LYS:HD3	1.97	0.46
2:H:50:ARG:HE	2:H:51:THR:HG23	1.79	0.46
2:I:978:SER:HB2	2:I:1025:GLY:HA3	1.97	0.46
2:K:3:ASN:HA	2:K:7:VAL:HA	1.98	0.46
2:L:36:ALA:HB3	2:L:87:LYS:HD3	1.97	0.46
1:b:1207:ARG:HH21	1:b:1250:VAL:HG23	1.80	0.46
1:c:251:ASP:OD2	1:c:980:SER:N	2.46	0.46
1:c:341:THR:OG1	1:c:342:GLU:OE1	2.32	0.46
1:e:484:THR:HG23	1:e:493:VAL:HG12	1.97	0.46
1:3:129:ASN:ND2	1:3:132:GLU:OE1	2.48	0.46
1:A:338:LEU:HG	1:A:339:LEU:HG	1.97	0.46
1:A:1034:GLU:HB3	1:A:1037:LEU:HD23	1.97	0.46
1:C:224:ILE:O	1:C:228:GLN:HB3	2.15	0.46
1:E:303:ARG:HG2	1:E:1209:LEU:HA	1.98	0.46
2:H:3:ASN:HA	2:H:7:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:765:ARG:HH22	2:I:856:GLN:HE22	1.63	0.46
2:K:50:ARG:HE	2:K:51:THR:HG23	1.79	0.46
3:R:411:ILE:HD11	3:R:652:SER:HB2	1.97	0.46
1:a:1081:CYS:HB2	1:a:1094:ILE:HD11	1.96	0.46
1:3:131:ASN:OD1	1:D:503:ARG:NH1	2.38	0.46
1:E:606:THR:HA	1:E:875:LEU:HB3	1.96	0.46
2:J:486:ASP:HA	2:J:489:VAL:HG12	1.97	0.46
2:K:578:VAL:HG21	5:K:1301:SAM:C5	2.36	0.46
2:L:518:SER:HB3	5:L:1301:SAM:HB2	1.96	0.46
4:U:512:ARG:HE	4:U:538:ASN:H	1.63	0.46
1:b:366:VAL:HG23	1:b:461:ILE:HD13	1.96	0.46
1:b:776:VAL:HG12	1:b:790:VAL:HG23	1.98	0.46
1:d:588:PHE:HE1	1:d:884:VAL:HG13	1.80	0.46
1:d:1049:ARG:O	1:d:1136:ARG:NH2	2.48	0.46
1:e:662:ILE:HD11	1:e:702:LEU:HG	1.97	0.46
1:4:8:THR:OG1	1:d:978:ASP:OD1	2.34	0.46
1:A:295:PRO:HB3	1:A:405:ILE:HA	1.96	0.46
1:C:543:LEU:HD21	1:C:595:LEU:HD23	1.97	0.46
1:D:770:GLU:OE2	1:D:801:LYS:NZ	2.48	0.46
1:E:854:ARG:NH1	1:E:866:THR:OG1	2.48	0.46
2:I:549:GLN:HE21	2:I:556:LYS:HB2	1.80	0.46
2:J:687:ILE:HG12	2:J:992:LYS:HB3	1.97	0.46
2:J:991:THR:HG22	2:J:995:LEU:HD23	1.96	0.46
2:K:687:ILE:HG12	2:K:992:LYS:HB3	1.97	0.46
2:L:552:TYR:H	5:L:1301:SAM:C2	2.28	0.46
3:R:625:SER:HB2	3:R:646:ASN:HD21	1.80	0.46
3:R:1126:SER:HB3	3:R:1174:ARG:HB3	1.96	0.46
1:b:472:MET:HA	1:b:508:ARG:HB3	1.97	0.46
1:c:504:LEU:HD23	1:c:506:PRO:HD3	1.96	0.46
1:d:935:VAL:HA	1:d:938:ILE:HG12	1.97	0.46
1:5:4:ILE:HG21	1:e:254:ARG:NH2	2.19	0.46
1:B:776:VAL:HG23	1:B:782:GLN:HE21	1.80	0.46
1:D:1084:SER:HB3	1:D:1093:MET:HB3	1.96	0.46
1:E:304:ILE:HG23	1:E:1210:PHE:HB2	1.98	0.46
2:H:455:GLN:HE22	2:H:621:ARG:HG3	1.81	0.46
2:J:19:GLU:HB2	2:J:279:LEU:HD21	1.97	0.46
2:L:812:ASN:HB3	2:L:839:LEU:HD21	1.97	0.46
1:d:328:THR:OG1	1:d:329:GLU:OE1	2.33	0.46
1:d:939:SER:HB3	1:d:957:ALA:HB3	1.98	0.46
1:e:419:ILE:HD11	1:e:1214:SER:HB2	1.97	0.46
1:5:13:SER:O	1:5:13:SER:OG	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:ARG:NH2	2:L:99:ARG:HH12	2.13	0.46
2:H:708:ILE:HG22	2:H:755:THR:HA	1.96	0.46
2:H:757:ARG:NE	2:H:794:LEU:O	2.45	0.46
2:H:812:ASN:HB3	2:H:839:LEU:HD21	1.97	0.46
2:J:331:VAL:HA	2:J:334:VAL:HG12	1.98	0.46
2:K:36:ALA:HB3	2:K:87:LYS:HD3	1.97	0.46
2:K:559:ILE:HG21	2:L:785:ARG:HH22	1.81	0.46
2:L:331:VAL:HA	2:L:334:VAL:HG12	1.98	0.46
3:R:232:ASP:OD2	3:R:266:TYR:OH	2.32	0.46
1:a:258:TRP:HH2	1:a:1262:TYR:HB2	1.80	0.46
1:a:1067:PHE:O	1:a:1138:ARG:NH1	2.49	0.46
1:B:1068:ASP:OD1	1:B:1071:THR:OG1	2.31	0.46
1:D:533:GLN:HE21	1:D:537:GLN:HE21	1.62	0.46
2:K:552:TYR:CE1	2:L:782:VAL:HG11	2.51	0.46
2:L:486:ASP:HA	2:L:489:VAL:HG12	1.97	0.46
2:L:549:GLN:HE21	2:L:556:LYS:HB2	1.80	0.46
4:U:333:ILE:HG23	4:U:338:TYR:HE2	1.80	0.46
1:a:603:VAL:HB	1:a:831:PHE:HZ	1.80	0.46
1:b:588:PHE:HE1	1:b:884:VAL:HG13	1.81	0.46
1:c:1027:THR:HA	1:c:1030:VAL:HG22	1.97	0.46
1:d:752:THR:HG21	1:d:809:MET:HG3	1.98	0.46
1:e:567:THR:O	1:e:569:GLN:N	2.49	0.46
1:5:11:LYS:NZ	1:5:11:LYS:HB3	2.27	0.46
1:5:72:PRO:HD3	1:e:249:HIS:HB3	1.98	0.46
1:B:326:PRO:HA	1:B:327:PRO:HD3	1.80	0.46
1:B:746:GLN:OE1	1:B:812:GLN:NE2	2.45	0.46
1:B:865:SER:HA	1:B:1000:GLN:HE22	1.81	0.46
1:B:1211:CYS:SG	1:B:1212:THR:N	2.89	0.46
1:D:381:ASP:OD1	1:D:410:ARG:NH2	2.48	0.46
1:D:818:GLU:HA	1:D:821:VAL:HG22	1.98	0.46
1:E:497:TYR:H	1:d:869:THR:HG23	1.79	0.46
1:E:529:ALA:HA	1:E:532:ILE:HG22	1.98	0.46
1:E:933:THR:HG21	1:E:1021:ALA:HB1	1.98	0.46
2:I:562:LEU:HG	5:I:1301:SAM:C2	2.45	0.46
2:K:991:THR:HG22	2:K:995:LEU:HD23	1.96	0.46
2:L:978:SER:HB2	2:L:1025:GLY:HA3	1.97	0.46
1:a:1058:PRO:HG2	1:a:1182:VAL:HG12	1.97	0.46
1:a:1232:TYR:HE1	1:a:1253:LEU:HB2	1.80	0.46
1:1:87:THR:OG1	1:1:146:ASN:OD1	2.31	0.46
1:A:603:VAL:HG23	1:A:604:VAL:HG23	1.98	0.46
1:B:571:LEU:HD13	1:B:623:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:THR:OG1	1:c:1079:ARG:NH1	2.49	0.46
1:D:529:ALA:HA	1:D:532:ILE:HB	1.96	0.46
2:H:331:VAL:HA	2:H:334:VAL:HG12	1.98	0.46
2:H:687:ILE:HG12	2:H:992:LYS:HB3	1.97	0.46
2:H:978:SER:HB2	2:H:1025:GLY:HA3	1.97	0.46
3:R:21:ASP:OD1	3:R:881:PHE:N	2.49	0.46
4:U:50:MET:HE1	4:U:162:ILE:HG12	1.98	0.46
1:b:1107:ASN:HA	1:b:1136:ARG:HB2	1.98	0.46
1:e:793:MET:HE2	1:e:793:MET:HB2	1.84	0.46
1:A:402:TRP:HA	1:A:405:ILE:HG22	1.98	0.46
1:E:613:TYR:CE2	1:E:676:SER:HB3	2.49	0.46
2:I:331:VAL:HA	2:I:334:VAL:HG12	1.98	0.46
2:J:812:ASN:HB3	2:J:839:LEU:HD21	1.97	0.46
2:L:455:GLN:HE22	2:L:621:ARG:HG3	1.81	0.46
2:L:733:ASN:O	2:L:762:SER:OG	2.33	0.46
3:R:435:ARG:NE	3:R:548:TYR:OH	2.48	0.46
4:U:455:THR:O	4:U:458:HIS:N	2.36	0.46
1:e:649:PHE:HD1	1:e:705:TRP:HD1	1.63	0.46
1:e:840:ARG:NH2	1:e:1004:TYR:OH	2.49	0.46
1:2:98:ALA:HA	1:2:101:GLU:HG2	1.98	0.45
1:B:176:SER:H	1:B:194:LEU:HD13	1.80	0.45
2:H:765:ARG:HH22	2:H:856:GLN:HE22	1.63	0.45
2:K:97:VAL:HA	2:K:100:ILE:HG22	1.99	0.45
2:L:757:ARG:NE	2:L:794:LEU:O	2.45	0.45
2:L:765:ARG:HH22	2:L:856:GLN:HE22	1.63	0.45
3:R:11:PRO:HB2	3:R:26:VAL:HG21	1.98	0.45
1:a:552:ASP:HB2	1:a:554:THR:HG22	1.98	0.45
1:e:455:ASP:OD1	1:e:455:ASP:N	2.47	0.45
1:2:53:TYR:OH	1:b:903:ASP:OD2	2.23	0.45
1:5:7:LYS:NZ	1:5:7:LYS:CB	2.72	0.45
1:A:220:ILE:HD13	3:R:1236:VAL:HG23	1.98	0.45
2:I:3:ASN:HA	2:I:7:VAL:HA	1.97	0.45
2:J:3:ASN:HA	2:J:7:VAL:HA	1.97	0.45
2:J:455:GLN:HE22	2:J:621:ARG:HG3	1.81	0.45
3:R:103:LEU:HA	3:R:115:LEU:HA	1.97	0.45
3:R:717:LEU:HA	3:R:720:MET:HG3	1.99	0.45
4:U:528:ALA:HB3	4:U:534:LEU:HD11	1.97	0.45
1:a:599:LEU:HA	1:a:832:GLN:HE21	1.81	0.45
1:b:436:ARG:HA	1:b:448:VAL:HA	1.97	0.45
1:5:10:GLY:HA3	1:e:319:ASP:HB3	1.89	0.45
1:B:1207:ARG:NH2	1:B:1249:GLU:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:ILE:O	1:C:703:ARG:NH1	2.50	0.45
1:D:220:ILE:HD12	1:D:557:SER:HB2	1.98	0.45
2:H:97:VAL:HA	2:H:100:ILE:HG22	1.99	0.45
2:H:240:GLN:HA	2:H:250:ASN:HA	1.98	0.45
2:J:577:ASP:C	2:J:615:LYS:HD3	2.40	0.45
2:J:765:ARG:HH22	2:J:856:GLN:HE22	1.63	0.45
2:K:978:SER:HB2	2:K:1025:GLY:HA3	1.97	0.45
2:L:551:GLY:HA2	5:L:1301:SAM:H2	1.98	0.45
1:d:906:TYR:O	1:d:910:ALA:HB2	2.16	0.45
1:e:359:LEU:HD21	1:e:949:LEU:HD21	1.98	0.45
1:5:144:GLY:HA3	1:A:377:GLY:HA2	1.98	0.45
1:C:853:SER:N	1:C:994:MET:O	2.41	0.45
1:D:269:VAL:HG11	1:D:326:PRO:HG3	1.98	0.45
1:D:956:ARG:HE	1:d:750:VAL:HG22	1.81	0.45
1:E:731:ASN:ND2	1:E:735:PRO:O	2.40	0.45
2:J:559:ILE:HG21	2:K:785:ARG:HH22	1.81	0.45
2:L:454:PRO:HG3	2:L:675:VAL:HG22	1.99	0.45
2:L:552:TYR:CE1	5:L:1301:SAM:N9	2.84	0.45
3:R:93:TYR:OH	3:R:379:ARG:NH2	2.50	0.45
3:R:97:CYS:O	3:R:136:TYR:OH	2.31	0.45
4:U:438:PRO:HD2	4:U:441:HIS:CE1	2.52	0.45
1:e:307:HIS:CD2	1:e:323:ILE:HG22	2.50	0.45
1:A:1241:PRO:HG2	1:A:1244:GLN:HB2	1.99	0.45
1:C:493:VAL:HA	1:C:1273:GLY:HA2	1.98	0.45
1:D:457:LEU:HD11	1:D:1030:VAL:HG21	1.97	0.45
1:D:729:SER:OG	1:D:731:ASN:OD1	2.34	0.45
2:J:925:GLN:HA	2:J:1018:ILE:HG22	1.99	0.45
2:L:3:ASN:HA	2:L:7:VAL:HA	1.98	0.45
2:L:517:ALA:HA	5:L:1301:SAM:OXT	2.17	0.45
4:U:301:LEU:HD21	4:U:391:ILE:HB	1.99	0.45
1:b:707:GLU:HG3	1:b:711:ARG:HH21	1.81	0.45
1:d:1117:MET:HB2	1:d:1122:PHE:HE2	1.81	0.45
1:5:158:THR:OG1	1:e:342:GLU:OE2	2.25	0.45
1:E:355:ARG:NH2	1:E:952:ILE:O	2.50	0.45
2:I:578:VAL:CG2	5:I:1301:SAM:C1'	2.92	0.45
2:K:925:GLN:HA	2:K:1018:ILE:HG22	1.99	0.45
3:R:278:PRO:HA	3:R:369:MET:HE1	1.99	0.45
3:R:889:SER:OG	3:R:890:TRP:N	2.49	0.45
1:a:1112:LEU:HD21	1:a:1175:ILE:HD11	1.99	0.45
1:b:544:GLN:HA	1:b:592:ARG:HE	1.82	0.45
1:d:1052:SER:OG	1:d:1053:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:PRO:HB2	1:B:627:TRP:HZ2	1.82	0.45
1:B:849:VAL:O	1:B:869:THR:N	2.47	0.45
1:C:1186:SER:HB3	1:C:1221:ALA:HB3	1.99	0.45
1:E:704:GLN:OE1	1:E:774:ASN:ND2	2.49	0.45
2:I:486:ASP:HA	2:I:489:VAL:HG12	1.97	0.45
2:L:97:VAL:HA	2:L:100:ILE:HG22	1.99	0.45
3:R:168:TYR:O	3:R:836:GLN:NE2	2.49	0.45
3:R:877:LEU:HD13	3:R:880:VAL:HG21	1.98	0.45
1:a:649:PHE:HD1	1:a:705:TRP:HD1	1.65	0.45
1:a:929:GLN:HB2	1:a:1015:MET:HE2	1.98	0.45
1:b:1034:GLU:OE2	1:b:1207:ARG:NH2	2.50	0.45
1:c:468:ARG:HB2	1:c:1019:VAL:HG21	1.99	0.45
1:d:898:ASN:ND2	1:d:1274:VAL:O	2.44	0.45
1:d:1212:THR:OG1	1:d:1224:ASP:OD1	2.34	0.45
1:e:299:ALA:O	1:e:1214:SER:OG	2.34	0.45
1:e:548:PRO:HG3	1:e:900:TRP:CD1	2.52	0.45
1:1:150:MET:HE1	1:B:379:SER:HA	1.99	0.45
1:2:165:HIS:HB3	1:b:1120:ARG:HD3	1.98	0.45
1:B:335:PHE:O	1:B:357:ASN:ND2	2.49	0.45
1:B:523:MET:HE2	1:B:523:MET:HB3	1.89	0.45
1:B:569:GLN:HA	1:C:566:SER:HA	1.99	0.45
1:B:692:GLN:HA	1:B:703:ARG:HH12	1.80	0.45
1:E:625:ASN:HB3	1:E:655:MET:HE1	1.99	0.45
1:E:719:ILE:HG22	1:E:739:LEU:HB3	1.99	0.45
2:H:486:ASP:HA	2:H:489:VAL:HG12	1.97	0.45
2:J:354:ALA:HB3	2:J:357:SER:HB2	1.99	0.45
2:K:331:VAL:HA	2:K:334:VAL:HG12	1.98	0.45
1:d:853:SER:N	1:d:995:THR:OG1	2.49	0.45
1:e:223:PHE:HD2	1:e:910:ALA:HA	1.81	0.45
1:e:430:ARG:O	1:e:1254:TYR:OH	2.32	0.45
1:1:3:ARG:HH22	1:a:313:ASN:HD21	1.65	0.45
1:A:601:ASN:ND2	1:A:833:VAL:O	2.40	0.45
1:B:1027:THR:HA	1:B:1030:VAL:HG12	1.99	0.45
1:C:920:ARG:HH22	1:C:982:MET:HB3	1.82	0.45
1:D:272:VAL:HG23	1:D:300:ALA:HB3	1.98	0.45
2:I:455:GLN:HE22	2:I:621:ARG:HG3	1.81	0.45
2:L:354:ALA:HB3	2:L:357:SER:HB2	1.99	0.45
1:a:737:GLU:HG2	1:a:738:VAL:HG13	1.98	0.45
1:c:853:SER:OG	1:c:854:ARG:N	2.46	0.45
1:1:128:ASN:ND2	1:B:494:THR:O	2.49	0.45
1:B:416:VAL:HG22	1:a:1082:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:HD11	1:D:469:LEU:HD22	1.99	0.45
2:H:851:ILE:HG22	2:H:871:ASP:HA	1.99	0.45
2:I:97:VAL:HA	2:I:100:ILE:HG22	1.98	0.45
1:a:306:VAL:HG12	1:a:324:MET:HE2	1.99	0.45
1:b:1045:ILE:HG12	1:b:1141:MET:HE2	1.99	0.45
1:d:713:TRP:HD1	1:d:837:ARG:HG3	1.82	0.45
1:e:330:ASN:HA	1:e:1147:MET:HE1	1.99	0.45
1:e:379:SER:N	1:e:391:LEU:O	2.49	0.45
1:e:1123:ASN:OD1	1:e:1124:GLN:N	2.50	0.45
1:5:163:SER:HB3	1:e:1120:ARG:HG3	2.00	0.44
1:A:382:HIS:HD2	1:e:353:MET:HE3	1.81	0.44
1:B:1116:GLN:HB3	1:B:1172:PRO:HA	1.99	0.44
1:C:416:VAL:HG21	1:b:1084:SER:HB3	1.99	0.44
1:E:913:GLU:HA	1:E:916:SER:HB2	2.00	0.44
2:J:97:VAL:HA	2:J:100:ILE:HG22	1.98	0.44
2:L:525:ASP:OD1	2:L:525:ASP:N	2.51	0.44
3:R:407:PRO:HD2	3:R:630:GLU:HB3	1.97	0.44
1:a:222:GLU:HB3	1:a:233:VAL:HG23	1.98	0.44
1:a:634:LEU:HD23	1:a:883:THR:HG23	2.00	0.44
1:b:505:MET:N	1:b:505:MET:SD	2.90	0.44
1:e:326:PRO:HA	1:e:327:PRO:HD3	1.86	0.44
1:B:318:ARG:NH1	1:B:370:LEU:O	2.50	0.44
1:B:528:ASN:HD22	1:B:531:VAL:HG23	1.82	0.44
1:B:818:GLU:OE2	1:B:901:TYR:OH	2.33	0.44
1:C:234:GLN:NE2	1:C:235:VAL:O	2.51	0.44
1:C:668:ILE:HG13	1:D:750:VAL:HG11	2.00	0.44
1:C:1027:THR:HA	1:C:1030:VAL:HG12	2.00	0.44
1:D:303:ARG:HH12	1:D:1148:LEU:HD11	1.82	0.44
2:I:731:CYS:HA	2:I:734:VAL:HG12	1.99	0.44
2:J:240:GLN:HA	2:J:250:ASN:HA	1.99	0.44
2:J:702:SER:OG	2:J:704:THR:O	2.28	0.44
4:U:97:ASN:ND2	4:U:130:VAL:O	2.50	0.44
1:a:1171:THR:HG23	1:a:1174:SER:H	1.81	0.44
1:c:948:TYR:HE2	1:c:1025:GLN:HB3	1.83	0.44
1:3:125:THR:HG22	1:c:876:ALA:HB2	2.00	0.44
2:H:454:PRO:HG3	2:H:675:VAL:HG22	1.99	0.44
2:H:560:VAL:HG22	2:I:397:LEU:HB2	1.99	0.44
2:J:562:LEU:HB2	5:J:1301:SAM:N1	2.31	0.44
2:J:731:CYS:HA	2:J:734:VAL:HG12	1.99	0.44
2:J:1009:ALA:HA	2:J:1012:MET:HE2	2.00	0.44
4:U:55:GLU:HG2	4:U:57:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:414:PRO:HB2	4:U:552:THR:HG21	1.99	0.44
1:b:746:GLN:HB3	1:b:813:GLN:HG3	1.99	0.44
1:e:705:TRP:HE3	1:e:771:LEU:HD13	1.83	0.44
1:5:6:ARG:CD	1:5:6:ARG:N	2.72	0.44
1:A:341:THR:HG23	1:A:342:GLU:HG2	2.00	0.44
1:A:669:TYR:HE1	1:a:783:PRO:HB3	1.82	0.44
1:B:634:LEU:HD23	1:B:883:THR:HG23	1.98	0.44
1:C:570:THR:OG1	1:D:564:SER:OG	2.24	0.44
1:C:719:ILE:HG22	1:C:739:LEU:HB3	1.99	0.44
1:C:810:TYR:OH	1:C:818:GLU:OE1	2.34	0.44
1:C:1207:ARG:HH22	1:C:1250:VAL:HG12	1.83	0.44
2:H:354:ALA:HB3	2:H:357:SER:HB2	1.99	0.44
2:I:240:GLN:HA	2:I:250:ASN:HA	1.99	0.44
2:I:925:GLN:HA	2:I:1018:ILE:HG22	1.99	0.44
2:K:354:ALA:HB3	2:K:357:SER:HB2	1.99	0.44
2:K:514:TYR:HB3	2:K:549:GLN:HA	2.00	0.44
2:L:731:CYS:HA	2:L:734:VAL:HG12	1.99	0.44
3:R:24:ASN:HA	3:R:867:MET:HE3	1.99	0.44
1:b:647:LYS:NZ	1:b:675:ALA:O	2.47	0.44
1:b:717:SER:OG	1:b:718:GLN:N	2.51	0.44
1:e:701:ILE:HD13	1:e:781:TYR:HE2	1.83	0.44
1:A:420:CYS:HA	1:A:423:VAL:HG12	1.99	0.44
1:A:620:VAL:HG12	1:A:655:MET:HG3	2.00	0.44
1:A:1096:ASP:OD1	1:A:1097:GLU:N	2.51	0.44
1:C:313:ASN:HD22	1:C:395:PRO:HG2	1.82	0.44
2:J:454:PRO:HG3	2:J:675:VAL:HG22	1.99	0.44
2:J:691:LEU:HD12	2:J:692:PRO:HD2	1.99	0.44
2:K:240:GLN:HA	2:K:250:ASN:HA	1.99	0.44
2:K:733:ASN:O	2:K:762:SER:OG	2.33	0.44
2:K:851:ILE:HG22	2:K:871:ASP:HA	2.00	0.44
2:K:1009:ALA:HA	2:K:1012:MET:HE2	2.00	0.44
2:L:514:TYR:HB3	2:L:549:GLN:HA	2.00	0.44
3:R:593:ILE:HA	3:R:598:PHE:HD2	1.81	0.44
3:R:892:MET:HA	3:R:1232:THR:HG22	1.99	0.44
4:U:219:SER:OG	4:U:220:GLY:N	2.51	0.44
1:b:543:LEU:HA	1:b:546:ILE:HG22	1.98	0.44
1:c:326:PRO:HA	1:c:327:PRO:HD3	1.88	0.44
1:3:166:PRO:HG3	1:D:290:TYR:HE1	1.82	0.44
1:C:217:GLN:HA	1:C:220:ILE:HG12	2.00	0.44
1:C:1241:PRO:HG2	1:C:1244:GLN:HB2	1.98	0.44
1:D:620:VAL:HG21	1:D:656:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:454:PRO:HG3	2:I:675:VAL:HG22	1.99	0.44
2:K:455:GLN:HE22	2:K:621:ARG:HG3	1.81	0.44
3:R:81:VAL:HG21	3:R:135:THR:HG21	1.99	0.44
3:R:95:PRO:O	3:R:224:SER:OG	2.35	0.44
3:R:1114:LYS:HG2	3:R:1116:VAL:HG22	2.00	0.44
1:b:330:ASN:HD21	1:b:332:ILE:HG22	1.82	0.44
1:b:958:SER:OG	1:b:959:ALA:N	2.51	0.44
1:b:1026:LEU:HD21	1:b:1247:LEU:HD21	1.99	0.44
2:I:514:TYR:HB3	2:I:549:GLN:HA	2.00	0.44
2:L:851:ILE:HG22	2:L:871:ASP:HA	2.00	0.44
2:L:925:GLN:HA	2:L:1018:ILE:HG22	1.99	0.44
1:c:303:ARG:NH1	1:c:1208:SER:OG	2.51	0.44
1:c:306:VAL:HG21	1:c:1038:PHE:HD1	1.83	0.44
1:e:349:ALA:N	1:e:1175:ILE:O	2.51	0.44
1:e:577:ILE:HD13	1:e:627:TRP:HB3	2.00	0.44
1:e:755:LEU:HD21	1:e:802:LEU:HB2	1.99	0.44
1:e:985:GLU:HA	1:e:988:LEU:HD13	2.00	0.44
1:C:1085:PHE:HE1	1:c:496:PRO:HB2	1.83	0.44
1:E:409:THR:OG1	1:E:428:ARG:NH2	2.41	0.44
1:E:958:SER:H	1:E:961:THR:HG1	1.61	0.44
2:H:691:LEU:HD12	2:H:692:PRO:HD2	1.99	0.44
2:H:925:GLN:HA	2:H:1018:ILE:HG22	1.99	0.44
2:H:940:LEU:HD21	2:H:1016:MET:HE1	2.00	0.44
2:K:446:ARG:HG3	2:K:668:SER:HB3	2.00	0.44
2:K:454:PRO:HG3	2:K:675:VAL:HG22	1.99	0.44
4:U:5:ALA:HB2	4:U:208:PRO:HB3	2.00	0.44
1:a:505:MET:HB2	1:a:507:TYR:HE2	1.83	0.44
1:b:1033:HIS:HB3	1:b:1207:ARG:HH12	1.81	0.44
1:c:684:TRP:HB3	1:c:689:MET:HE3	1.99	0.44
1:e:961:THR:O	1:e:964:THR:OG1	2.35	0.44
1:5:7:LYS:HB3	1:5:7:LYS:HZ3	1.81	0.44
1:A:1078:GLY:H	1:A:1097:GLU:HB2	1.83	0.44
1:A:1152:ASP:HB3	1:A:1155:GLN:HE22	1.83	0.44
1:A:1218:GLN:HE22	1:A:1220:ILE:HG13	1.83	0.44
1:E:417:SER:HA	1:E:1217:PRO:HA	2.00	0.44
2:I:354:ALA:HB3	2:I:357:SER:HB2	1.99	0.44
2:I:559:ILE:HG21	2:J:785:ARG:HH22	1.82	0.44
2:K:935:THR:HB	2:K:942:ILE:HG12	2.00	0.44
2:L:240:GLN:HA	2:L:250:ASN:HA	1.99	0.44
2:L:446:ARG:HG3	2:L:668:SER:HB3	2.00	0.44
3:R:146:GLN:HE22	3:R:804:GLU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:500:SER:H	1:a:503:ARG:HH12	1.66	0.44
1:a:521:ARG:HB3	1:a:828:PHE:CE1	2.52	0.44
1:a:1065:LEU:HD22	1:a:1200:ILE:HD11	1.99	0.44
1:B:304:ILE:HG23	1:B:1210:PHE:HB2	2.00	0.43
1:D:802:LEU:HD23	1:D:802:LEU:HA	1.86	0.43
2:H:709:ILE:HD11	2:H:727:ILE:HD13	2.00	0.43
2:I:446:ARG:HG3	2:I:668:SER:HB3	2.00	0.43
2:I:935:THR:HB	2:I:942:ILE:HG12	2.00	0.43
2:J:912:ARG:O	2:J:915:THR:OG1	2.30	0.43
2:K:731:CYS:HA	2:K:734:VAL:HG12	1.99	0.43
2:K:873:LEU:HD23	2:K:899:LYS:HZ2	1.82	0.43
3:R:1067:ARG:HE	3:R:1196:HIS:CG	2.36	0.43
4:U:96:ASP:HA	4:U:103:ARG:HH22	1.83	0.43
1:a:742:PRO:HG2	1:a:743:ILE:HD12	2.00	0.43
1:b:606:THR:HG1	1:b:640:THR:H	1.62	0.43
1:e:609:ASP:HB3	1:e:876:ALA:HB1	2.00	0.43
1:e:713:TRP:HB3	1:e:837:ARG:HE	1.83	0.43
1:e:748:ALA:HA	1:e:813:GLN:HB3	2.00	0.43
1:4:6:ARG:NH2	1:d:978:ASP:OD1	2.51	0.43
1:A:598:TRP:O	1:A:835:TYR:OH	2.36	0.43
1:B:259:ASP:OD2	1:B:462:ARG:NH1	2.43	0.43
1:B:706:ALA:O	1:B:710:HIS:ND1	2.35	0.43
1:B:842:ARG:HH12	2:I:291:TYR:HE2	1.65	0.43
1:D:468:ARG:CZ	1:D:471:ARG:HH21	2.31	0.43
1:E:1204:TYR:CZ	1:E:1206:ASP:HB2	2.53	0.43
2:H:912:ARG:O	2:H:915:THR:OG1	2.30	0.43
2:K:181:ASP:OD1	2:L:91:ARG:NH2	2.51	0.43
3:R:586:ILE:HD13	3:R:589:CYS:HA	2.00	0.43
3:R:814:TRP:CD2	3:R:852:GLN:HG3	2.53	0.43
3:R:826:PHE:O	3:R:830:HIS:ND1	2.44	0.43
4:U:168:LEU:HD13	4:U:175:TYR:HE2	1.84	0.43
4:U:451:GLN:HE22	4:U:514:PHE:HB2	1.80	0.43
1:a:1036:ASN:HD22	1:a:1207:ARG:HB2	1.82	0.43
1:b:186:CYS:SG	1:b:203:HIS:NE2	2.86	0.43
1:c:785:TRP:CD2	1:c:789:LEU:HD12	2.53	0.43
1:e:1188:HIS:HA	1:e:1220:ILE:HD12	1.98	0.43
1:B:1213:ASN:O	1:B:1215:SER:N	2.51	0.43
1:C:933:THR:HG21	1:C:1021:ALA:HB1	1.99	0.43
1:D:836:VAL:HG21	1:D:842:ARG:HB2	2.00	0.43
1:D:1096:ASP:HB3	1:D:1100:MET:H	1.82	0.43
1:D:1115:TRP:CZ2	1:D:1167:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ARG:NH2	1:E:950:ASP:O	2.51	0.43
2:H:731:CYS:HA	2:H:734:VAL:HG12	1.99	0.43
2:H:1009:ALA:HA	2:H:1012:MET:HE2	2.00	0.43
2:I:691:LEU:HD12	2:I:692:PRO:HD2	2.00	0.43
2:J:567:PRO:HG3	2:K:854:THR:HA	2.00	0.43
2:K:757:ARG:NE	2:K:794:LEU:O	2.45	0.43
2:K:926:VAL:HG11	2:K:966:LEU:HD11	2.00	0.43
3:R:4:MET:O	3:R:7:THR:OG1	2.29	0.43
3:R:308:PHE:CD2	3:R:569:PRO:HB2	2.53	0.43
3:R:381:PRO:O	3:R:384:THR:OG1	2.30	0.43
3:R:603:MET:HA	3:R:606:ILE:HG22	2.00	0.43
4:U:531:ASP:OD2	4:U:545:ARG:NE	2.46	0.43
1:a:236:SER:OG	1:a:237:ALA:N	2.50	0.43
1:b:1077:PHE:HD2	1:b:1110:PHE:HE1	1.67	0.43
1:d:483:LEU:HA	1:d:486:CYS:HB3	1.99	0.43
1:d:746:GLN:HB2	1:d:813:GLN:HB3	2.00	0.43
1:B:468:ARG:HB2	1:B:1019:VAL:HG11	2.01	0.43
1:B:960:ALA:HB2	1:b:806:MET:HE1	2.01	0.43
1:C:352:LEU:O	1:C:955:LEU:N	2.51	0.43
1:C:853:SER:OG	1:C:854:ARG:N	2.51	0.43
1:D:762:THR:HG22	1:D:765:ARG:HH22	1.83	0.43
1:E:501:VAL:HG23	1:E:502:ASN:H	1.83	0.43
2:I:466:GLN:HA	2:I:469:ARG:HG2	2.01	0.43
2:I:912:ARG:O	2:I:915:THR:OG1	2.30	0.43
2:J:478:VAL:HG21	2:J:481:ARG:HG3	2.00	0.43
3:R:295:PRO:HG3	3:R:1075:LEU:HD21	1.99	0.43
4:U:458:HIS:HA	4:U:461:MET:HE2	2.01	0.43
1:b:542:LEU:HD11	1:b:908:MET:HE2	1.98	0.43
1:b:1033:HIS:O	1:b:1207:ARG:NH1	2.52	0.43
1:c:674:ARG:HG3	1:c:676:SER:H	1.83	0.43
1:c:1095:ARG:HE	1:c:1099:GLY:HA2	1.83	0.43
1:c:1186:SER:OG	1:c:1187:ASP:N	2.51	0.43
1:d:932:VAL:HG12	1:d:994:MET:HG3	2.00	0.43
1:A:958:SER:O	1:A:961:THR:OG1	2.32	0.43
1:C:606:THR:HB	1:C:877:LEU:HD11	2.01	0.43
1:D:1096:ASP:OD1	1:D:1097:GLU:N	2.51	0.43
1:E:224:ILE:O	1:E:228:GLN:NE2	2.52	0.43
1:E:809:MET:HE3	1:E:809:MET:HB2	1.67	0.43
2:H:525:ASP:N	2:H:525:ASP:OD1	2.51	0.43
2:I:926:VAL:HG11	2:I:966:LEU:HD11	2.00	0.43
2:I:1009:ALA:HA	2:I:1012:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:525:ASP:OD1	2:J:525:ASP:N	2.51	0.43
2:J:873:LEU:HD23	2:J:899:LYS:HZ2	1.83	0.43
2:K:709:ILE:HD11	2:K:727:ILE:HD13	2.01	0.43
2:L:745:GLU:HA	2:L:750:ARG:HA	2.01	0.43
3:R:189:CYS:O	3:R:193:ILE:HG12	2.18	0.43
3:R:610:VAL:HG22	3:R:614:SER:HB3	2.00	0.43
1:a:752:THR:HG21	1:a:813:GLN:HE22	1.83	0.43
1:2:69:ALA:HA	1:b:538:ASP:HB3	1.99	0.43
1:A:230:HIS:HB3	1:A:233:VAL:HG22	2.01	0.43
1:A:949:LEU:HD12	1:A:952:ILE:HD12	2.01	0.43
1:B:518:GLN:NE2	1:B:829:PRO:HG2	2.34	0.43
1:E:399:ALA:HA	1:E:402:TRP:HD1	1.83	0.43
1:E:1171:THR:HG22	1:E:1173:THR:H	1.82	0.43
1:E:1201:SER:OG	1:E:1202:THR:N	2.51	0.43
2:H:706:ILE:HA	2:H:757:ARG:HA	2.01	0.43
2:J:583:ASP:OD2	5:J:1301:SAM:N6	2.49	0.43
2:J:745:GLU:HA	2:J:750:ARG:HA	2.01	0.43
2:K:478:VAL:HG21	2:K:481:ARG:HG3	2.00	0.43
2:K:691:LEU:HD12	2:K:692:PRO:HD2	1.99	0.43
2:L:691:LEU:HD12	2:L:692:PRO:HD2	2.00	0.43
2:L:940:LEU:HD21	2:L:1016:MET:HE1	2.00	0.43
3:R:269:PHE:O	3:R:273:THR:HB	2.19	0.43
3:R:452:ARG:NH2	3:R:620:MET:SD	2.91	0.43
3:R:1193:PHE:HE1	3:R:1224:PHE:HA	1.84	0.43
4:U:77:LEU:N	4:U:156:THR:O	2.47	0.43
1:a:507:TYR:CE1	1:a:915:PHE:HB3	2.53	0.43
1:a:609:ASP:O	1:a:612:SER:OG	2.35	0.43
1:4:70:GLU:HG2	1:d:249:HIS:HB2	2.01	0.43
1:A:219:HIS:HB3	3:R:1066:ALA:HB2	2.00	0.43
1:B:762:THR:HG23	1:B:765:ARG:HH21	1.83	0.43
1:C:749:ASN:HD21	2:J:154:SER:H	1.65	0.43
2:H:516:GLY:N	2:H:550:PHE:O	2.52	0.43
2:I:259:SER:OG	2:I:281:GLN:O	2.37	0.43
2:J:466:GLN:HA	2:J:469:ARG:HG2	2.01	0.43
2:J:940:LEU:HD21	2:J:1016:MET:HE1	2.00	0.43
2:K:466:GLN:HA	2:K:469:ARG:HG2	2.01	0.43
2:K:516:GLY:N	2:K:550:PHE:O	2.52	0.43
3:R:919:TYR:HD2	3:R:936:CYS:HB3	1.83	0.43
1:a:474:ILE:HD12	1:a:507:TYR:HB2	2.00	0.43
1:a:1056:TRP:CZ3	1:a:1058:PRO:HA	2.53	0.43
1:b:1246:GLN:NE2	1:b:1252:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:223:PHE:HD2	1:d:910:ALA:HA	1.83	0.43
1:d:1095:ARG:HA	1:d:1101:MET:HG3	1.99	0.43
1:A:452:GLU:OE2	1:A:1259:ARG:NH2	2.49	0.43
1:A:584:SER:OG	1:A:585:ASN:N	2.48	0.43
1:B:327:PRO:HB2	1:B:1148:LEU:HD12	2.01	0.43
2:H:446:ARG:HG3	2:H:668:SER:HB3	2.00	0.43
2:I:886:VAL:HB	2:I:922:LEU:HB2	2.01	0.43
2:L:194:ASP:OD1	2:L:194:ASP:N	2.51	0.43
3:R:34:PHE:O	3:R:153:LYS:NZ	2.50	0.43
1:b:870:THR:OG1	1:b:871:VAL:N	2.52	0.43
1:c:515:GLN:HG2	1:c:730:ALA:HA	2.00	0.43
1:c:1049:ARG:NH1	1:c:1131:LYS:O	2.51	0.43
1:d:632:LEU:HD23	1:d:651:THR:HG21	2.01	0.43
1:2:89:GLY:HA3	1:2:137:GLY:HA3	2.01	0.43
1:A:214:SER:HA	1:A:217:GLN:NE2	2.33	0.43
1:B:324:MET:HE3	1:B:331:ASN:HD21	1.83	0.43
1:C:212:THR:H	1:C:217:GLN:HE22	1.67	0.43
1:C:1044:ASP:HB3	1:C:1141:MET:H	1.83	0.43
1:E:382:HIS:HD2	1:d:353:MET:HE3	1.83	0.43
2:H:407:VAL:HA	2:H:772:LEU:HD23	2.01	0.43
2:I:525:ASP:OD1	2:I:525:ASP:N	2.51	0.43
2:J:552:TYR:HA	2:J:559:ILE:HG22	1.99	0.43
2:J:709:ILE:HD11	2:J:727:ILE:HD13	2.00	0.43
2:K:577:ASP:CG	5:K:1301:SAM:N	2.70	0.43
2:L:466:GLN:HA	2:L:469:ARG:HG2	2.01	0.43
2:L:1009:ALA:HA	2:L:1012:MET:HE2	2.00	0.43
3:R:1225:LEU:HD13	3:R:1225:LEU:HA	1.90	0.43
1:b:283:TYR:HB2	1:b:290:TYR:HB2	2.01	0.43
1:c:306:VAL:HG21	1:c:1038:PHE:CD1	2.54	0.43
1:e:398:ASP:HB2	1:e:401:LYS:HG2	2.01	0.43
1:5:11:LYS:HD3	1:e:321:SER:H	1.84	0.43
1:5:82:ASP:OD1	1:5:85:GLY:N	2.48	0.43
1:A:192:SER:HB3	1:A:195:ASP:HB2	2.01	0.43
1:A:390:ASN:OD1	1:A:433:ARG:NH2	2.52	0.43
1:A:731:ASN:HD22	1:A:737:GLU:H	1.66	0.43
1:B:572:SER:OG	3:R:1205:ARG:NH2	2.52	0.43
1:C:546:ILE:HD13	1:C:822:ILE:HD11	2.00	0.43
1:D:438:GLN:NE2	1:D:440:MET:O	2.52	0.43
1:E:761:LEU:HD13	1:E:761:LEU:HA	1.83	0.43
2:H:578:VAL:CG2	5:H:1301:SAM:C4	2.60	0.43
2:I:512:VAL:HG12	2:I:573:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:940:LEU:HD21	2:I:1016:MET:HE1	2.00	0.43
2:J:851:ILE:HG22	2:J:871:ASP:HA	2.00	0.43
2:K:407:VAL:HA	2:K:772:LEU:HD23	2.01	0.43
2:L:709:ILE:HD11	2:L:727:ILE:HD13	2.01	0.43
2:L:926:VAL:HG11	2:L:966:LEU:HD11	2.00	0.43
1:a:1119:THR:O	1:a:1123:ASN:HB2	2.19	0.43
1:b:430:ARG:O	1:b:1254:TYR:OH	2.36	0.43
1:c:339:LEU:HD23	1:c:353:MET:HE3	2.01	0.43
1:e:308:THR:HG21	1:e:322:VAL:H	1.84	0.43
1:e:1094:ILE:HB	1:e:1104:PHE:HE1	1.84	0.43
1:A:1052:SER:OG	1:A:1054:HIS:ND1	2.42	0.42
1:B:562:THR:OG1	1:B:799:LYS:NZ	2.36	0.42
1:C:713:TRP:HD1	1:C:837:ARG:HG3	1.84	0.42
1:D:1027:THR:HA	1:D:1030:VAL:HG22	2.01	0.42
2:I:194:ASP:OD1	2:I:194:ASP:N	2.51	0.42
3:R:509:ILE:HG13	3:R:510:LEU:HD22	2.01	0.42
3:R:700:GLU:HB2	3:R:725:ILE:HD13	1.99	0.42
1:e:524:ASN:HA	1:e:986:PRO:HG2	2.02	0.42
1:A:278:GLN:HE21	1:A:281:LEU:HB3	1.84	0.42
1:C:199:HIS:O	1:C:202:SER:OG	2.31	0.42
1:C:1002:GLN:HE22	1:C:1004:TYR:HA	1.84	0.42
1:E:684:TRP:HB3	1:E:689:MET:HE3	2.02	0.42
2:H:259:SER:OG	2:H:281:GLN:O	2.37	0.42
2:H:397:LEU:HB2	2:L:560:VAL:HG22	2.00	0.42
2:H:512:VAL:HG12	2:H:573:PHE:HB3	2.01	0.42
2:H:935:THR:HB	2:H:942:ILE:HG12	2.00	0.42
2:I:516:GLY:N	2:I:550:PHE:O	2.52	0.42
2:I:709:ILE:HD11	2:I:727:ILE:HD13	2.00	0.42
2:I:745:GLU:HA	2:I:750:ARG:HA	2.01	0.42
2:J:407:VAL:HA	2:J:772:LEU:HD23	2.01	0.42
2:J:516:GLY:N	2:J:550:PHE:O	2.52	0.42
2:L:886:VAL:HB	2:L:922:LEU:HB2	2.01	0.42
3:R:586:ILE:HD12	3:R:769:TRP:HE3	1.85	0.42
4:U:135:ILE:HG23	4:U:136:SER:H	1.84	0.42
4:U:377:MET:HA	4:U:378:PRO:HD3	1.78	0.42
1:e:186:CYS:HB3	1:e:203:HIS:CE1	2.55	0.42
1:e:417:SER:HB2	1:e:1215:SER:HA	2.01	0.42
1:e:638:LEU:HD11	1:e:886:LEU:HD11	2.00	0.42
1:B:440:MET:HE1	1:B:499:PRO:HB2	2.01	0.42
1:C:565:GLU:HG2	1:C:792:SER:HB2	2.00	0.42
1:E:483:LEU:HD21	1:E:915:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:926:VAL:HG11	2:H:966:LEU:HD11	2.00	0.42
2:I:407:VAL:HA	2:I:772:LEU:HD23	2.01	0.42
2:I:478:VAL:HG21	2:I:481:ARG:HG3	2.00	0.42
2:I:851:ILE:HG22	2:I:871:ASP:HA	2.00	0.42
2:J:446:ARG:HG3	2:J:668:SER:HB3	2.00	0.42
2:J:926:VAL:HG11	2:J:966:LEU:HD11	2.00	0.42
2:J:935:THR:HB	2:J:942:ILE:HG12	2.00	0.42
2:K:745:GLU:HA	2:K:750:ARG:HA	2.01	0.42
3:R:82:ARG:HH21	3:R:386:LEU:HD13	1.84	0.42
3:R:706:TRP:CZ3	3:R:763:TYR:HB2	2.54	0.42
3:R:1215:MET:HE1	3:R:1253:GLY:HA3	2.01	0.42
4:U:210:ILE:HG21	4:U:242:HIS:CD2	2.55	0.42
1:a:588:PHE:HE1	1:a:884:VAL:HG13	1.84	0.42
1:b:363:LEU:O	1:b:367:LEU:HB3	2.19	0.42
1:b:852:GLN:HG3	1:b:858:THR:HG21	2.01	0.42
1:b:1049:ARG:HG3	1:b:1198:TYR:HE1	1.84	0.42
1:b:1204:TYR:CZ	1:b:1206:ASP:HB3	2.54	0.42
1:e:1034:GLU:OE2	1:e:1207:ARG:NH2	2.52	0.42
1:A:664:MET:HE3	1:A:664:MET:HB2	1.91	0.42
1:B:704:GLN:HE22	1:B:774:ASN:ND2	2.17	0.42
1:B:858:THR:HG23	1:B:942:GLN:HB2	2.02	0.42
1:B:1169:GLU:HB2	1:B:1176:PRO:HG3	2.00	0.42
1:C:1207:ARG:NH2	1:C:1249:GLU:O	2.52	0.42
1:D:307:HIS:CD2	1:D:323:ILE:HG23	2.55	0.42
1:D:721:TYR:CD1	1:D:739:LEU:HB2	2.55	0.42
1:D:852:GLN:HA	1:D:995:THR:HA	2.01	0.42
2:H:542:PRO:HA	2:H:543:PRO:HD3	1.90	0.42
2:J:542:PRO:HA	2:J:543:PRO:HD3	1.89	0.42
2:K:525:ASP:OD1	2:K:525:ASP:N	2.51	0.42
2:K:886:VAL:HB	2:K:922:LEU:HB2	2.01	0.42
2:L:259:SER:OG	2:L:281:GLN:O	2.37	0.42
3:R:210:LEU:HG	3:R:212:ALA:H	1.84	0.42
3:R:470:LEU:HA	3:R:473:ILE:HG12	2.00	0.42
3:R:586:ILE:HD12	3:R:769:TRP:CE3	2.54	0.42
1:a:600:TYR:OH	1:a:828:PHE:O	2.34	0.42
1:b:1096:ASP:OD1	1:b:1097:GLU:N	2.53	0.42
1:d:340:ASN:OD1	1:d:350:ASN:HB2	2.19	0.42
1:B:350:ASN:ND2	1:B:353:MET:SD	2.93	0.42
1:C:435:ASP:HB3	1:C:449:ASP:HB2	2.00	0.42
1:C:1171:THR:HG22	1:C:1173:THR:H	1.84	0.42
2:H:194:ASP:N	2:H:194:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:478:VAL:HG21	2:H:481:ARG:HG3	2.01	0.42
2:H:572:GLN:HE22	2:I:956:ARG:HG2	1.84	0.42
2:I:706:ILE:HA	2:I:757:ARG:HA	2.01	0.42
2:J:886:VAL:HB	2:J:922:LEU:HB2	2.01	0.42
2:K:47:ARG:HB3	2:K:54:ILE:HD13	2.01	0.42
2:L:47:ARG:HB3	2:L:54:ILE:HD13	2.01	0.42
3:R:362:VAL:HG22	3:R:1079:ALA:HB2	2.01	0.42
3:R:948:MET:HA	3:R:951:LEU:HD23	2.01	0.42
1:a:1018:SER:OG	1:a:1019:VAL:N	2.52	0.42
1:c:945:VAL:HG13	1:c:947:ARG:HE	1.85	0.42
1:d:1047:ILE:HD11	1:d:1166:TRP:HZ3	1.84	0.42
1:e:392:ARG:HH12	1:e:1259:ARG:CZ	2.33	0.42
1:e:536:LEU:HD12	1:e:593:VAL:HG23	2.00	0.42
1:e:1066:VAL:HG21	1:e:1202:THR:HG22	2.00	0.42
1:B:313:ASN:HD22	1:B:395:PRO:HG2	1.84	0.42
1:B:714:PRO:HA	1:B:760:GLU:OE2	2.19	0.42
1:E:785:TRP:HD1	1:E:789:LEU:HD23	1.85	0.42
1:E:1130:ILE:HG23	1:E:1160:TRP:HH2	1.84	0.42
2:I:47:ARG:HB3	2:I:54:ILE:HD13	2.01	0.42
2:K:567:PRO:HB2	2:L:832:PRO:HB3	2.01	0.42
1:a:1031:PHE:HZ	1:a:1040:ILE:HD12	1.84	0.42
1:b:776:VAL:HG11	1:b:793:MET:HG2	2.02	0.42
1:c:366:VAL:HG11	1:c:1024:VAL:HG22	2.02	0.42
1:d:306:VAL:HG21	1:d:1038:PHE:CD1	2.55	0.42
1:d:1082:ARG:H	1:d:1095:ARG:HB3	1.83	0.42
1:d:1151:TYR:CZ	1:d:1183:PRO:HB3	2.54	0.42
1:e:464:ARG:NH2	1:e:1022:ASP:OD2	2.49	0.42
1:e:729:SER:OG	1:e:731:ASN:OD1	2.33	0.42
1:3:11:LYS:HB2	1:c:320:SER:HA	2.01	0.42
1:A:244:THR:HG21	1:A:534:PRO:HG2	2.02	0.42
1:A:457:LEU:O	1:A:460:SER:OG	2.36	0.42
1:A:686:ARG:HA	1:A:689:MET:HB2	2.01	0.42
1:C:276:VAL:HG13	1:C:277:PRO:HD3	2.01	0.42
1:C:459:VAL:HG21	1:C:1255:ASN:HD21	1.85	0.42
1:D:608:ILE:HD12	1:D:608:ILE:HA	1.89	0.42
2:H:514:TYR:HB3	2:H:549:GLN:HA	2.00	0.42
2:I:44:ARG:NH2	2:I:58:GLN:OE1	2.49	0.42
2:I:181:ASP:OD1	2:J:91:ARG:NH2	2.52	0.42
2:L:407:VAL:HA	2:L:772:LEU:HD23	2.01	0.42
2:L:478:VAL:HG21	2:L:481:ARG:HG3	2.01	0.42
3:R:714:PRO:O	3:R:718:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:405:PHE:HB2	4:U:407:LYS:NZ	2.34	0.42
1:b:504:LEU:HD23	1:b:506:PRO:HD3	2.02	0.42
1:c:559:THR:HG22	1:c:799:LYS:HD3	2.01	0.42
1:c:963:ALA:HA	1:c:992:PRO:HG3	2.02	0.42
1:c:1166:TRP:CD1	1:c:1176:PRO:HG2	2.54	0.42
1:d:649:PHE:HA	1:d:705:TRP:HE1	1.83	0.42
1:e:1095:ARG:NH2	1:e:1099:GLY:HA2	2.35	0.42
1:4:133:LEU:O	1:d:527:ASN:ND2	2.52	0.42
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.90	0.42
1:C:392:ARG:HH12	1:C:1259:ARG:HE	1.67	0.42
1:E:346:VAL:HG13	1:E:347:ARG:HG3	2.02	0.42
2:H:886:VAL:HB	2:H:922:LEU:HB2	2.01	0.42
2:I:552:TYR:CZ	2:J:782:VAL:HG11	2.55	0.42
2:I:733:ASN:O	2:I:762:SER:OG	2.33	0.42
2:J:259:SER:OG	2:J:281:GLN:O	2.37	0.42
2:J:512:VAL:HG12	2:J:573:PHE:HB3	2.01	0.42
2:J:908:GLN:HA	2:J:911:VAL:HG12	2.02	0.42
2:K:706:ILE:HA	2:K:757:ARG:HA	2.01	0.42
2:L:516:GLY:N	2:L:550:PHE:O	2.52	0.42
3:R:486:LYS:HB3	3:R:486:LYS:HE3	1.80	0.42
3:R:659:PHE:CE2	3:R:681:PRO:HD3	2.54	0.42
3:R:1173:ALA:HB1	3:R:1178:LEU:HB3	2.02	0.42
4:U:301:LEU:O	4:U:388:THR:OG1	2.35	0.42
4:U:532:SER:HA	4:U:535:LEU:HB2	2.01	0.42
1:a:1220:ILE:HG22	1:a:1221:ALA:H	1.83	0.42
1:c:515:GLN:O	1:c:519:ILE:HG12	2.20	0.42
1:c:588:PHE:HE1	1:c:884:VAL:HG13	1.85	0.42
1:c:1233:ASN:ND2	1:c:1244:GLN:OE1	2.52	0.42
1:e:306:VAL:HG21	1:e:1038:PHE:CD1	2.54	0.42
1:e:560:MET:HG3	1:e:578:LEU:HD21	2.01	0.42
1:1:86:ASN:ND2	1:1:151:SER:H	2.17	0.42
1:4:149:PRO:O	1:4:152:THR:OG1	2.34	0.42
1:A:457:LEU:HD12	1:A:1030:VAL:HG11	2.02	0.42
1:A:777:ASP:OD1	1:A:794:ARG:NH2	2.48	0.42
1:D:482:ALA:HB1	1:D:723:THR:HG21	2.02	0.42
1:E:243:LYS:HD3	1:E:524:ASN:HD21	1.84	0.42
1:E:1096:ASP:OD1	1:E:1097:GLU:N	2.53	0.42
2:H:485:LYS:NZ	2:H:643:PRO:O	2.53	0.42
2:H:745:GLU:HA	2:H:750:ARG:HA	2.01	0.42
2:K:143:ILE:HD12	2:K:146:LEU:HD23	2.02	0.42
2:L:542:PRO:HA	2:L:543:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:914:MET:HE3	3:R:914:MET:HB3	1.75	0.42
3:R:1183:THR:HG1	3:R:1184:TRP:CD1	2.38	0.42
4:U:685:ALA:N	4:U:709:TYR:OH	2.52	0.42
4:U:693:PRO:HB2	4:U:695:LYS:HG3	2.02	0.42
1:a:653:ALA:HB1	1:a:671:GLN:HE21	1.85	0.42
1:a:686:ARG:HA	1:a:689:MET:HE2	2.01	0.42
1:c:608:ILE:HD12	1:c:636:LEU:HD23	2.01	0.42
1:1:106:THR:HG22	1:1:122:TYR:H	1.85	0.42
1:B:1186:SER:OG	1:B:1187:ASP:N	2.52	0.42
1:C:514:ARG:HH12	1:C:727:PHE:HD2	1.67	0.42
1:E:409:THR:HG1	1:E:428:ARG:HH21	1.65	0.42
1:E:705:TRP:HE3	1:E:771:LEU:HD13	1.84	0.42
1:E:1058:PRO:HD2	1:E:1182:VAL:HB	2.02	0.42
2:H:221:LEU:HB2	2:H:234:ILE:HB	2.02	0.42
2:H:466:GLN:HA	2:H:469:ARG:HG2	2.01	0.42
2:K:702:SER:OG	2:K:704:THR:O	2.28	0.42
4:U:212:THR:OG1	4:U:215:CYS:HB2	2.20	0.42
1:a:505:MET:HB2	1:a:507:TYR:CE2	2.55	0.42
1:a:851:ARG:NH1	1:a:990:GLY:O	2.53	0.42
1:c:1115:TRP:HZ3	1:c:1126:PHE:HD2	1.68	0.42
1:1:63:GLN:HA	1:1:66:THR:HG22	2.02	0.41
1:1:154:ILE:HA	1:1:157:ALA:HB3	2.02	0.41
1:A:864:LEU:HD21	1:A:1000:GLN:HG2	2.02	0.41
1:B:1083:ILE:HD12	1:B:1121:TYR:CE2	2.55	0.41
1:E:849:VAL:O	1:E:869:THR:N	2.52	0.41
2:I:908:GLN:HA	2:I:911:VAL:HG12	2.02	0.41
2:I:1012:MET:HE2	2:I:1012:MET:HB3	1.90	0.41
2:J:47:ARG:HB3	2:J:54:ILE:HD13	2.01	0.41
2:K:940:LEU:HD21	2:K:1016:MET:HE1	2.00	0.41
2:L:150:GLY:HA2	1:d:698:ASP:CG	2.45	0.41
3:R:277:PHE:O	3:R:281:THR:OG1	2.27	0.41
3:R:369:MET:HG3	3:R:792:ILE:HG21	2.02	0.41
4:U:668:ILE:HB	4:U:684:LYS:HB2	2.01	0.41
1:a:518:GLN:NE2	1:a:829:PRO:O	2.52	0.41
1:c:600:TYR:OH	1:c:828:PHE:O	2.33	0.41
1:d:273:PRO:HA	1:d:299:ALA:HB1	2.02	0.41
1:d:860:PRO:HB2	1:d:862:LEU:HD23	2.01	0.41
1:d:1048:GLY:HA3	1:d:1136:ARG:HD3	2.01	0.41
1:e:436:ARG:HA	1:e:448:VAL:HA	2.02	0.41
1:e:841:ASP:HA	1:e:1004:TYR:HB3	2.02	0.41
1:A:793:MET:HE2	1:A:793:MET:HB2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:MET:HE3	1:C:809:MET:HB2	1.83	0.41
1:D:859:GLN:HA	1:D:860:PRO:HD3	1.91	0.41
2:H:143:ILE:HD12	2:H:146:LEU:HD23	2.02	0.41
2:K:221:LEU:HB2	2:K:234:ILE:HB	2.02	0.41
3:R:106:HIS:HE1	3:R:108:THR:HG22	1.85	0.41
3:R:821:ILE:HD13	3:R:824:ILE:HD12	2.02	0.41
3:R:881:PHE:HD2	3:R:910:MET:HG2	1.85	0.41
1:a:468:ARG:NH1	1:a:471:ARG:HH21	2.17	0.41
1:b:338:LEU:HD13	1:b:357:ASN:HA	2.01	0.41
1:b:418:LYS:NZ	1:b:1212:THR:OG1	2.53	0.41
1:b:649:PHE:HA	1:b:705:TRP:NE1	2.34	0.41
1:b:1002:GLN:HB3	1:b:1008:THR:HG22	2.02	0.41
1:b:1003:GLN:HE21	1:b:1007:ARG:HB2	1.85	0.41
1:c:858:THR:OG1	1:c:859:GLN:N	2.53	0.41
1:c:926:GLU:HB3	1:c:1020:ILE:HD12	2.01	0.41
1:c:1213:ASN:O	1:c:1216:SER:OG	2.34	0.41
1:d:1096:ASP:OD1	1:d:1097:GLU:N	2.53	0.41
1:A:190:LEU:HA	1:B:550:GLN:HE22	1.86	0.41
1:C:503:ARG:HH11	1:C:1270:VAL:HG22	1.85	0.41
1:C:660:GLU:HG3	1:C:699:ALA:HB2	2.03	0.41
1:E:362:LEU:HD22	1:E:1027:THR:HG22	2.02	0.41
1:E:755:LEU:HA	1:E:809:MET:HE1	2.02	0.41
2:H:511:SER:OG	2:H:572:GLN:OE1	2.39	0.41
2:H:516:GLY:O	5:H:1301:SAM:HG2	2.19	0.41
2:H:562:LEU:HG	5:H:1301:SAM:H2	2.02	0.41
4:U:444:ASP:OD1	4:U:445:SER:N	2.53	0.41
1:a:581:LEU:O	1:a:880:ARG:NH1	2.50	0.41
1:a:807:THR:HG21	1:a:886:LEU:HA	2.02	0.41
1:d:193:PRO:HA	1:d:196:LEU:HB2	2.03	0.41
1:d:306:VAL:HG21	1:d:1038:PHE:HD1	1.86	0.41
1:d:705:TRP:HE3	1:d:771:LEU:HD13	1.85	0.41
1:1:142:GLU:OE2	1:a:958:SER:OG	2.26	0.41
1:2:110:ALA:HB2	1:2:118:ALA:HB2	2.02	0.41
1:3:3:ARG:NH1	1:c:314:VAL:O	2.53	0.41
1:4:120:VAL:HG11	1:d:593:VAL:HG21	2.03	0.41
1:A:314:VAL:HG22	1:A:316:PHE:H	1.85	0.41
1:A:854:ARG:HD2	1:a:757:PHE:CE2	2.55	0.41
1:B:406:MET:HA	1:B:453:THR:HG22	2.03	0.41
2:H:903:PHE:HE2	2:H:927:ASN:HB3	1.85	0.41
2:I:511:SER:OG	2:I:572:GLN:OE1	2.39	0.41
2:K:578:VAL:HG23	5:K:1301:SAM:C2'	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:327:PRO:HB2	1:a:1148:LEU:HD23	2.02	0.41
1:a:406:MET:HB3	1:a:406:MET:HE2	1.87	0.41
1:b:858:THR:OG1	1:b:859:GLN:OE1	2.38	0.41
1:e:1201:SER:OG	1:e:1202:THR:N	2.53	0.41
1:2:74:LYS:HE2	1:b:530:THR:HG22	2.02	0.41
1:A:207:GLY:HA3	1:C:184:HIS:HB2	2.02	0.41
1:A:457:LEU:O	1:A:461:ILE:HG12	2.21	0.41
1:E:829:PRO:HA	1:E:830:PRO:HD3	1.93	0.41
2:I:221:LEU:HB2	2:I:234:ILE:HB	2.02	0.41
2:J:706:ILE:HA	2:J:757:ARG:HA	2.01	0.41
2:J:915:THR:HG22	2:J:974:TRP:HE1	1.85	0.41
2:K:512:VAL:HG12	2:K:573:PHE:HB3	2.01	0.41
2:L:613:VAL:HG22	2:L:654:VAL:HG13	2.03	0.41
3:R:404:TRP:C	3:R:415:LYS:HZ2	2.28	0.41
3:R:819:ASP:OD1	3:R:953:ARG:NH1	2.53	0.41
3:R:874:GLY:HA3	3:R:894:THR:HG22	2.02	0.41
3:R:919:TYR:CD2	3:R:936:CYS:HB3	2.55	0.41
4:U:574:TYR:HA	4:U:577:LYS:HZ2	1.85	0.41
1:c:1057:SER:HB3	1:c:1223:PRO:HB3	2.03	0.41
1:d:478:GLU:OE1	1:d:508:ARG:NH2	2.53	0.41
1:e:1059:LEU:HD12	1:e:1205:ASN:HB3	2.00	0.41
1:4:127:ILE:HD11	1:d:607:VAL:HG11	2.01	0.41
1:A:807:THR:HG21	1:A:886:LEU:HA	2.02	0.41
1:C:417:SER:OG	1:C:420:CYS:SG	2.76	0.41
1:D:230:HIS:ND1	1:D:232:ILE:HG12	2.36	0.41
1:D:338:LEU:HG	1:D:339:LEU:HG	2.02	0.41
2:H:25:TYR:CE1	2:H:30:PHE:HB2	2.56	0.41
2:H:908:GLN:HA	2:H:911:VAL:HG12	2.02	0.41
2:I:915:THR:HG22	2:I:974:TRP:HE1	1.85	0.41
2:L:100:ILE:HG21	2:L:133:LEU:HD21	2.03	0.41
2:L:903:PHE:HE2	2:L:927:ASN:HB3	1.85	0.41
1:b:480:GLU:HB2	1:b:493:VAL:HG23	2.03	0.41
1:d:427:VAL:HG22	1:d:1235:LEU:HB2	2.02	0.41
1:d:455:ASP:OD1	1:d:455:ASP:N	2.51	0.41
1:d:577:ILE:HD12	1:d:627:TRP:CZ3	2.55	0.41
1:d:1166:TRP:NE1	1:d:1176:PRO:O	2.51	0.41
1:4:133:LEU:HD22	1:d:864:LEU:HG	2.02	0.41
1:C:732:LEU:HD23	1:C:999:ILE:HG21	2.01	0.41
1:C:853:SER:HB3	1:C:994:MET:HB3	2.03	0.41
1:D:507:TYR:CE1	1:D:915:PHE:HB3	2.55	0.41
1:E:278:GLN:HE21	1:E:281:LEU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ARG:HB3	2:H:54:ILE:HD13	2.01	0.41
2:I:100:ILE:HG21	2:I:133:LEU:HD21	2.03	0.41
2:J:25:TYR:CE1	2:J:30:PHE:HB2	2.56	0.41
2:J:44:ARG:NH2	2:J:58:GLN:OE1	2.49	0.41
2:K:194:ASP:N	2:K:194:ASP:OD1	2.51	0.41
2:K:259:SER:OG	2:K:281:GLN:O	2.37	0.41
2:K:485:LYS:NZ	2:K:643:PRO:O	2.53	0.41
2:K:511:SER:OG	2:K:572:GLN:OE1	2.39	0.41
2:K:903:PHE:HE2	2:K:927:ASN:HB3	1.85	0.41
2:L:221:LEU:HB2	2:L:234:ILE:HB	2.02	0.41
2:L:512:VAL:HG12	2:L:573:PHE:HB3	2.01	0.41
3:R:325:PRO:HD3	3:R:754:GLN:NE2	2.36	0.41
3:R:910:MET:O	3:R:914:MET:HG2	2.21	0.41
1:a:399:ALA:HA	1:a:402:TRP:HD1	1.86	0.41
1:a:846:MET:SD	1:a:1002:GLN:NE2	2.93	0.41
1:c:713:TRP:HD1	1:c:837:ARG:HG3	1.86	0.41
1:e:599:LEU:HD11	1:e:819:LEU:HD22	2.02	0.41
1:1:77:ASP:OD1	1:1:80:THR:OG1	2.29	0.41
1:3:97:GLU:OE1	1:3:136:SER:OG	2.32	0.41
1:A:1085:PHE:HE1	1:a:496:PRO:HB2	1.86	0.41
1:A:1171:THR:HG22	1:A:1173:THR:H	1.86	0.41
1:B:742:PRO:HB2	1:B:743:ILE:HD12	2.03	0.41
1:B:807:THR:HG21	1:B:886:LEU:HA	2.01	0.41
1:D:433:ARG:HA	1:D:450:VAL:HG12	2.01	0.41
2:I:25:TYR:CE1	2:I:30:PHE:HB2	2.56	0.41
2:J:511:SER:OG	2:J:572:GLN:OE1	2.39	0.41
2:K:25:TYR:CE1	2:K:30:PHE:HB2	2.56	0.41
2:K:100:ILE:HG21	2:K:133:LEU:HD21	2.03	0.41
2:K:830:THR:H	2:K:850:ASP:HB2	1.86	0.41
2:K:908:GLN:HA	2:K:911:VAL:HG12	2.02	0.41
3:R:417:THR:HG21	1:e:554:THR:HG22	2.03	0.41
3:R:1245:ILE:HD12	3:R:1252:LEU:HD13	2.02	0.41
1:a:821:VAL:HG11	1:a:905:ILE:HD12	2.01	0.41
1:b:723:THR:OG1	1:b:725:ASN:OD1	2.38	0.41
1:c:548:PRO:HG3	1:c:900:TRP:CD1	2.56	0.41
1:d:543:LEU:HA	1:d:546:ILE:HG22	2.03	0.41
1:d:1056:TRP:CZ3	1:d:1058:PRO:HA	2.56	0.41
1:A:192:SER:HA	1:A:193:PRO:HD3	1.88	0.41
1:A:739:LEU:HD12	1:A:832:GLN:HE22	1.86	0.41
1:A:1272:MET:SD	1:A:1272:MET:N	2.94	0.41
1:B:457:LEU:O	1:B:461:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:ASN:HB3	1:B:781:TYR:HD2	1.86	0.41
1:C:219:HIS:HA	1:C:222:GLU:HG2	2.02	0.41
1:C:713:TRP:CD1	1:C:837:ARG:HG3	2.56	0.41
1:C:970:ASN:HD22	1:C:988:LEU:HD11	1.86	0.41
1:D:476:PRO:HA	1:D:479:ILE:HD12	2.03	0.41
1:D:670:THR:OG1	1:D:671:GLN:N	2.54	0.41
1:D:993:ARG:NH2	1:d:752:THR:O	2.49	0.41
1:E:249:HIS:CE1	4:U:241:ILE:HD11	2.55	0.41
2:I:282:CYS:HB3	2:I:305:SER:HB2	2.03	0.41
2:I:903:PHE:HE2	2:I:927:ASN:HB3	1.85	0.41
2:J:194:ASP:OD1	2:J:194:ASP:N	2.51	0.41
2:J:474:LEU:HD21	2:K:274:GLN:HE21	1.86	0.41
2:K:112:ASN:HD22	2:K:115:VAL:HG23	1.86	0.41
2:K:912:ARG:O	2:K:915:THR:OG1	2.30	0.41
2:L:25:TYR:CE1	2:L:30:PHE:HB2	2.56	0.41
2:L:706:ILE:HA	2:L:757:ARG:HA	2.01	0.41
2:L:935:THR:HB	2:L:942:ILE:HG12	2.01	0.41
3:R:135:THR:HG22	3:R:668:SER:HA	2.02	0.41
1:b:552:ASP:OD2	1:b:890:LYS:NZ	2.54	0.41
1:b:604:VAL:HG23	1:b:873:VAL:HG23	2.02	0.41
1:b:858:THR:HG1	1:b:859:GLN:H	1.68	0.41
1:b:1052:SER:OG	1:b:1054:HIS:ND1	2.44	0.41
1:c:621:THR:HG22	1:c:783:PRO:HD2	2.02	0.41
1:c:931:LEU:HD12	1:c:984:LEU:HD13	2.03	0.41
1:c:1037:LEU:HD13	1:c:1037:LEU:HA	1.96	0.41
1:c:1120:ARG:HH22	1:c:1168:GLU:HA	1.85	0.41
1:c:1163:THR:HG23	1:c:1199:ILE:HD11	2.03	0.41
1:e:332:ILE:HD11	1:e:1177:SER:HB2	2.03	0.41
1:e:536:LEU:HD13	1:e:536:LEU:HA	1.96	0.41
1:e:1096:ASP:OD1	1:e:1097:GLU:N	2.54	0.41
1:e:1150:TYR:HB3	1:e:1184:ILE:HD11	2.02	0.41
1:2:11:LYS:NZ	1:b:364:GLU:OE2	2.43	0.41
1:4:135:ARG:HB3	1:d:864:LEU:HD21	2.03	0.41
1:5:101:GLU:OE1	1:e:529:ALA:N	2.54	0.41
1:C:521:ARG:HA	1:C:524:ASN:HD22	1.85	0.41
1:C:721:TYR:CE1	1:C:739:LEU:HB2	2.55	0.41
1:C:1166:TRP:CD1	1:C:1176:PRO:HG2	2.56	0.41
1:D:306:VAL:HG21	1:D:1038:PHE:CD1	2.56	0.41
1:D:601:ASN:OD1	1:D:602:GLY:N	2.54	0.41
1:E:253:PRO:HB3	1:E:979:LEU:HD11	2.03	0.41
1:E:402:TRP:O	1:E:406:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:282:CYS:HB3	2:J:305:SER:HB2	2.03	0.41
2:J:485:LYS:NZ	2:J:643:PRO:O	2.53	0.41
2:K:514:TYR:N	2:K:548:ARG:O	2.47	0.41
2:K:562:LEU:CG	5:K:1301:SAM:C2	2.98	0.41
2:L:207:LEU:HD23	2:L:207:LEU:HA	1.95	0.41
2:L:830:THR:H	2:L:850:ASP:HB2	1.86	0.41
2:L:908:GLN:HA	2:L:911:VAL:HG12	2.02	0.41
4:U:341:ARG:HH21	4:U:347:PHE:HE1	1.69	0.41
1:a:455:ASP:HB3	1:a:1253:LEU:HD23	2.03	0.41
1:a:711:ARG:HH11	1:a:711:ARG:HD3	1.75	0.41
1:a:1050:VAL:HG21	1:a:1065:LEU:HD11	2.03	0.41
1:b:1148:LEU:HD23	1:b:1180:PHE:HB2	2.02	0.41
1:d:490:TYR:HE2	1:d:817:VAL:HG11	1.85	0.41
1:2:131:ASN:HB2	1:C:498:ALA:HB3	2.04	0.40
1:3:86:ASN:OD1	1:3:150:MET:N	2.54	0.40
1:5:11:LYS:HD2	1:e:320:SER:CA	2.33	0.40
1:A:515:GLN:O	1:A:519:ILE:HG12	2.22	0.40
1:B:529:ALA:HA	1:B:532:ILE:HG22	2.02	0.40
1:B:1096:ASP:OD1	1:B:1097:GLU:N	2.54	0.40
1:C:399:ALA:HA	1:C:402:TRP:HD1	1.85	0.40
1:C:543:LEU:HA	1:C:546:ILE:HG12	2.04	0.40
2:I:764:ARG:HD2	2:I:841:PRO:HA	2.03	0.40
2:J:112:ASN:HD22	2:J:115:VAL:HG23	1.86	0.40
2:J:560:VAL:HG22	2:K:397:LEU:HB2	2.02	0.40
2:J:903:PHE:HE2	2:J:927:ASN:HB3	1.85	0.40
3:R:470:LEU:HD12	3:R:473:ILE:HD11	2.03	0.40
4:U:100:ARG:HH22	1:d:564:SER:HA	1.86	0.40
1:a:468:ARG:HH12	1:a:471:ARG:HH21	1.68	0.40
1:d:186:CYS:HB3	1:d:203:HIS:HE1	1.86	0.40
1:A:582:ARG:HH12	3:R:1191:THR:HG23	1.86	0.40
1:B:518:GLN:HE22	1:B:829:PRO:HG2	1.86	0.40
1:B:1067:PHE:CE2	1:B:1107:ASN:HB3	2.56	0.40
1:B:1166:TRP:HE3	1:B:1167:LEU:HD22	1.85	0.40
1:C:263:CYS:SG	1:C:462:ARG:NH1	2.94	0.40
1:D:416:VAL:HG21	1:c:1084:SER:HB3	2.03	0.40
2:H:282:CYS:HB3	2:H:305:SER:HB2	2.03	0.40
2:H:514:TYR:N	2:H:548:ARG:O	2.47	0.40
2:H:764:ARG:HD2	2:H:841:PRO:HA	2.03	0.40
2:H:1011:LEU:HA	2:H:1014:LYS:HZ3	1.85	0.40
2:L:578:VAL:HA	5:L:1301:SAM:H5'2	2.03	0.40
1:a:1049:ARG:NH1	1:a:1131:LYS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:1109:ILE:HG12	1:c:1138:ARG:HB3	2.03	0.40
1:c:1149:HIS:N	1:c:1180:PHE:O	2.54	0.40
1:d:225:SER:OG	1:d:226:SER:N	2.50	0.40
1:d:261:GLY:HA3	1:d:312:SER:HA	2.02	0.40
1:d:351:PRO:HA	1:d:354:PHE:CE2	2.56	0.40
1:d:521:ARG:HB3	1:d:828:PHE:HE1	1.86	0.40
1:e:1241:PRO:HB2	1:e:1244:GLN:HB3	2.03	0.40
1:5:3:ARG:O	1:5:3:ARG:CG	2.70	0.40
1:A:307:HIS:ND1	1:A:310:TRP:HB3	2.37	0.40
1:A:610:ASP:HA	1:A:613:TYR:HD2	1.87	0.40
1:B:381:ASP:OD1	1:B:382:HIS:N	2.55	0.40
1:B:422:PHE:HE1	1:B:1229:VAL:HG12	1.86	0.40
1:B:954:SER:OG	1:B:955:LEU:N	2.54	0.40
1:C:620:VAL:HG11	1:C:656:MET:HG2	2.04	0.40
1:D:309:ARG:HE	1:D:368:ASP:CG	2.28	0.40
1:D:505:MET:HB2	1:D:507:TYR:HE2	1.85	0.40
1:D:645:PRO:HG3	1:D:713:TRP:CE2	2.57	0.40
1:D:1241:PRO:HA	1:D:1242:PRO:HD3	1.94	0.40
1:E:287:THR:OG1	1:E:298:GLU:OE2	2.39	0.40
1:E:509:ILE:HG12	1:E:918:LEU:HD12	2.02	0.40
2:I:809:MET:HG2	2:I:994:ALA:HB2	2.03	0.40
2:J:518:SER:N	5:J:1301:SAM:O	2.45	0.40
2:J:809:MET:HG2	2:J:994:ALA:HB2	2.03	0.40
2:L:485:LYS:NZ	2:L:643:PRO:O	2.53	0.40
3:R:776:ASP:OD1	3:R:776:ASP:N	2.54	0.40
4:U:460:VAL:HG13	4:U:568:PHE:HZ	1.86	0.40
1:a:1083:ILE:HD12	1:a:1121:TYR:CE2	2.56	0.40
1:a:1118:ASN:OD1	1:a:1118:ASN:N	2.54	0.40
1:A:334:LEU:HB3	1:A:361:MET:HE1	2.03	0.40
1:B:610:ASP:HB3	1:B:674:ARG:HH21	1.87	0.40
1:C:339:LEU:HB2	1:C:353:MET:HG2	2.03	0.40
1:D:686:ARG:CZ	2:L:99:ARG:HH22	2.35	0.40
2:H:613:VAL:HG22	2:H:654:VAL:HG13	2.03	0.40
2:H:830:THR:H	2:H:850:ASP:HB2	1.86	0.40
2:H:915:THR:HG22	2:H:974:TRP:HE1	1.85	0.40
2:I:486:ASP:HB2	2:I:529:VAL:HG11	2.04	0.40
2:J:221:LEU:HB2	2:J:234:ILE:HB	2.02	0.40
2:K:915:THR:HG22	2:K:974:TRP:HE1	1.85	0.40
2:L:112:ASN:HD22	2:L:115:VAL:HG23	1.86	0.40
2:L:143:ILE:HD12	2:L:146:LEU:HD23	2.03	0.40
2:L:282:CYS:HB3	2:L:305:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:709:ILE:HD13	1:c:764:TRP:HH2	1.86	0.40
1:c:927:ALA:HB1	1:c:984:LEU:HD11	2.03	0.40
1:d:1204:TYR:CZ	1:d:1206:ASP:HB3	2.57	0.40
1:e:562:THR:HG22	1:e:578:LEU:HG	2.04	0.40
1:B:1209:LEU:HD22	1:B:1225:LYS:HB3	2.04	0.40
1:C:293:GLN:HE22	1:C:400:GLU:CD	2.30	0.40
1:D:1243:THR:HG22	1:D:1256:VAL:HG11	2.02	0.40
2:H:533:TRP:HD1	2:H:541:VAL:HG21	1.87	0.40
2:K:282:CYS:HB3	2:K:305:SER:HB2	2.03	0.40
2:K:566:PHE:CE2	2:L:397:LEU:HD13	2.56	0.40
2:K:613:VAL:HG22	2:K:654:VAL:HG13	2.03	0.40
2:L:44:ARG:NH2	2:L:58:GLN:OE1	2.49	0.40
2:L:511:SER:OG	2:L:572:GLN:OE1	2.39	0.40
4:U:105:ARG:HH21	4:U:118:TYR:HB2	1.86	0.40
1:a:669:TYR:HB3	1:a:673:ARG:HD2	2.03	0.40
1:b:599:LEU:HD12	1:b:830:PRO:HB3	2.02	0.40
1:b:994:MET:HE1	1:b:997:LEU:HD22	2.03	0.40
1:d:803:ILE:HG13	1:d:887:LEU:HD21	2.04	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%)	120 (88%)	16 (12%)	0	100	100
1	2	134/1275 (10%)	119 (89%)	15 (11%)	0	100	100
1	3	133/1275 (10%)	124 (93%)	9 (7%)	0	100	100
1	4	122/1275 (10%)	108 (88%)	14 (12%)	0	100	100
1	5	135/1275 (11%)	124 (92%)	11 (8%)	0	100	100
1	A	1126/1275 (88%)	1030 (92%)	94 (8%)	2 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1069/1275 (84%)	978 (92%)	90 (8%)	1 (0%)	48	78
1	C	1076/1275 (84%)	985 (92%)	90 (8%)	1 (0%)	48	78
1	D	1046/1275 (82%)	961 (92%)	85 (8%)	0	100	100
1	E	1058/1275 (83%)	974 (92%)	83 (8%)	1 (0%)	48	78
1	a	1084/1275 (85%)	987 (91%)	95 (9%)	2 (0%)	43	71
1	b	1083/1275 (85%)	994 (92%)	89 (8%)	0	100	100
1	c	1074/1275 (84%)	989 (92%)	84 (8%)	1 (0%)	48	78
1	d	1081/1275 (85%)	995 (92%)	84 (8%)	2 (0%)	43	71
1	e	1071/1275 (84%)	970 (91%)	101 (9%)	0	100	100
2	H	1022/1289 (79%)	926 (91%)	95 (9%)	1 (0%)	48	78
2	I	1022/1289 (79%)	925 (90%)	96 (9%)	1 (0%)	48	78
2	J	1022/1289 (79%)	924 (90%)	97 (10%)	1 (0%)	48	78
2	K	1022/1289 (79%)	926 (91%)	95 (9%)	1 (0%)	48	78
2	L	1022/1289 (79%)	925 (90%)	96 (9%)	1 (0%)	48	78
3	R	1249/1267 (99%)	1129 (90%)	119 (10%)	1 (0%)	48	78
4	U	658/736 (89%)	587 (89%)	65 (10%)	6 (1%)	14	42
All	All	18445/27573 (67%)	16800 (91%)	1623 (9%)	22 (0%)	49	78

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	TRP
1	a	310	TRP
1	E	787	GLN
4	U	588	PHE
1	B	1214	SER
1	C	614	PRO
2	H	1003	SER
2	I	1003	SER
2	J	1003	SER
2	K	1003	SER
2	L	1003	SER
1	A	584	SER
4	U	136	SER
4	U	471	ASP
1	a	339	LEU

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Mol	Chain	Res	Type
4	U	133	PRO
3	R	633	VAL
4	U	134	LEU
4	U	456	PHE
1	d	1066	VAL
1	c	1058	PRO
1	d	1057	SER

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	110/1113 (10%)	110 (100%)	0	100	100
1	3	110/1113 (10%)	110 (100%)	0	100	100
1	4	103/1113 (9%)	103 (100%)	0	100	100
1	5	112/1113 (10%)	107 (96%)	5 (4%)	24	51
1	A	994/1113 (89%)	992 (100%)	2 (0%)	87	85
1	B	945/1113 (85%)	944 (100%)	1 (0%)	88	89
1	C	958/1113 (86%)	958 (100%)	0	100	100
1	D	931/1113 (84%)	929 (100%)	2 (0%)	87	85
1	E	939/1113 (84%)	936 (100%)	3 (0%)	86	84
1	a	961/1113 (86%)	960 (100%)	1 (0%)	88	89
1	b	960/1113 (86%)	959 (100%)	1 (0%)	88	89
1	c	953/1113 (86%)	951 (100%)	2 (0%)	87	85
1	d	959/1113 (86%)	959 (100%)	0	100	100
1	e	951/1113 (85%)	945 (99%)	6 (1%)	78	80
2	H	884/1118 (79%)	880 (100%)	4 (0%)	81	81
2	I	884/1118 (79%)	880 (100%)	4 (0%)	81	81
2	J	884/1118 (79%)	878 (99%)	6 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	884/1118 (79%)	880 (100%)	4 (0%)	81	81
2	L	884/1118 (79%)	880 (100%)	4 (0%)	81	81
3	R	1074/1084 (99%)	1071 (100%)	3 (0%)	86	84
4	U	592/650 (91%)	591 (100%)	1 (0%)	87	85
All	All	16184/24019 (67%)	16135 (100%)	49 (0%)	84	84

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	4	ILE
1	5	6	ARG
1	5	7	LYS
1	5	8	THR
1	5	11	LYS
1	A	217	GLN
1	A	413	THR
1	B	967	GLU
1	D	416	VAL
1	D	501	VAL
1	E	479	ILE
1	E	761	LEU
1	E	771	LEU
2	H	222	VAL
2	H	351	VAL
2	H	552	TYR
2	H	814	GLU
2	I	222	VAL
2	I	351	VAL
2	I	552	TYR
2	I	814	GLU
2	J	222	VAL
2	J	351	VAL
2	J	577	ASP
2	J	578	VAL
2	J	580	GLN
2	J	814	GLU
2	K	222	VAL
2	K	351	VAL
2	K	552	TYR
2	K	814	GLU
2	L	222	VAL

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Mol	Chain	Res	Type
2	L	351	VAL
2	L	552	TYR
2	L	814	GLU
3	R	468	GLU
3	R	760	ILE
3	R	1057	LEU
4	U	212	THR
1	a	945	VAL
1	b	636	LEU
1	c	822	ILE
1	c	923	ILE
1	e	315	ASP
1	e	319	ASP
1	e	323	ILE
1	e	739	LEU
1	e	843	VAL
1	e	945	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	63	GLN
1	1	76	ASN
1	1	86	ASN
1	2	63	GLN
1	2	119	GLN
1	3	95	HIS
1	3	109	GLN
1	3	141	ASN
1	4	146	ASN
1	5	63	GLN
1	5	131	ASN
1	A	219	HIS
1	A	228	GLN
1	A	278	GLN
1	A	382	HIS
1	A	421	ASN
1	A	569	GLN
1	A	718	GLN
1	A	731	ASN
1	A	779	GLN
1	A	917	ASN

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Mol	Chain	Res	Type
1	A	929	GLN
1	A	1036	ASN
1	A	1107	ASN
1	A	1116	GLN
1	A	1124	GLN
1	A	1125	GLN
1	A	1149	HIS
1	A	1197	GLN
1	A	1213	ASN
1	A	1218	GLN
1	A	1233	ASN
1	B	182	GLN
1	B	293	GLN
1	B	331	ASN
1	B	337	GLN
1	B	357	ASN
1	B	518	GLN
1	B	533	GLN
1	B	544	GLN
1	B	550	GLN
1	B	671	GLN
1	B	704	GLN
1	B	749	ASN
1	B	937	GLN
1	B	996	GLN
1	B	1000	GLN
1	B	1002	GLN
1	B	1025	GLN
1	B	1075	HIS
1	B	1116	GLN
1	B	1197	GLN
1	C	182	GLN
1	C	275	GLN
1	C	278	GLN
1	C	293	GLN
1	C	313	ASN
1	C	337	GLN
1	C	340	ASN
1	C	357	ASN
1	C	524	ASN
1	C	527	ASN
1	C	749	ASN

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Mol	Chain	Res	Type
1	C	832	GLN
1	C	970	ASN
1	C	996	GLN
1	C	1036	ASN
1	C	1213	ASN
1	C	1237	ASN
1	D	278	GLN
1	D	340	ASN
1	D	421	ASN
1	D	441	ASN
1	D	537	GLN
1	D	544	GLN
1	D	718	GLN
1	D	779	GLN
1	D	996	GLN
1	D	1000	GLN
1	D	1002	GLN
1	D	1075	HIS
1	D	1116	GLN
1	D	1123	ASN
1	D	1233	ASN
1	E	219	HIS
1	E	228	GLN
1	E	234	GLN
1	E	246	GLN
1	E	380	GLN
1	E	382	HIS
1	E	558	ASN
1	E	704	GLN
1	E	718	GLN
1	E	731	ASN
1	E	774	ASN
1	E	779	GLN
1	E	782	GLN
1	E	970	ASN
1	E	1002	GLN
1	E	1036	ASN
1	E	1051	GLN
1	E	1116	GLN
1	E	1123	ASN
1	E	1149	HIS
2	H	64	GLN

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Mol	Chain	Res	Type
2	H	112	ASN
2	H	117	ASN
2	H	127	GLN
2	H	223	HIS
2	H	267	ASN
2	H	313	GLN
2	H	321	GLN
2	H	455	GLN
2	H	549	GLN
2	H	617	ASN
2	H	856	GLN
2	H	862	ASN
2	I	64	GLN
2	I	112	ASN
2	I	117	ASN
2	I	127	GLN
2	I	155	GLN
2	I	223	HIS
2	I	267	ASN
2	I	313	GLN
2	I	321	GLN
2	I	455	GLN
2	I	549	GLN
2	I	585	HIS
2	I	617	ASN
2	I	856	GLN
2	I	862	ASN
2	I	925	GLN
2	J	49	GLN
2	J	64	GLN
2	J	112	ASN
2	J	117	ASN
2	J	223	HIS
2	J	267	ASN
2	J	274	GLN
2	J	313	GLN
2	J	321	GLN
2	J	455	GLN
2	J	549	GLN
2	J	580	GLN
2	J	617	ASN
2	J	856	GLN

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Mol	Chain	Res	Type
2	J	862	ASN
2	K	64	GLN
2	K	112	ASN
2	K	117	ASN
2	K	127	GLN
2	K	223	HIS
2	K	267	ASN
2	K	274	GLN
2	K	281	GLN
2	K	310	ASN
2	K	313	GLN
2	K	321	GLN
2	K	455	GLN
2	K	549	GLN
2	K	617	ASN
2	K	629	GLN
2	K	856	GLN
2	K	862	ASN
2	L	64	GLN
2	L	112	ASN
2	L	117	ASN
2	L	223	HIS
2	L	267	ASN
2	L	274	GLN
2	L	281	GLN
2	L	313	GLN
2	L	321	GLN
2	L	455	GLN
2	L	549	GLN
2	L	617	ASN
2	L	856	GLN
2	L	862	ASN
2	L	925	GLN
3	R	79	ASN
3	R	121	ASN
3	R	143	GLN
3	R	535	GLN
3	R	550	ASN
3	R	649	GLN
3	R	675	HIS
3	R	695	ASN
3	R	726	GLN

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Mol	Chain	Res	Type
3	R	836	GLN
3	R	969	GLN
3	R	1100	GLN
3	R	1144	GLN
3	R	1208	ASN
4	U	82	GLN
4	U	119	ASN
4	U	451	GLN
4	U	621	HIS
1	a	293	GLN
1	a	390	ASN
1	a	518	GLN
1	a	527	ASN
1	a	779	GLN
1	a	832	GLN
1	a	970	ASN
1	a	996	GLN
1	a	1003	GLN
1	a	1036	ASN
1	a	1075	HIS
1	a	1124	GLN
1	a	1125	GLN
1	a	1149	HIS
1	a	1205	ASN
1	b	228	GLN
1	b	340	ASN
1	b	527	ASN
1	b	667	GLN
1	b	763	ASN
1	b	774	ASN
1	b	868	ASN
1	b	929	GLN
1	b	970	ASN
1	b	1002	GLN
1	b	1123	ASN
1	b	1255	ASN
1	c	246	GLN
1	c	357	ASN
1	c	375	HIS
1	c	731	ASN
1	c	868	ASN
1	c	1003	GLN

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Mol	Chain	Res	Type
1	c	1036	ASN
1	c	1233	ASN
1	c	1244	GLN
1	d	184	HIS
1	d	234	GLN
1	d	246	GLN
1	d	357	ASN
1	d	369	ASN
1	d	438	GLN
1	d	515	GLN
1	d	550	GLN
1	d	746	GLN
1	d	787	GLN
1	d	937	GLN
1	d	1025	GLN
1	d	1036	ASN
1	d	1075	HIS
1	d	1255	ASN
1	e	229	ASN
1	e	278	GLN
1	e	307	HIS
1	e	382	HIS
1	e	763	ASN
1	e	778	ASN
1	e	942	GLN
1	e	1002	GLN
1	e	1036	ASN
1	e	1054	HIS
1	e	1118	ASN
1	e	1125	GLN
1	e	1149	HIS
1	e	1197	GLN
1	e	1205	ASN
1	e	1226	HIS
1	e	1233	ASN
1	e	1237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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$
5	SAM	J	1301	-	27,29,29	1.43	6 (22%)	34,42,42	2.25	11 (32%)
5	SAM	I	1301	-	27,29,29	1.47	7 (25%)	34,42,42	2.24	13 (38%)
5	SAM	K	1301	-	27,29,29	1.42	5 (18%)	34,42,42	2.33	11 (32%)
5	SAM	L	1301	-	27,29,29	1.56	5 (18%)	34,42,42	2.41	15 (44%)
5	SAM	H	1301	-	27,29,29	1.47	6 (22%)	34,42,42	2.07	10 (29%)

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
5	SAM	J	1301	-	-	4/17/33/33	0/3/3/3
5	SAM	I	1301	-	-	5/17/33/33	0/3/3/3
5	SAM	K	1301	-	-	4/17/33/33	0/3/3/3
5	SAM	L	1301	-	-	8/17/33/33	0/3/3/3
5	SAM	H	1301	-	-	5/17/33/33	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1301	SAM	C5-C4	5.07	1.48	1.39
5	I	1301	SAM	C5-C4	4.16	1.46	1.39
5	H	1301	SAM	C5-C4	4.16	1.46	1.39
5	K	1301	SAM	C5-C4	4.14	1.46	1.39
5	J	1301	SAM	C5-C4	4.13	1.46	1.39
5	L	1301	SAM	C8-N7	3.47	1.38	1.31
5	K	1301	SAM	C5-N7	-2.85	1.33	1.39
5	H	1301	SAM	C5-N7	-2.73	1.34	1.39
5	I	1301	SAM	C5-N7	-2.68	1.34	1.39
5	J	1301	SAM	C5-N7	-2.64	1.34	1.39
5	L	1301	SAM	C5-C6	2.57	1.48	1.41
5	I	1301	SAM	OXT-C	-2.50	1.22	1.30
5	J	1301	SAM	C5-C6	2.44	1.47	1.41
5	I	1301	SAM	C5-C6	2.40	1.47	1.41
5	K	1301	SAM	C5-C6	2.40	1.47	1.41
5	H	1301	SAM	C5-C6	2.37	1.47	1.41
5	L	1301	SAM	OXT-C	-2.33	1.23	1.30
5	H	1301	SAM	C8-N7	2.23	1.36	1.31
5	I	1301	SAM	C8-N7	2.17	1.35	1.31
5	H	1301	SAM	C4-N9	-2.17	1.33	1.37
5	J	1301	SAM	C8-N7	2.15	1.35	1.31
5	K	1301	SAM	C8-N7	2.14	1.35	1.31
5	J	1301	SAM	OXT-C	-2.09	1.24	1.30
5	H	1301	SAM	OXT-C	-2.09	1.24	1.30
5	J	1301	SAM	C4-N9	-2.08	1.33	1.37
5	I	1301	SAM	C4-N9	-2.06	1.33	1.37
5	I	1301	SAM	CE-SD	-2.03	1.66	1.78
5	K	1301	SAM	OXT-C	-2.01	1.24	1.30
5	L	1301	SAM	CE-SD	-2.01	1.66	1.78

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1301	SAM	C5-C4-N3	-6.25	118.12	126.72
5	K	1301	SAM	CG-SD-C5'	6.05	118.23	103.43
5	J	1301	SAM	C5-C4-N3	-6.03	118.42	126.72
5	I	1301	SAM	C5-C4-N3	-5.93	118.55	126.72
5	L	1301	SAM	C5-C4-N3	-5.91	118.58	126.72
5	H	1301	SAM	C5-C4-N3	-5.88	118.62	126.72
5	J	1301	SAM	CG-SD-C5'	5.19	116.13	103.43
5	L	1301	SAM	C4-C5-N7	-4.69	105.22	110.58
5	H	1301	SAM	N3-C4-N9	4.57	134.94	127.17
5	K	1301	SAM	N3-C4-N9	4.56	134.93	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1301	SAM	N3-C4-N9	4.56	134.92	127.17
5	I	1301	SAM	N3-C4-N9	4.47	134.76	127.17
5	I	1301	SAM	CB-CA-N	4.21	121.10	110.12
5	K	1301	SAM	C2-N3-C4	4.08	121.79	111.83
5	J	1301	SAM	C2-N3-C4	3.98	121.56	111.83
5	L	1301	SAM	CG-SD-C5'	3.95	113.08	103.43
5	I	1301	SAM	C2-N3-C4	3.93	121.42	111.83
5	H	1301	SAM	C2-N3-C4	3.91	121.37	111.83
5	H	1301	SAM	N3-C2-N1	-3.85	122.75	128.58
5	K	1301	SAM	N3-C2-N1	-3.82	122.79	128.58
5	L	1301	SAM	N3-C4-N9	3.74	133.53	127.17
5	J	1301	SAM	N3-C2-N1	-3.72	122.95	128.58
5	I	1301	SAM	N3-C2-N1	-3.68	123.00	128.58
5	K	1301	SAM	C4-C5-N7	-3.65	106.41	110.58
5	L	1301	SAM	C2-N3-C4	3.61	120.64	111.83
5	J	1301	SAM	C4-C5-N7	-3.55	106.52	110.58
5	L	1301	SAM	C5-N7-C8	3.55	109.03	103.45
5	I	1301	SAM	C4-C5-N7	-3.46	106.63	110.58
5	L	1301	SAM	C6-C5-N7	3.45	138.75	132.09
5	I	1301	SAM	CB-CA-C	3.39	119.44	110.45
5	H	1301	SAM	C4-C5-N7	-3.30	106.81	110.58
5	L	1301	SAM	N9-C8-N7	-3.10	109.54	113.94
5	L	1301	SAM	C4-N9-C1'	-2.88	119.89	126.63
5	K	1301	SAM	C5-N7-C8	2.83	107.90	103.45
5	L	1301	SAM	N3-C2-N1	-2.76	124.41	128.58
5	J	1301	SAM	C5-N7-C8	2.72	107.73	103.45
5	I	1301	SAM	C5-N7-C8	2.68	107.66	103.45
5	H	1301	SAM	C4-N9-C8	2.61	108.48	105.74
5	H	1301	SAM	C5-N7-C8	2.58	107.50	103.45
5	H	1301	SAM	CG-SD-C5'	2.56	109.70	103.43
5	L	1301	SAM	C3'-C2'-C1'	2.51	106.21	101.46
5	J	1301	SAM	C4-N9-C8	2.46	108.32	105.74
5	L	1301	SAM	C4-N9-C8	2.42	108.28	105.74
5	I	1301	SAM	CG-SD-C5'	2.40	109.31	103.43
5	I	1301	SAM	C4-N9-C8	2.32	108.18	105.74
5	L	1301	SAM	C2'-C3'-C4'	2.25	106.96	102.61
5	H	1301	SAM	N9-C8-N7	-2.23	110.77	113.94
5	J	1301	SAM	N9-C8-N7	-2.23	110.77	113.94
5	J	1301	SAM	CE-SD-C5'	2.22	118.02	100.54
5	I	1301	SAM	N9-C8-N7	-2.17	110.85	113.94
5	L	1301	SAM	C1'-N9-C8	2.13	131.83	127.09
5	H	1301	SAM	C2-N1-C6	2.11	122.19	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1301	SAM	C6-C5-N7	2.09	136.12	132.09
5	K	1301	SAM	N9-C8-N7	-2.09	110.98	113.94
5	L	1301	SAM	CB-CA-C	2.05	115.88	110.45
5	K	1301	SAM	C6-C5-N7	2.04	136.03	132.09
5	I	1301	SAM	C6-C5-N7	2.04	136.02	132.09
5	K	1301	SAM	C2-N1-C6	2.03	122.06	118.73
5	K	1301	SAM	CE-SD-C5'	2.03	116.46	100.54
5	I	1301	SAM	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

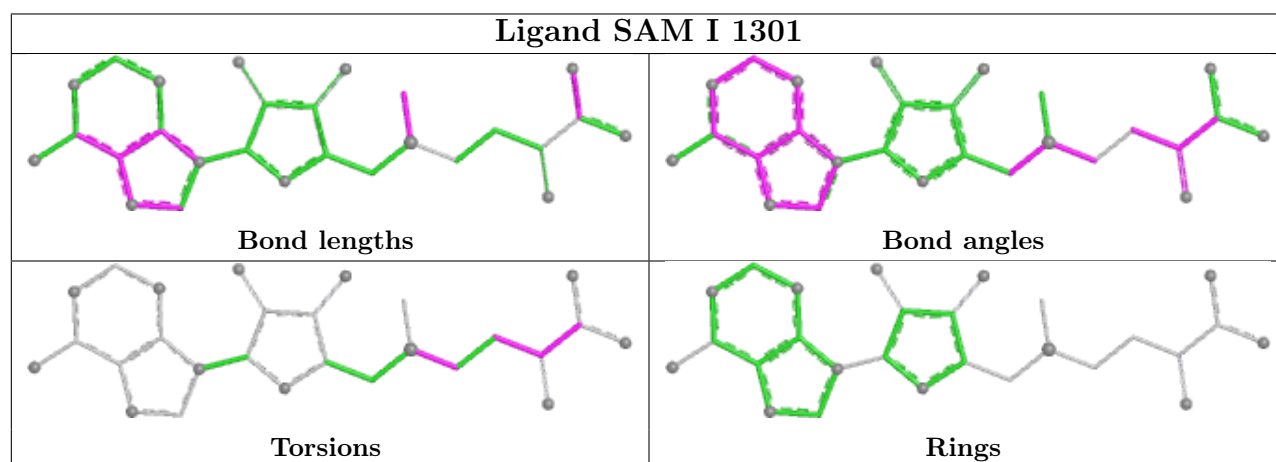
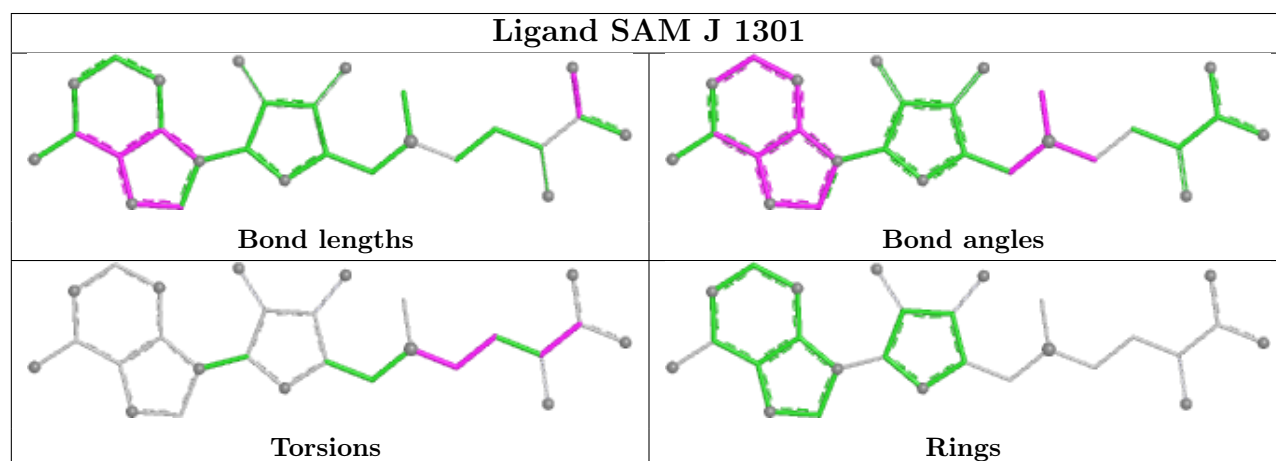
Mol	Chain	Res	Type	Atoms
5	I	1301	SAM	N-CA-CB-CG
5	J	1301	SAM	CA-CB-CG-SD
5	K	1301	SAM	CB-CG-SD-C5'
5	L	1301	SAM	N-CA-CB-CG
5	L	1301	SAM	C-CA-CB-CG
5	L	1301	SAM	C4'-C5'-SD-CE
5	L	1301	SAM	C2'-C1'-N9-C8
5	H	1301	SAM	CB-CG-SD-CE
5	I	1301	SAM	CB-CG-SD-CE
5	L	1301	SAM	CB-CG-SD-CE
5	H	1301	SAM	OXT-C-CA-CB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

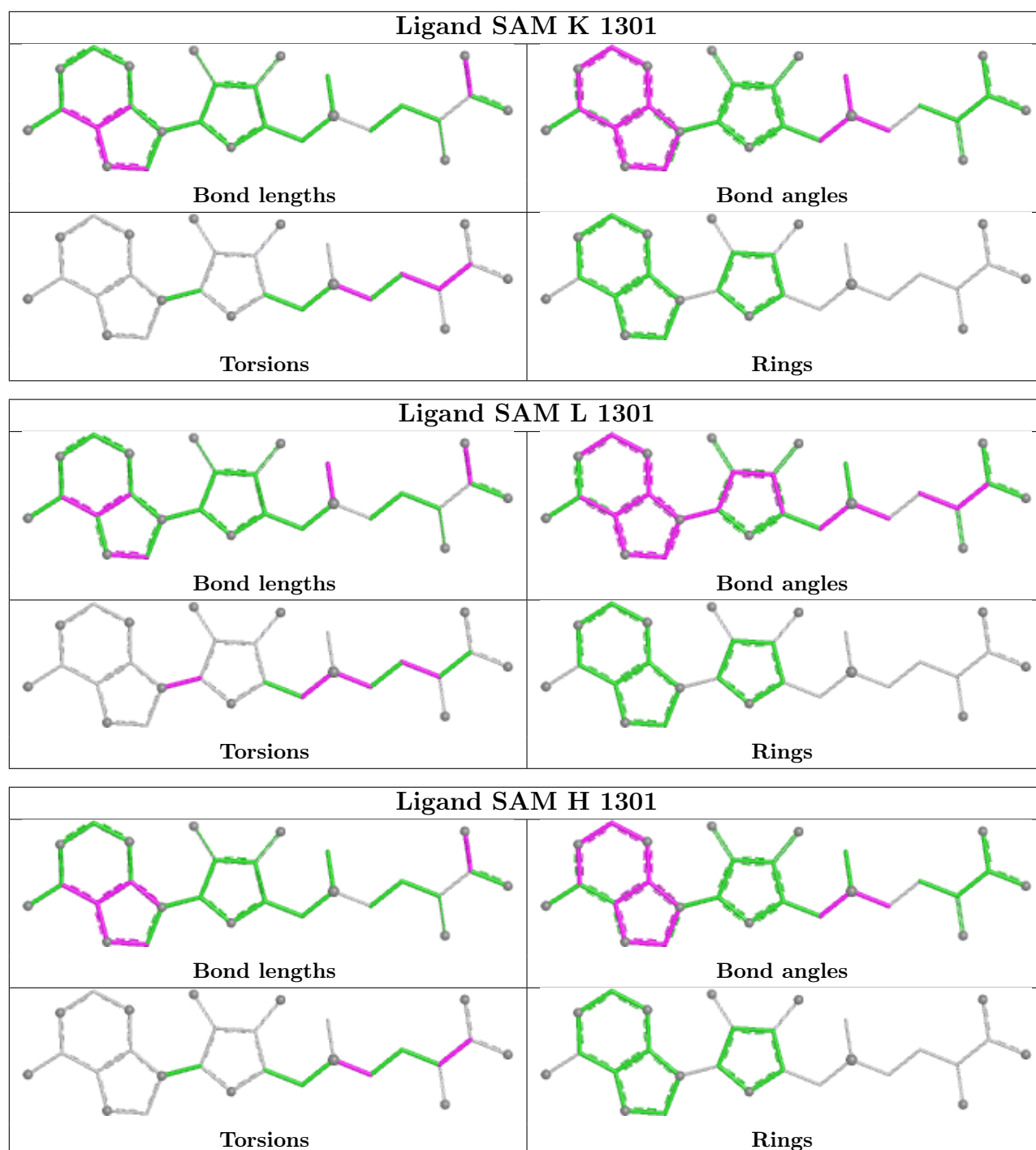
There are no ring outliers.

5 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1301	SAM	11	0
5	I	1301	SAM	22	0
5	K	1301	SAM	37	0
5	L	1301	SAM	19	0
5	H	1301	SAM	27	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.

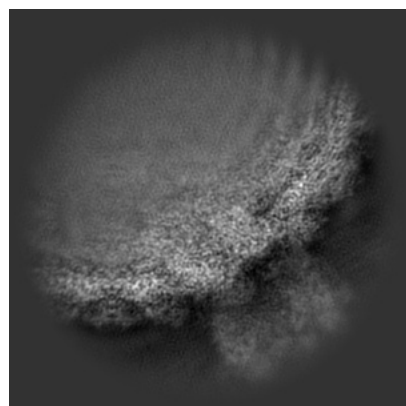
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33779. These allow visual inspection of the internal detail of the map and identification of artifacts.

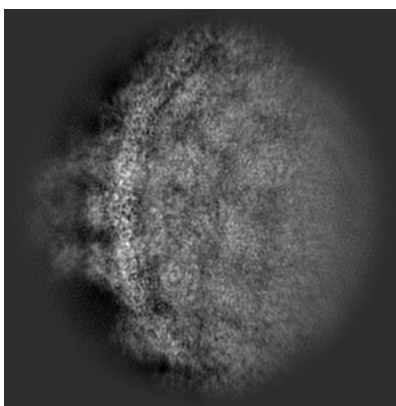
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

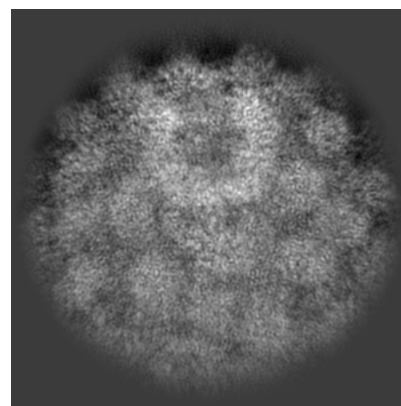
6.1.1 Primary map



X

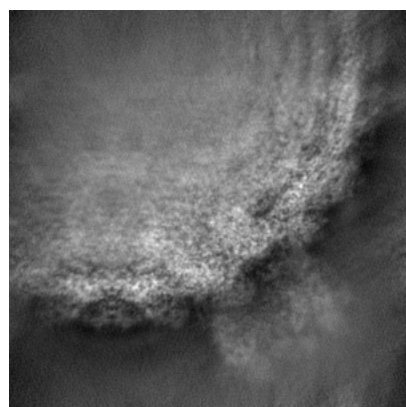


Y

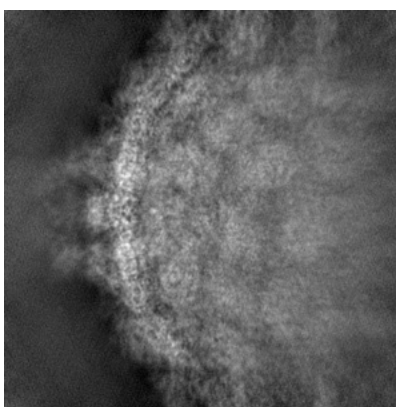


Z

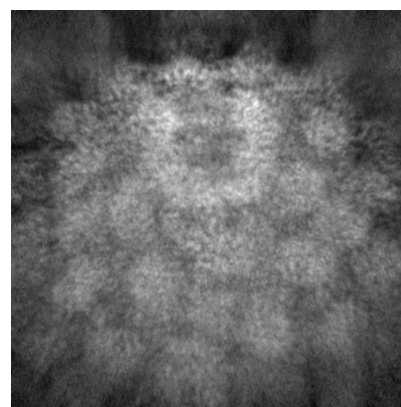
6.1.2 Raw map



X



Y

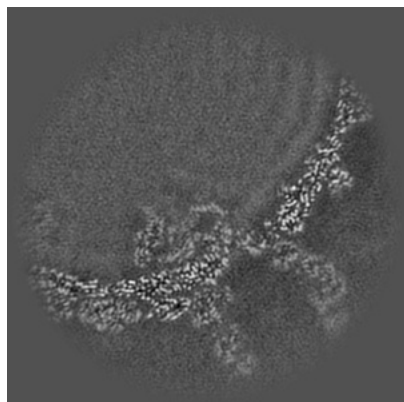


Z

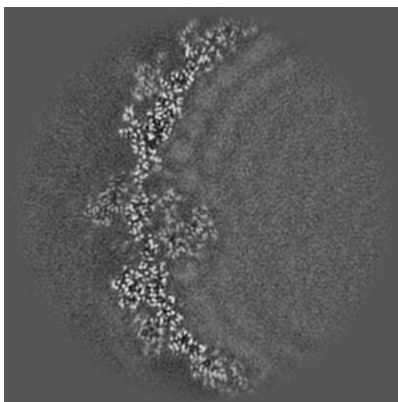
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

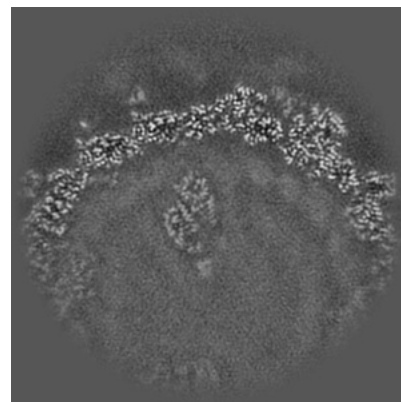
6.2.1 Primary map



X Index: 160

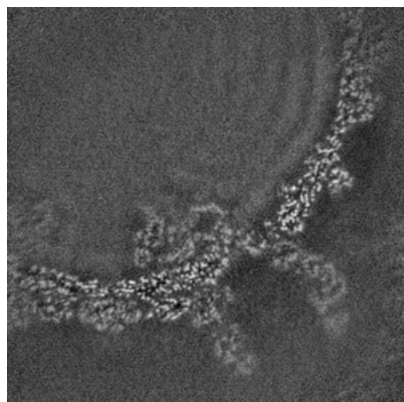


Y Index: 160

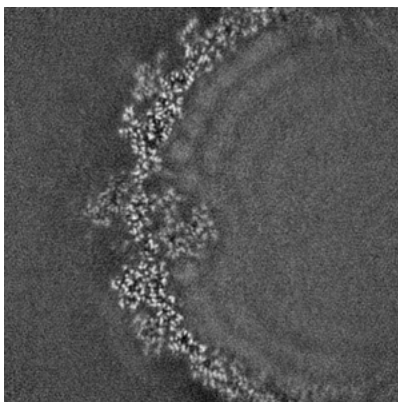


Z Index: 160

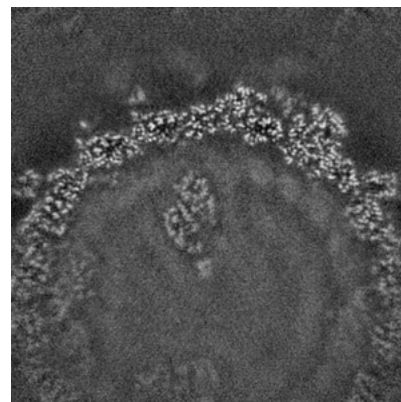
6.2.2 Raw map



X Index: 160



Y Index: 160

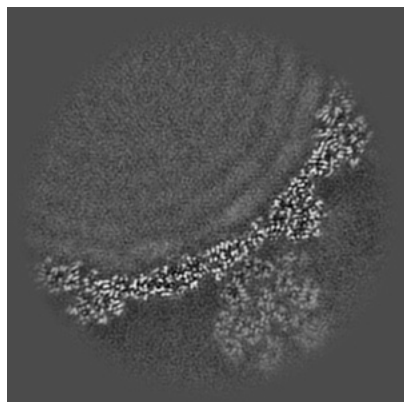


Z Index: 160

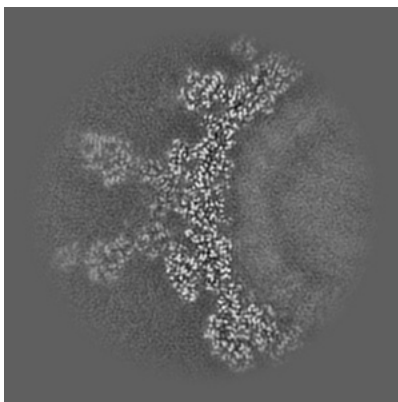
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

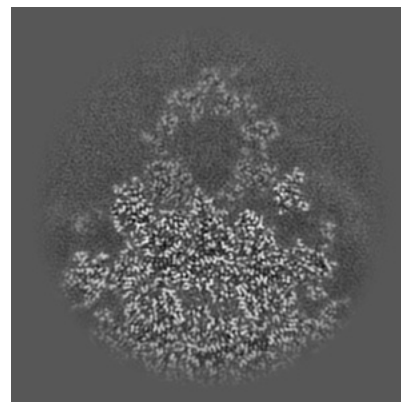
6.3.1 Primary map



X Index: 196

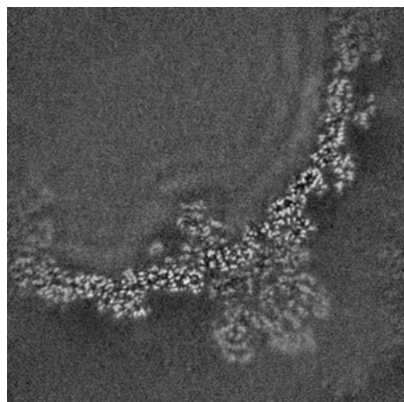


Y Index: 227

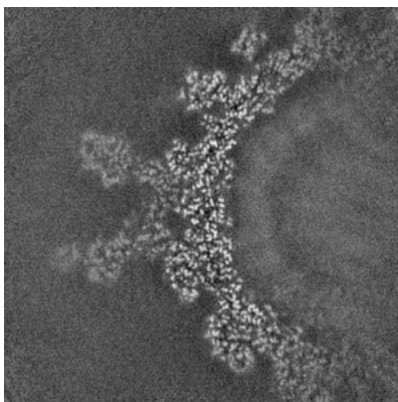


Z Index: 99

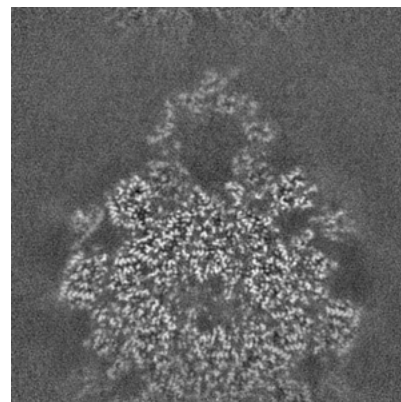
6.3.2 Raw map



X Index: 125



Y Index: 228

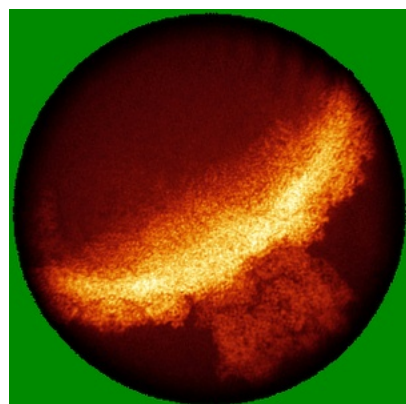


Z Index: 102

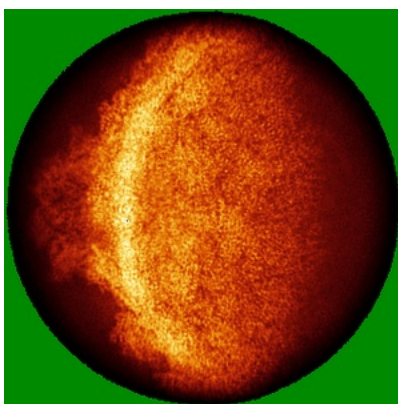
The images above show the largest variance slices of the map in three orthogonal directions.

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

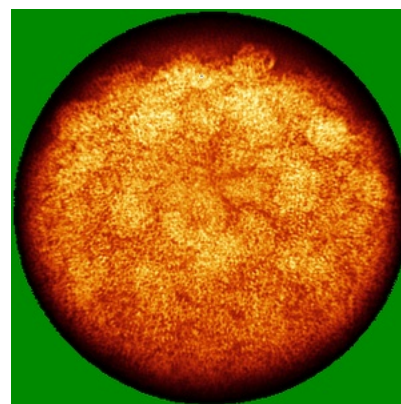
6.4.1 Primary map



X

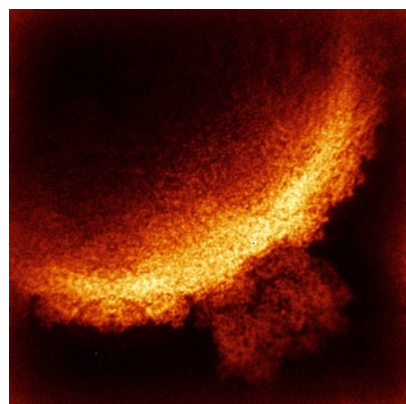


Y

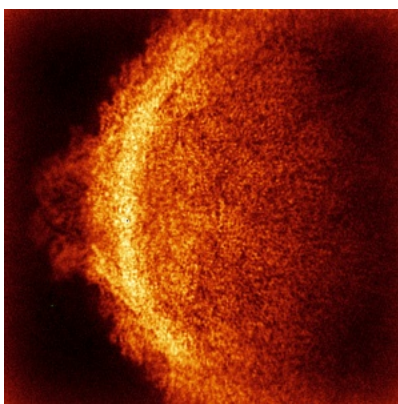


Z

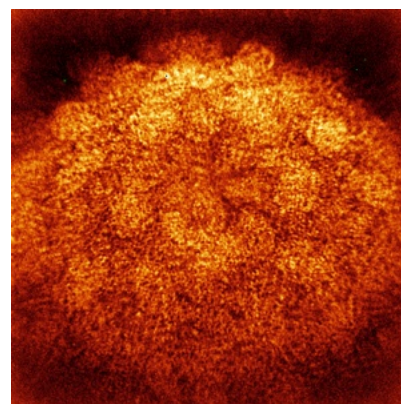
6.4.2 Raw map



X



Y

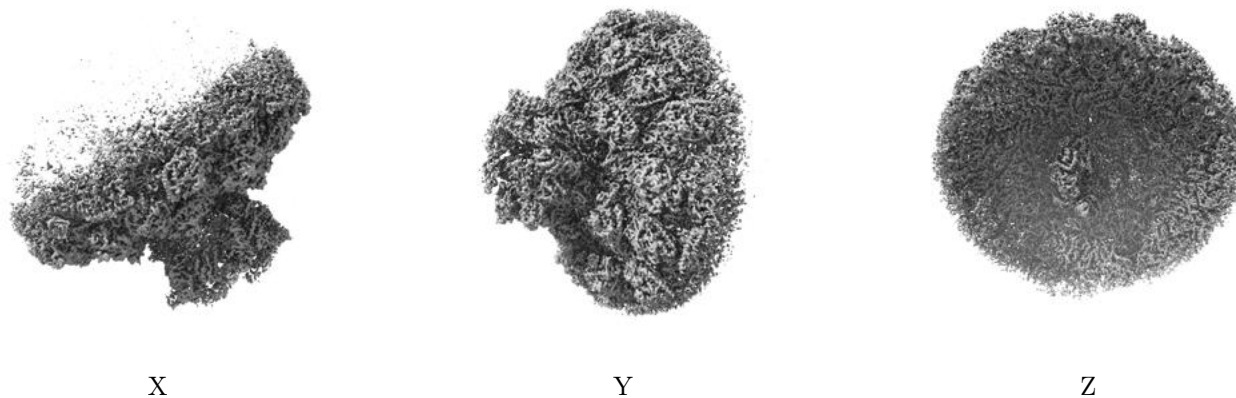


Z

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.

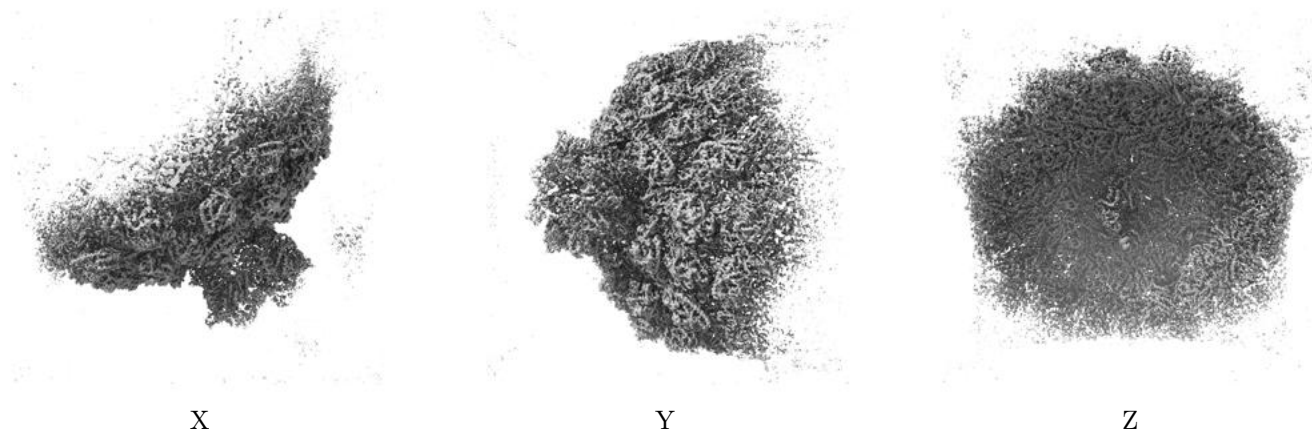
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

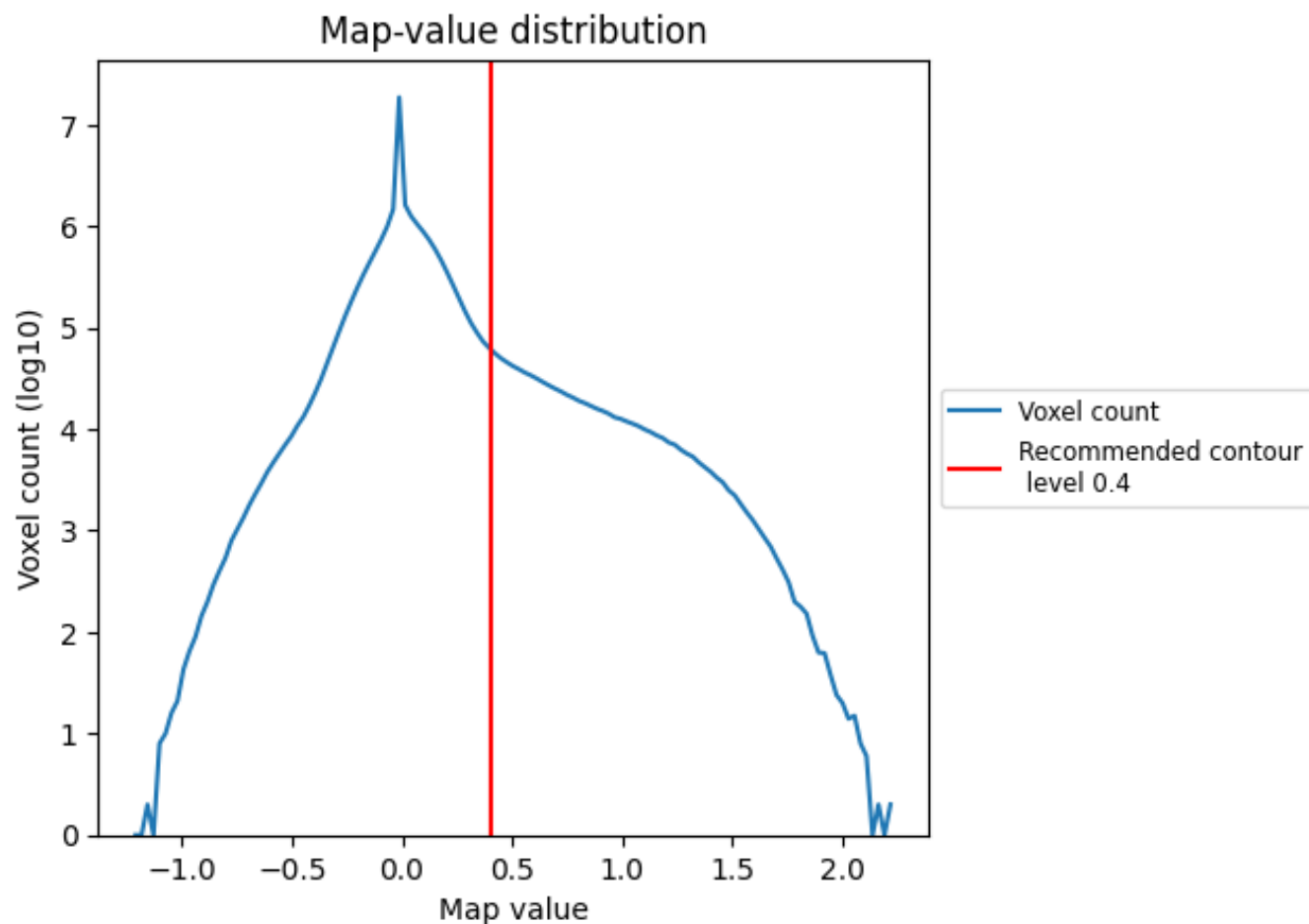
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

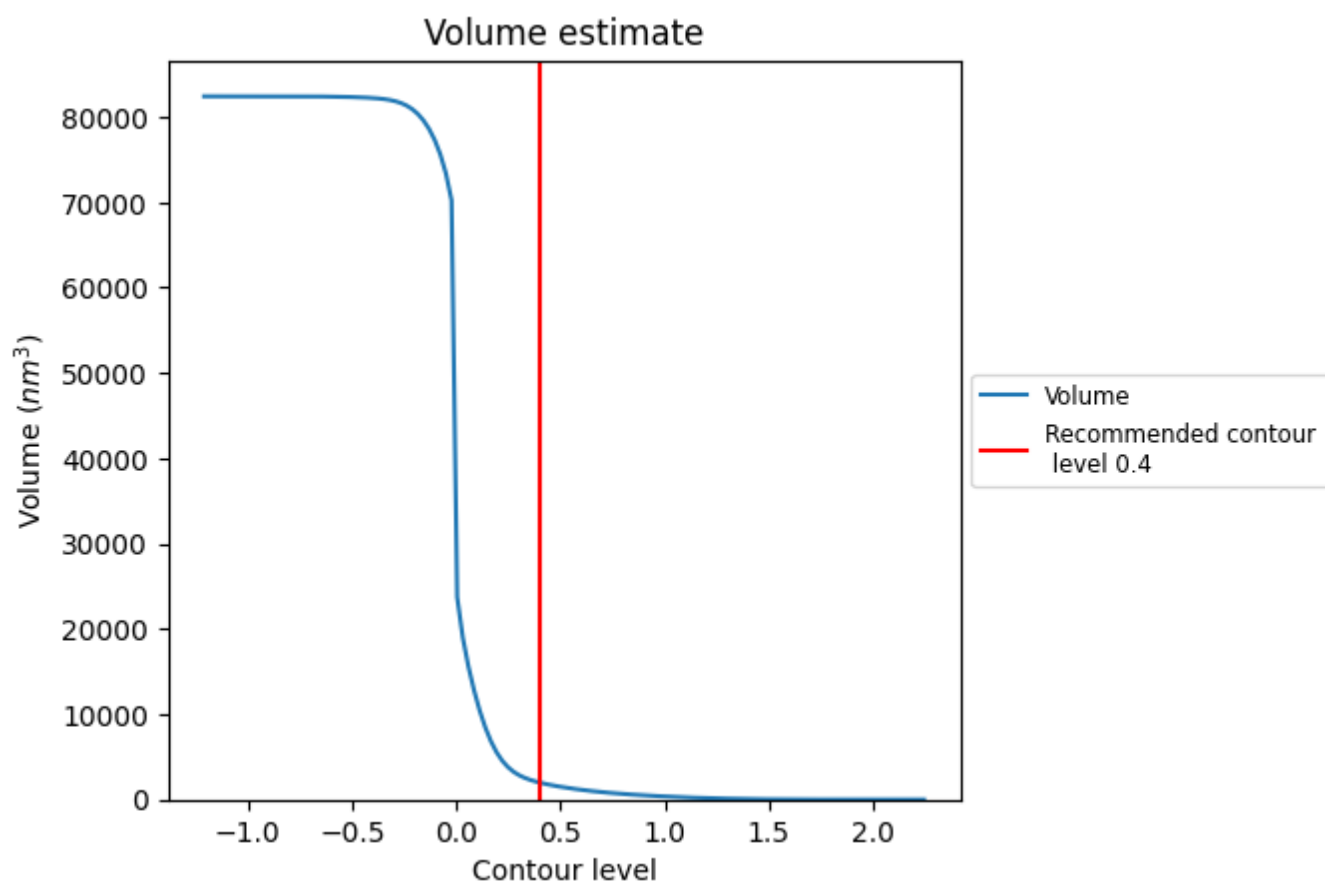
This section contains the results of statistical analysis of the map.

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.

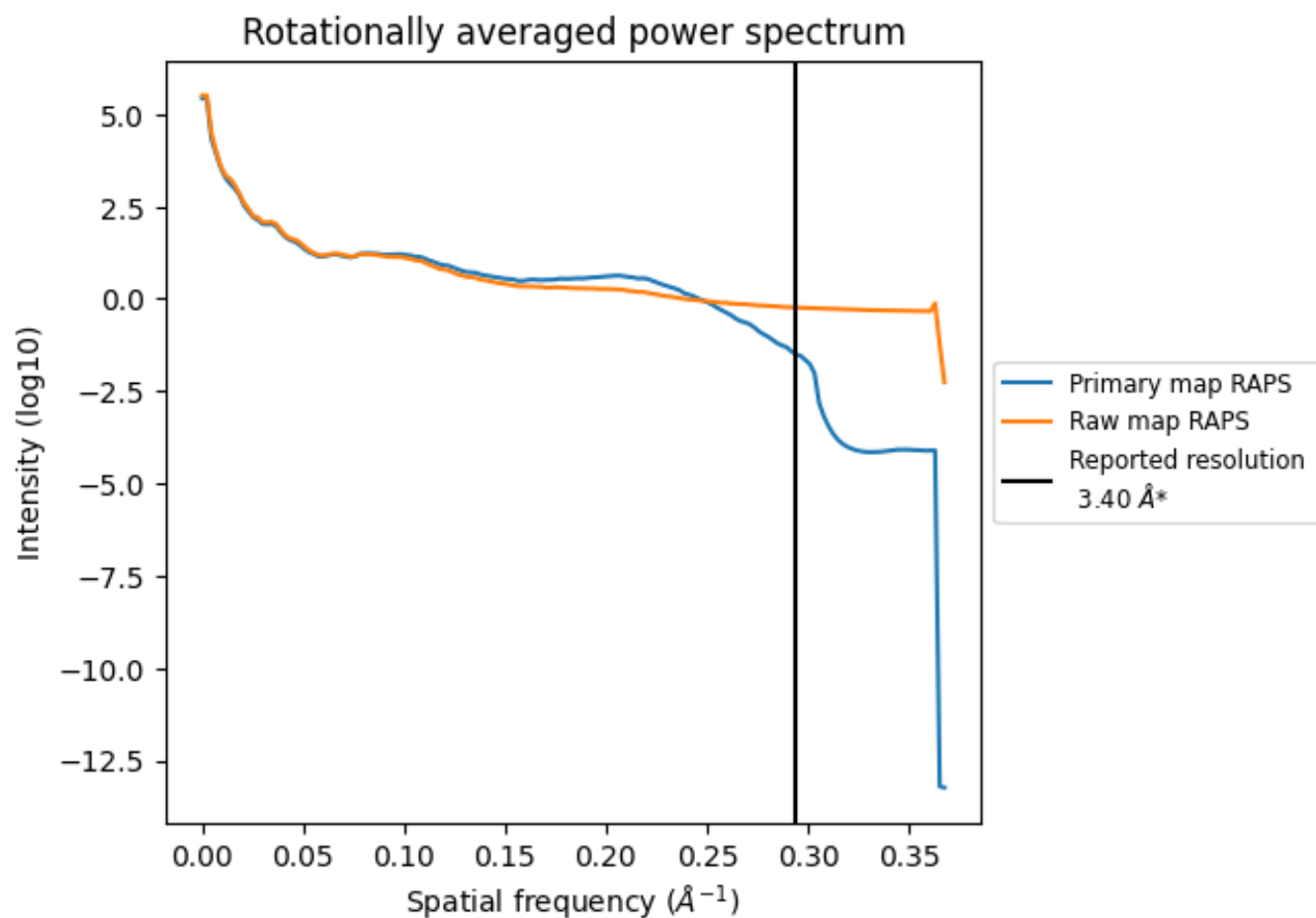
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1994 nm³; this corresponds to an approximate mass of 1801 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 ⓘ

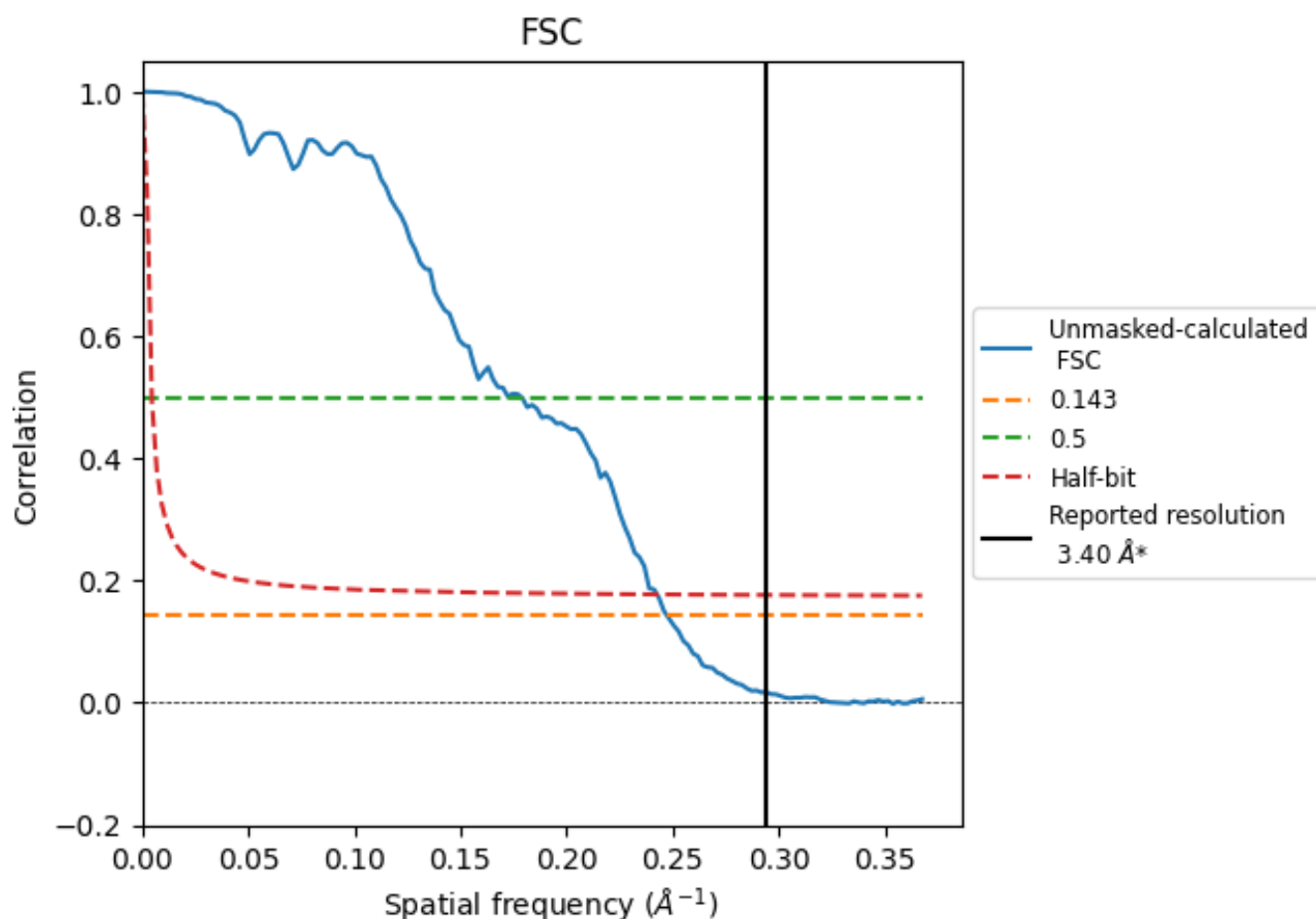


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

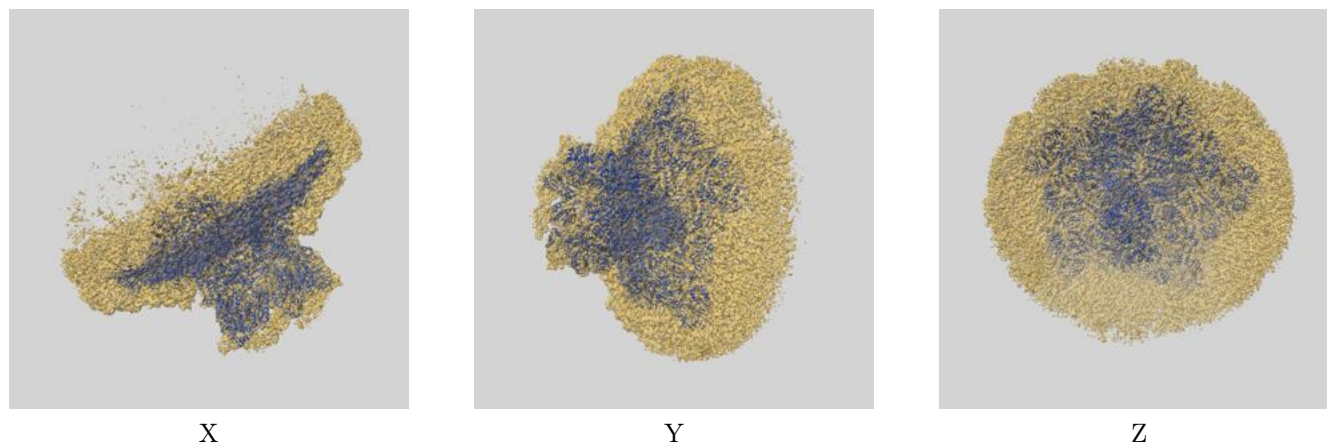
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	5.60	4.12

*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 4.05 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

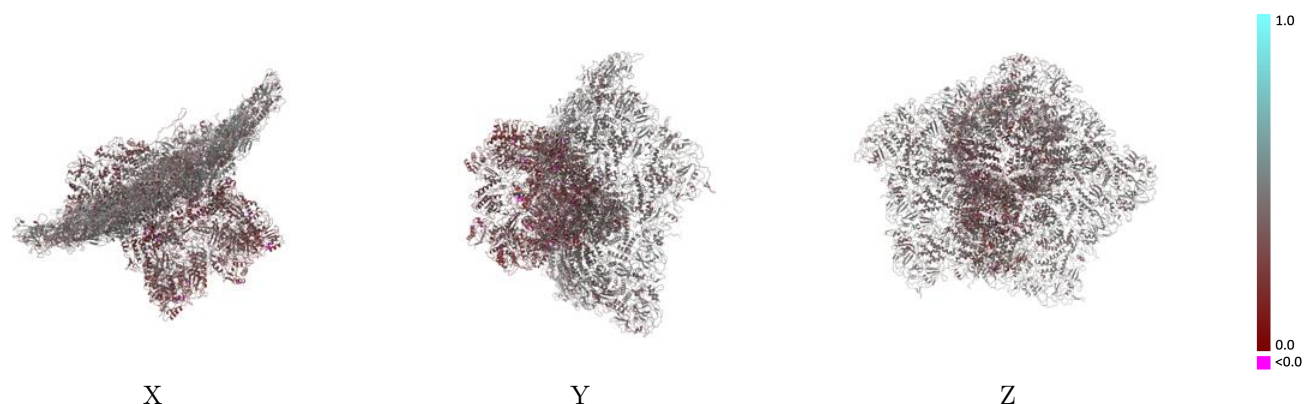
This section contains information regarding the fit between EMDB map EMD-33779 and PDB model 7YEZ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



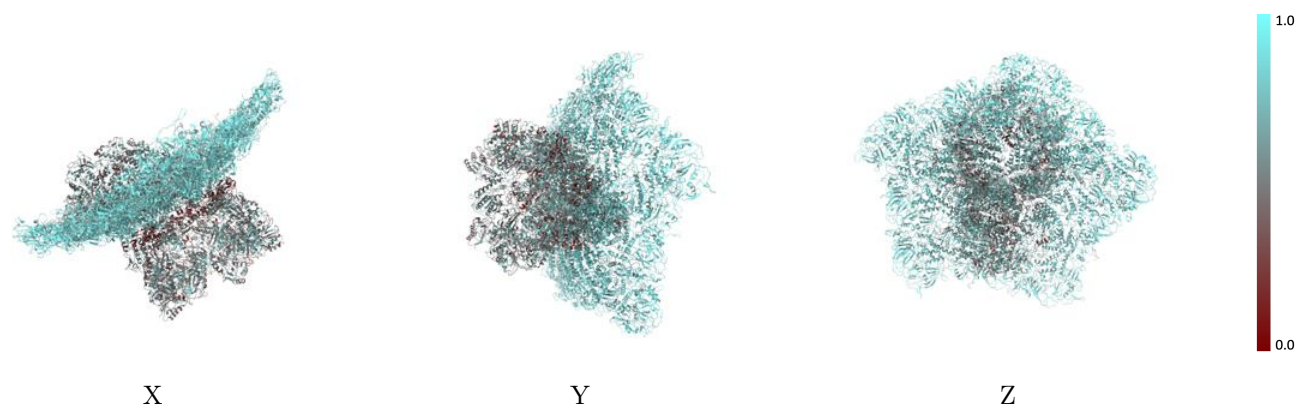
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



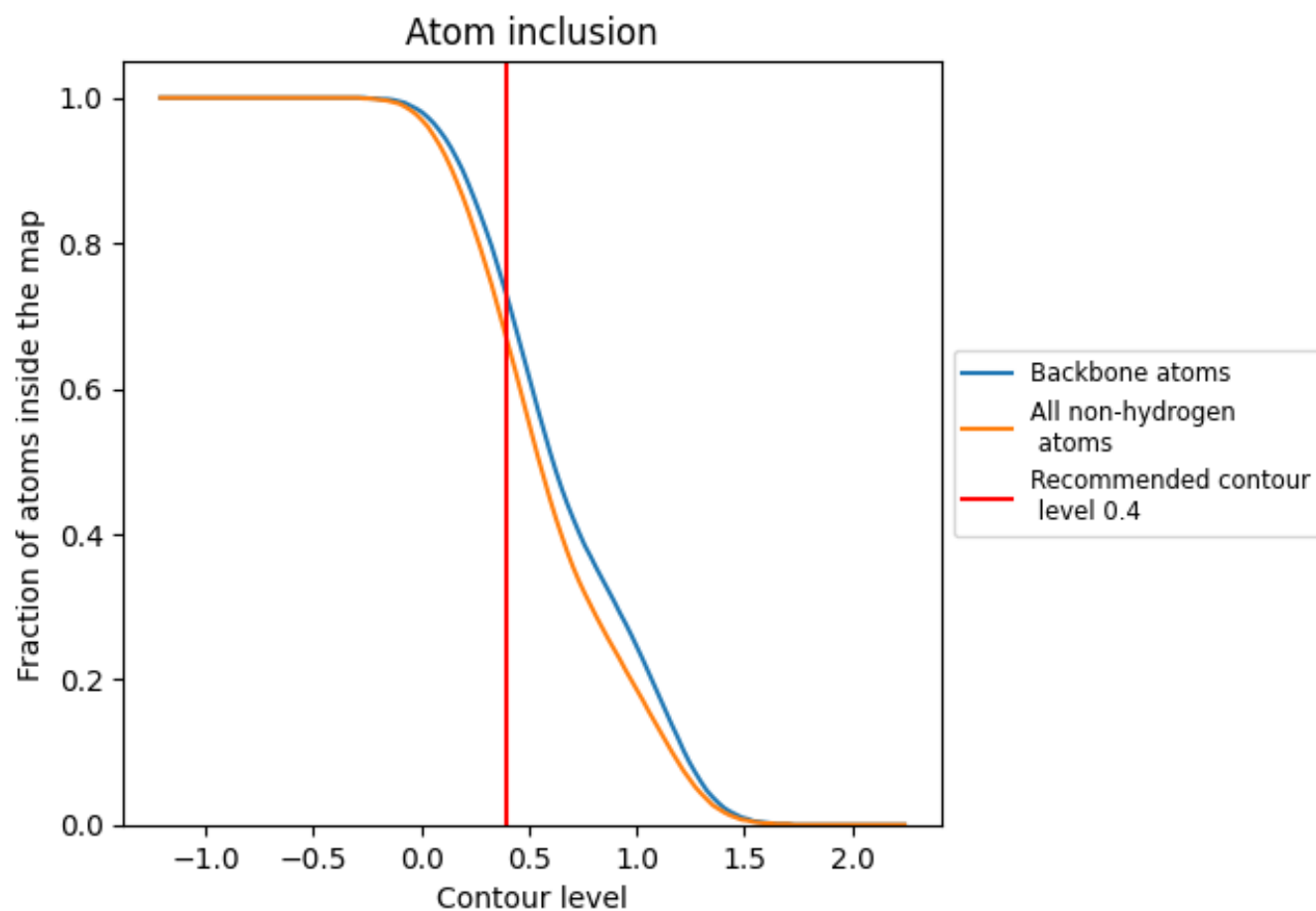
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.3840
1	 0.6430	 0.4010
2	 0.7100	 0.4080
3	 0.6880	 0.4160
4	 0.5910	 0.3840
5	 0.5930	 0.3750
A	 0.7530	 0.4170
B	 0.7750	 0.4250
C	 0.7790	 0.4230
D	 0.7860	 0.4280
E	 0.7720	 0.4250
H	 0.4800	 0.2980
I	 0.4610	 0.2860
J	 0.4700	 0.3070
K	 0.4750	 0.3130
L	 0.4790	 0.3100
R	 0.5820	 0.3460
U	 0.5690	 0.3640
a	 0.7880	 0.4250
b	 0.7970	 0.4330
c	 0.7920	 0.4320
d	 0.7980	 0.4310
e	 0.7970	 0.4270

