Full wwPDB EM Validation Report ⓘ

Mar 4, 2023 – 06:16 PM EST

PDB ID	:	8FNV
EMDB ID	:	EMD-29327
Title	:	Structure of RdrB from Escherichia coli RADAR defense system
Authors	:	Duncan-Lowey, B.; Johnson, A.G.; Rawson, S.; Mayer, M.L.; Kranzusch, P.J.
Deposited on	:	2022-12-28
Resolution	:	2.11 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:

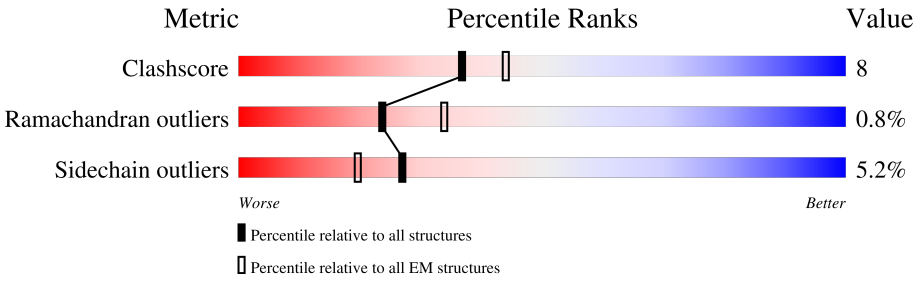
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	798	9% 73% 20%
1	B	798	9% 73% 20%
1	C	798	9% 73% 20%
1	D	798	9% 73% 20%
1	E	798	9% 72% 21%
1	F	798	9% 73% 20%
1	G	798	9% 72% 21%
1	H	798	9% 73% 20%

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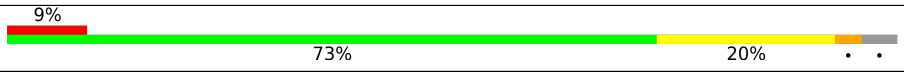
Mol	Chain	Length	Quality of chain
1	I	798	
1	J	798	
1	K	798	
1	L	798	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 74928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	B	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	C	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	D	767	Total	C	N	O	S	0	0
			6221	3989	1078	1120	34		
1	E	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	F	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	G	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	H	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	I	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	J	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	K	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		
1	L	770	Total	C	N	O	S	0	0
			6245	4002	1082	1127	34		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	THR	ILE	conflict	UNP A0A8E2SFD7
B	274	THR	ILE	conflict	UNP A0A8E2SFD7
C	274	THR	ILE	conflict	UNP A0A8E2SFD7
D	274	THR	ILE	conflict	UNP A0A8E2SFD7
E	274	THR	ILE	conflict	UNP A0A8E2SFD7
F	274	THR	ILE	conflict	UNP A0A8E2SFD7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	THR	ILE	conflict	UNP A0A8E2SFD7
H	274	THR	ILE	conflict	UNP A0A8E2SFD7
I	274	THR	ILE	conflict	UNP A0A8E2SFD7
J	274	THR	ILE	conflict	UNP A0A8E2SFD7
K	274	THR	ILE	conflict	UNP A0A8E2SFD7
L	274	THR	ILE	conflict	UNP A0A8E2SFD7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

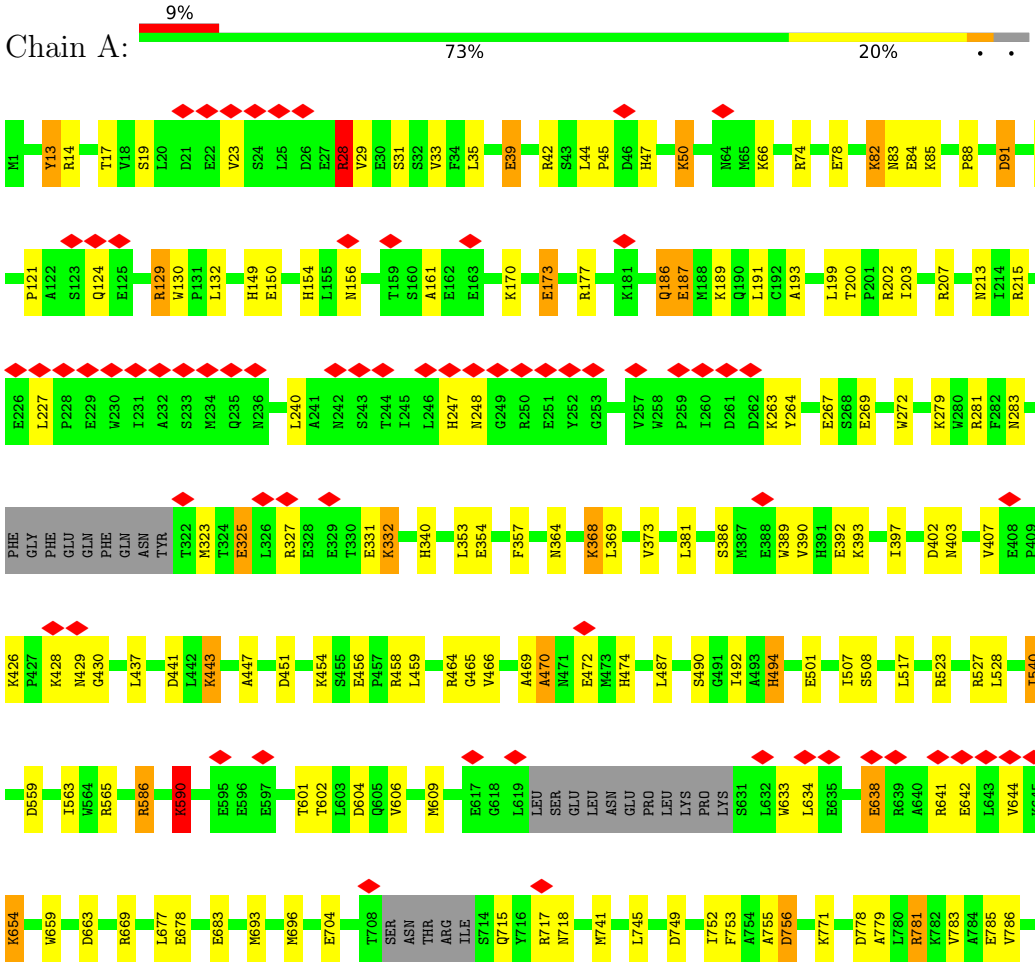
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0
2	E	1	Total Zn 1 1	0
2	F	1	Total Zn 1 1	0
2	G	1	Total Zn 1 1	0
2	H	1	Total Zn 1 1	0
2	I	1	Total Zn 1 1	0
2	J	1	Total Zn 1 1	0
2	K	1	Total Zn 1 1	0
2	L	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

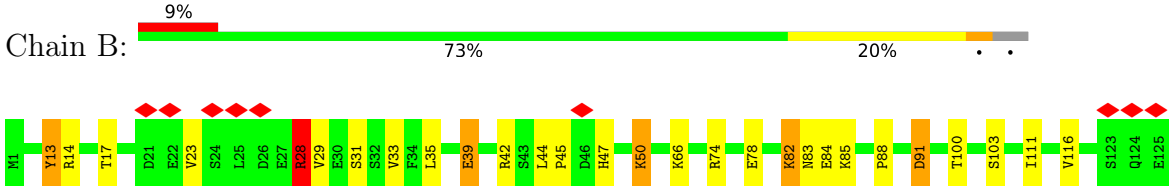
• Molecule 1: Adenosine deaminase

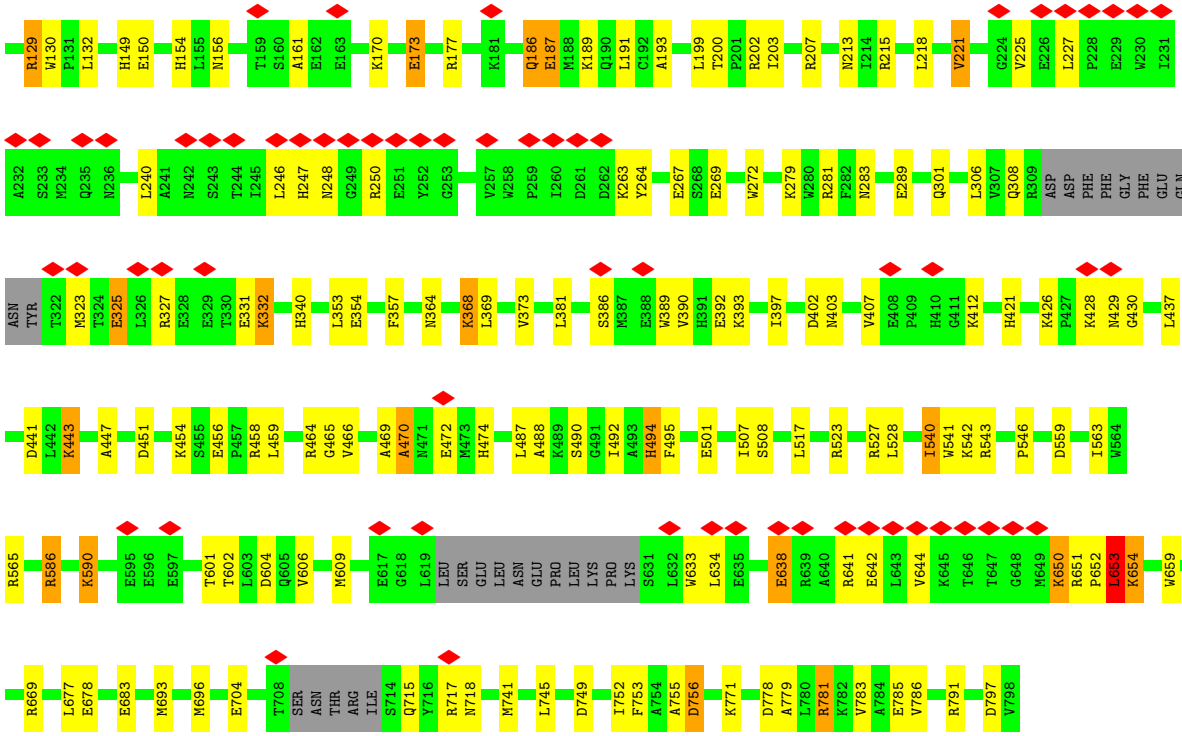
Chain A:



• Molecule 1: Adenosine deaminase

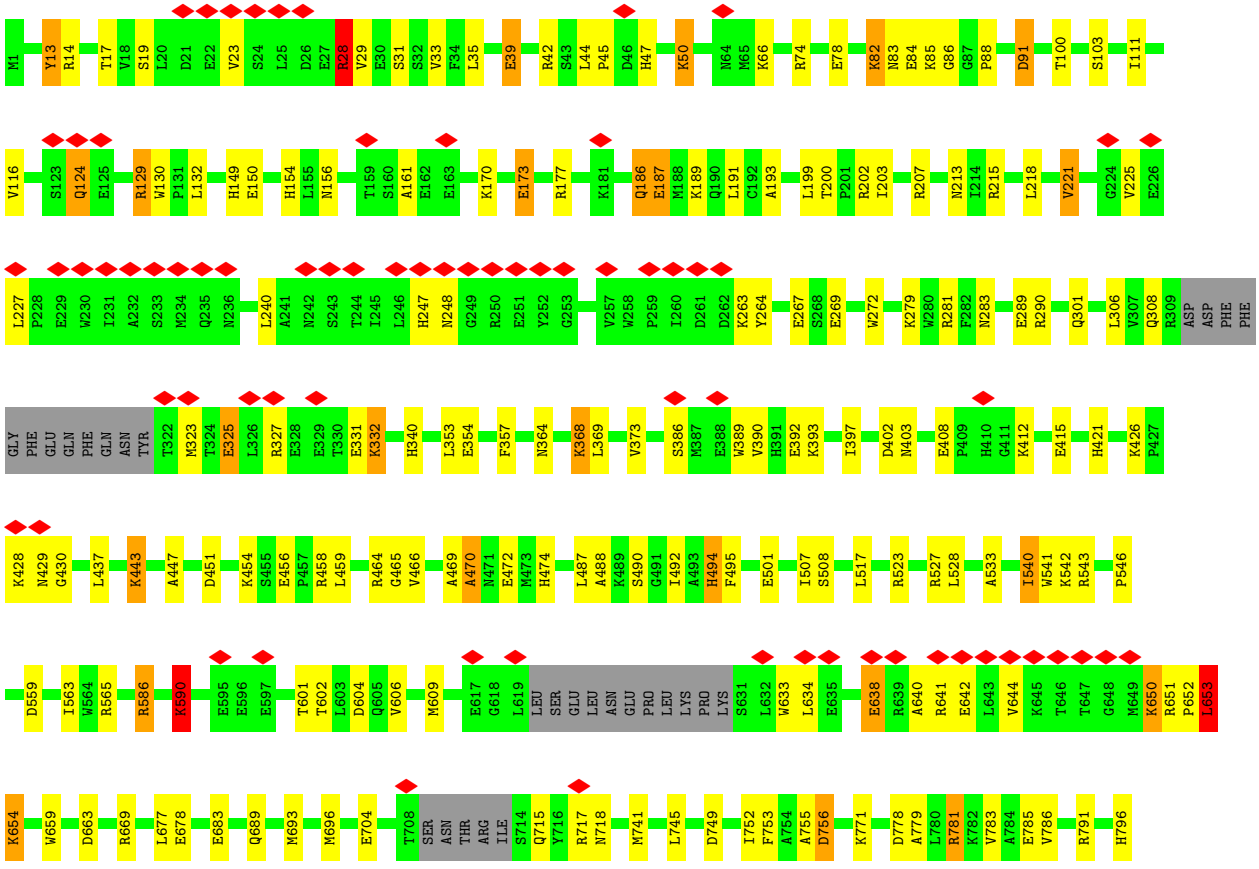
Chain B:





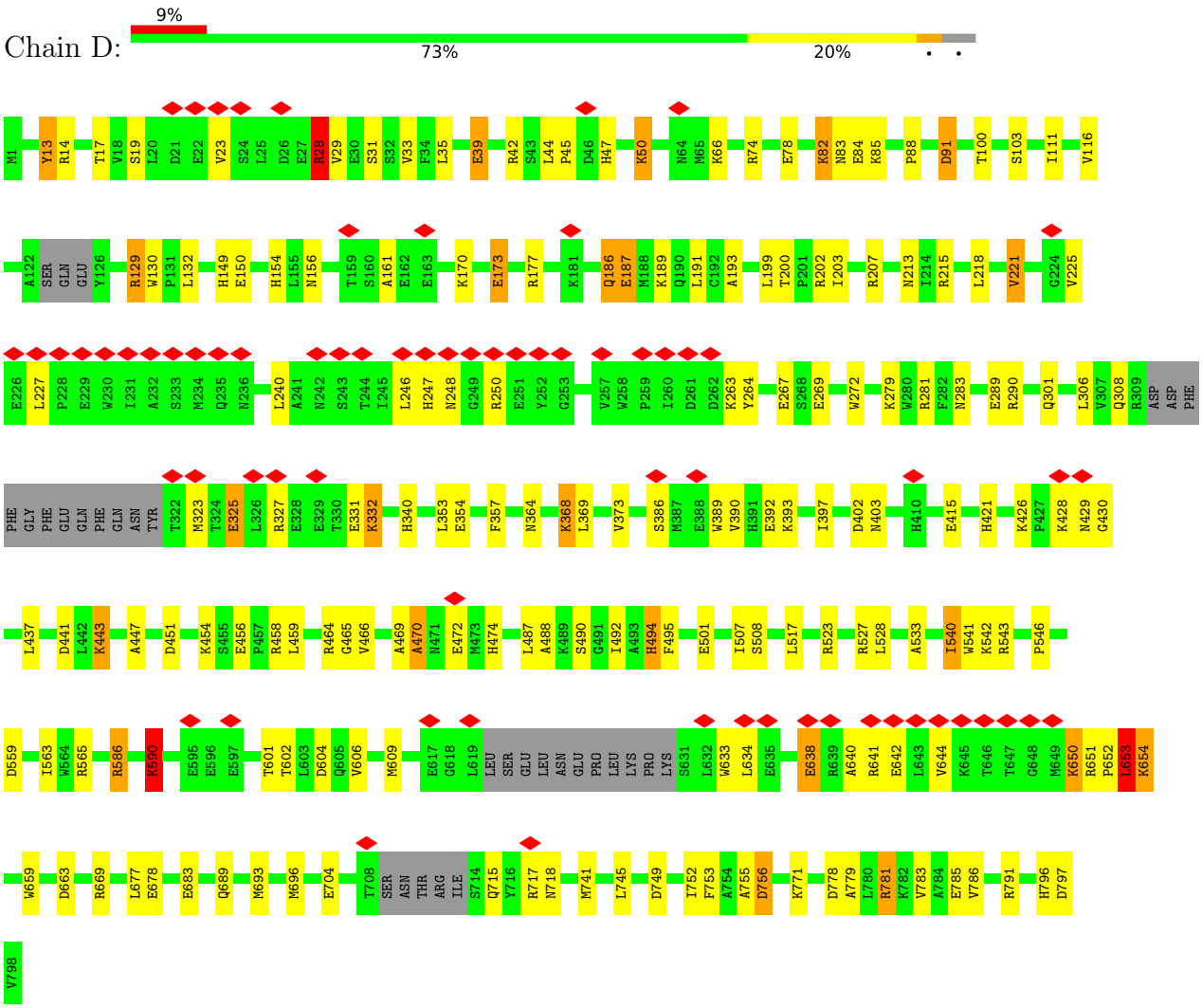
• Molecule 1: Adenosine deaminase

Chain C:



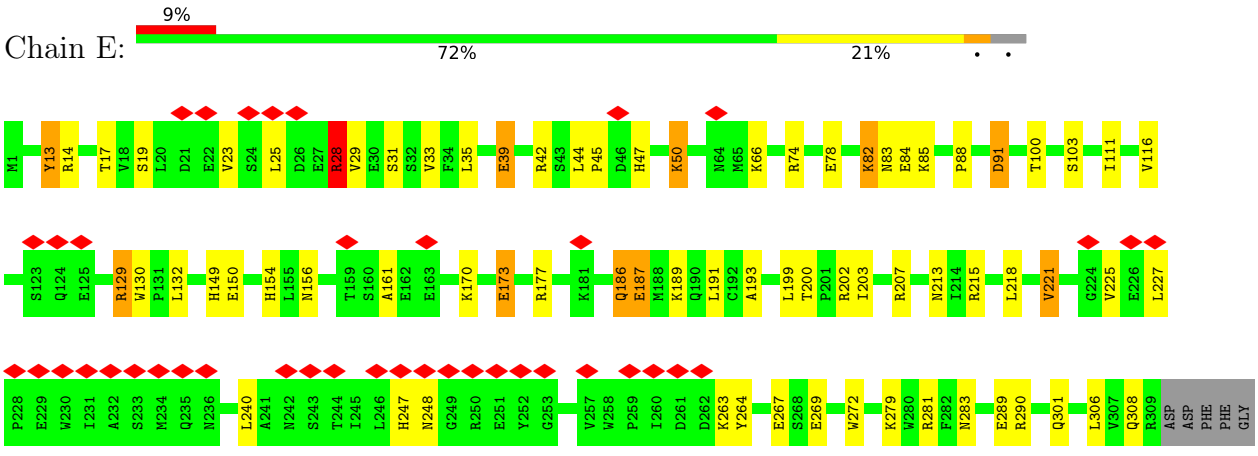
• Molecule 1: Adenosine deaminase

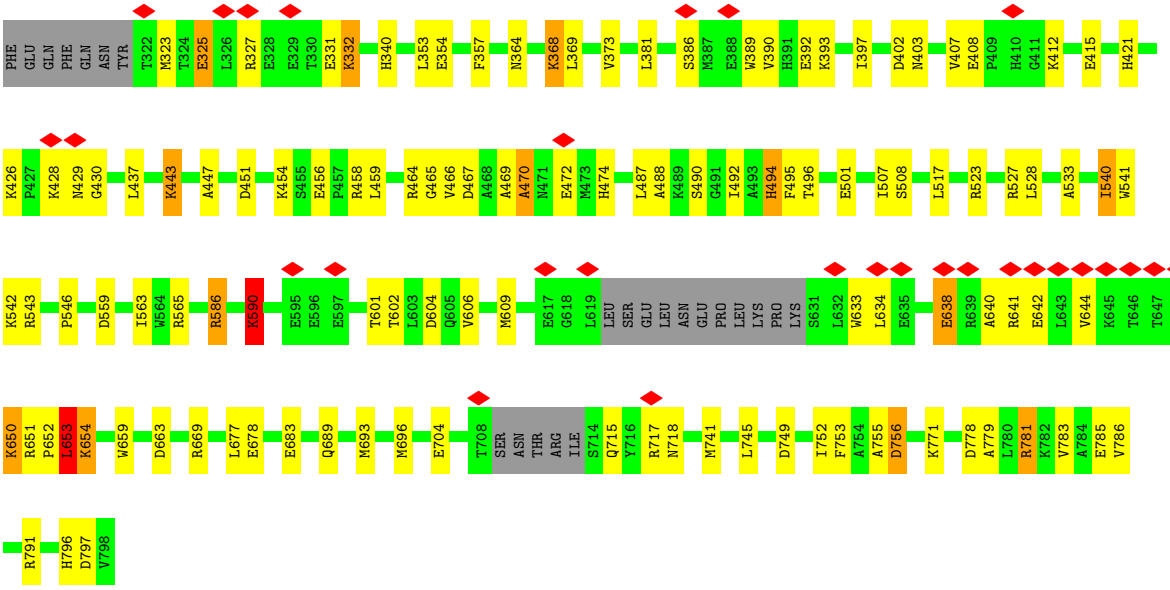
Chain D:



• Molecule 1: Adenosine deaminase

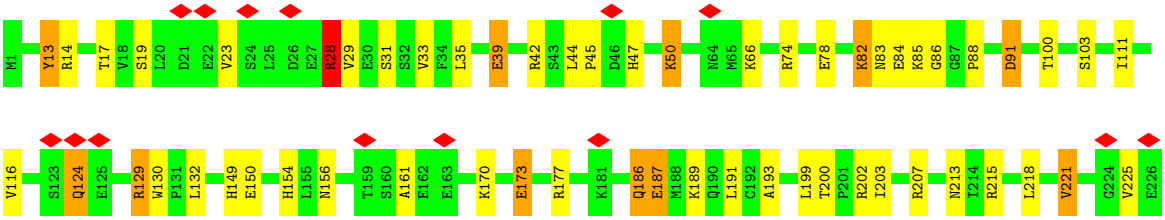
Chain E:

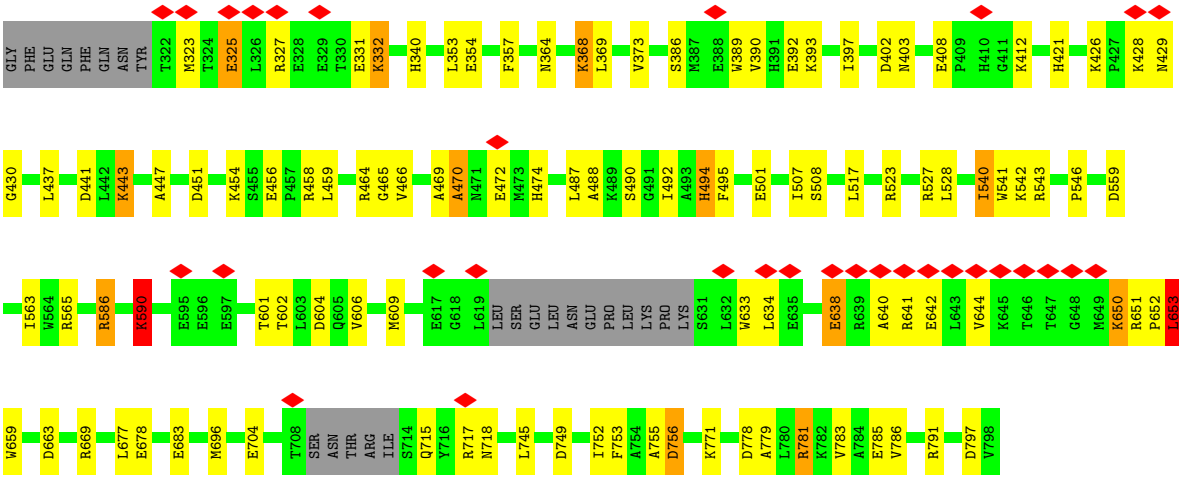




• Molecule 1: Adenosine deaminase

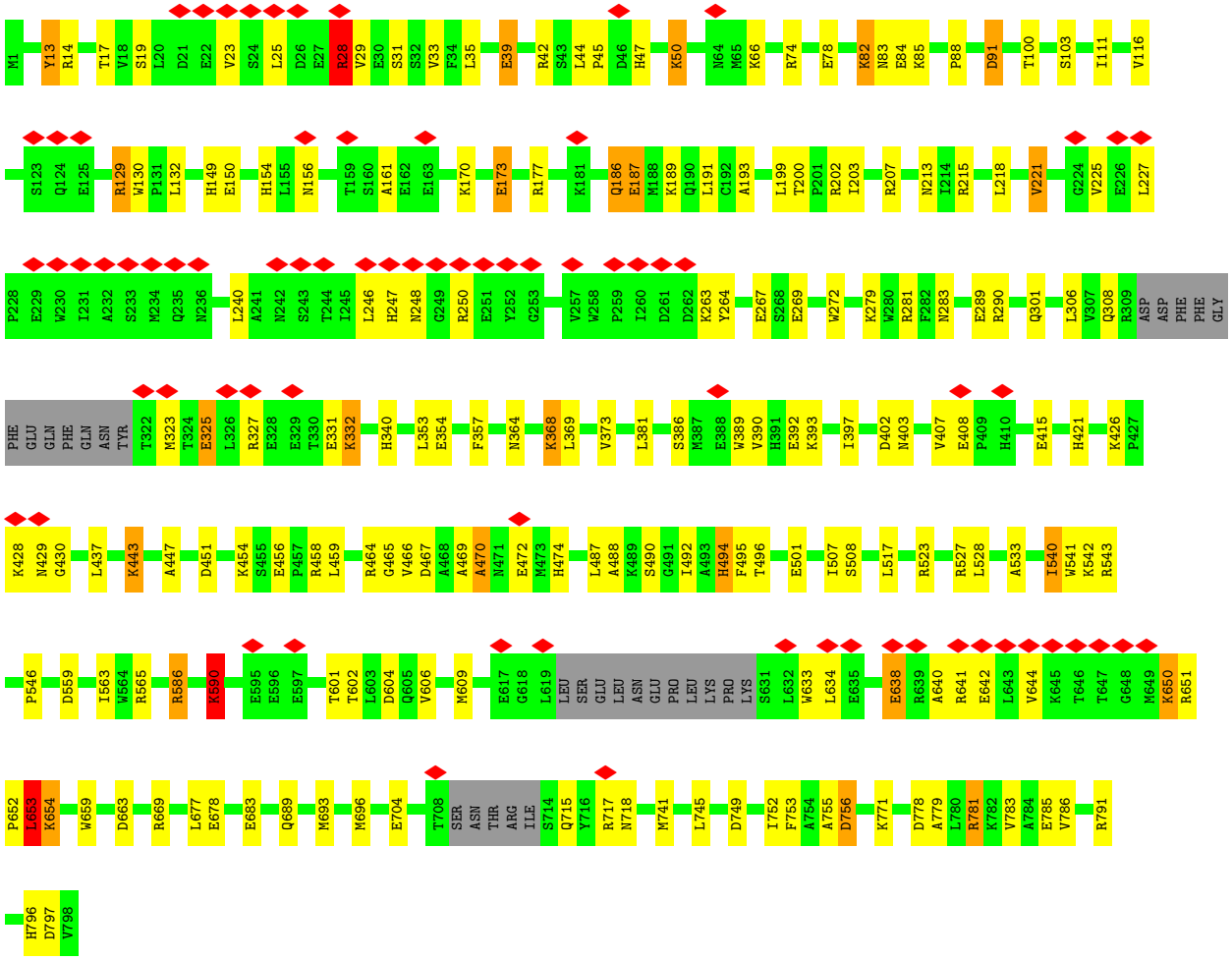
Chain F:





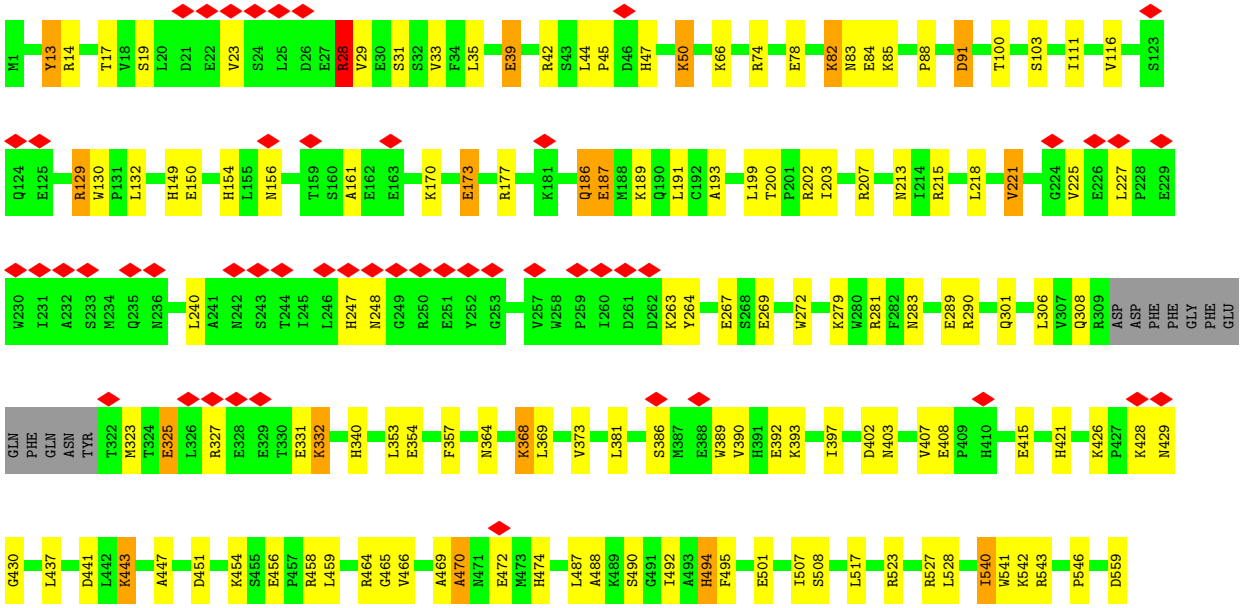
• Molecule 1: Adenosine deaminase

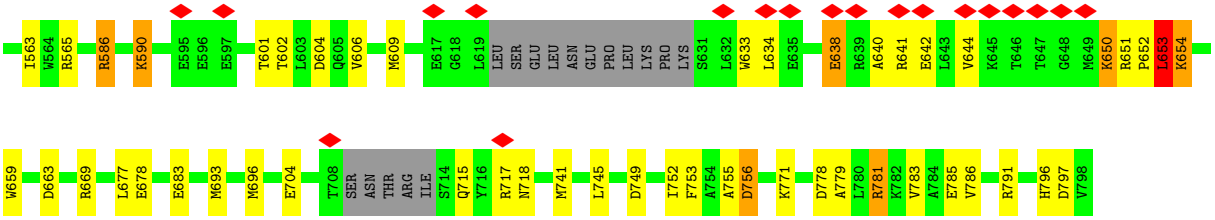
Chain G:



• Molecule 1: Adenosine deaminase

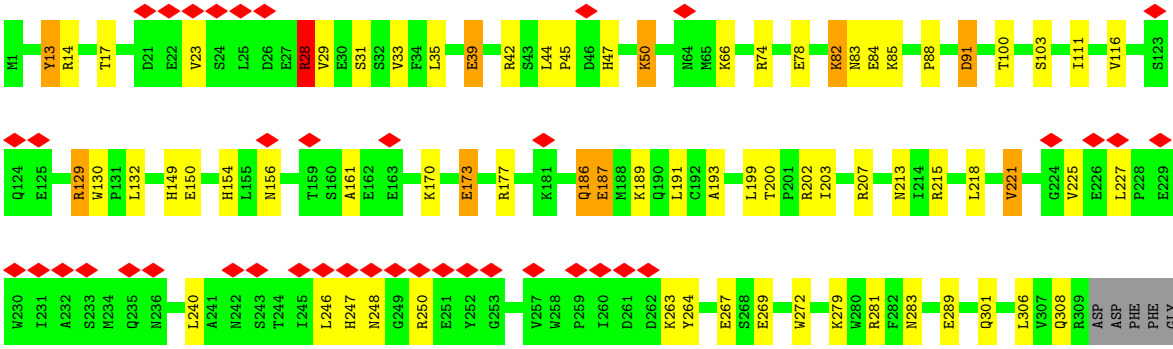
Chain H:

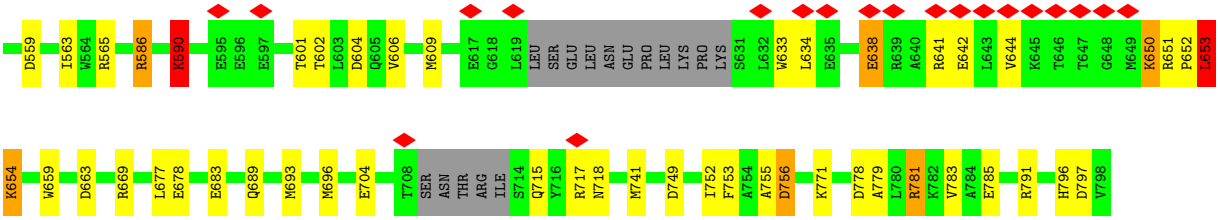




• Molecule 1: Adenosine deaminase

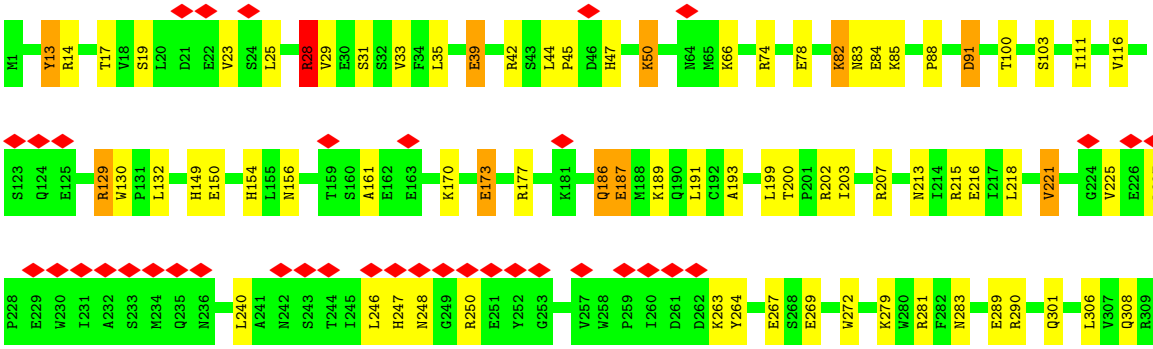
Chain I:

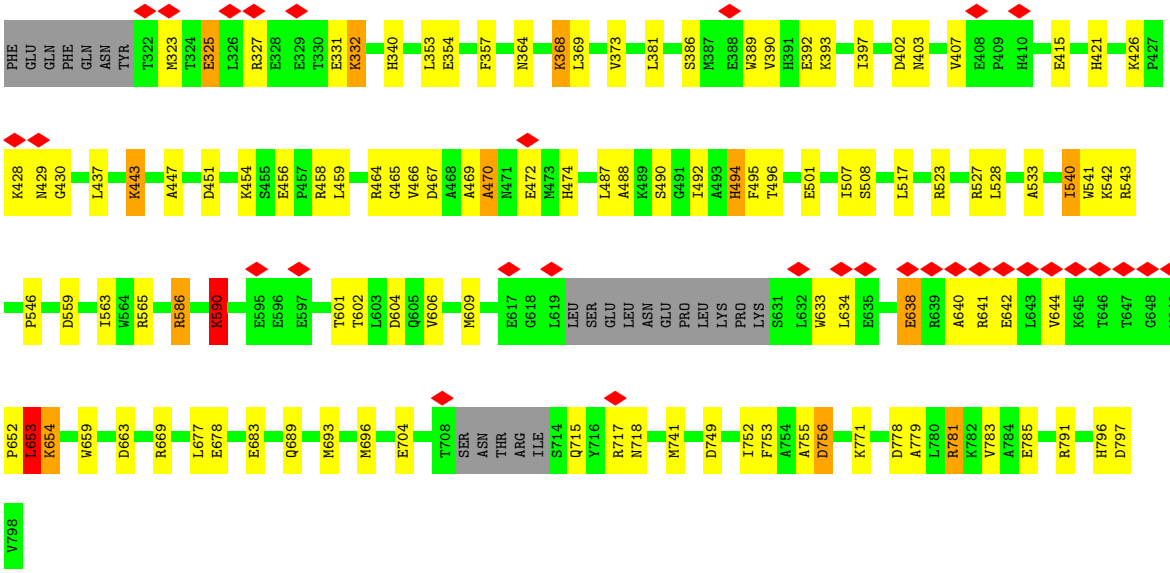




• Molecule 1: Adenosine deaminase

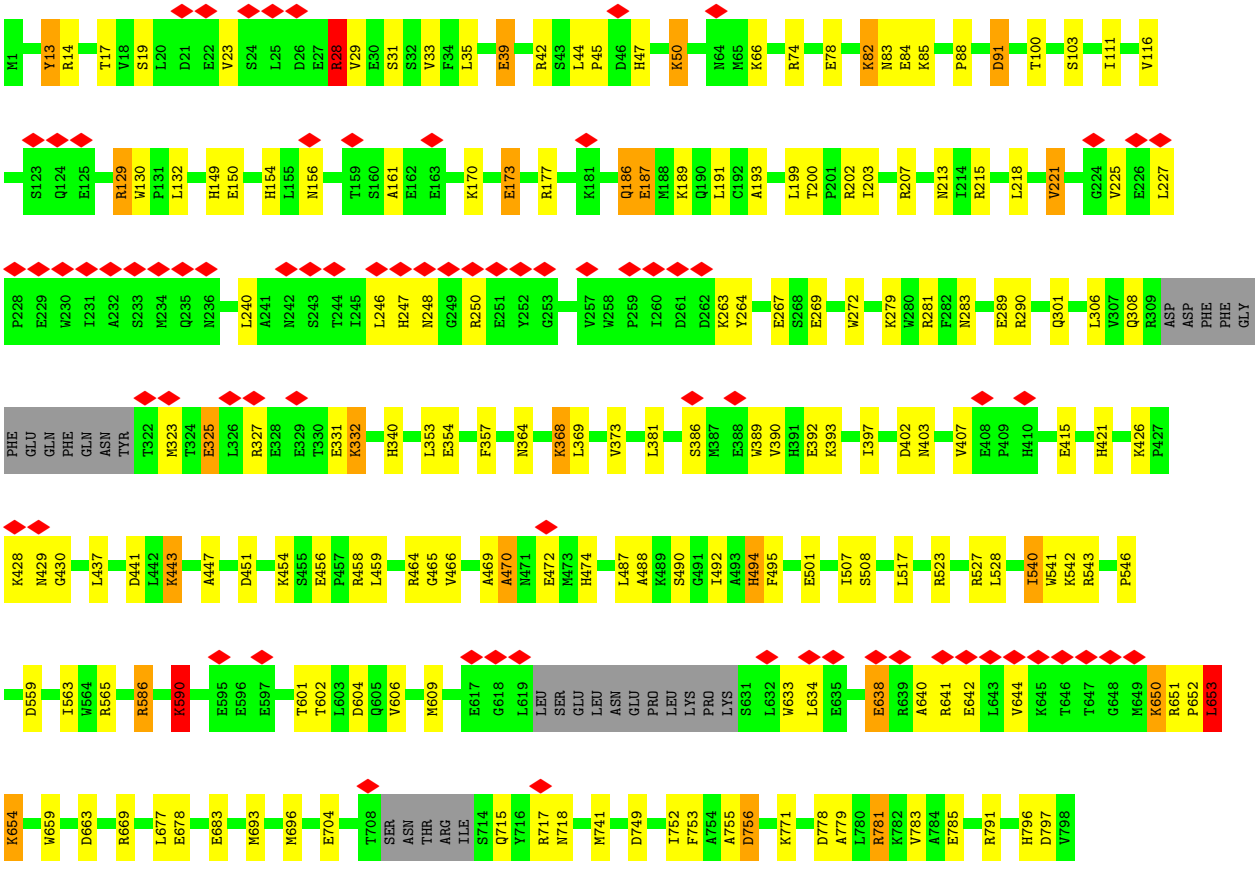
Chain J:





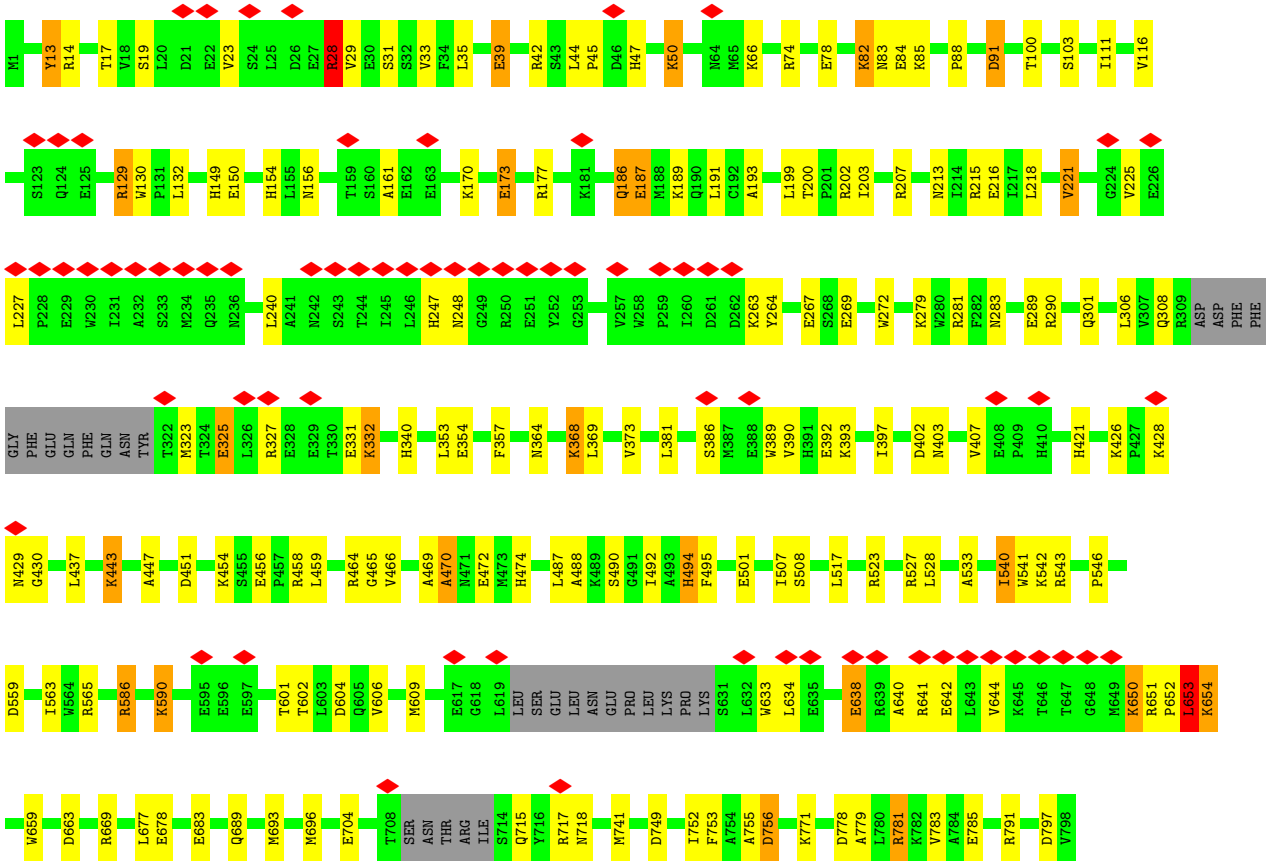
• Molecule 1: Adenosine deaminase

Chain K:



• Molecule 1: Adenosine deaminase

Chain L:


M1 Y13 R14 T17 V18 S19 L20 D21 E22 V23 S24 L25 D26 E27 R28 V29 E30 S31 S32 V33 F34 L35 E39 R42 S43 L44 P45 D46 H47 K50 N64 M65 K66 R74 E78 K82 N83 E84 K85 P88 D91 T100 S103 I111 V116
S123 Q124 E125 R129 W130 P131 L132 H149 E150 H154 L155 N156 T159 S160 A161 E162 E163 K170 E173 R177 K181 Q186 E187 M188 K189 Q190 L191 C192 A193 L199 T200 P201 R202 I203 R207 N213 I214 R215 E216 I217 L218 V221 G224 V225 E226
L227 P228 E229 W230 I231 A232 S233 M234 Q235 N236 L240 A241 N242 S243 T244 I245 L246 H247 N248 G249 R250 E251 Y252 G253 V257 W258 P259 I260 D261 D262 K263 Y264 E267 S268 E269 W272 K279 W280 R281 F282 N283 E289 R290 Q301 L306 V307 Q308 R309 ASP ASP PHE PHE
GLY PHE GLU GLN PHE GLN ASN TYR T322 M323 T324 E325 L326 R327 E328 E329 T330 E331 K332 H340 L353 E354 F357 N364 K368 L369 V373 L381 S386 M387 E388 W389 V390 H391 E392 K393 I397 D402 N403 V407 E408 P409 H410 H421 K426 P427 K428
N429 G430 L437 K443 A447 D451 K454 S455 E456 P457 R458 L459 R464 G465 V466 A469 A470 N471 E472 M473 H474 L487 A488 K489 S490 G491 I492 A493 H494 F495 E501 I507 S508 L517 R523 R527 L528 A533 I540 W541 K542 R543 P546
D559 I563 W564 R565 R586 K590 E595 E596 E597 T601 T602 L603 D604 Q605 V606 M609 E617 G618 L619 LEU SER GLU LEU ASN GLU PRO LEU LYS PRO LYS S631 L632 W633 L634 E635 E638 R639 A640 R641 E642 L643 V644 K645 T646 T647 G648 M649 K650 R651 P652 L653 K654
W659 D663 R669 L677 E678 E683 Q689 M693 M696 E704 T708 SER ASN THR ARG ILE S714 Q715 Y716 R717 N718 M741 D749 I752 F753 A754 A755 D756 K771 D778 A779 L780 R781 K782 V783 A784 E785 R791 D797 V798

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	233454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.050	Depositor
Minimum map value	-2.537	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	B	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	C	0.41	4/6400 (0.1%)	0.75	24/8672 (0.3%)
1	D	0.41	4/6375 (0.1%)	0.75	25/8637 (0.3%)
1	E	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	F	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	G	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	H	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	I	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	J	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	K	0.41	4/6400 (0.1%)	0.75	25/8672 (0.3%)
1	L	0.41	4/6400 (0.1%)	0.75	24/8672 (0.3%)
All	All	0.41	48/76775 (0.1%)	0.75	298/104029 (0.3%)

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	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
1	G	0	5
1	H	0	5
1	I	0	5
1	J	0	5
1	K	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	5
All	All	0	60

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	13	TYR	CD2-CE2	10.63	1.55	1.39
1	I	13	TYR	CD2-CE2	10.62	1.55	1.39
1	F	13	TYR	CD2-CE2	10.62	1.55	1.39
1	C	13	TYR	CD2-CE2	10.61	1.55	1.39
1	J	13	TYR	CD2-CE2	10.60	1.55	1.39
1	E	13	TYR	CD2-CE2	10.59	1.55	1.39
1	K	13	TYR	CD2-CE2	10.59	1.55	1.39
1	B	13	TYR	CD2-CE2	10.59	1.55	1.39
1	D	13	TYR	CD2-CE2	10.58	1.55	1.39
1	L	13	TYR	CD2-CE2	10.58	1.55	1.39
1	H	13	TYR	CD2-CE2	10.57	1.55	1.39
1	A	13	TYR	CD2-CE2	10.56	1.55	1.39
1	B	187	GLU	CB-CG	7.36	1.66	1.52
1	D	187	GLU	CB-CG	7.35	1.66	1.52
1	A	187	GLU	CB-CG	7.35	1.66	1.52
1	K	187	GLU	CB-CG	7.34	1.66	1.52
1	F	187	GLU	CB-CG	7.32	1.66	1.52
1	E	187	GLU	CB-CG	7.31	1.66	1.52
1	L	187	GLU	CB-CG	7.31	1.66	1.52
1	G	187	GLU	CB-CG	7.30	1.66	1.52
1	H	187	GLU	CB-CG	7.29	1.66	1.52
1	C	187	GLU	CB-CG	7.29	1.66	1.52
1	J	187	GLU	CB-CG	7.29	1.66	1.52
1	I	187	GLU	CB-CG	7.28	1.66	1.52
1	H	13	TYR	CE2-CZ	6.15	1.46	1.38
1	B	13	TYR	CE2-CZ	6.15	1.46	1.38
1	D	13	TYR	CE2-CZ	6.15	1.46	1.38
1	E	13	TYR	CE2-CZ	6.14	1.46	1.38
1	I	13	TYR	CE2-CZ	6.12	1.46	1.38
1	J	13	TYR	CE2-CZ	6.11	1.46	1.38
1	L	13	TYR	CE2-CZ	6.11	1.46	1.38
1	K	13	TYR	CE2-CZ	6.10	1.46	1.38
1	F	13	TYR	CE2-CZ	6.10	1.46	1.38
1	C	13	TYR	CE2-CZ	6.09	1.46	1.38
1	A	13	TYR	CE2-CZ	6.07	1.46	1.38
1	G	13	TYR	CE2-CZ	6.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	590	LYS	CB-CG	-5.52	1.37	1.52
1	A	590	LYS	CB-CG	-5.50	1.37	1.52
1	H	590	LYS	CB-CG	-5.50	1.37	1.52
1	E	590	LYS	CB-CG	-5.50	1.37	1.52
1	B	590	LYS	CB-CG	-5.50	1.37	1.52
1	D	590	LYS	CB-CG	-5.50	1.37	1.52
1	J	590	LYS	CB-CG	-5.49	1.37	1.52
1	I	590	LYS	CB-CG	-5.49	1.37	1.52
1	C	590	LYS	CB-CG	-5.48	1.37	1.52
1	G	590	LYS	CB-CG	-5.47	1.37	1.52
1	K	590	LYS	CB-CG	-5.47	1.37	1.52
1	L	590	LYS	CB-CG	-5.47	1.37	1.52

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	590	LYS	CD-CE-NZ	14.73	145.58	111.70
1	I	590	LYS	CD-CE-NZ	14.72	145.56	111.70
1	K	590	LYS	CD-CE-NZ	14.72	145.55	111.70
1	G	590	LYS	CD-CE-NZ	14.71	145.54	111.70
1	J	590	LYS	CD-CE-NZ	14.71	145.54	111.70
1	L	590	LYS	CD-CE-NZ	14.71	145.54	111.70
1	D	590	LYS	CD-CE-NZ	14.71	145.54	111.70
1	H	590	LYS	CD-CE-NZ	14.71	145.53	111.70
1	C	590	LYS	CD-CE-NZ	14.71	145.53	111.70
1	E	590	LYS	CD-CE-NZ	14.71	145.52	111.70
1	F	590	LYS	CD-CE-NZ	14.70	145.52	111.70
1	B	590	LYS	CD-CE-NZ	14.69	145.49	111.70
1	F	129	ARG	CG-CD-NE	14.44	142.11	111.80
1	H	129	ARG	CG-CD-NE	14.43	142.11	111.80
1	E	129	ARG	CG-CD-NE	14.43	142.10	111.80
1	D	129	ARG	CG-CD-NE	14.43	142.09	111.80
1	K	129	ARG	CG-CD-NE	14.42	142.08	111.80
1	B	129	ARG	CG-CD-NE	14.42	142.07	111.80
1	G	129	ARG	CG-CD-NE	14.41	142.07	111.80
1	A	129	ARG	CG-CD-NE	14.41	142.06	111.80
1	I	129	ARG	CG-CD-NE	14.41	142.06	111.80
1	L	129	ARG	CG-CD-NE	14.41	142.06	111.80
1	C	129	ARG	CG-CD-NE	14.41	142.05	111.80
1	J	129	ARG	CG-CD-NE	14.40	142.03	111.80
1	C	654	LYS	CD-CE-NZ	11.55	138.26	111.70
1	J	654	LYS	CD-CE-NZ	11.54	138.24	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	654	LYS	CD-CE-NZ	11.53	138.23	111.70
1	K	654	LYS	CD-CE-NZ	11.54	138.23	111.70
1	A	654	LYS	CD-CE-NZ	11.53	138.22	111.70
1	H	654	LYS	CD-CE-NZ	11.53	138.22	111.70
1	B	654	LYS	CD-CE-NZ	11.53	138.22	111.70
1	G	654	LYS	CD-CE-NZ	11.52	138.20	111.70
1	E	654	LYS	CD-CE-NZ	11.52	138.19	111.70
1	L	654	LYS	CD-CE-NZ	11.52	138.18	111.70
1	D	654	LYS	CD-CE-NZ	11.51	138.17	111.70
1	I	654	LYS	CD-CE-NZ	11.51	138.17	111.70
1	L	650	LYS	CD-CE-NZ	11.39	137.90	111.70
1	C	650	LYS	CD-CE-NZ	11.39	137.89	111.70
1	A	650	LYS	CD-CE-NZ	11.38	137.88	111.70
1	I	650	LYS	CD-CE-NZ	11.38	137.88	111.70
1	D	650	LYS	CD-CE-NZ	11.38	137.88	111.70
1	B	650	LYS	CD-CE-NZ	11.38	137.87	111.70
1	F	650	LYS	CD-CE-NZ	11.37	137.85	111.70
1	G	650	LYS	CD-CE-NZ	11.37	137.85	111.70
1	H	650	LYS	CD-CE-NZ	11.36	137.83	111.70
1	J	650	LYS	CD-CE-NZ	11.36	137.83	111.70
1	K	650	LYS	CD-CE-NZ	11.36	137.83	111.70
1	E	650	LYS	CD-CE-NZ	11.34	137.78	111.70
1	I	771	LYS	CD-CE-NZ	10.97	136.94	111.70
1	J	771	LYS	CD-CE-NZ	10.97	136.93	111.70
1	C	771	LYS	CD-CE-NZ	10.97	136.92	111.70
1	H	771	LYS	CD-CE-NZ	10.96	136.92	111.70
1	D	771	LYS	CD-CE-NZ	10.96	136.91	111.70
1	E	771	LYS	CD-CE-NZ	10.96	136.91	111.70
1	G	771	LYS	CD-CE-NZ	10.96	136.91	111.70
1	B	771	LYS	CD-CE-NZ	10.96	136.91	111.70
1	A	771	LYS	CD-CE-NZ	10.96	136.90	111.70
1	F	771	LYS	CD-CE-NZ	10.95	136.90	111.70
1	K	771	LYS	CD-CE-NZ	10.95	136.87	111.70
1	L	771	LYS	CD-CE-NZ	10.95	136.88	111.70
1	D	28	ARG	CB-CG-CD	8.19	132.90	111.60
1	K	28	ARG	CB-CG-CD	8.19	132.90	111.60
1	A	28	ARG	CG-CD-NE	8.18	128.98	111.80
1	G	28	ARG	CB-CG-CD	8.18	132.87	111.60
1	H	28	ARG	CG-CD-NE	8.18	128.98	111.80
1	L	28	ARG	CB-CG-CD	8.18	132.87	111.60
1	C	28	ARG	CB-CG-CD	8.18	132.87	111.60
1	F	28	ARG	CB-CG-CD	8.18	132.87	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	28	ARG	CG-CD-NE	8.18	128.98	111.80
1	I	28	ARG	CB-CG-CD	8.18	132.86	111.60
1	C	28	ARG	CG-CD-NE	8.18	128.97	111.80
1	B	28	ARG	CG-CD-NE	8.17	128.97	111.80
1	A	28	ARG	CB-CG-CD	8.17	132.84	111.60
1	H	28	ARG	CB-CG-CD	8.17	132.83	111.60
1	I	28	ARG	CG-CD-NE	8.17	128.95	111.80
1	D	28	ARG	CG-CD-NE	8.16	128.94	111.80
1	E	28	ARG	CG-CD-NE	8.16	128.94	111.80
1	L	28	ARG	CG-CD-NE	8.16	128.94	111.80
1	E	28	ARG	CB-CG-CD	8.16	132.81	111.60
1	G	28	ARG	CG-CD-NE	8.16	128.94	111.80
1	J	28	ARG	CB-CG-CD	8.16	132.82	111.60
1	B	28	ARG	CB-CG-CD	8.16	132.81	111.60
1	F	28	ARG	CG-CD-NE	8.15	128.93	111.80
1	K	28	ARG	CG-CD-NE	8.15	128.92	111.80
1	J	393	LYS	CD-CE-NZ	6.65	126.99	111.70
1	C	393	LYS	CD-CE-NZ	6.65	126.99	111.70
1	L	393	LYS	CD-CE-NZ	6.65	126.99	111.70
1	G	393	LYS	CD-CE-NZ	6.64	126.98	111.70
1	F	393	LYS	CD-CE-NZ	6.64	126.98	111.70
1	H	393	LYS	CD-CE-NZ	6.64	126.97	111.70
1	E	393	LYS	CD-CE-NZ	6.64	126.97	111.70
1	K	393	LYS	CD-CE-NZ	6.63	126.95	111.70
1	A	393	LYS	CD-CE-NZ	6.63	126.95	111.70
1	B	393	LYS	CD-CE-NZ	6.63	126.95	111.70
1	D	393	LYS	CD-CE-NZ	6.62	126.94	111.70
1	I	393	LYS	CD-CE-NZ	6.62	126.92	111.70
1	G	129	ARG	CB-CG-CD	-6.55	94.56	111.60
1	A	129	ARG	CB-CG-CD	-6.55	94.56	111.60
1	J	129	ARG	CB-CG-CD	-6.55	94.56	111.60
1	C	129	ARG	CB-CG-CD	-6.55	94.57	111.60
1	B	129	ARG	CB-CG-CD	-6.54	94.59	111.60
1	D	129	ARG	CB-CG-CD	-6.54	94.59	111.60
1	I	129	ARG	CB-CG-CD	-6.54	94.59	111.60
1	L	129	ARG	CB-CG-CD	-6.54	94.59	111.60
1	F	129	ARG	CB-CG-CD	-6.53	94.61	111.60
1	H	129	ARG	CB-CG-CD	-6.53	94.61	111.60
1	K	129	ARG	CB-CG-CD	-6.53	94.61	111.60
1	E	129	ARG	CB-CG-CD	-6.53	94.62	111.60
1	H	443	LYS	CD-CE-NZ	6.53	126.72	111.70
1	C	443	LYS	CD-CE-NZ	6.53	126.71	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	443	LYS	CD-CE-NZ	6.53	126.71	111.70
1	L	443	LYS	CD-CE-NZ	6.52	126.70	111.70
1	I	443	LYS	CD-CE-NZ	6.52	126.69	111.70
1	J	443	LYS	CD-CE-NZ	6.52	126.69	111.70
1	A	443	LYS	CD-CE-NZ	6.52	126.69	111.70
1	D	443	LYS	CD-CE-NZ	6.51	126.68	111.70
1	F	443	LYS	CD-CE-NZ	6.51	126.68	111.70
1	B	443	LYS	CD-CE-NZ	6.51	126.67	111.70
1	K	443	LYS	CD-CE-NZ	6.51	126.67	111.70
1	G	443	LYS	CD-CE-NZ	6.50	126.65	111.70
1	L	454	LYS	CD-CE-NZ	6.44	126.52	111.70
1	F	454	LYS	CD-CE-NZ	6.43	126.50	111.70
1	K	454	LYS	CD-CE-NZ	6.43	126.49	111.70
1	D	454	LYS	CD-CE-NZ	6.43	126.49	111.70
1	E	454	LYS	CD-CE-NZ	6.43	126.49	111.70
1	A	454	LYS	CD-CE-NZ	6.42	126.46	111.70
1	H	454	LYS	CD-CE-NZ	6.42	126.46	111.70
1	G	454	LYS	CD-CE-NZ	6.41	126.45	111.70
1	I	454	LYS	CD-CE-NZ	6.41	126.45	111.70
1	C	454	LYS	CD-CE-NZ	6.41	126.44	111.70
1	B	454	LYS	CD-CE-NZ	6.41	126.44	111.70
1	J	454	LYS	CD-CE-NZ	6.40	126.43	111.70
1	I	129	ARG	CD-NE-CZ	6.37	132.52	123.60
1	K	129	ARG	CD-NE-CZ	6.37	132.52	123.60
1	J	129	ARG	CD-NE-CZ	6.36	132.51	123.60
1	C	129	ARG	CD-NE-CZ	6.36	132.50	123.60
1	B	129	ARG	CD-NE-CZ	6.36	132.50	123.60
1	L	129	ARG	CD-NE-CZ	6.35	132.49	123.60
1	G	129	ARG	CD-NE-CZ	6.34	132.47	123.60
1	H	129	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	129	ARG	CD-NE-CZ	6.33	132.47	123.60
1	E	129	ARG	CD-NE-CZ	6.33	132.46	123.60
1	D	129	ARG	CD-NE-CZ	6.32	132.44	123.60
1	F	129	ARG	CD-NE-CZ	6.32	132.44	123.60
1	J	187	GLU	CA-CB-CG	6.29	127.23	113.40
1	A	187	GLU	CA-CB-CG	6.28	127.22	113.40
1	I	187	GLU	CA-CB-CG	6.28	127.22	113.40
1	G	187	GLU	CA-CB-CG	6.27	127.20	113.40
1	K	187	GLU	CA-CB-CG	6.27	127.20	113.40
1	E	187	GLU	CA-CB-CG	6.27	127.20	113.40
1	H	187	GLU	CA-CB-CG	6.27	127.20	113.40
1	F	187	GLU	CA-CB-CG	6.27	127.19	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	187	GLU	CA-CB-CG	6.26	127.17	113.40
1	B	187	GLU	CA-CB-CG	6.26	127.17	113.40
1	C	187	GLU	CA-CB-CG	6.25	127.16	113.40
1	L	187	GLU	CA-CB-CG	6.25	127.16	113.40
1	K	653	LEU	CB-CG-CD2	6.06	121.30	111.00
1	B	653	LEU	CB-CG-CD2	6.05	121.29	111.00
1	F	653	LEU	CB-CG-CD2	6.05	121.29	111.00
1	J	653	LEU	CB-CG-CD2	6.04	121.28	111.00
1	D	653	LEU	CB-CG-CD2	6.04	121.27	111.00
1	L	653	LEU	CB-CG-CD2	6.04	121.26	111.00
1	I	653	LEU	CB-CG-CD2	6.04	121.26	111.00
1	A	653	LEU	CB-CG-CD2	6.03	121.25	111.00
1	G	653	LEU	CB-CG-CD2	6.03	121.25	111.00
1	E	653	LEU	CB-CG-CD2	6.02	121.24	111.00
1	C	653	LEU	CB-CG-CD2	6.02	121.23	111.00
1	H	653	LEU	CB-CG-CD2	6.02	121.23	111.00
1	F	13	TYR	CZ-CE2-CD2	-5.97	114.42	119.80
1	I	13	TYR	CZ-CE2-CD2	-5.97	114.43	119.80
1	D	13	TYR	CZ-CE2-CD2	-5.96	114.43	119.80
1	J	13	TYR	CZ-CE2-CD2	-5.96	114.44	119.80
1	C	13	TYR	CZ-CE2-CD2	-5.96	114.44	119.80
1	A	13	TYR	CZ-CE2-CD2	-5.95	114.45	119.80
1	B	13	TYR	CZ-CE2-CD2	-5.95	114.45	119.80
1	H	13	TYR	CZ-CE2-CD2	-5.94	114.45	119.80
1	E	13	TYR	CZ-CE2-CD2	-5.94	114.45	119.80
1	G	13	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	K	13	TYR	CZ-CE2-CD2	-5.91	114.48	119.80
1	L	13	TYR	CZ-CE2-CD2	-5.88	114.50	119.80
1	B	187	GLU	CG-CD-OE2	-5.84	106.61	118.30
1	D	187	GLU	CG-CD-OE2	-5.84	106.61	118.30
1	H	187	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	A	187	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	F	187	GLU	CG-CD-OE2	-5.84	106.63	118.30
1	I	187	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	L	187	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	C	187	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	E	187	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	G	156	ASN	N-CA-CB	5.83	121.09	110.60
1	I	156	ASN	N-CA-CB	5.83	121.09	110.60
1	K	187	GLU	CG-CD-OE2	-5.83	106.65	118.30
1	C	156	ASN	N-CA-CB	5.83	121.09	110.60
1	K	156	ASN	N-CA-CB	5.82	121.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	187	GLU	CG-CD-OE2	-5.82	106.66	118.30
1	D	156	ASN	N-CA-CB	5.82	121.07	110.60
1	J	156	ASN	N-CA-CB	5.81	121.06	110.60
1	J	187	GLU	CG-CD-OE2	-5.81	106.67	118.30
1	F	156	ASN	N-CA-CB	5.81	121.06	110.60
1	B	156	ASN	N-CA-CB	5.81	121.06	110.60
1	E	156	ASN	N-CA-CB	5.81	121.06	110.60
1	H	156	ASN	N-CA-CB	5.80	121.04	110.60
1	L	156	ASN	N-CA-CB	5.79	121.03	110.60
1	A	156	ASN	N-CA-CB	5.79	121.03	110.60
1	B	590	LYS	CB-CG-CD	5.61	126.19	111.60
1	F	590	LYS	CB-CG-CD	5.61	126.19	111.60
1	I	590	LYS	CB-CG-CD	5.61	126.18	111.60
1	J	590	LYS	CB-CG-CD	5.61	126.18	111.60
1	G	590	LYS	CB-CG-CD	5.60	126.17	111.60
1	K	590	LYS	CB-CG-CD	5.60	126.16	111.60
1	C	590	LYS	CB-CG-CD	5.60	126.16	111.60
1	A	590	LYS	CB-CG-CD	5.60	126.15	111.60
1	D	590	LYS	CB-CG-CD	5.60	126.15	111.60
1	H	590	LYS	CB-CG-CD	5.60	126.15	111.60
1	E	590	LYS	CB-CG-CD	5.59	126.14	111.60
1	L	590	LYS	CB-CG-CD	5.58	126.12	111.60
1	D	129	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	129	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	129	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	129	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	J	129	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	H	129	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	L	129	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	G	129	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	129	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	K	129	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	I	129	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	129	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	J	66	LYS	CD-CE-NZ	5.25	123.77	111.70
1	A	156	ASN	N-CA-C	-5.24	96.86	111.00
1	B	66	LYS	CD-CE-NZ	5.24	123.74	111.70
1	B	156	ASN	N-CA-C	-5.24	96.86	111.00
1	F	156	ASN	N-CA-C	-5.24	96.86	111.00
1	C	66	LYS	CD-CE-NZ	5.23	123.74	111.70
1	G	66	LYS	CD-CE-NZ	5.23	123.74	111.70
1	J	156	ASN	N-CA-C	-5.23	96.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	156	ASN	N-CA-C	-5.23	96.88	111.00
1	E	156	ASN	N-CA-C	-5.23	96.89	111.00
1	H	156	ASN	N-CA-C	-5.23	96.89	111.00
1	K	66	LYS	CD-CE-NZ	5.23	123.72	111.70
1	G	156	ASN	N-CA-C	-5.22	96.90	111.00
1	C	156	ASN	N-CA-C	-5.22	96.90	111.00
1	F	66	LYS	CD-CE-NZ	5.22	123.71	111.70
1	D	156	ASN	N-CA-C	-5.22	96.91	111.00
1	L	156	ASN	N-CA-C	-5.22	96.91	111.00
1	A	66	LYS	CD-CE-NZ	5.22	123.70	111.70
1	L	66	LYS	CD-CE-NZ	5.22	123.70	111.70
1	E	66	LYS	CD-CE-NZ	5.21	123.69	111.70
1	I	156	ASN	N-CA-C	-5.21	96.92	111.00
1	H	66	LYS	CD-CE-NZ	5.21	123.68	111.70
1	D	66	LYS	CD-CE-NZ	5.21	123.68	111.70
1	I	66	LYS	CD-CE-NZ	5.20	123.65	111.70
1	A	586	ARG	CD-NE-CZ	5.18	130.85	123.60
1	F	586	ARG	CD-NE-CZ	5.16	130.83	123.60
1	D	586	ARG	CD-NE-CZ	5.16	130.82	123.60
1	H	586	ARG	CD-NE-CZ	5.15	130.81	123.60
1	G	586	ARG	CD-NE-CZ	5.15	130.80	123.60
1	E	586	ARG	CD-NE-CZ	5.14	130.79	123.60
1	J	586	ARG	CD-NE-CZ	5.13	130.79	123.60
1	C	586	ARG	CD-NE-CZ	5.13	130.78	123.60
1	B	586	ARG	CD-NE-CZ	5.11	130.76	123.60
1	I	586	ARG	CD-NE-CZ	5.11	130.75	123.60
1	L	586	ARG	CD-NE-CZ	5.11	130.75	123.60
1	K	586	ARG	CD-NE-CZ	5.11	130.75	123.60
1	G	189	LYS	CD-CE-NZ	5.06	123.34	111.70
1	D	189	LYS	CD-CE-NZ	5.06	123.34	111.70
1	F	189	LYS	CD-CE-NZ	5.06	123.33	111.70
1	H	189	LYS	CD-CE-NZ	5.06	123.34	111.70
1	F	441	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	189	LYS	CD-CE-NZ	5.05	123.32	111.70
1	I	189	LYS	CD-CE-NZ	5.05	123.31	111.70
1	B	189	LYS	CD-CE-NZ	5.05	123.31	111.70
1	L	50	LYS	CD-CE-NZ	5.05	123.31	111.70
1	E	189	LYS	CD-CE-NZ	5.04	123.30	111.70
1	J	189	LYS	CD-CE-NZ	5.04	123.30	111.70
1	K	189	LYS	CD-CE-NZ	5.04	123.30	111.70
1	L	189	LYS	CD-CE-NZ	5.04	123.30	111.70
1	C	189	LYS	CD-CE-NZ	5.04	123.29	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	50	LYS	CD-CE-NZ	5.03	123.28	111.70
1	F	50	LYS	CD-CE-NZ	5.03	123.27	111.70
1	J	50	LYS	CD-CE-NZ	5.03	123.27	111.70
1	K	50	LYS	CD-CE-NZ	5.03	123.27	111.70
1	B	50	LYS	CD-CE-NZ	5.03	123.26	111.70
1	H	441	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	441	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	50	LYS	CD-CE-NZ	5.02	123.25	111.70
1	G	25	LEU	CB-CG-CD2	5.02	119.54	111.00
1	C	50	LYS	CD-CE-NZ	5.02	123.24	111.70
1	D	50	LYS	CD-CE-NZ	5.02	123.24	111.70
1	I	50	LYS	CD-CE-NZ	5.02	123.24	111.70
1	E	50	LYS	CD-CE-NZ	5.01	123.23	111.70
1	K	441	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	G	50	LYS	CD-CE-NZ	5.01	123.23	111.70
1	D	441	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	I	441	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	441	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	J	25	LEU	CB-CG-CD2	5.01	119.51	111.00
1	E	25	LEU	CB-CG-CD2	5.00	119.51	111.00

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	540	ILE	Peptide
1	A	586	ARG	Sidechain
1	A	781	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	540	ILE	Peptide
1	B	586	ARG	Sidechain
1	B	781	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	28	ARG	Sidechain
1	C	540	ILE	Peptide
1	C	586	ARG	Sidechain
1	C	781	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	540	ILE	Peptide
1	D	586	ARG	Sidechain
1	D	781	ARG	Sidechain
1	E	177	ARG	Sidechain
1	E	28	ARG	Sidechain
1	E	540	ILE	Peptide
1	E	586	ARG	Sidechain
1	E	781	ARG	Sidechain
1	F	177	ARG	Sidechain
1	F	28	ARG	Sidechain
1	F	540	ILE	Peptide
1	F	586	ARG	Sidechain
1	F	781	ARG	Sidechain
1	G	177	ARG	Sidechain
1	G	28	ARG	Sidechain
1	G	540	ILE	Peptide
1	G	586	ARG	Sidechain
1	G	781	ARG	Sidechain
1	H	177	ARG	Sidechain
1	H	28	ARG	Sidechain
1	H	540	ILE	Peptide
1	H	586	ARG	Sidechain
1	H	781	ARG	Sidechain
1	I	177	ARG	Sidechain
1	I	28	ARG	Sidechain
1	I	540	ILE	Peptide
1	I	586	ARG	Sidechain
1	I	781	ARG	Sidechain
1	J	177	ARG	Sidechain
1	J	28	ARG	Sidechain
1	J	540	ILE	Peptide
1	J	586	ARG	Sidechain
1	J	781	ARG	Sidechain
1	K	177	ARG	Sidechain
1	K	28	ARG	Sidechain
1	K	540	ILE	Peptide
1	K	586	ARG	Sidechain
1	K	781	ARG	Sidechain
1	L	177	ARG	Sidechain
1	L	28	ARG	Sidechain
1	L	540	ILE	Peptide
1	L	586	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	781	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6245	0	6229	109	0
1	B	6245	0	6229	110	0
1	C	6245	0	6229	111	0
1	D	6221	0	6209	112	0
1	E	6245	0	6229	113	0
1	F	6245	0	6229	109	0
1	G	6245	0	6229	113	0
1	H	6245	0	6229	109	0
1	I	6245	0	6229	109	0
1	J	6245	0	6229	112	0
1	K	6245	0	6229	110	0
1	L	6245	0	6229	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	74928	0	74728	1240	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 (1240) 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)
1:C:472:GLU:OE2	1:C:501:GLU:N	2.02	0.93
1:F:472:GLU:OE2	1:F:501:GLU:N	2.02	0.93
1:H:472:GLU:OE2	1:H:501:GLU:N	2.02	0.92
1:D:472:GLU:OE2	1:D:501:GLU:N	2.02	0.92
1:L:472:GLU:OE2	1:L:501:GLU:N	2.02	0.92
1:C:389:TRP:O	1:C:403:ASN:ND2	2.03	0.92
1:E:472:GLU:OE2	1:E:501:GLU:N	2.02	0.92
1:G:472:GLU:OE2	1:G:501:GLU:N	2.02	0.92
1:A:472:GLU:OE2	1:A:501:GLU:N	2.02	0.92
1:H:389:TRP:O	1:H:403:ASN:ND2	2.03	0.92
1:J:389:TRP:O	1:J:403:ASN:ND2	2.03	0.92
1:L:389:TRP:O	1:L:403:ASN:ND2	2.03	0.92
1:I:389:TRP:O	1:I:403:ASN:ND2	2.03	0.92
1:D:389:TRP:O	1:D:403:ASN:ND2	2.03	0.91
1:I:472:GLU:OE2	1:I:501:GLU:N	2.02	0.91
1:A:389:TRP:O	1:A:403:ASN:ND2	2.03	0.91
1:E:389:TRP:O	1:E:403:ASN:ND2	2.03	0.91
1:K:472:GLU:OE2	1:K:501:GLU:N	2.02	0.91
1:J:472:GLU:OE2	1:J:501:GLU:N	2.02	0.91
1:F:389:TRP:O	1:F:403:ASN:ND2	2.03	0.91
1:G:389:TRP:O	1:G:403:ASN:ND2	2.03	0.91
1:C:42:ARG:NH2	1:D:39:GLU:O	2.04	0.91
1:B:389:TRP:O	1:B:403:ASN:ND2	2.03	0.91
1:B:472:GLU:OE2	1:B:501:GLU:N	2.02	0.91
1:J:42:ARG:NH2	1:K:39:GLU:O	2.03	0.91
1:H:39:GLU:O	1:I:42:ARG:NH2	2.04	0.90
1:J:39:GLU:O	1:K:42:ARG:NH2	2.03	0.90
1:C:39:GLU:O	1:D:42:ARG:NH2	2.04	0.90
1:A:39:GLU:O	1:L:42:ARG:NH2	2.04	0.90
1:A:42:ARG:NH2	1:L:39:GLU:O	2.04	0.90
1:F:39:GLU:O	1:G:42:ARG:NH2	2.04	0.90
1:K:389:TRP:O	1:K:403:ASN:ND2	2.03	0.90
1:B:42:ARG:NH2	1:E:39:GLU:O	2.04	0.90
1:B:39:GLU:O	1:E:42:ARG:NH2	2.04	0.89
1:F:42:ARG:NH2	1:G:39:GLU:O	2.05	0.89
1:H:42:ARG:NH2	1:I:39:GLU:O	2.05	0.89
1:I:778:ASP:OD2	1:I:781:ARG:NH2	2.07	0.88
1:J:778:ASP:OD2	1:J:781:ARG:NH2	2.07	0.88
1:D:778:ASP:OD2	1:D:781:ARG:NH2	2.07	0.88
1:H:778:ASP:OD2	1:H:781:ARG:NH2	2.07	0.87
1:G:778:ASP:OD2	1:G:781:ARG:NH2	2.07	0.87
1:K:778:ASP:OD2	1:K:781:ARG:NH2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:ASP:OD2	1:B:781:ARG:NH2	2.07	0.87
1:L:778:ASP:OD2	1:L:781:ARG:NH2	2.07	0.87
1:E:778:ASP:OD2	1:E:781:ARG:NH2	2.07	0.87
1:A:778:ASP:OD2	1:A:781:ARG:NH2	2.07	0.87
1:C:778:ASP:OD2	1:C:781:ARG:NH2	2.07	0.86
1:F:778:ASP:OD2	1:F:781:ARG:NH2	2.07	0.86
1:E:368:LYS:HE3	1:E:368:LYS:HA	1.63	0.81
1:L:368:LYS:HE3	1:L:368:LYS:HA	1.63	0.81
1:H:368:LYS:HE3	1:H:368:LYS:HA	1.63	0.81
1:I:368:LYS:HA	1:I:368:LYS:HE3	1.63	0.81
1:A:368:LYS:HE3	1:A:368:LYS:HA	1.63	0.80
1:J:368:LYS:HE3	1:J:368:LYS:HA	1.63	0.80
1:C:368:LYS:HE3	1:C:368:LYS:HA	1.63	0.80
1:D:368:LYS:HA	1:D:368:LYS:HE3	1.63	0.80
1:D:215:ARG:NH2	1:D:263:LYS:O	2.15	0.80
1:E:215:ARG:NH2	1:E:263:LYS:O	2.15	0.80
1:F:42:ARG:NH2	1:G:39:GLU:OE2	2.15	0.80
1:B:39:GLU:OE2	1:E:42:ARG:NH2	2.15	0.79
1:I:215:ARG:NH2	1:I:263:LYS:O	2.15	0.79
1:C:39:GLU:OE2	1:D:42:ARG:NH2	2.15	0.79
1:J:39:GLU:OE2	1:K:42:ARG:NH2	2.15	0.79
1:A:215:ARG:NH2	1:A:263:LYS:O	2.15	0.79
1:F:368:LYS:HE3	1:F:368:LYS:HA	1.63	0.79
1:G:215:ARG:NH2	1:G:263:LYS:O	2.15	0.79
1:A:39:GLU:OE2	1:L:42:ARG:NH2	2.14	0.79
1:F:215:ARG:NH2	1:F:263:LYS:O	2.15	0.79
1:K:368:LYS:HA	1:K:368:LYS:HE3	1.63	0.79
1:L:215:ARG:NH2	1:L:263:LYS:O	2.15	0.79
1:K:215:ARG:NH2	1:K:263:LYS:O	2.15	0.79
1:B:368:LYS:HE3	1:B:368:LYS:HA	1.63	0.78
1:J:215:ARG:NH2	1:J:263:LYS:O	2.15	0.78
1:B:215:ARG:NH2	1:B:263:LYS:O	2.15	0.78
1:G:368:LYS:HE3	1:G:368:LYS:HA	1.63	0.78
1:H:215:ARG:NH2	1:H:263:LYS:O	2.15	0.78
1:A:13:TYR:CE1	1:A:17:THR:HG21	2.19	0.78
1:A:100:THR:O	1:A:103:SER:OG	2.02	0.78
1:J:42:ARG:NH2	1:K:39:GLU:OE2	2.17	0.78
1:F:13:TYR:CE1	1:F:17:THR:HG21	2.19	0.78
1:H:42:ARG:NH2	1:I:39:GLU:OE2	2.15	0.78
1:L:13:TYR:CE1	1:L:17:THR:HG21	2.19	0.78
1:C:42:ARG:NH2	1:D:39:GLU:OE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:TYR:CE1	1:E:17:THR:HG21	2.19	0.78
1:F:100:THR:O	1:F:103:SER:OG	2.01	0.78
1:I:100:THR:O	1:I:103:SER:OG	2.01	0.78
1:K:13:TYR:CE1	1:K:17:THR:HG21	2.19	0.78
1:C:215:ARG:NH2	1:C:263:LYS:O	2.15	0.78
1:I:13:TYR:CE1	1:I:17:THR:HG21	2.19	0.77
1:D:100:THR:O	1:D:103:SER:OG	2.02	0.77
1:G:100:THR:O	1:G:103:SER:OG	2.02	0.77
1:A:325:GLU:N	1:A:325:GLU:OE1	2.18	0.77
1:B:42:ARG:NH2	1:E:39:GLU:OE2	2.17	0.77
1:B:100:THR:O	1:B:103:SER:OG	2.01	0.77
1:D:13:TYR:CE1	1:D:17:THR:HG21	2.19	0.77
1:H:39:GLU:OE2	1:I:42:ARG:NH2	2.18	0.77
1:J:13:TYR:CE1	1:J:17:THR:HG21	2.19	0.77
1:K:100:THR:O	1:K:103:SER:OG	2.02	0.77
1:C:13:TYR:CE1	1:C:17:THR:HG21	2.19	0.77
1:E:325:GLU:N	1:E:325:GLU:OE1	2.18	0.77
1:G:13:TYR:CE1	1:G:17:THR:HG21	2.19	0.77
1:H:13:TYR:CE1	1:H:17:THR:HG21	2.19	0.77
1:L:325:GLU:OE1	1:L:325:GLU:N	2.18	0.77
1:B:325:GLU:OE1	1:B:325:GLU:N	2.18	0.77
1:E:100:THR:O	1:E:103:SER:OG	2.02	0.77
1:L:100:THR:O	1:L:103:SER:OG	2.02	0.77
1:C:100:THR:O	1:C:103:SER:OG	2.01	0.77
1:F:325:GLU:N	1:F:325:GLU:OE1	2.18	0.77
1:H:325:GLU:N	1:H:325:GLU:OE1	2.18	0.77
1:B:13:TYR:CE1	1:B:17:THR:HG21	2.19	0.76
1:F:39:GLU:OE2	1:G:42:ARG:NH2	2.18	0.76
1:H:100:THR:O	1:H:103:SER:OG	2.02	0.76
1:A:42:ARG:NH2	1:L:39:GLU:OE2	2.18	0.76
1:I:325:GLU:OE1	1:I:325:GLU:N	2.18	0.76
1:J:100:THR:O	1:J:103:SER:OG	2.01	0.76
1:G:325:GLU:OE1	1:G:325:GLU:N	2.18	0.76
1:J:325:GLU:N	1:J:325:GLU:OE1	2.18	0.76
1:K:325:GLU:N	1:K:325:GLU:OE1	2.18	0.76
1:C:325:GLU:N	1:C:325:GLU:OE1	2.18	0.76
1:D:325:GLU:OE1	1:D:325:GLU:N	2.18	0.76
1:J:541:TRP:O	1:J:715:GLN:NE2	2.22	0.73
1:B:541:TRP:O	1:B:715:GLN:NE2	2.22	0.73
1:G:541:TRP:O	1:G:715:GLN:NE2	2.22	0.73
1:E:541:TRP:O	1:E:715:GLN:NE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:TRP:O	1:C:715:GLN:NE2	2.22	0.73
1:H:402:ASP:OD1	1:H:458:ARG:NH1	2.22	0.73
1:I:541:TRP:O	1:I:715:GLN:NE2	2.22	0.73
1:E:402:ASP:OD1	1:E:458:ARG:NH1	2.22	0.73
1:D:402:ASP:OD1	1:D:458:ARG:NH1	2.22	0.73
1:F:541:TRP:O	1:F:715:GLN:NE2	2.22	0.72
1:C:402:ASP:OD1	1:C:458:ARG:NH1	2.22	0.72
1:L:541:TRP:O	1:L:715:GLN:NE2	2.22	0.72
1:A:541:TRP:O	1:A:715:GLN:NE2	2.22	0.72
1:D:541:TRP:O	1:D:715:GLN:NE2	2.22	0.72
1:H:541:TRP:O	1:H:715:GLN:NE2	2.22	0.72
1:K:402:ASP:OD1	1:K:458:ARG:NH1	2.22	0.72
1:K:541:TRP:O	1:K:715:GLN:NE2	2.22	0.72
1:B:402:ASP:OD1	1:B:458:ARG:NH1	2.22	0.71
1:L:402:ASP:OD1	1:L:458:ARG:NH1	2.22	0.71
1:F:402:ASP:OD1	1:F:458:ARG:NH1	2.22	0.70
1:G:402:ASP:OD1	1:G:458:ARG:NH1	2.22	0.70
1:J:402:ASP:OD1	1:J:458:ARG:NH1	2.22	0.70
1:F:606:VAL:HG22	1:F:652:PRO:HA	1.74	0.70
1:B:606:VAL:HG22	1:B:652:PRO:HA	1.74	0.70
1:E:606:VAL:HG22	1:E:652:PRO:HA	1.74	0.70
1:C:606:VAL:HG22	1:C:652:PRO:HA	1.74	0.70
1:H:606:VAL:HG22	1:H:652:PRO:HA	1.74	0.70
1:J:606:VAL:HG22	1:J:652:PRO:HA	1.74	0.70
1:G:606:VAL:HG22	1:G:652:PRO:HA	1.74	0.70
1:I:606:VAL:HG22	1:I:652:PRO:HA	1.74	0.70
1:I:402:ASP:OD1	1:I:458:ARG:NH1	2.22	0.69
1:A:606:VAL:HG22	1:A:652:PRO:HA	1.74	0.69
1:D:606:VAL:HG22	1:D:652:PRO:HA	1.74	0.69
1:E:642:GLU:N	1:E:642:GLU:OE1	2.26	0.69
1:K:642:GLU:N	1:K:642:GLU:OE1	2.26	0.69
1:F:14:ARG:NH1	1:F:31:SER:OG	2.26	0.69
1:K:606:VAL:HG22	1:K:652:PRO:HA	1.74	0.69
1:E:14:ARG:NH1	1:E:31:SER:OG	2.26	0.69
1:L:14:ARG:NH1	1:L:31:SER:OG	2.26	0.69
1:A:642:GLU:OE1	1:A:642:GLU:N	2.26	0.68
1:H:642:GLU:OE1	1:H:642:GLU:N	2.26	0.68
1:A:402:ASP:OD1	1:A:458:ARG:NH1	2.22	0.68
1:I:14:ARG:NH1	1:I:31:SER:OG	2.26	0.68
1:L:606:VAL:HG22	1:L:652:PRO:HA	1.74	0.68
1:C:642:GLU:OE1	1:C:642:GLU:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ARG:NH1	1:C:31:SER:OG	2.26	0.68
1:D:642:GLU:N	1:D:642:GLU:OE1	2.26	0.68
1:L:683:GLU:OE1	1:L:683:GLU:N	2.22	0.68
1:J:642:GLU:N	1:J:642:GLU:OE1	2.26	0.68
1:H:14:ARG:NH1	1:H:31:SER:OG	2.26	0.68
1:D:14:ARG:NH1	1:D:31:SER:OG	2.26	0.68
1:G:642:GLU:N	1:G:642:GLU:OE1	2.26	0.68
1:K:14:ARG:NH1	1:K:31:SER:OG	2.26	0.68
1:A:14:ARG:NH1	1:A:31:SER:OG	2.26	0.67
1:A:683:GLU:OE1	1:A:683:GLU:N	2.21	0.67
1:L:642:GLU:N	1:L:642:GLU:OE1	2.26	0.67
1:G:14:ARG:NH1	1:G:31:SER:OG	2.26	0.67
1:J:14:ARG:NH1	1:J:31:SER:OG	2.26	0.67
1:F:642:GLU:OE1	1:F:642:GLU:N	2.26	0.67
1:K:683:GLU:OE1	1:K:683:GLU:N	2.21	0.67
1:B:14:ARG:NH1	1:B:31:SER:OG	2.26	0.67
1:I:642:GLU:N	1:I:642:GLU:OE1	2.26	0.67
1:B:642:GLU:N	1:B:642:GLU:OE1	2.26	0.67
1:L:225:VAL:HG23	1:L:225:VAL:O	1.95	0.67
1:B:225:VAL:HG23	1:B:225:VAL:O	1.95	0.67
1:E:225:VAL:HG23	1:E:225:VAL:O	1.95	0.67
1:I:225:VAL:HG23	1:I:225:VAL:O	1.95	0.67
1:A:225:VAL:O	1:A:225:VAL:HG23	1.95	0.67
1:D:225:VAL:HG23	1:D:225:VAL:O	1.95	0.66
1:C:225:VAL:O	1:C:225:VAL:HG23	1.95	0.66
1:E:683:GLU:OE1	1:E:683:GLU:N	2.21	0.66
1:H:225:VAL:O	1:H:225:VAL:HG23	1.95	0.66
1:J:225:VAL:HG23	1:J:225:VAL:O	1.95	0.66
1:G:225:VAL:HG23	1:G:225:VAL:O	1.95	0.65
1:D:683:GLU:OE1	1:D:683:GLU:N	2.21	0.65
1:F:225:VAL:HG23	1:F:225:VAL:O	1.95	0.65
1:K:225:VAL:HG23	1:K:225:VAL:O	1.95	0.65
1:J:683:GLU:OE1	1:J:683:GLU:N	2.21	0.65
1:G:368:LYS:HE3	1:G:368:LYS:CA	2.27	0.64
1:B:542:LYS:HB2	1:B:677:LEU:HD21	1.80	0.64
1:F:683:GLU:OE1	1:F:683:GLU:N	2.21	0.64
1:G:683:GLU:OE1	1:G:683:GLU:N	2.21	0.64
1:B:368:LYS:HE3	1:B:368:LYS:CA	2.27	0.64
1:G:542:LYS:HB2	1:G:677:LEU:HD21	1.80	0.64
1:L:368:LYS:HE3	1:L:368:LYS:CA	2.27	0.64
1:K:542:LYS:HB2	1:K:677:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HE3	1:A:368:LYS:CA	2.27	0.64
1:J:542:LYS:HB2	1:J:677:LEU:HD21	1.79	0.64
1:A:542:LYS:HB2	1:A:677:LEU:HD21	1.80	0.64
1:F:368:LYS:HE3	1:F:368:LYS:CA	2.27	0.64
1:C:35:LEU:HD21	1:D:193:ALA:HB1	1.80	0.64
1:H:456:GLU:HB3	1:H:459:LEU:HD12	1.80	0.64
1:L:542:LYS:HB2	1:L:677:LEU:HD21	1.80	0.64
1:B:456:GLU:HB3	1:B:459:LEU:HD12	1.80	0.64
1:H:683:GLU:OE1	1:H:683:GLU:N	2.22	0.64
1:J:456:GLU:HB3	1:J:459:LEU:HD12	1.80	0.64
1:K:456:GLU:HB3	1:K:459:LEU:HD12	1.80	0.64
1:B:227:LEU:HD12	1:B:227:LEU:O	1.98	0.63
1:D:456:GLU:HB3	1:D:459:LEU:HD12	1.80	0.63
1:E:227:LEU:HD12	1:E:227:LEU:O	1.98	0.63
1:L:227:LEU:HD12	1:L:227:LEU:O	1.98	0.63
1:E:542:LYS:HB2	1:E:677:LEU:HD21	1.79	0.63
1:F:542:LYS:HB2	1:F:677:LEU:HD21	1.80	0.63
1:G:227:LEU:HD12	1:G:227:LEU:O	1.98	0.63
1:G:456:GLU:HB3	1:G:459:LEU:HD12	1.80	0.63
1:I:456:GLU:HB3	1:I:459:LEU:HD12	1.80	0.63
1:F:456:GLU:HB3	1:F:459:LEU:HD12	1.80	0.63
1:E:456:GLU:HB3	1:E:459:LEU:HD12	1.80	0.63
1:H:542:LYS:HB2	1:H:677:LEU:HD21	1.79	0.63
1:J:227:LEU:HD12	1:J:227:LEU:O	1.98	0.63
1:I:542:LYS:HB2	1:I:677:LEU:HD21	1.80	0.63
1:C:227:LEU:HD12	1:C:227:LEU:O	1.98	0.63
1:C:542:LYS:HB2	1:C:677:LEU:HD21	1.80	0.63
1:D:227:LEU:HD12	1:D:227:LEU:O	1.98	0.63
1:K:227:LEU:O	1:K:227:LEU:HD12	1.98	0.63
1:A:456:GLU:HB3	1:A:459:LEU:HD12	1.80	0.63
1:C:456:GLU:HB3	1:C:459:LEU:HD12	1.80	0.63
1:F:227:LEU:O	1:F:227:LEU:HD12	1.98	0.63
1:D:207:ARG:NH1	1:D:301:GLN:OE1	2.32	0.62
1:A:227:LEU:O	1:A:227:LEU:HD12	1.98	0.62
1:F:207:ARG:NH1	1:F:301:GLN:OE1	2.32	0.62
1:I:227:LEU:HD12	1:I:227:LEU:O	1.98	0.62
1:C:193:ALA:HB1	1:D:35:LEU:HD21	1.79	0.62
1:D:542:LYS:HB2	1:D:677:LEU:HD21	1.79	0.62
1:H:207:ARG:NH1	1:H:301:GLN:OE1	2.32	0.62
1:G:207:ARG:NH1	1:G:301:GLN:OE1	2.32	0.62
1:L:456:GLU:HB3	1:L:459:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:LYS:HE3	1:E:368:LYS:CA	2.27	0.62
1:A:193:ALA:HB1	1:L:35:LEU:HD21	1.81	0.62
1:B:35:LEU:HD21	1:E:193:ALA:HB1	1.82	0.62
1:H:193:ALA:HB1	1:I:35:LEU:HD21	1.81	0.62
1:H:227:LEU:HD12	1:H:227:LEU:O	1.98	0.62
1:I:368:LYS:HE3	1:I:368:LYS:CA	2.27	0.62
1:L:207:ARG:NH1	1:L:301:GLN:OE1	2.32	0.62
1:B:207:ARG:NH1	1:B:301:GLN:OE1	2.32	0.62
1:A:207:ARG:NH1	1:A:301:GLN:OE1	2.32	0.62
1:B:683:GLU:OE1	1:B:683:GLU:N	2.21	0.62
1:H:35:LEU:HD21	1:I:193:ALA:HB1	1.80	0.62
1:K:207:ARG:NH1	1:K:301:GLN:OE1	2.32	0.62
1:E:207:ARG:NH1	1:E:301:GLN:OE1	2.32	0.62
1:J:207:ARG:NH1	1:J:301:GLN:OE1	2.32	0.62
1:J:35:LEU:HD21	1:K:193:ALA:HB1	1.81	0.61
1:C:207:ARG:NH1	1:C:301:GLN:OE1	2.32	0.61
1:I:207:ARG:NH1	1:I:301:GLN:OE1	2.32	0.61
1:B:193:ALA:HB1	1:E:35:LEU:HD21	1.81	0.61
1:C:340:HIS:NE2	1:C:756:ASP:OD1	2.34	0.61
1:E:340:HIS:NE2	1:E:756:ASP:OD1	2.34	0.61
1:J:340:HIS:NE2	1:J:756:ASP:OD1	2.34	0.61
1:B:340:HIS:NE2	1:B:756:ASP:OD1	2.34	0.61
1:F:193:ALA:HB1	1:G:35:LEU:HD21	1.83	0.61
1:A:35:LEU:HD21	1:L:193:ALA:HB1	1.83	0.61
1:F:35:LEU:HD21	1:G:193:ALA:HB1	1.82	0.61
1:K:340:HIS:NE2	1:K:756:ASP:OD1	2.34	0.60
1:L:340:HIS:NE2	1:L:756:ASP:OD1	2.34	0.60
1:A:116:VAL:O	1:A:281:ARG:NH2	2.35	0.60
1:E:749:ASP:HB3	1:E:752:ILE:HG22	1.83	0.60
1:F:340:HIS:NE2	1:F:756:ASP:OD1	2.34	0.60
1:H:340:HIS:NE2	1:H:756:ASP:OD1	2.34	0.60
1:B:749:ASP:HB3	1:B:752:ILE:HG22	1.83	0.60
1:D:116:VAL:O	1:D:281:ARG:NH2	2.35	0.60
1:G:749:ASP:HB3	1:G:752:ILE:HG22	1.83	0.60
1:I:340:HIS:NE2	1:I:756:ASP:OD1	2.34	0.60
1:E:116:VAL:O	1:E:281:ARG:NH2	2.35	0.60
1:B:116:VAL:O	1:B:281:ARG:NH2	2.35	0.60
1:C:683:GLU:OE1	1:C:683:GLU:N	2.21	0.60
1:J:193:ALA:HB1	1:K:35:LEU:HD21	1.81	0.60
1:A:340:HIS:NE2	1:A:756:ASP:OD1	2.34	0.60
1:H:749:ASP:HB3	1:H:752:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:VAL:O	1:K:281:ARG:NH2	2.35	0.60
1:C:749:ASP:HB3	1:C:752:ILE:HG22	1.83	0.60
1:D:340:HIS:NE2	1:D:756:ASP:OD1	2.34	0.60
1:I:116:VAL:O	1:I:281:ARG:NH2	2.35	0.60
1:A:749:ASP:HB3	1:A:752:ILE:HG22	1.83	0.60
1:D:749:ASP:HB3	1:D:752:ILE:HG22	1.83	0.60
1:J:749:ASP:HB3	1:J:752:ILE:HG22	1.83	0.60
1:L:116:VAL:O	1:L:281:ARG:NH2	2.35	0.59
1:F:116:VAL:O	1:F:281:ARG:NH2	2.35	0.59
1:H:331:GLU:O	1:H:332:LYS:HE2	2.03	0.59
1:I:683:GLU:OE1	1:I:683:GLU:N	2.21	0.59
1:K:331:GLU:O	1:K:332:LYS:HE2	2.03	0.59
1:G:116:VAL:O	1:G:281:ARG:NH2	2.35	0.59
1:J:116:VAL:O	1:J:281:ARG:NH2	2.35	0.59
1:J:368:LYS:HE3	1:J:368:LYS:CA	2.27	0.59
1:B:331:GLU:O	1:B:332:LYS:HE2	2.03	0.59
1:F:749:ASP:HB3	1:F:752:ILE:HG22	1.83	0.59
1:H:116:VAL:O	1:H:281:ARG:NH2	2.35	0.59
1:J:331:GLU:O	1:J:332:LYS:HE2	2.03	0.59
1:C:116:VAL:O	1:C:281:ARG:NH2	2.35	0.59
1:G:340:HIS:NE2	1:G:756:ASP:OD1	2.34	0.59
1:I:749:ASP:HB3	1:I:752:ILE:HG22	1.83	0.59
1:K:749:ASP:HB3	1:K:752:ILE:HG22	1.83	0.59
1:G:331:GLU:O	1:G:332:LYS:HE2	2.03	0.59
1:H:368:LYS:HE3	1:H:368:LYS:CA	2.27	0.59
1:C:331:GLU:O	1:C:332:LYS:HE2	2.03	0.58
1:D:331:GLU:O	1:D:332:LYS:HE2	2.03	0.58
1:I:331:GLU:O	1:I:332:LYS:HE2	2.03	0.58
1:L:749:ASP:HB3	1:L:752:ILE:HG22	1.83	0.58
1:L:331:GLU:O	1:L:332:LYS:HE2	2.03	0.58
1:F:331:GLU:O	1:F:332:LYS:HE2	2.03	0.58
1:A:331:GLU:O	1:A:332:LYS:HE2	2.03	0.58
1:E:331:GLU:O	1:E:332:LYS:HE2	2.03	0.58
1:H:508:SER:OG	1:H:559:ASP:OD2	2.22	0.58
1:A:429:ASN:OD1	1:A:430:GLY:N	2.37	0.57
1:D:429:ASN:OD1	1:D:430:GLY:N	2.37	0.57
1:J:429:ASN:OD1	1:J:430:GLY:N	2.37	0.57
1:E:429:ASN:OD1	1:E:430:GLY:N	2.37	0.57
1:G:429:ASN:OD1	1:G:430:GLY:N	2.37	0.57
1:K:508:SER:OG	1:K:559:ASP:OD2	2.22	0.57
1:K:368:LYS:HE3	1:K:368:LYS:CA	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ASN:OD1	1:B:430:GLY:N	2.37	0.57
1:C:429:ASN:OD1	1:C:430:GLY:N	2.37	0.57
1:F:508:SER:OG	1:F:559:ASP:OD2	2.22	0.57
1:F:429:ASN:OD1	1:F:430:GLY:N	2.37	0.57
1:L:429:ASN:OD1	1:L:430:GLY:N	2.37	0.57
1:C:86:GLY:HA2	1:C:124:GLN:HE22	1.70	0.57
1:F:638:GLU:N	1:F:638:GLU:OE2	2.38	0.57
1:J:508:SER:OG	1:J:559:ASP:OD2	2.22	0.57
1:K:429:ASN:OD1	1:K:430:GLY:N	2.37	0.57
1:L:638:GLU:OE2	1:L:638:GLU:N	2.38	0.57
1:A:508:SER:OG	1:A:559:ASP:OD2	2.22	0.57
1:B:508:SER:OG	1:B:559:ASP:OD2	2.22	0.57
1:C:368:LYS:HE3	1:C:368:LYS:CA	2.27	0.57
1:I:429:ASN:OD1	1:I:430:GLY:N	2.37	0.57
1:J:752:ILE:HG21	1:J:755:ALA:HB2	1.87	0.57
1:G:638:GLU:OE2	1:G:638:GLU:N	2.38	0.56
1:K:638:GLU:N	1:K:638:GLU:OE2	2.38	0.56
1:A:213:ASN:ND2	1:A:240:LEU:O	2.39	0.56
1:D:638:GLU:N	1:D:638:GLU:OE2	2.38	0.56
1:D:752:ILE:HG21	1:D:755:ALA:HB2	1.87	0.56
1:H:638:GLU:OE2	1:H:638:GLU:N	2.38	0.56
1:K:213:ASN:ND2	1:K:240:LEU:O	2.39	0.56
1:K:752:ILE:HG21	1:K:755:ALA:HB2	1.87	0.56
1:H:429:ASN:OD1	1:H:430:GLY:N	2.37	0.56
1:F:752:ILE:HG21	1:F:755:ALA:HB2	1.87	0.56
1:H:752:ILE:HG21	1:H:755:ALA:HB2	1.87	0.56
1:J:638:GLU:OE2	1:J:638:GLU:N	2.38	0.56
1:B:638:GLU:N	1:B:638:GLU:OE2	2.38	0.56
1:C:638:GLU:OE2	1:C:638:GLU:N	2.38	0.56
1:E:213:ASN:ND2	1:E:240:LEU:O	2.39	0.56
1:B:213:ASN:ND2	1:B:240:LEU:O	2.39	0.56
1:C:213:ASN:ND2	1:C:240:LEU:O	2.39	0.56
1:E:638:GLU:OE2	1:E:638:GLU:N	2.38	0.56
1:L:213:ASN:ND2	1:L:240:LEU:O	2.39	0.56
1:D:634:LEU:CD2	1:D:638:GLU:OE1	2.54	0.56
1:I:213:ASN:ND2	1:I:240:LEU:O	2.39	0.56
1:I:752:ILE:HG21	1:I:755:ALA:HB2	1.87	0.56
1:J:213:ASN:ND2	1:J:240:LEU:O	2.39	0.56
1:C:634:LEU:CD2	1:C:638:GLU:OE1	2.54	0.56
1:E:508:SER:OG	1:E:559:ASP:OD2	2.22	0.56
1:G:634:LEU:CD2	1:G:638:GLU:OE1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:GLU:N	1:A:638:GLU:OE2	2.38	0.55
1:F:213:ASN:ND2	1:F:240:LEU:O	2.39	0.55
1:H:634:LEU:CD2	1:H:638:GLU:OE1	2.54	0.55
1:I:638:GLU:N	1:I:638:GLU:OE2	2.38	0.55
1:K:634:LEU:CD2	1:K:638:GLU:OE1	2.54	0.55
1:L:508:SER:OG	1:L:559:ASP:OD2	2.22	0.55
1:D:508:SER:OG	1:D:559:ASP:OD2	2.22	0.55
1:G:752:ILE:HG21	1:G:755:ALA:HB2	1.87	0.55
1:B:111:ILE:HG12	1:B:132:LEU:HD11	1.88	0.55
1:H:213:ASN:ND2	1:H:240:LEU:O	2.39	0.55
1:I:111:ILE:HG12	1:I:132:LEU:HD11	1.88	0.55
1:J:111:ILE:HG12	1:J:132:LEU:HD11	1.88	0.55
1:D:213:ASN:ND2	1:D:240:LEU:O	2.39	0.55
1:E:542:LYS:CB	1:E:677:LEU:HD21	2.37	0.55
1:E:634:LEU:CD2	1:E:638:GLU:OE1	2.54	0.55
1:E:752:ILE:HG21	1:E:755:ALA:HB2	1.87	0.55
1:I:634:LEU:CD2	1:I:638:GLU:OE1	2.54	0.55
1:B:752:ILE:HG21	1:B:755:ALA:HB2	1.87	0.55
1:C:542:LYS:CB	1:C:677:LEU:HD21	2.37	0.55
1:C:752:ILE:HG21	1:C:755:ALA:HB2	1.87	0.55
1:D:111:ILE:HG12	1:D:132:LEU:HD11	1.88	0.55
1:G:111:ILE:HG12	1:G:132:LEU:HD11	1.88	0.55
1:L:111:ILE:HG12	1:L:132:LEU:HD11	1.88	0.55
1:C:191:LEU:HD11	1:C:308:GLN:HB3	1.89	0.55
1:D:82:LYS:NZ	1:D:91:ASP:OD2	2.40	0.55
1:F:634:LEU:CD2	1:F:638:GLU:OE1	2.54	0.55
1:G:542:LYS:CB	1:G:677:LEU:HD21	2.37	0.55
1:H:191:LEU:HD11	1:H:308:GLN:HB3	1.89	0.55
1:J:82:LYS:NZ	1:J:91:ASP:OD2	2.40	0.55
1:E:191:LEU:HD11	1:E:308:GLN:HB3	1.89	0.55
1:G:213:ASN:ND2	1:G:240:LEU:O	2.39	0.55
1:I:466:VAL:HG11	1:I:487:LEU:HD13	1.89	0.55
1:J:191:LEU:HD11	1:J:308:GLN:HB3	1.89	0.55
1:L:634:LEU:CD2	1:L:638:GLU:OE1	2.54	0.55
1:L:752:ILE:HG21	1:L:755:ALA:HB2	1.87	0.55
1:A:111:ILE:HG12	1:A:132:LEU:HD11	1.88	0.55
1:D:191:LEU:HD11	1:D:308:GLN:HB3	1.89	0.55
1:F:82:LYS:NZ	1:F:91:ASP:OD2	2.40	0.55
1:H:542:LYS:CB	1:H:677:LEU:HD21	2.37	0.55
1:I:191:LEU:HD11	1:I:308:GLN:HB3	1.89	0.55
1:I:508:SER:OG	1:I:559:ASP:OD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ILE:HG21	1:A:755:ALA:HB2	1.87	0.55
1:H:466:VAL:HG11	1:H:487:LEU:HD13	1.89	0.55
1:K:111:ILE:HG12	1:K:132:LEU:HD11	1.88	0.55
1:A:191:LEU:HD11	1:A:308:GLN:HB3	1.89	0.54
1:B:634:LEU:CD2	1:B:638:GLU:OE1	2.54	0.54
1:C:111:ILE:HG12	1:C:132:LEU:HD11	1.88	0.54
1:G:191:LEU:HD11	1:G:308:GLN:HB3	1.89	0.54
1:H:82:LYS:NZ	1:H:91:ASP:OD2	2.40	0.54
1:I:542:LYS:CB	1:I:677:LEU:HD21	2.37	0.54
1:A:634:LEU:CD2	1:A:638:GLU:OE1	2.54	0.54
1:E:466:VAL:HG11	1:E:487:LEU:HD13	1.89	0.54
1:H:546:PRO:HD3	1:I:44:LEU:HD21	1.89	0.54
1:E:82:LYS:NZ	1:E:91:ASP:OD2	2.40	0.54
1:J:634:LEU:CD2	1:J:638:GLU:OE1	2.54	0.54
1:A:542:LYS:CB	1:A:677:LEU:HD21	2.37	0.54
1:B:82:LYS:NZ	1:B:91:ASP:OD2	2.40	0.54
1:B:466:VAL:HG11	1:B:487:LEU:HD13	1.89	0.54
1:C:82:LYS:NZ	1:C:91:ASP:OD2	2.40	0.54
1:C:466:VAL:HG11	1:C:487:LEU:HD13	1.89	0.54
1:F:111:ILE:HG12	1:F:132:LEU:HD11	1.88	0.54
1:J:44:LEU:HD21	1:K:546:PRO:HD3	1.90	0.54
1:K:191:LEU:HD11	1:K:308:GLN:HB3	1.89	0.54
1:L:191:LEU:HD11	1:L:308:GLN:HB3	1.89	0.54
1:B:191:LEU:HD11	1:B:308:GLN:HB3	1.89	0.54
1:B:779:ALA:O	1:B:783:VAL:HG23	2.08	0.54
1:D:779:ALA:O	1:D:783:VAL:HG23	2.08	0.54
1:F:191:LEU:HD11	1:F:308:GLN:HB3	1.89	0.54
1:I:779:ALA:O	1:I:783:VAL:HG23	2.08	0.54
1:K:542:LYS:CB	1:K:677:LEU:HD21	2.37	0.54
1:A:464:ARG:NH2	1:A:797:ASP:OD2	2.41	0.54
1:B:542:LYS:CB	1:B:677:LEU:HD21	2.37	0.54
1:D:466:VAL:HG11	1:D:487:LEU:HD13	1.89	0.54
1:F:542:LYS:CB	1:F:677:LEU:HD21	2.37	0.54
1:F:779:ALA:O	1:F:783:VAL:HG23	2.08	0.54
1:K:82:LYS:NZ	1:K:91:ASP:OD2	2.40	0.54
1:L:542:LYS:CB	1:L:677:LEU:HD21	2.37	0.54
1:B:199:LEU:O	1:B:203:ILE:HB	2.08	0.54
1:F:464:ARG:NH2	1:F:797:ASP:OD2	2.41	0.54
1:J:466:VAL:HG11	1:J:487:LEU:HD13	1.89	0.54
1:J:542:LYS:CB	1:J:677:LEU:HD21	2.37	0.54
1:L:517:LEU:HD11	1:L:696:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:NZ	1:A:91:ASP:OD2	2.40	0.54
1:D:542:LYS:CB	1:D:677:LEU:HD21	2.37	0.54
1:H:199:LEU:O	1:H:203:ILE:HB	2.08	0.54
1:J:464:ARG:NH2	1:J:797:ASP:OD2	2.41	0.54
1:C:527:ARG:NH1	1:C:704:GLU:OE2	2.39	0.54
1:G:82:LYS:NZ	1:G:91:ASP:OD2	2.40	0.54
1:H:111:ILE:HG12	1:H:132:LEU:HD11	1.88	0.54
1:A:369:LEU:O	1:A:373:VAL:HG23	2.08	0.54
1:C:464:ARG:NH2	1:C:797:ASP:OD2	2.41	0.54
1:D:369:LEU:O	1:D:373:VAL:HG23	2.08	0.54
1:E:111:ILE:HG12	1:E:132:LEU:HD11	1.88	0.54
1:E:779:ALA:O	1:E:783:VAL:HG23	2.08	0.54
1:H:779:ALA:O	1:H:783:VAL:HG23	2.08	0.54
1:I:82:LYS:NZ	1:I:91:ASP:OD2	2.40	0.54
1:J:517:LEU:HD11	1:J:696:MET:HG2	1.90	0.54
1:K:779:ALA:O	1:K:783:VAL:HG23	2.08	0.54
1:L:82:LYS:NZ	1:L:91:ASP:OD2	2.40	0.54
1:L:779:ALA:O	1:L:783:VAL:HG23	2.08	0.54
1:D:199:LEU:O	1:D:203:ILE:HB	2.08	0.53
1:E:369:LEU:O	1:E:373:VAL:HG23	2.09	0.53
1:G:369:LEU:O	1:G:373:VAL:HG23	2.09	0.53
1:J:199:LEU:O	1:J:203:ILE:HB	2.08	0.53
1:J:546:PRO:HD3	1:K:44:LEU:HD21	1.90	0.53
1:K:466:VAL:HG11	1:K:487:LEU:HD13	1.89	0.53
1:K:517:LEU:HD11	1:K:696:MET:HG2	1.90	0.53
1:C:199:LEU:O	1:C:203:ILE:HB	2.08	0.53
1:D:464:ARG:NH2	1:D:797:ASP:OD2	2.41	0.53
1:J:369:LEU:O	1:J:373:VAL:HG23	2.09	0.53
1:L:199:LEU:O	1:L:203:ILE:HB	2.08	0.53
1:A:779:ALA:O	1:A:783:VAL:HG23	2.08	0.53
1:E:199:LEU:O	1:E:203:ILE:HB	2.08	0.53
1:E:507:ILE:HG21	1:E:563:ILE:HD11	1.91	0.53
1:G:466:VAL:HG11	1:G:487:LEU:HD13	1.89	0.53
1:H:369:LEU:O	1:H:373:VAL:HG23	2.09	0.53
1:I:464:ARG:NH2	1:I:797:ASP:OD2	2.41	0.53
1:K:369:LEU:O	1:K:373:VAL:HG23	2.08	0.53
1:L:369:LEU:O	1:L:373:VAL:HG23	2.08	0.53
1:L:464:ARG:NH2	1:L:797:ASP:OD2	2.41	0.53
1:G:199:LEU:O	1:G:203:ILE:HB	2.08	0.53
1:G:517:LEU:HD11	1:G:696:MET:HG2	1.90	0.53
1:G:718:ASN:OD1	1:G:718:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:779:ALA:O	1:G:783:VAL:HG23	2.08	0.53
1:H:527:ARG:NH1	1:H:704:GLU:OE2	2.40	0.53
1:I:517:LEU:HD11	1:I:696:MET:HG2	1.90	0.53
1:B:464:ARG:NH2	1:B:797:ASP:OD2	2.41	0.53
1:C:517:LEU:HD11	1:C:696:MET:HG2	1.90	0.53
1:D:368:LYS:HE3	1:D:368:LYS:CA	2.27	0.53
1:F:369:LEU:O	1:F:373:VAL:HG23	2.08	0.53
1:F:546:PRO:HD3	1:G:44:LEU:HD21	1.89	0.53
1:J:527:ARG:NH1	1:J:704:GLU:OE2	2.39	0.53
1:A:466:VAL:HG11	1:A:487:LEU:HD13	1.89	0.53
1:A:527:ARG:NH1	1:A:704:GLU:OE2	2.39	0.53
1:C:508:SER:OG	1:C:559:ASP:OD2	2.22	0.53
1:C:779:ALA:O	1:C:783:VAL:HG23	2.08	0.53
1:E:464:ARG:NH2	1:E:797:ASP:OD2	2.41	0.53
1:F:44:LEU:HD21	1:G:546:PRO:HD3	1.91	0.53
1:F:199:LEU:O	1:F:203:ILE:HB	2.08	0.53
1:I:718:ASN:N	1:I:718:ASN:OD1	2.42	0.53
1:K:464:ARG:NH2	1:K:797:ASP:OD2	2.41	0.53
1:A:199:LEU:O	1:A:203:ILE:HB	2.08	0.53
1:A:447:ALA:O	1:A:451:ASP:OD2	2.27	0.53
1:G:447:ALA:O	1:G:451:ASP:OD2	2.27	0.53
1:I:369:LEU:O	1:I:373:VAL:HG23	2.09	0.53
1:B:507:ILE:HG21	1:B:563:ILE:HD11	1.91	0.53
1:E:718:ASN:OD1	1:E:718:ASN:N	2.42	0.53
1:F:86:GLY:HA2	1:F:124:GLN:HE22	1.74	0.53
1:G:464:ARG:NH2	1:G:797:ASP:OD2	2.41	0.53
1:H:718:ASN:OD1	1:H:718:ASN:N	2.42	0.53
1:I:199:LEU:O	1:I:203:ILE:HB	2.08	0.53
1:J:779:ALA:O	1:J:783:VAL:HG23	2.08	0.53
1:K:527:ARG:NH1	1:K:704:GLU:OE2	2.39	0.53
1:L:466:VAL:HG11	1:L:487:LEU:HD13	1.89	0.53
1:L:527:ARG:NH1	1:L:704:GLU:OE2	2.40	0.53
1:A:44:LEU:HD21	1:L:546:PRO:HD3	1.89	0.53
1:D:447:ALA:O	1:D:451:ASP:OD2	2.27	0.53
1:E:517:LEU:HD11	1:E:696:MET:HG2	1.90	0.53
1:F:466:VAL:HG11	1:F:487:LEU:HD13	1.89	0.53
1:G:508:SER:OG	1:G:559:ASP:OD2	2.22	0.53
1:H:447:ALA:O	1:H:451:ASP:OD2	2.27	0.53
1:J:507:ILE:HG21	1:J:563:ILE:HD11	1.91	0.53
1:K:199:LEU:O	1:K:203:ILE:HB	2.08	0.53
1:D:718:ASN:OD1	1:D:718:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:447:ALA:O	1:J:451:ASP:OD2	2.27	0.53
1:A:517:LEU:HD11	1:A:696:MET:HG2	1.90	0.52
1:B:369:LEU:O	1:B:373:VAL:HG23	2.08	0.52
1:D:517:LEU:HD11	1:D:696:MET:HG2	1.90	0.52
1:H:464:ARG:NH2	1:H:797:ASP:OD2	2.41	0.52
1:B:527:ARG:NH1	1:B:704:GLU:OE2	2.39	0.52
1:F:718:ASN:OD1	1:F:718:ASN:N	2.42	0.52
1:G:507:ILE:HG21	1:G:563:ILE:HD11	1.91	0.52
1:H:507:ILE:HG21	1:H:563:ILE:HD11	1.91	0.52
1:B:44:LEU:HD21	1:E:546:PRO:HD3	1.90	0.52
1:B:447:ALA:O	1:B:451:ASP:OD2	2.27	0.52
1:C:507:ILE:HG21	1:C:563:ILE:HD11	1.91	0.52
1:H:44:LEU:HD21	1:I:546:PRO:HD3	1.91	0.52
1:C:412:LYS:NZ	1:F:408:GLU:OE2	2.38	0.52
1:F:447:ALA:O	1:F:451:ASP:OD2	2.27	0.52
1:H:517:LEU:HD11	1:H:696:MET:HG2	1.90	0.52
1:I:447:ALA:O	1:I:451:ASP:OD2	2.27	0.52
1:L:447:ALA:O	1:L:451:ASP:OD2	2.27	0.52
1:L:507:ILE:HG21	1:L:563:ILE:HD11	1.91	0.52
1:B:517:LEU:HD11	1:B:696:MET:HG2	1.90	0.52
1:F:517:LEU:HD11	1:F:696:MET:HG2	1.90	0.52
1:G:527:ARG:NH1	1:G:704:GLU:OE2	2.39	0.52
1:C:44:LEU:HD21	1:D:546:PRO:HD3	1.91	0.52
1:K:447:ALA:O	1:K:451:ASP:OD2	2.27	0.52
1:B:718:ASN:OD1	1:B:718:ASN:N	2.42	0.52
1:B:546:PRO:HD3	1:E:44:LEU:HD21	1.91	0.52
1:I:507:ILE:HG21	1:I:563:ILE:HD11	1.91	0.52
1:J:718:ASN:OD1	1:J:718:ASN:N	2.42	0.52
1:L:718:ASN:OD1	1:L:718:ASN:N	2.42	0.52
1:A:507:ILE:HG21	1:A:563:ILE:HD11	1.91	0.52
1:E:447:ALA:O	1:E:451:ASP:OD2	2.27	0.52
1:E:527:ARG:NH1	1:E:704:GLU:OE2	2.39	0.52
1:F:507:ILE:HG21	1:F:563:ILE:HD11	1.91	0.52
1:K:507:ILE:HG21	1:K:563:ILE:HD11	1.91	0.51
1:C:447:ALA:O	1:C:451:ASP:OD2	2.27	0.51
1:D:507:ILE:HG21	1:D:563:ILE:HD11	1.91	0.51
1:A:357:PHE:CD2	1:A:369:LEU:HD21	2.46	0.51
1:A:546:PRO:HD3	1:L:44:LEU:HD21	1.91	0.51
1:C:369:LEU:O	1:C:373:VAL:HG23	2.09	0.51
1:H:357:PHE:CD2	1:H:369:LEU:HD21	2.46	0.51
1:H:283:ASN:N	1:H:283:ASN:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:357:PHE:CD2	1:J:369:LEU:HD21	2.46	0.51
1:L:283:ASN:OD1	1:L:283:ASN:N	2.44	0.51
1:B:283:ASN:OD1	1:B:283:ASN:N	2.44	0.51
1:C:546:PRO:HD3	1:D:44:LEU:HD21	1.92	0.51
1:K:718:ASN:N	1:K:718:ASN:OD1	2.42	0.51
1:B:609:MET:HE1	1:B:653:LEU:HA	1.93	0.51
1:C:283:ASN:N	1:C:283:ASN:OD1	2.44	0.51
1:D:527:ARG:NH1	1:D:704:GLU:OE2	2.39	0.51
1:F:527:ARG:NH1	1:F:704:GLU:OE2	2.39	0.51
1:G:443:LYS:HE3	1:G:633:TRP:CE2	2.46	0.51
1:H:443:LYS:HE3	1:H:633:TRP:CE2	2.46	0.51
1:I:283:ASN:OD1	1:I:283:ASN:N	2.44	0.51
1:K:443:LYS:HE3	1:K:633:TRP:CE2	2.46	0.51
1:A:718:ASN:OD1	1:A:718:ASN:N	2.42	0.51
1:E:45:PRO:O	1:E:47:HIS:ND1	2.44	0.51
1:E:357:PHE:CD2	1:E:369:LEU:HD21	2.46	0.51
1:G:283:ASN:OD1	1:G:283:ASN:N	2.44	0.51
1:H:45:PRO:O	1:H:47:HIS:ND1	2.44	0.51
1:I:527:ARG:NH1	1:I:704:GLU:OE2	2.39	0.51
1:L:443:LYS:HE3	1:L:633:TRP:CE2	2.46	0.51
1:E:283:ASN:N	1:E:283:ASN:OD1	2.44	0.51
1:E:443:LYS:HE3	1:E:633:TRP:CE2	2.46	0.51
1:K:357:PHE:CD2	1:K:369:LEU:HD21	2.46	0.51
1:L:357:PHE:CD2	1:L:369:LEU:HD21	2.46	0.51
1:A:45:PRO:O	1:A:47:HIS:ND1	2.44	0.50
1:C:45:PRO:O	1:C:47:HIS:ND1	2.44	0.50
1:F:357:PHE:CD2	1:F:369:LEU:HD21	2.46	0.50
1:G:357:PHE:CD2	1:G:369:LEU:HD21	2.46	0.50
1:I:45:PRO:O	1:I:47:HIS:ND1	2.44	0.50
1:G:45:PRO:O	1:G:47:HIS:ND1	2.44	0.50
1:H:215:ARG:NH1	1:H:269:GLU:OE1	2.45	0.50
1:C:215:ARG:NH1	1:C:269:GLU:OE1	2.45	0.50
1:C:408:GLU:OE2	1:E:412:LYS:NZ	2.39	0.50
1:F:283:ASN:OD1	1:F:283:ASN:N	2.44	0.50
1:F:443:LYS:HE3	1:F:633:TRP:CE2	2.46	0.50
1:G:634:LEU:HD22	1:G:638:GLU:OE1	2.12	0.50
1:I:357:PHE:CD2	1:I:369:LEU:HD21	2.46	0.50
1:I:443:LYS:HE3	1:I:633:TRP:CE2	2.46	0.50
1:K:634:LEU:HD22	1:K:638:GLU:OE1	2.12	0.50
1:B:215:ARG:NH1	1:B:269:GLU:OE1	2.45	0.50
1:B:357:PHE:CD2	1:B:369:LEU:HD21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:PHE:CD2	1:D:369:LEU:HD21	2.46	0.50
1:D:443:LYS:HE3	1:D:633:TRP:CE2	2.46	0.50
1:A:215:ARG:NH1	1:A:269:GLU:OE1	2.45	0.50
1:F:215:ARG:NH1	1:F:269:GLU:OE1	2.45	0.50
1:L:466:VAL:HG13	1:L:492:ILE:HG21	1.94	0.50
1:L:634:LEU:HD22	1:L:638:GLU:OE1	2.12	0.50
1:A:443:LYS:HE3	1:A:633:TRP:CE2	2.46	0.50
1:C:443:LYS:HE3	1:C:633:TRP:CE2	2.46	0.50
1:D:215:ARG:NH1	1:D:269:GLU:OE1	2.45	0.50
1:E:634:LEU:HD22	1:E:638:GLU:OE1	2.12	0.50
1:I:634:LEU:HD22	1:I:638:GLU:OE1	2.12	0.50
1:K:215:ARG:NH1	1:K:269:GLU:OE1	2.45	0.50
1:A:634:LEU:HD22	1:A:638:GLU:OE1	2.12	0.50
1:C:357:PHE:CD2	1:C:369:LEU:HD21	2.46	0.50
1:E:466:VAL:HG13	1:E:492:ILE:HG21	1.94	0.50
1:F:634:LEU:HD22	1:F:638:GLU:OE1	2.12	0.50
1:H:466:VAL:HG13	1:H:492:ILE:HG21	1.94	0.50
1:H:634:LEU:HD22	1:H:638:GLU:OE1	2.12	0.50
1:I:466:VAL:HG13	1:I:492:ILE:HG21	1.94	0.50
1:J:45:PRO:O	1:J:47:HIS:ND1	2.44	0.50
1:J:443:LYS:HE3	1:J:633:TRP:CE2	2.46	0.50
1:K:466:VAL:HG13	1:K:492:ILE:HG21	1.94	0.50
1:L:45:PRO:O	1:L:47:HIS:ND1	2.44	0.50
1:A:121:PRO:HD2	1:A:124:GLN:HE21	1.77	0.50
1:D:283:ASN:OD1	1:D:283:ASN:N	2.44	0.50
1:I:215:ARG:NH1	1:I:269:GLU:OE1	2.45	0.50
1:J:634:LEU:HD22	1:J:638:GLU:OE1	2.12	0.50
1:K:283:ASN:OD1	1:K:283:ASN:N	2.44	0.50
1:K:327:ARG:HA	1:K:327:ARG:NE	2.27	0.50
1:L:327:ARG:HA	1:L:327:ARG:NE	2.27	0.50
1:B:443:LYS:HE3	1:B:633:TRP:CE2	2.46	0.50
1:K:45:PRO:O	1:K:47:HIS:ND1	2.44	0.50
1:G:466:VAL:HG13	1:G:492:ILE:HG21	1.94	0.49
1:I:327:ARG:HA	1:I:327:ARG:NE	2.27	0.49
1:C:327:ARG:NE	1:C:327:ARG:HA	2.27	0.49
1:D:634:LEU:HD22	1:D:638:GLU:OE1	2.12	0.49
1:B:45:PRO:O	1:B:47:HIS:ND1	2.44	0.49
1:D:466:VAL:HG13	1:D:492:ILE:HG21	1.94	0.49
1:G:215:ARG:NH1	1:G:269:GLU:OE1	2.45	0.49
1:G:327:ARG:HA	1:G:327:ARG:NE	2.27	0.49
1:D:45:PRO:O	1:D:47:HIS:ND1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ARG:HA	1:D:327:ARG:NE	2.27	0.49
1:F:466:VAL:HG13	1:F:492:ILE:HG21	1.94	0.49
1:H:602:THR:O	1:H:606:VAL:HG23	2.13	0.49
1:J:283:ASN:N	1:J:283:ASN:OD1	2.44	0.49
1:J:327:ARG:HA	1:J:327:ARG:NE	2.27	0.49
1:E:327:ARG:HA	1:E:327:ARG:NE	2.27	0.49
1:E:368:LYS:HA	1:E:368:LYS:CE	2.37	0.49
1:E:408:GLU:OE2	1:F:412:LYS:NZ	2.36	0.49
1:E:602:THR:O	1:E:606:VAL:HG23	2.13	0.49
1:C:634:LEU:HD22	1:C:638:GLU:OE1	2.12	0.49
1:E:215:ARG:NH1	1:E:269:GLU:OE1	2.45	0.49
1:F:609:MET:HE1	1:F:653:LEU:HA	1.95	0.49
1:B:465:GLY:HA2	1:B:494:HIS:O	2.13	0.49
1:C:465:GLY:HA2	1:C:494:HIS:O	2.13	0.49
1:C:466:VAL:HG13	1:C:492:ILE:HG21	1.94	0.49
1:E:465:GLY:HA2	1:E:494:HIS:O	2.13	0.49
1:I:150:GLU:HB3	1:I:353:LEU:HD12	1.95	0.49
1:I:602:THR:O	1:I:606:VAL:HG23	2.13	0.49
1:L:602:THR:O	1:L:606:VAL:HG23	2.13	0.49
1:A:283:ASN:OD1	1:A:283:ASN:N	2.44	0.49
1:B:634:LEU:HD22	1:B:638:GLU:OE1	2.12	0.49
1:D:465:GLY:HA2	1:D:494:HIS:O	2.13	0.49
1:G:609:MET:HE1	1:G:653:LEU:HA	1.93	0.49
1:H:327:ARG:NE	1:H:327:ARG:HA	2.27	0.49
1:J:150:GLU:HB3	1:J:353:LEU:HD12	1.95	0.49
1:K:428:LYS:HD2	1:K:437:LEU:HD12	1.95	0.49
1:K:602:THR:O	1:K:606:VAL:HG23	2.13	0.49
1:L:216:GLU:OE2	1:L:263:LYS:NZ	2.38	0.49
1:A:465:GLY:HA2	1:A:494:HIS:O	2.13	0.49
1:B:466:VAL:HG13	1:B:492:ILE:HG21	1.94	0.49
1:D:609:MET:HE1	1:D:653:LEU:HA	1.94	0.49
1:G:150:GLU:HB3	1:G:353:LEU:HD12	1.95	0.49
1:J:215:ARG:NH1	1:J:269:GLU:OE1	2.45	0.49
1:C:609:MET:HE1	1:C:653:LEU:HA	1.95	0.48
1:C:718:ASN:OD1	1:C:718:ASN:N	2.42	0.48
1:D:150:GLU:HB3	1:D:353:LEU:HD12	1.95	0.48
1:H:465:GLY:HA2	1:H:494:HIS:O	2.13	0.48
1:H:609:MET:HE1	1:H:653:LEU:HA	1.95	0.48
1:K:150:GLU:HB3	1:K:353:LEU:HD12	1.95	0.48
1:A:150:GLU:HB3	1:A:353:LEU:HD12	1.95	0.48
1:B:602:THR:O	1:B:606:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:LYS:HD2	1:G:437:LEU:HD12	1.95	0.48
1:G:602:THR:O	1:G:606:VAL:HG23	2.13	0.48
1:J:602:THR:O	1:J:606:VAL:HG23	2.13	0.48
1:L:215:ARG:NH1	1:L:269:GLU:OE1	2.45	0.48
1:A:466:VAL:HG13	1:A:492:ILE:HG21	1.94	0.48
1:B:428:LYS:HD2	1:B:437:LEU:HD12	1.95	0.48
1:F:602:THR:O	1:F:606:VAL:HG23	2.13	0.48
1:H:150:GLU:HB3	1:H:353:LEU:HD12	1.94	0.48
1:I:465:GLY:HA2	1:I:494:HIS:O	2.13	0.48
1:L:428:LYS:HD2	1:L:437:LEU:HD12	1.95	0.48
1:L:609:MET:HE1	1:L:653:LEU:HA	1.94	0.48
1:A:602:THR:O	1:A:606:VAL:HG23	2.13	0.48
1:E:428:LYS:HD2	1:E:437:LEU:HD12	1.95	0.48
1:H:428:LYS:HD2	1:H:437:LEU:HD12	1.95	0.48
1:A:327:ARG:NE	1:A:327:ARG:HA	2.27	0.48
1:A:590:LYS:H	1:A:590:LYS:HG3	1.61	0.48
1:B:150:GLU:HB3	1:B:353:LEU:HD12	1.95	0.48
1:C:428:LYS:HD2	1:C:437:LEU:HD12	1.95	0.48
1:D:602:THR:O	1:D:606:VAL:HG23	2.13	0.48
1:F:327:ARG:NE	1:F:327:ARG:HA	2.27	0.48
1:G:465:GLY:HA2	1:G:494:HIS:O	2.13	0.48
1:J:466:VAL:HG13	1:J:492:ILE:HG21	1.94	0.48
1:L:465:GLY:HA2	1:L:494:HIS:O	2.13	0.48
1:C:150:GLU:HB3	1:C:353:LEU:HD12	1.95	0.48
1:H:29:VAL:O	1:H:33:VAL:HG23	2.14	0.48
1:B:327:ARG:HA	1:B:327:ARG:NE	2.27	0.48
1:D:29:VAL:O	1:D:33:VAL:HG23	2.14	0.48
1:E:150:GLU:HB3	1:E:353:LEU:HD12	1.95	0.48
1:F:465:GLY:HA2	1:F:494:HIS:O	2.13	0.48
1:J:29:VAL:O	1:J:33:VAL:HG23	2.14	0.48
1:L:29:VAL:O	1:L:33:VAL:HG23	2.14	0.48
1:I:609:MET:HE1	1:I:653:LEU:HA	1.95	0.48
1:D:327:ARG:HA	1:D:327:ARG:HE	1.79	0.48
1:F:150:GLU:HB3	1:F:353:LEU:HD12	1.95	0.48
1:J:428:LYS:HD2	1:J:437:LEU:HD12	1.95	0.48
1:L:150:GLU:HB3	1:L:353:LEU:HD12	1.95	0.48
1:C:29:VAL:O	1:C:33:VAL:HG23	2.14	0.48
1:C:602:THR:O	1:C:606:VAL:HG23	2.13	0.48
1:G:173:GLU:H	1:G:173:GLU:CD	2.18	0.48
1:A:428:LYS:HD2	1:A:437:LEU:HD12	1.95	0.47
1:B:29:VAL:O	1:B:33:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:VAL:O	1:E:33:VAL:HG23	2.14	0.47
1:F:173:GLU:CD	1:F:173:GLU:H	2.18	0.47
1:K:29:VAL:O	1:K:33:VAL:HG23	2.14	0.47
1:A:327:ARG:HA	1:A:327:ARG:HE	1.79	0.47
1:B:74:ARG:O	1:B:78:GLU:HG3	2.15	0.47
1:C:74:ARG:O	1:C:78:GLU:HG3	2.15	0.47
1:I:173:GLU:CD	1:I:173:GLU:H	2.18	0.47
1:C:327:ARG:HA	1:C:327:ARG:HE	1.79	0.47
1:E:609:MET:HE1	1:E:653:LEU:HA	1.95	0.47
1:G:29:VAL:O	1:G:33:VAL:HG23	2.14	0.47
1:H:327:ARG:HA	1:H:327:ARG:HE	1.79	0.47
1:J:609:MET:HE1	1:J:653:LEU:HA	1.96	0.47
1:K:465:GLY:HA2	1:K:494:HIS:O	2.13	0.47
1:L:173:GLU:H	1:L:173:GLU:CD	2.18	0.47
1:A:173:GLU:CD	1:A:173:GLU:H	2.18	0.47
1:C:186:GLN:OE1	1:C:186:GLN:HA	2.15	0.47
1:I:428:LYS:HD2	1:I:437:LEU:HD12	1.95	0.47
1:J:465:GLY:HA2	1:J:494:HIS:O	2.13	0.47
1:L:74:ARG:O	1:L:78:GLU:HG3	2.15	0.47
1:L:186:GLN:HA	1:L:186:GLN:OE1	2.15	0.47
1:E:173:GLU:H	1:E:173:GLU:CD	2.18	0.47
1:F:186:GLN:OE1	1:F:186:GLN:HA	2.15	0.47
1:F:428:LYS:HD2	1:F:437:LEU:HD12	1.95	0.47
1:H:173:GLU:CD	1:H:173:GLU:H	2.18	0.47
1:D:428:LYS:HD2	1:D:437:LEU:HD12	1.95	0.47
1:F:45:PRO:O	1:F:47:HIS:ND1	2.44	0.47
1:I:29:VAL:O	1:I:33:VAL:HG23	2.14	0.47
1:I:327:ARG:HA	1:I:327:ARG:HE	1.79	0.47
1:K:173:GLU:CD	1:K:173:GLU:H	2.18	0.47
1:C:528:LEU:HD12	1:C:696:MET:SD	2.55	0.47
1:E:218:LEU:HA	1:E:221:VAL:HG13	1.97	0.47
1:E:327:ARG:HA	1:E:327:ARG:HE	1.79	0.47
1:E:528:LEU:HD12	1:E:696:MET:SD	2.55	0.47
1:E:590:LYS:H	1:E:590:LYS:HG3	1.61	0.47
1:G:186:GLN:HA	1:G:186:GLN:OE1	2.15	0.47
1:G:327:ARG:HA	1:G:327:ARG:HE	1.79	0.47
1:H:218:LEU:HA	1:H:221:VAL:HG13	1.97	0.47
1:H:528:LEU:HD12	1:H:696:MET:SD	2.55	0.47
1:J:528:LEU:HD12	1:J:696:MET:SD	2.55	0.47
1:K:186:GLN:OE1	1:K:186:GLN:HA	2.15	0.47
1:K:528:LEU:HD12	1:K:696:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:609:MET:HE1	1:K:653:LEU:HA	1.96	0.47
1:B:327:ARG:HA	1:B:327:ARG:HE	1.79	0.47
1:B:412:LYS:NZ	1:H:408:GLU:OE2	2.39	0.47
1:C:170:LYS:HG3	1:C:264:TYR:HD1	1.80	0.47
1:K:170:LYS:HG3	1:K:264:TYR:HD1	1.80	0.47
1:K:218:LEU:HA	1:K:221:VAL:HG13	1.97	0.47
1:L:170:LYS:HG3	1:L:264:TYR:HD1	1.80	0.47
1:L:368:LYS:HA	1:L:368:LYS:CE	2.37	0.47
1:A:528:LEU:HD12	1:A:696:MET:SD	2.55	0.47
1:B:173:GLU:CD	1:B:173:GLU:H	2.18	0.47
1:B:218:LEU:HA	1:B:221:VAL:HG13	1.97	0.47
1:D:74:ARG:O	1:D:78:GLU:HG3	2.15	0.47
1:F:170:LYS:HG3	1:F:264:TYR:HD1	1.80	0.47
1:F:528:LEU:HD12	1:F:696:MET:SD	2.55	0.47
1:J:74:ARG:O	1:J:78:GLU:HG3	2.15	0.47
1:L:752:ILE:CG2	1:L:755:ALA:HB2	2.45	0.47
1:A:170:LYS:HG3	1:A:264:TYR:HD1	1.80	0.47
1:B:528:LEU:HD12	1:B:696:MET:SD	2.55	0.47
1:C:173:GLU:CD	1:C:173:GLU:H	2.18	0.47
1:F:29:VAL:O	1:F:33:VAL:HG23	2.14	0.47
1:G:74:ARG:O	1:G:78:GLU:HG3	2.15	0.47
1:H:659:TRP:O	1:H:669:ARG:NH1	2.47	0.47
1:I:170:LYS:HG3	1:I:264:TYR:HD1	1.80	0.47
1:J:659:TRP:O	1:J:669:ARG:NH1	2.47	0.47
1:K:74:ARG:O	1:K:78:GLU:HG3	2.14	0.47
1:C:651:ARG:N	1:C:652:PRO:CD	2.79	0.46
1:E:186:GLN:OE1	1:E:186:GLN:HA	2.15	0.46
1:F:590:LYS:H	1:F:590:LYS:HG3	1.61	0.46
1:I:186:GLN:HA	1:I:186:GLN:OE1	2.15	0.46
1:L:528:LEU:HD12	1:L:696:MET:SD	2.55	0.46
1:D:173:GLU:CD	1:D:173:GLU:H	2.18	0.46
1:D:659:TRP:O	1:D:669:ARG:NH1	2.47	0.46
1:F:651:ARG:N	1:F:652:PRO:CD	2.79	0.46
1:I:218:LEU:HA	1:I:221:VAL:HG13	1.97	0.46
1:J:173:GLU:CD	1:J:173:GLU:H	2.18	0.46
1:J:186:GLN:OE1	1:J:186:GLN:HA	2.15	0.46
1:J:218:LEU:HA	1:J:221:VAL:HG13	1.97	0.46
1:A:247:HIS:O	1:A:248:ASN:OD1	2.34	0.46
1:A:641:ARG:HA	1:A:644:VAL:HG22	1.98	0.46
1:A:752:ILE:CG2	1:A:755:ALA:HB2	2.45	0.46
1:C:752:ILE:CG2	1:C:755:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLN:HA	1:D:186:GLN:OE1	2.15	0.46
1:D:247:HIS:O	1:D:248:ASN:OD1	2.34	0.46
1:F:74:ARG:O	1:F:78:GLU:HG3	2.15	0.46
1:H:641:ARG:HA	1:H:644:VAL:HG22	1.98	0.46
1:I:74:ARG:O	1:I:78:GLU:HG3	2.15	0.46
1:I:528:LEU:HD12	1:I:696:MET:SD	2.55	0.46
1:L:354:GLU:OE2	1:L:527:ARG:NH2	2.48	0.46
1:A:659:TRP:O	1:A:669:ARG:NH1	2.47	0.46
1:E:641:ARG:HA	1:E:644:VAL:HG22	1.98	0.46
1:F:641:ARG:HA	1:F:644:VAL:HG22	1.98	0.46
1:F:659:TRP:O	1:F:669:ARG:NH1	2.47	0.46
1:G:170:LYS:HG3	1:G:264:TYR:HD1	1.80	0.46
1:G:528:LEU:HD12	1:G:696:MET:SD	2.55	0.46
1:G:651:ARG:N	1:G:652:PRO:CD	2.79	0.46
1:G:752:ILE:CG2	1:G:755:ALA:HB2	2.45	0.46
1:L:218:LEU:HA	1:L:221:VAL:HG13	1.97	0.46
1:L:327:ARG:HA	1:L:327:ARG:HE	1.79	0.46
1:L:641:ARG:HA	1:L:644:VAL:HG22	1.98	0.46
1:D:170:LYS:HG3	1:D:264:TYR:HD1	1.80	0.46
1:I:651:ARG:N	1:I:652:PRO:CD	2.79	0.46
1:K:651:ARG:N	1:K:652:PRO:CD	2.79	0.46
1:K:752:ILE:CG2	1:K:755:ALA:HB2	2.45	0.46
1:B:752:ILE:CG2	1:B:755:ALA:HB2	2.45	0.46
1:E:74:ARG:O	1:E:78:GLU:HG3	2.15	0.46
1:E:170:LYS:HG3	1:E:264:TYR:HD1	1.80	0.46
1:I:590:LYS:H	1:I:590:LYS:HG3	1.61	0.46
1:J:752:ILE:CG2	1:J:755:ALA:HB2	2.45	0.46
1:A:29:VAL:O	1:A:33:VAL:HG23	2.14	0.46
1:A:74:ARG:O	1:A:78:GLU:HG3	2.14	0.46
1:A:218:LEU:HA	1:A:221:VAL:HG13	1.97	0.46
1:C:247:HIS:O	1:C:248:ASN:OD1	2.34	0.46
1:C:659:TRP:O	1:C:669:ARG:NH1	2.47	0.46
1:D:528:LEU:HD12	1:D:696:MET:SD	2.55	0.46
1:E:247:HIS:O	1:E:248:ASN:OD1	2.34	0.46
1:E:651:ARG:N	1:E:652:PRO:CD	2.79	0.46
1:F:752:ILE:CG2	1:F:755:ALA:HB2	2.45	0.46
1:G:218:LEU:HA	1:G:221:VAL:HG13	1.97	0.46
1:G:354:GLU:OE2	1:G:527:ARG:NH2	2.48	0.46
1:G:659:TRP:O	1:G:669:ARG:NH1	2.47	0.46
1:H:170:LYS:HG3	1:H:264:TYR:HD1	1.80	0.46
1:E:752:ILE:CG2	1:E:755:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:GLN:OE1	1:H:186:GLN:HA	2.15	0.46
1:H:247:HIS:O	1:H:248:ASN:OD1	2.34	0.46
1:H:651:ARG:N	1:H:652:PRO:CD	2.79	0.46
1:I:641:ARG:HA	1:I:644:VAL:HG22	1.98	0.46
1:J:641:ARG:HA	1:J:644:VAL:HG22	1.98	0.46
1:D:218:LEU:HA	1:D:221:VAL:HG13	1.97	0.46
1:E:354:GLU:OE2	1:E:527:ARG:NH2	2.48	0.46
1:F:327:ARG:HA	1:F:327:ARG:HE	1.79	0.46
1:A:186:GLN:OE1	1:A:186:GLN:HA	2.15	0.46
1:B:186:GLN:HA	1:B:186:GLN:OE1	2.15	0.46
1:B:368:LYS:HA	1:B:368:LYS:CE	2.37	0.46
1:C:590:LYS:H	1:C:590:LYS:HG3	1.61	0.46
1:F:218:LEU:HA	1:F:221:VAL:HG13	1.97	0.46
1:G:641:ARG:HA	1:G:644:VAL:HG22	1.98	0.46
1:I:752:ILE:CG2	1:I:755:ALA:HB2	2.45	0.46
1:J:170:LYS:HG3	1:J:264:TYR:HD1	1.80	0.46
1:J:327:ARG:HA	1:J:327:ARG:HE	1.79	0.46
1:L:651:ARG:N	1:L:652:PRO:CD	2.79	0.46
1:L:659:TRP:O	1:L:669:ARG:NH1	2.47	0.46
1:B:651:ARG:N	1:B:652:PRO:CD	2.79	0.45
1:C:218:LEU:HA	1:C:221:VAL:HG13	1.97	0.45
1:D:651:ARG:N	1:D:652:PRO:CD	2.79	0.45
1:K:641:ARG:HA	1:K:644:VAL:HG22	1.98	0.45
1:B:659:TRP:O	1:B:669:ARG:NH1	2.47	0.45
1:G:247:HIS:O	1:G:248:ASN:OD1	2.34	0.45
1:H:74:ARG:O	1:H:78:GLU:HG3	2.15	0.45
1:H:752:ILE:CG2	1:H:755:ALA:HB2	2.45	0.45
1:K:247:HIS:O	1:K:248:ASN:OD1	2.34	0.45
1:K:327:ARG:HA	1:K:327:ARG:HE	1.79	0.45
1:B:247:HIS:O	1:B:248:ASN:OD1	2.34	0.45
1:B:641:ARG:HA	1:B:644:VAL:HG22	1.98	0.45
1:A:651:ARG:N	1:A:652:PRO:CD	2.79	0.45
1:B:634:LEU:CD1	1:B:638:GLU:OE1	2.65	0.45
1:F:247:HIS:O	1:F:248:ASN:OD1	2.34	0.45
1:I:247:HIS:O	1:I:248:ASN:OD1	2.34	0.45
1:A:354:GLU:OE2	1:A:527:ARG:NH2	2.48	0.45
1:A:634:LEU:CD1	1:A:638:GLU:OE1	2.65	0.45
1:B:354:GLU:OE2	1:B:527:ARG:NH2	2.48	0.45
1:C:634:LEU:CD1	1:C:638:GLU:OE1	2.65	0.45
1:E:634:LEU:CD1	1:E:638:GLU:OE1	2.65	0.45
1:I:634:LEU:CD1	1:I:638:GLU:OE1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:247:HIS:O	1:L:248:ASN:OD1	2.34	0.45
1:C:45:PRO:HB2	1:C:47:HIS:CE1	2.52	0.45
1:D:752:ILE:CG2	1:D:755:ALA:HB2	2.45	0.45
1:I:45:PRO:HB2	1:I:47:HIS:CE1	2.52	0.45
1:I:659:TRP:O	1:I:669:ARG:NH1	2.47	0.45
1:J:354:GLU:OE2	1:J:527:ARG:NH2	2.48	0.45
1:B:170:LYS:HG3	1:B:264:TYR:HD1	1.80	0.45
1:F:634:LEU:CD1	1:F:638:GLU:OE1	2.65	0.45
1:G:634:LEU:CD1	1:G:638:GLU:OE1	2.65	0.45
1:J:651:ARG:N	1:J:652:PRO:CD	2.79	0.45
1:L:45:PRO:HB2	1:L:47:HIS:CE1	2.52	0.45
1:L:634:LEU:CD1	1:L:638:GLU:OE1	2.65	0.45
1:D:45:PRO:HB2	1:D:47:HIS:CE1	2.52	0.45
1:D:641:ARG:HA	1:D:644:VAL:HG22	1.98	0.45
1:F:354:GLU:OE2	1:F:527:ARG:NH2	2.48	0.45
1:G:45:PRO:HB2	1:G:47:HIS:CE1	2.52	0.45
1:J:247:HIS:O	1:J:248:ASN:OD1	2.34	0.45
1:A:45:PRO:HB2	1:A:47:HIS:CE1	2.52	0.45
1:D:634:LEU:CD1	1:D:638:GLU:OE1	2.65	0.45
1:E:45:PRO:HB2	1:E:47:HIS:CE1	2.52	0.45
1:E:523:ARG:NH1	1:F:84:GLU:HA	2.32	0.45
1:K:634:LEU:CD1	1:K:638:GLU:OE1	2.65	0.45
1:D:354:GLU:OE2	1:D:527:ARG:NH2	2.48	0.45
1:J:216:GLU:OE2	1:J:263:LYS:NZ	2.38	0.45
1:B:130:TRP:O	1:B:340:HIS:HE1	2.00	0.44
1:C:641:ARG:HA	1:C:644:VAL:HG22	1.98	0.44
1:E:659:TRP:O	1:E:669:ARG:NH1	2.47	0.44
1:J:45:PRO:HB2	1:J:47:HIS:CE1	2.52	0.44
1:H:634:LEU:CD1	1:H:638:GLU:OE1	2.65	0.44
1:J:717:ARG:CZ	1:K:717:ARG:CZ	2.95	0.44
1:K:45:PRO:HB2	1:K:47:HIS:CE1	2.52	0.44
1:F:130:TRP:O	1:F:340:HIS:HE1	2.00	0.44
1:G:523:ARG:NH1	1:I:84:GLU:HA	2.32	0.44
1:C:130:TRP:O	1:C:340:HIS:HE1	2.00	0.44
1:K:659:TRP:O	1:K:669:ARG:NH1	2.47	0.44
1:A:609:MET:HE1	1:A:653:LEU:HA	1.99	0.44
1:B:45:PRO:HB2	1:B:47:HIS:CE1	2.52	0.44
1:E:225:VAL:O	1:E:225:VAL:CG2	2.66	0.44
1:D:130:TRP:O	1:D:340:HIS:HE1	2.00	0.44
1:D:590:LYS:H	1:D:590:LYS:HG3	1.61	0.44
1:H:130:TRP:O	1:H:340:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:TRP:O	1:I:340:HIS:HE1	2.00	0.44
1:J:634:LEU:CD1	1:J:638:GLU:OE1	2.65	0.44
1:K:590:LYS:H	1:K:590:LYS:HG3	1.61	0.44
1:B:13:TYR:CE1	1:B:17:THR:CG2	2.98	0.44
1:F:45:PRO:HB2	1:F:47:HIS:CE1	2.52	0.44
1:G:130:TRP:O	1:G:340:HIS:HE1	2.00	0.44
1:H:45:PRO:HB2	1:H:47:HIS:CE1	2.52	0.44
1:J:590:LYS:H	1:J:590:LYS:HG3	1.61	0.44
1:L:785:GLU:OE1	1:L:785:GLU:HA	2.18	0.44
1:H:161:ALA:HB1	1:H:306:LEU:HD23	2.00	0.44
1:L:130:TRP:O	1:L:340:HIS:HE1	2.00	0.44
1:A:785:GLU:HA	1:A:785:GLU:OE1	2.18	0.43
1:B:225:VAL:O	1:B:225:VAL:CG2	2.66	0.43
1:I:565:ARG:HD2	1:I:604:ASP:OD1	2.18	0.43
1:K:130:TRP:O	1:K:340:HIS:HE1	2.00	0.43
1:A:565:ARG:HD2	1:A:604:ASP:OD1	2.19	0.43
1:D:225:VAL:O	1:D:225:VAL:CG2	2.65	0.43
1:D:368:LYS:HA	1:D:368:LYS:CE	2.37	0.43
1:G:785:GLU:OE1	1:G:785:GLU:HA	2.18	0.43
1:H:354:GLU:OE2	1:H:527:ARG:NH2	2.48	0.43
1:D:84:GLU:HA	1:L:523:ARG:NH1	2.33	0.43
1:F:785:GLU:HA	1:F:785:GLU:OE1	2.18	0.43
1:G:84:GLU:HA	1:J:523:ARG:NH1	2.33	0.43
1:I:785:GLU:HA	1:I:785:GLU:OE1	2.18	0.43
1:J:565:ARG:HD2	1:J:604:ASP:OD1	2.19	0.43
1:D:565:ARG:HD2	1:D:604:ASP:OD1	2.19	0.43
1:E:130:TRP:O	1:E:340:HIS:HE1	2.00	0.43
1:H:540:ILE:HD12	1:H:543:ARG:NH1	2.34	0.43
1:J:540:ILE:HD12	1:J:543:ARG:NH1	2.34	0.43
1:L:540:ILE:HD12	1:L:543:ARG:NH1	2.34	0.43
1:A:161:ALA:HB1	1:A:306:LEU:HD23	2.00	0.43
1:C:161:ALA:HB1	1:C:306:LEU:HD23	2.00	0.43
1:C:354:GLU:OE2	1:C:527:ARG:NH2	2.48	0.43
1:C:540:ILE:HD12	1:C:543:ARG:NH1	2.34	0.43
1:D:540:ILE:HD12	1:D:543:ARG:NH1	2.34	0.43
1:E:565:ARG:HD2	1:E:604:ASP:OD1	2.19	0.43
1:H:565:ARG:HD2	1:H:604:ASP:OD1	2.19	0.43
1:A:130:TRP:O	1:A:340:HIS:HE1	2.00	0.43
1:B:565:ARG:HD2	1:B:604:ASP:OD1	2.19	0.43
1:G:565:ARG:HD2	1:G:604:ASP:OD1	2.19	0.43
1:J:785:GLU:OE1	1:J:785:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:523:ARG:NH1	1:L:84:GLU:HA	2.33	0.43
1:L:161:ALA:HB1	1:L:306:LEU:HD23	2.00	0.43
1:K:540:ILE:HD12	1:K:543:ARG:NH1	2.34	0.43
1:K:785:GLU:HA	1:K:785:GLU:OE1	2.18	0.43
1:A:523:ARG:NH1	1:H:84:GLU:HA	2.34	0.43
1:D:161:ALA:HB1	1:D:306:LEU:HD23	2.00	0.43
1:D:523:ARG:NH1	1:K:84:GLU:HA	2.34	0.43
1:D:785:GLU:HA	1:D:785:GLU:OE1	2.18	0.43
1:E:13:TYR:CE1	1:E:17:THR:CG2	2.98	0.43
1:G:540:ILE:HD12	1:G:543:ARG:NH1	2.34	0.43
1:I:523:ARG:NH1	1:J:84:GLU:HA	2.34	0.43
1:J:533:ALA:O	1:J:689:GLN:NE2	2.50	0.43
1:A:84:GLU:HA	1:B:523:ARG:NH1	2.34	0.43
1:C:523:ARG:NH1	1:E:84:GLU:HA	2.34	0.43
1:C:565:ARG:HD2	1:C:604:ASP:OD1	2.19	0.43
1:G:590:LYS:H	1:G:590:LYS:HG3	1.61	0.43
1:J:130:TRP:O	1:J:340:HIS:HE1	2.00	0.43
1:L:565:ARG:HD2	1:L:604:ASP:OD1	2.19	0.43
1:A:149:HIS:CD2	1:A:791:ARG:HB2	2.54	0.43
1:A:540:ILE:HD12	1:A:543:ARG:NH1	2.34	0.43
1:A:717:ARG:CZ	1:L:717:ARG:CZ	2.97	0.43
1:J:149:HIS:CD2	1:J:791:ARG:HB2	2.54	0.43
1:J:161:ALA:HB1	1:J:306:LEU:HD23	2.00	0.43
1:F:149:HIS:CD2	1:F:791:ARG:HB2	2.54	0.42
1:F:565:ARG:HD2	1:F:604:ASP:OD1	2.19	0.42
1:G:82:LYS:O	1:G:88:PRO:HA	2.19	0.42
1:I:82:LYS:O	1:I:88:PRO:HA	2.19	0.42
1:L:82:LYS:O	1:L:88:PRO:HA	2.19	0.42
1:B:28:ARG:HH11	1:B:28:ARG:HD2	1.72	0.42
1:B:469:ALA:O	1:B:470:ALA:HB3	2.20	0.42
1:B:785:GLU:OE1	1:B:785:GLU:HA	2.18	0.42
1:F:469:ALA:O	1:F:470:ALA:HB3	2.19	0.42
1:F:540:ILE:HD12	1:F:543:ARG:NH1	2.34	0.42
1:G:523:ARG:HH11	1:I:84:GLU:HA	1.84	0.42
1:H:82:LYS:O	1:H:88:PRO:HA	2.19	0.42
1:H:717:ARG:CZ	1:I:717:ARG:CZ	2.97	0.42
1:H:785:GLU:OE1	1:H:785:GLU:HA	2.18	0.42
1:I:161:ALA:HB1	1:I:306:LEU:HD23	2.00	0.42
1:J:469:ALA:O	1:J:470:ALA:HB3	2.20	0.42
1:K:161:ALA:HB1	1:K:306:LEU:HD23	2.00	0.42
1:K:469:ALA:O	1:K:470:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:GLU:OE1	1:C:785:GLU:HA	2.18	0.42
1:E:161:ALA:HB1	1:E:306:LEU:HD23	2.00	0.42
1:E:149:HIS:CD2	1:E:791:ARG:HB2	2.54	0.42
1:G:149:HIS:CD2	1:G:791:ARG:HB2	2.54	0.42
1:I:540:ILE:HD12	1:I:543:ARG:NH1	2.34	0.42
1:L:149:HIS:CD2	1:L:791:ARG:HB2	2.54	0.42
1:L:389:TRP:HB2	1:L:392:GLU:OE2	2.20	0.42
1:A:28:ARG:HH11	1:A:28:ARG:HD2	1.71	0.42
1:C:82:LYS:O	1:C:88:PRO:HA	2.19	0.42
1:E:540:ILE:HD12	1:E:543:ARG:NH1	2.34	0.42
1:F:161:ALA:HB1	1:F:306:LEU:HD23	2.00	0.42
1:H:149:HIS:CD2	1:H:791:ARG:HB2	2.54	0.42
1:K:354:GLU:OE2	1:K:527:ARG:NH2	2.48	0.42
1:A:368:LYS:HA	1:A:368:LYS:CE	2.37	0.42
1:A:389:TRP:HB2	1:A:392:GLU:OE2	2.20	0.42
1:A:469:ALA:O	1:A:470:ALA:HB3	2.20	0.42
1:C:717:ARG:CZ	1:D:717:ARG:CZ	2.98	0.42
1:D:469:ALA:O	1:D:470:ALA:HB3	2.20	0.42
1:E:785:GLU:OE1	1:E:785:GLU:HA	2.18	0.42
1:G:161:ALA:HB1	1:G:306:LEU:HD23	2.00	0.42
1:G:389:TRP:HB2	1:G:392:GLU:OE2	2.20	0.42
1:J:389:TRP:HB2	1:J:392:GLU:OE2	2.20	0.42
1:K:368:LYS:HA	1:K:368:LYS:CE	2.37	0.42
1:B:154:HIS:HB2	1:B:421:HIS:NE2	2.35	0.42
1:B:540:ILE:HD12	1:B:543:ARG:NH1	2.34	0.42
1:E:469:ALA:O	1:E:470:ALA:HB3	2.19	0.42
1:E:533:ALA:O	1:E:689:GLN:NE2	2.50	0.42
1:F:154:HIS:HB2	1:F:421:HIS:NE2	2.35	0.42
1:F:397:ILE:HG21	1:F:459:LEU:HD11	2.02	0.42
1:J:82:LYS:O	1:J:88:PRO:HA	2.20	0.42
1:A:13:TYR:CE1	1:A:17:THR:CG2	2.98	0.42
1:A:82:LYS:O	1:A:88:PRO:HA	2.19	0.42
1:B:82:LYS:O	1:B:88:PRO:HA	2.19	0.42
1:B:149:HIS:CD2	1:B:791:ARG:HB2	2.54	0.42
1:B:717:ARG:CZ	1:E:717:ARG:CZ	2.97	0.42
1:C:415:GLU:O	1:C:796:HIS:NE2	2.53	0.42
1:D:149:HIS:CD2	1:D:791:ARG:HB2	2.54	0.42
1:D:154:HIS:HB2	1:D:421:HIS:NE2	2.35	0.42
1:E:389:TRP:HB2	1:E:392:GLU:OE2	2.20	0.42
1:I:523:ARG:HH11	1:J:84:GLU:HA	1.85	0.42
1:C:397:ILE:HG21	1:C:459:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:O	1:D:88:PRO:HA	2.19	0.42
1:G:408:GLU:OE2	1:I:412:LYS:NZ	2.36	0.42
1:H:543:ARG:HD3	1:I:717:ARG:NH2	2.35	0.42
1:I:397:ILE:HG21	1:I:459:LEU:HD11	2.02	0.42
1:J:397:ILE:HG21	1:J:459:LEU:HD11	2.02	0.42
1:J:415:GLU:O	1:J:796:HIS:NE2	2.53	0.42
1:K:149:HIS:CD2	1:K:791:ARG:HB2	2.54	0.42
1:K:154:HIS:HB2	1:K:421:HIS:NE2	2.35	0.42
1:K:397:ILE:HG21	1:K:459:LEU:HD11	2.02	0.42
1:K:565:ARG:HD2	1:K:604:ASP:OD1	2.19	0.42
1:L:154:HIS:HB2	1:L:421:HIS:NE2	2.35	0.42
1:B:84:GLU:HA	1:H:523:ARG:NH1	2.35	0.42
1:E:82:LYS:O	1:E:88:PRO:HA	2.19	0.42
1:F:389:TRP:HB2	1:F:392:GLU:OE2	2.20	0.42
1:G:154:HIS:HB2	1:G:421:HIS:NE2	2.35	0.42
1:H:469:ALA:O	1:H:470:ALA:HB3	2.20	0.42
1:I:149:HIS:CD2	1:I:791:ARG:HB2	2.54	0.42
1:J:28:ARG:HH11	1:J:28:ARG:HD2	1.71	0.42
1:K:82:LYS:O	1:K:88:PRO:HA	2.19	0.42
1:L:397:ILE:HG21	1:L:459:LEU:HD11	2.02	0.42
1:A:397:ILE:HG21	1:A:459:LEU:HD11	2.02	0.41
1:E:154:HIS:HB2	1:E:421:HIS:NE2	2.35	0.41
1:E:415:GLU:O	1:E:796:HIS:NE2	2.53	0.41
1:G:488:ALA:HB2	1:G:495:PHE:CZ	2.55	0.41
1:H:488:ALA:HB2	1:H:495:PHE:CZ	2.55	0.41
1:H:540:ILE:HD12	1:H:543:ARG:CZ	2.50	0.41
1:I:533:ALA:O	1:I:689:GLN:NE2	2.50	0.41
1:J:488:ALA:HB2	1:J:495:PHE:CZ	2.55	0.41
1:K:28:ARG:HH11	1:K:28:ARG:HD2	1.71	0.41
1:K:415:GLU:O	1:K:796:HIS:NE2	2.53	0.41
1:A:415:GLU:O	1:A:796:HIS:NE2	2.53	0.41
1:C:84:GLU:HA	1:F:523:ARG:NH1	2.35	0.41
1:C:154:HIS:HB2	1:C:421:HIS:NE2	2.35	0.41
1:F:82:LYS:O	1:F:88:PRO:HA	2.19	0.41
1:K:13:TYR:CE1	1:K:17:THR:CG2	2.98	0.41
1:L:469:ALA:O	1:L:470:ALA:HB3	2.20	0.41
1:B:161:ALA:HB1	1:B:306:LEU:HD23	2.00	0.41
1:D:13:TYR:CE1	1:D:17:THR:CG2	2.98	0.41
1:I:540:ILE:HD12	1:I:543:ARG:CZ	2.51	0.41
1:K:488:ALA:HB2	1:K:495:PHE:CZ	2.55	0.41
1:L:488:ALA:HB2	1:L:495:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:HIS:CD2	1:C:791:ARG:HB2	2.54	0.41
1:C:540:ILE:HD12	1:C:543:ARG:CZ	2.51	0.41
1:D:397:ILE:HG21	1:D:459:LEU:HD11	2.02	0.41
1:D:540:ILE:HD12	1:D:543:ARG:CZ	2.51	0.41
1:F:543:ARG:HD3	1:G:717:ARG:NH2	2.36	0.41
1:F:717:ARG:CZ	1:G:717:ARG:CZ	2.98	0.41
1:G:84:GLU:HA	1:J:523:ARG:HH11	1.85	0.41
1:G:415:GLU:O	1:G:796:HIS:NE2	2.53	0.41
1:H:225:VAL:O	1:H:225:VAL:CG2	2.66	0.41
1:I:154:HIS:HB2	1:I:421:HIS:NE2	2.35	0.41
1:J:540:ILE:HD12	1:J:543:ARG:CZ	2.51	0.41
1:B:389:TRP:HB2	1:B:392:GLU:OE2	2.20	0.41
1:B:397:ILE:HG21	1:B:459:LEU:HD11	2.02	0.41
1:B:488:ALA:HB2	1:B:495:PHE:CZ	2.55	0.41
1:B:745:LEU:HG	1:B:786:VAL:HG12	2.03	0.41
1:C:523:ARG:HH11	1:E:84:GLU:HA	1.86	0.41
1:D:84:GLU:HA	1:L:523:ARG:HH11	1.85	0.41
1:E:488:ALA:HB2	1:E:495:PHE:CZ	2.56	0.41
1:H:397:ILE:HG21	1:H:459:LEU:HD11	2.02	0.41
1:I:28:ARG:HH11	1:I:28:ARG:HD2	1.72	0.41
1:I:354:GLU:OE2	1:I:527:ARG:NH2	2.48	0.41
1:J:368:LYS:HA	1:J:368:LYS:CE	2.37	0.41
1:K:523:ARG:HH11	1:L:84:GLU:HA	1.85	0.41
1:B:381:LEU:HD13	1:B:407:VAL:HG21	2.03	0.41
1:C:469:ALA:O	1:C:470:ALA:HB3	2.20	0.41
1:C:640:ALA:O	1:C:644:VAL:HG13	2.21	0.41
1:D:415:GLU:O	1:D:796:HIS:NE2	2.53	0.41
1:I:469:ALA:O	1:I:470:ALA:HB3	2.20	0.41
1:C:19:SER:O	1:C:290:ARG:NH1	2.54	0.41
1:C:389:TRP:HB2	1:C:392:GLU:OE2	2.20	0.41
1:D:640:ALA:O	1:D:644:VAL:HG13	2.21	0.41
1:G:533:ALA:O	1:G:689:GLN:NE2	2.50	0.41
1:I:488:ALA:HB2	1:I:495:PHE:CZ	2.55	0.41
1:J:381:LEU:HD13	1:J:407:VAL:HG21	2.03	0.41
1:J:640:ALA:O	1:J:644:VAL:HG13	2.21	0.41
1:A:540:ILE:HD12	1:A:543:ARG:CZ	2.51	0.41
1:B:540:ILE:HD12	1:B:543:ARG:CZ	2.51	0.41
1:C:488:ALA:HB2	1:C:495:PHE:CZ	2.56	0.41
1:C:717:ARG:NH2	1:D:543:ARG:HD3	2.36	0.41
1:D:19:SER:O	1:D:290:ARG:NH1	2.54	0.41
1:E:381:LEU:HD13	1:E:407:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:SER:O	1:F:290:ARG:NH1	2.54	0.41
1:F:640:ALA:O	1:F:644:VAL:HG13	2.21	0.41
1:G:469:ALA:O	1:G:470:ALA:HB3	2.19	0.41
1:H:693:MET:HG2	1:H:741:MET:SD	2.61	0.41
1:I:381:LEU:HD13	1:I:407:VAL:HG21	2.03	0.41
1:I:389:TRP:HB2	1:I:392:GLU:OE2	2.20	0.41
1:J:154:HIS:HB2	1:J:421:HIS:NE2	2.35	0.41
1:A:154:HIS:HB2	1:A:421:HIS:NE2	2.35	0.41
1:B:82:LYS:HZ1	1:B:91:ASP:CG	2.24	0.41
1:B:634:LEU:HD13	1:B:638:GLU:OE1	2.21	0.41
1:B:693:MET:HG2	1:B:741:MET:SD	2.61	0.41
1:C:693:MET:HG2	1:C:741:MET:SD	2.61	0.41
1:D:246:LEU:HA	1:D:250:ARG:O	2.21	0.41
1:D:389:TRP:HB2	1:D:392:GLU:OE2	2.20	0.41
1:D:488:ALA:HB2	1:D:495:PHE:CZ	2.55	0.41
1:D:634:LEU:HD13	1:D:638:GLU:OE1	2.21	0.41
1:E:397:ILE:HG21	1:E:459:LEU:HD11	2.02	0.41
1:E:540:ILE:HD12	1:E:543:ARG:CZ	2.51	0.41
1:E:745:LEU:HG	1:E:786:VAL:HG12	2.03	0.41
1:F:488:ALA:HB2	1:F:495:PHE:CZ	2.55	0.41
1:G:693:MET:HG2	1:G:741:MET:SD	2.61	0.41
1:H:154:HIS:HB2	1:H:421:HIS:NE2	2.35	0.41
1:H:368:LYS:HA	1:H:368:LYS:CE	2.37	0.41
1:H:381:LEU:HD13	1:H:407:VAL:HG21	2.03	0.41
1:H:389:TRP:HB2	1:H:392:GLU:OE2	2.20	0.41
1:H:640:ALA:O	1:H:644:VAL:HG13	2.21	0.41
1:H:745:LEU:HG	1:H:786:VAL:HG12	2.03	0.41
1:H:749:ASP:HB3	1:H:752:ILE:CG2	2.51	0.41
1:I:415:GLU:O	1:I:796:HIS:NE2	2.53	0.41
1:J:19:SER:O	1:J:290:ARG:NH1	2.54	0.41
1:K:540:ILE:HD12	1:K:543:ARG:CZ	2.51	0.41
1:K:634:LEU:HD13	1:K:638:GLU:OE1	2.21	0.41
1:L:381:LEU:HD13	1:L:407:VAL:HG21	2.03	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.99	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.99	0.41
1:C:634:LEU:HD13	1:C:638:GLU:OE1	2.21	0.41
1:D:693:MET:HG2	1:D:741:MET:SD	2.61	0.41
1:E:467:ASP:HA	1:E:496:THR:O	2.21	0.41
1:E:523:ARG:HH11	1:F:84:GLU:HA	1.85	0.41
1:E:693:MET:HG2	1:E:741:MET:SD	2.61	0.41
1:F:634:LEU:HD13	1:F:638:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:540:ILE:HD12	1:G:543:ARG:CZ	2.51	0.41
1:G:634:LEU:HD13	1:G:638:GLU:OE1	2.21	0.41
1:K:389:TRP:HB2	1:K:392:GLU:OE2	2.20	0.41
1:A:19:SER:O	1:A:290:ARG:NH1	2.54	0.40
1:B:749:ASP:HB3	1:B:752:ILE:CG2	2.51	0.40
1:C:745:LEU:HG	1:C:786:VAL:HG12	2.03	0.40
1:E:19:SER:O	1:E:290:ARG:NH1	2.54	0.40
1:F:225:VAL:O	1:F:225:VAL:CG2	2.66	0.40
1:F:540:ILE:HD12	1:F:543:ARG:CZ	2.51	0.40
1:H:415:GLU:O	1:H:796:HIS:NE2	2.53	0.40
1:I:693:MET:HG2	1:I:741:MET:SD	2.61	0.40
1:J:246:LEU:HA	1:J:250:ARG:O	2.21	0.40
1:J:693:MET:HG2	1:J:741:MET:SD	2.61	0.40
1:K:640:ALA:O	1:K:644:VAL:HG13	2.21	0.40
1:L:540:ILE:HD12	1:L:543:ARG:CZ	2.51	0.40
1:A:381:LEU:HD13	1:A:407:VAL:HG21	2.03	0.40
1:A:693:MET:HG2	1:A:741:MET:SD	2.61	0.40
1:D:523:ARG:HH11	1:K:84:GLU:HA	1.86	0.40
1:G:19:SER:O	1:G:290:ARG:NH1	2.54	0.40
1:G:397:ILE:HG21	1:G:459:LEU:HD11	2.02	0.40
1:G:467:ASP:HA	1:G:496:THR:O	2.21	0.40
1:H:19:SER:O	1:H:290:ARG:NH1	2.54	0.40
1:H:82:LYS:HZ1	1:H:91:ASP:CG	2.25	0.40
1:K:693:MET:HG2	1:K:741:MET:SD	2.61	0.40
1:L:19:SER:O	1:L:290:ARG:NH1	2.54	0.40
1:L:640:ALA:O	1:L:644:VAL:HG13	2.21	0.40
1:C:533:ALA:O	1:C:689:GLN:NE2	2.50	0.40
1:E:640:ALA:O	1:E:644:VAL:HG13	2.21	0.40
1:G:640:ALA:O	1:G:644:VAL:HG13	2.21	0.40
1:L:533:ALA:O	1:L:689:GLN:NE2	2.50	0.40
1:L:693:MET:HG2	1:L:741:MET:SD	2.61	0.40
1:A:84:GLU:HA	1:B:523:ARG:HH11	1.86	0.40
1:B:246:LEU:HA	1:B:250:ARG:O	2.21	0.40
1:F:246:LEU:HA	1:F:250:ARG:O	2.21	0.40
1:G:44:LEU:HA	1:G:45:PRO:HD3	1.99	0.40
1:G:745:LEU:HG	1:G:786:VAL:HG12	2.03	0.40
1:K:246:LEU:HA	1:K:250:ARG:O	2.21	0.40
1:K:381:LEU:HD13	1:K:407:VAL:HG21	2.03	0.40
1:A:340:HIS:CE1	1:A:756:ASP:OD1	2.75	0.40
1:A:745:LEU:HG	1:A:786:VAL:HG12	2.03	0.40
1:D:533:ALA:O	1:D:689:GLN:NE2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:LEU:HG	1:D:786:VAL:HG12	2.03	0.40
1:F:745:LEU:HG	1:F:786:VAL:HG12	2.03	0.40
1:G:246:LEU:HA	1:G:250:ARG:O	2.21	0.40
1:G:381:LEU:HD13	1:G:407:VAL:HG21	2.03	0.40
1:I:246:LEU:HA	1:I:250:ARG:O	2.21	0.40
1:I:340:HIS:CE1	1:I:756:ASP:OD1	2.75	0.40
1:J:467:ASP:HA	1:J:496:THR:O	2.21	0.40
1:J:749:ASP:HB3	1:J:752:ILE:CG2	2.51	0.40
1:K:19:SER:O	1:K:290:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	B	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	C	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	D	757/798 (95%)	710 (94%)	41 (5%)	6 (1%)	19	14
1	E	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	F	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	G	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	H	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	I	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	J	762/798 (96%)	713 (94%)	43 (6%)	6 (1%)	19	14
1	K	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
1	L	762/798 (96%)	712 (93%)	44 (6%)	6 (1%)	19	14
All	All	9139/9576 (95%)	8543 (94%)	524 (6%)	72 (1%)	24	14

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	23	VAL
1	C	23	VAL
1	D	23	VAL
1	E	23	VAL
1	F	23	VAL
1	G	23	VAL
1	H	23	VAL
1	I	23	VAL
1	J	23	VAL
1	K	23	VAL
1	L	23	VAL
1	A	390	VAL
1	A	470	ALA
1	B	390	VAL
1	B	470	ALA
1	C	390	VAL
1	C	470	ALA
1	D	390	VAL
1	D	470	ALA
1	E	390	VAL
1	E	470	ALA
1	F	390	VAL
1	F	470	ALA
1	G	390	VAL
1	G	470	ALA
1	H	390	VAL
1	H	470	ALA
1	I	390	VAL
1	I	470	ALA
1	J	390	VAL
1	J	470	ALA
1	K	390	VAL
1	K	470	ALA
1	L	390	VAL
1	L	470	ALA
1	A	85	LYS
1	A	494	HIS
1	B	85	LYS
1	B	494	HIS
1	C	85	LYS
1	C	494	HIS

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Mol	Chain	Res	Type
1	D	85	LYS
1	D	494	HIS
1	E	85	LYS
1	E	494	HIS
1	F	85	LYS
1	F	494	HIS
1	G	85	LYS
1	G	494	HIS
1	H	85	LYS
1	H	494	HIS
1	I	85	LYS
1	I	494	HIS
1	J	85	LYS
1	J	494	HIS
1	K	85	LYS
1	K	494	HIS
1	L	85	LYS
1	L	494	HIS
1	A	200	THR
1	B	200	THR
1	C	200	THR
1	D	200	THR
1	E	200	THR
1	F	200	THR
1	G	200	THR
1	H	200	THR
1	I	200	THR
1	J	200	THR
1	K	200	THR
1	L	200	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	678/705 (96%)	643 (95%)	35 (5%)	23 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	C	678/705 (96%)	642 (95%)	36 (5%)	22	20
1	D	675/705 (96%)	640 (95%)	35 (5%)	23	20
1	E	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	F	678/705 (96%)	642 (95%)	36 (5%)	22	20
1	G	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	H	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	I	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	J	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	K	678/705 (96%)	643 (95%)	35 (5%)	23	20
1	L	678/705 (96%)	643 (95%)	35 (5%)	23	20
All	All	8133/8460 (96%)	7711 (95%)	422 (5%)	27	20

All (422) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	39	GLU
1	A	50	LYS
1	A	82	LYS
1	A	83	ASN
1	A	91	ASP
1	A	129	ARG
1	A	173	GLU
1	A	186	GLN
1	A	187	GLU
1	A	202	ARG
1	A	221	VAL
1	A	267	GLU
1	A	272	TRP
1	A	279	LYS
1	A	289	GLU
1	A	323	MET
1	A	325	GLU
1	A	332	LYS
1	A	364	ASN
1	A	368	LYS
1	A	386	SER

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Mol	Chain	Res	Type
1	A	426	LYS
1	A	474	HIS
1	A	490	SER
1	A	590	LYS
1	A	601	THR
1	A	638	GLU
1	A	650	LYS
1	A	653	LEU
1	A	654	LYS
1	A	663	ASP
1	A	678	GLU
1	A	753	PHE
1	A	756	ASP
1	B	28	ARG
1	B	39	GLU
1	B	50	LYS
1	B	82	LYS
1	B	83	ASN
1	B	91	ASP
1	B	129	ARG
1	B	173	GLU
1	B	186	GLN
1	B	187	GLU
1	B	202	ARG
1	B	221	VAL
1	B	267	GLU
1	B	272	TRP
1	B	279	LYS
1	B	289	GLU
1	B	323	MET
1	B	325	GLU
1	B	332	LYS
1	B	364	ASN
1	B	368	LYS
1	B	386	SER
1	B	426	LYS
1	B	474	HIS
1	B	490	SER
1	B	590	LYS
1	B	601	THR
1	B	638	GLU
1	B	650	LYS

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Mol	Chain	Res	Type
1	B	653	LEU
1	B	654	LYS
1	B	663	ASP
1	B	678	GLU
1	B	753	PHE
1	B	756	ASP
1	C	28	ARG
1	C	39	GLU
1	C	50	LYS
1	C	82	LYS
1	C	83	ASN
1	C	91	ASP
1	C	124	GLN
1	C	129	ARG
1	C	173	GLU
1	C	186	GLN
1	C	187	GLU
1	C	202	ARG
1	C	221	VAL
1	C	267	GLU
1	C	272	TRP
1	C	279	LYS
1	C	289	GLU
1	C	323	MET
1	C	325	GLU
1	C	332	LYS
1	C	364	ASN
1	C	368	LYS
1	C	386	SER
1	C	426	LYS
1	C	474	HIS
1	C	490	SER
1	C	590	LYS
1	C	601	THR
1	C	638	GLU
1	C	650	LYS
1	C	653	LEU
1	C	654	LYS
1	C	663	ASP
1	C	678	GLU
1	C	753	PHE
1	C	756	ASP

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Mol	Chain	Res	Type
1	D	28	ARG
1	D	39	GLU
1	D	50	LYS
1	D	82	LYS
1	D	83	ASN
1	D	91	ASP
1	D	129	ARG
1	D	173	GLU
1	D	186	GLN
1	D	187	GLU
1	D	202	ARG
1	D	221	VAL
1	D	267	GLU
1	D	272	TRP
1	D	279	LYS
1	D	289	GLU
1	D	323	MET
1	D	325	GLU
1	D	332	LYS
1	D	364	ASN
1	D	368	LYS
1	D	386	SER
1	D	426	LYS
1	D	474	HIS
1	D	490	SER
1	D	590	LYS
1	D	601	THR
1	D	638	GLU
1	D	650	LYS
1	D	653	LEU
1	D	654	LYS
1	D	663	ASP
1	D	678	GLU
1	D	753	PHE
1	D	756	ASP
1	E	28	ARG
1	E	39	GLU
1	E	50	LYS
1	E	82	LYS
1	E	83	ASN
1	E	91	ASP
1	E	129	ARG

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Mol	Chain	Res	Type
1	E	173	GLU
1	E	186	GLN
1	E	187	GLU
1	E	202	ARG
1	E	221	VAL
1	E	267	GLU
1	E	272	TRP
1	E	279	LYS
1	E	289	GLU
1	E	323	MET
1	E	325	GLU
1	E	332	LYS
1	E	364	ASN
1	E	368	LYS
1	E	386	SER
1	E	426	LYS
1	E	474	HIS
1	E	490	SER
1	E	590	LYS
1	E	601	THR
1	E	638	GLU
1	E	650	LYS
1	E	653	LEU
1	E	654	LYS
1	E	663	ASP
1	E	678	GLU
1	E	753	PHE
1	E	756	ASP
1	F	28	ARG
1	F	39	GLU
1	F	50	LYS
1	F	82	LYS
1	F	83	ASN
1	F	91	ASP
1	F	124	GLN
1	F	129	ARG
1	F	173	GLU
1	F	186	GLN
1	F	187	GLU
1	F	202	ARG
1	F	221	VAL
1	F	267	GLU

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Mol	Chain	Res	Type
1	F	272	TRP
1	F	279	LYS
1	F	289	GLU
1	F	323	MET
1	F	325	GLU
1	F	332	LYS
1	F	364	ASN
1	F	368	LYS
1	F	386	SER
1	F	426	LYS
1	F	474	HIS
1	F	490	SER
1	F	590	LYS
1	F	601	THR
1	F	638	GLU
1	F	650	LYS
1	F	653	LEU
1	F	654	LYS
1	F	663	ASP
1	F	678	GLU
1	F	753	PHE
1	F	756	ASP
1	G	28	ARG
1	G	39	GLU
1	G	50	LYS
1	G	82	LYS
1	G	83	ASN
1	G	91	ASP
1	G	129	ARG
1	G	173	GLU
1	G	186	GLN
1	G	187	GLU
1	G	202	ARG
1	G	221	VAL
1	G	267	GLU
1	G	272	TRP
1	G	279	LYS
1	G	289	GLU
1	G	323	MET
1	G	325	GLU
1	G	332	LYS
1	G	364	ASN

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Mol	Chain	Res	Type
1	G	368	LYS
1	G	386	SER
1	G	426	LYS
1	G	474	HIS
1	G	490	SER
1	G	590	LYS
1	G	601	THR
1	G	638	GLU
1	G	650	LYS
1	G	653	LEU
1	G	654	LYS
1	G	663	ASP
1	G	678	GLU
1	G	753	PHE
1	G	756	ASP
1	H	28	ARG
1	H	39	GLU
1	H	50	LYS
1	H	82	LYS
1	H	83	ASN
1	H	91	ASP
1	H	129	ARG
1	H	173	GLU
1	H	186	GLN
1	H	187	GLU
1	H	202	ARG
1	H	221	VAL
1	H	267	GLU
1	H	272	TRP
1	H	279	LYS
1	H	289	GLU
1	H	323	MET
1	H	325	GLU
1	H	332	LYS
1	H	364	ASN
1	H	368	LYS
1	H	386	SER
1	H	426	LYS
1	H	474	HIS
1	H	490	SER
1	H	590	LYS
1	H	601	THR

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Mol	Chain	Res	Type
1	H	638	GLU
1	H	650	LYS
1	H	653	LEU
1	H	654	LYS
1	H	663	ASP
1	H	678	GLU
1	H	753	PHE
1	H	756	ASP
1	I	28	ARG
1	I	39	GLU
1	I	50	LYS
1	I	82	LYS
1	I	83	ASN
1	I	91	ASP
1	I	129	ARG
1	I	173	GLU
1	I	186	GLN
1	I	187	GLU
1	I	202	ARG
1	I	221	VAL
1	I	267	GLU
1	I	272	TRP
1	I	279	LYS
1	I	289	GLU
1	I	323	MET
1	I	325	GLU
1	I	332	LYS
1	I	364	ASN
1	I	368	LYS
1	I	386	SER
1	I	426	LYS
1	I	474	HIS
1	I	490	SER
1	I	590	LYS
1	I	601	THR
1	I	638	GLU
1	I	650	LYS
1	I	653	LEU
1	I	654	LYS
1	I	663	ASP
1	I	678	GLU
1	I	753	PHE

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Mol	Chain	Res	Type
1	I	756	ASP
1	J	28	ARG
1	J	39	GLU
1	J	50	LYS
1	J	82	LYS
1	J	83	ASN
1	J	91	ASP
1	J	129	ARG
1	J	173	GLU
1	J	186	GLN
1	J	187	GLU
1	J	202	ARG
1	J	221	VAL
1	J	267	GLU
1	J	272	TRP
1	J	279	LYS
1	J	289	GLU
1	J	323	MET
1	J	325	GLU
1	J	332	LYS
1	J	364	ASN
1	J	368	LYS
1	J	386	SER
1	J	426	LYS
1	J	474	HIS
1	J	490	SER
1	J	590	LYS
1	J	601	THR
1	J	638	GLU
1	J	650	LYS
1	J	653	LEU
1	J	654	LYS
1	J	663	ASP
1	J	678	GLU
1	J	753	PHE
1	J	756	ASP
1	K	28	ARG
1	K	39	GLU
1	K	50	LYS
1	K	82	LYS
1	K	83	ASN
1	K	91	ASP

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Mol	Chain	Res	Type
1	K	129	ARG
1	K	173	GLU
1	K	186	GLN
1	K	187	GLU
1	K	202	ARG
1	K	221	VAL
1	K	267	GLU
1	K	272	TRP
1	K	279	LYS
1	K	289	GLU
1	K	323	MET
1	K	325	GLU
1	K	332	LYS
1	K	364	ASN
1	K	368	LYS
1	K	386	SER
1	K	426	LYS
1	K	474	HIS
1	K	490	SER
1	K	590	LYS
1	K	601	THR
1	K	638	GLU
1	K	650	LYS
1	K	653	LEU
1	K	654	LYS
1	K	663	ASP
1	K	678	GLU
1	K	753	PHE
1	K	756	ASP
1	L	28	ARG
1	L	39	GLU
1	L	50	LYS
1	L	82	LYS
1	L	83	ASN
1	L	91	ASP
1	L	129	ARG
1	L	173	GLU
1	L	186	GLN
1	L	187	GLU
1	L	202	ARG
1	L	221	VAL
1	L	267	GLU

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Mol	Chain	Res	Type
1	L	272	TRP
1	L	279	LYS
1	L	289	GLU
1	L	323	MET
1	L	325	GLU
1	L	332	LYS
1	L	364	ASN
1	L	368	LYS
1	L	386	SER
1	L	426	LYS
1	L	474	HIS
1	L	490	SER
1	L	590	LYS
1	L	601	THR
1	L	638	GLU
1	L	650	LYS
1	L	653	LEU
1	L	654	LYS
1	L	663	ASP
1	L	678	GLU
1	L	753	PHE
1	L	756	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	248	ASN
1	A	403	ASN
1	A	715	GLN
1	B	149	HIS
1	B	248	ASN
1	B	403	ASN
1	B	715	GLN
1	C	124	GLN
1	C	149	HIS
1	C	248	ASN
1	C	403	ASN
1	D	149	HIS
1	D	248	ASN
1	D	403	ASN
1	E	149	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	E	248	ASN
1	E	403	ASN
1	E	715	GLN
1	F	124	GLN
1	F	149	HIS
1	F	248	ASN
1	F	403	ASN
1	G	149	HIS
1	G	248	ASN
1	G	403	ASN
1	G	715	GLN
1	H	149	HIS
1	H	248	ASN
1	H	403	ASN
1	I	149	HIS
1	I	248	ASN
1	I	403	ASN
1	I	715	GLN
1	J	149	HIS
1	J	248	ASN
1	J	403	ASN
1	K	149	HIS
1	K	248	ASN
1	K	403	ASN
1	L	149	HIS
1	L	248	ASN
1	L	403	ASN
1	L	715	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

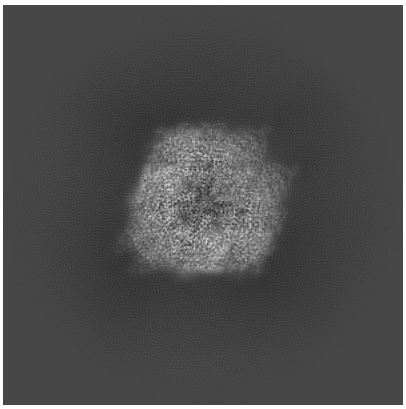
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29327. These allow visual inspection of the internal detail of the map and identification of artifacts.

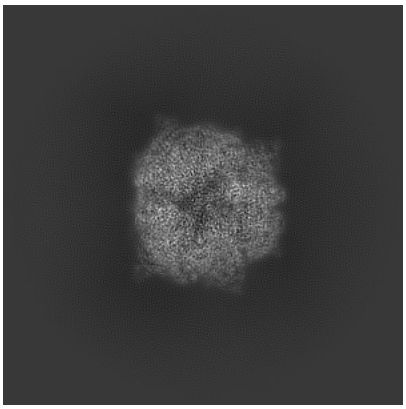
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

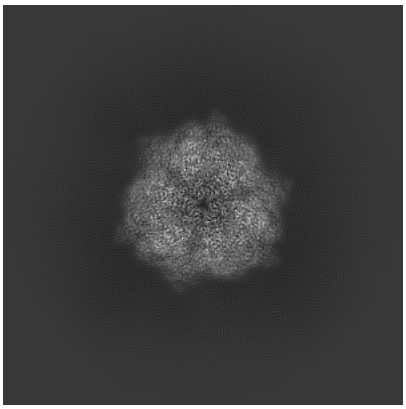
6.1.1 Primary map



X

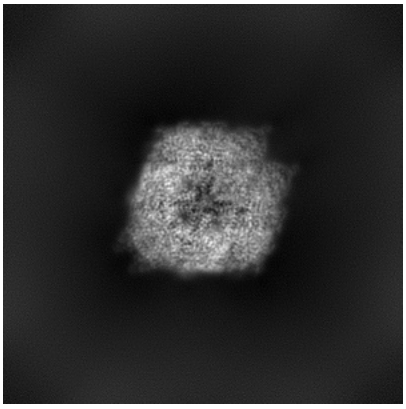


Y

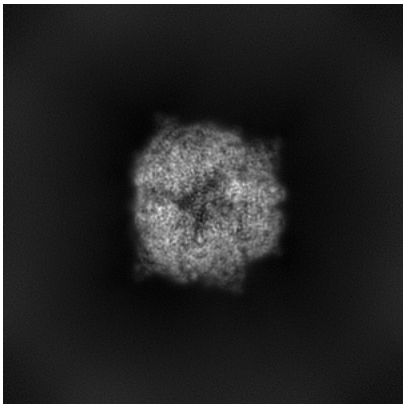


Z

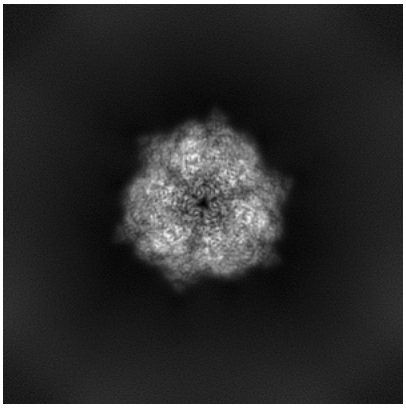
6.1.2 Raw map



X



Y

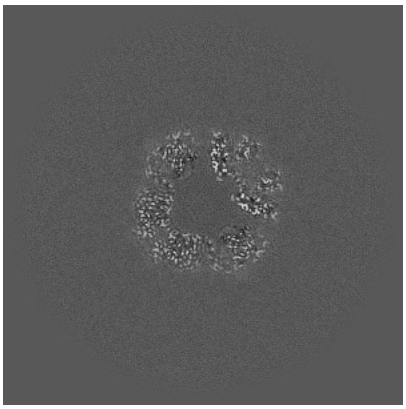


Z

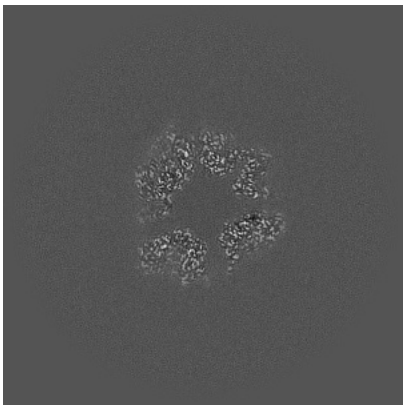
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

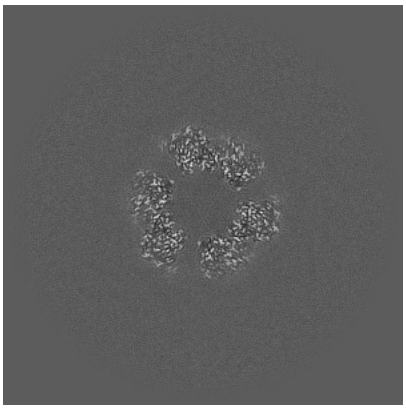
6.2.1 Primary map



X Index: 240

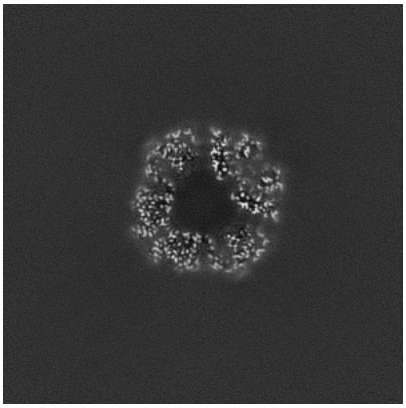


Y Index: 240

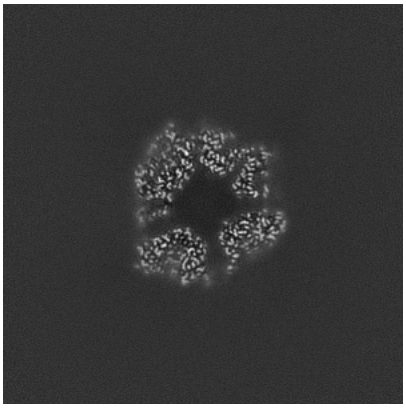


Z Index: 240

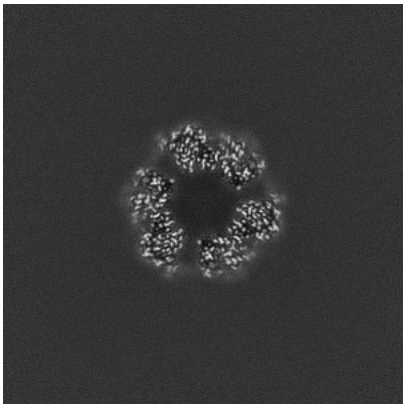
6.2.2 Raw map



X Index: 240



Y Index: 240

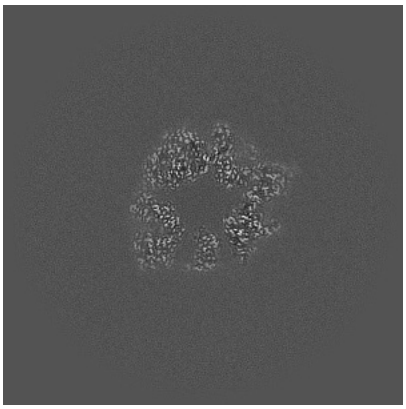


Z Index: 240

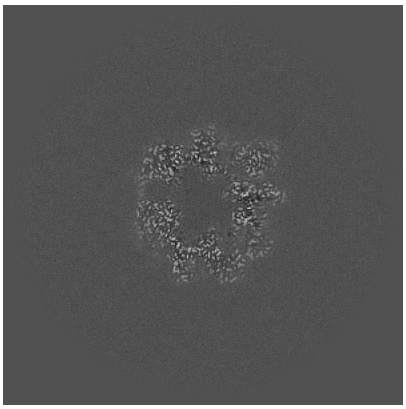
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

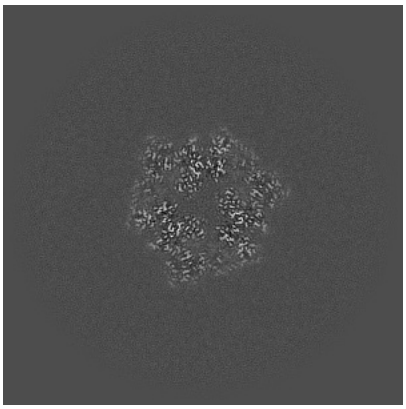
6.3.1 Primary map



X Index: 258

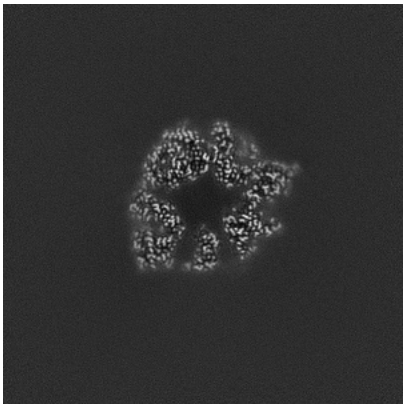


Y Index: 221

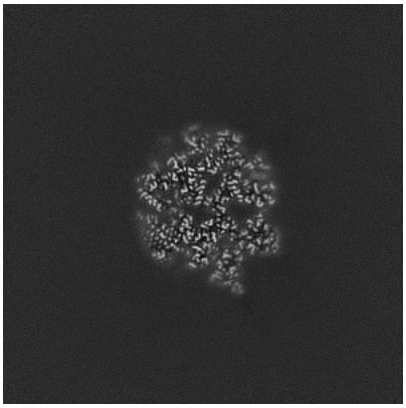


Z Index: 205

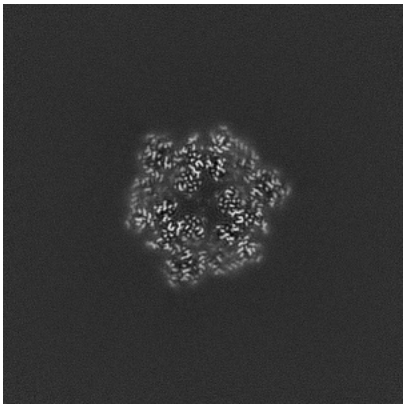
6.3.2 Raw map



X Index: 258



Y Index: 198

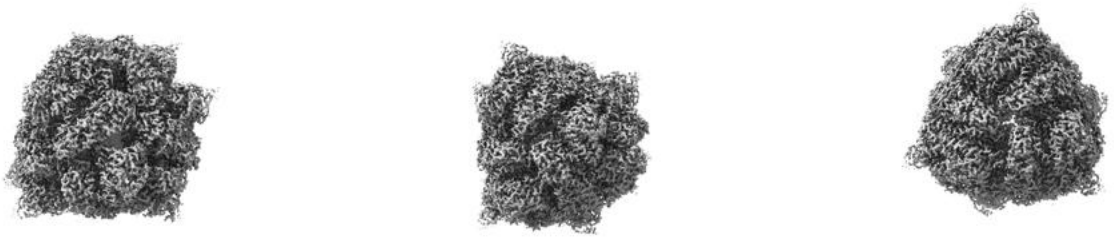


Z Index: 205

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

6.4 Orthogonal surface views (i)

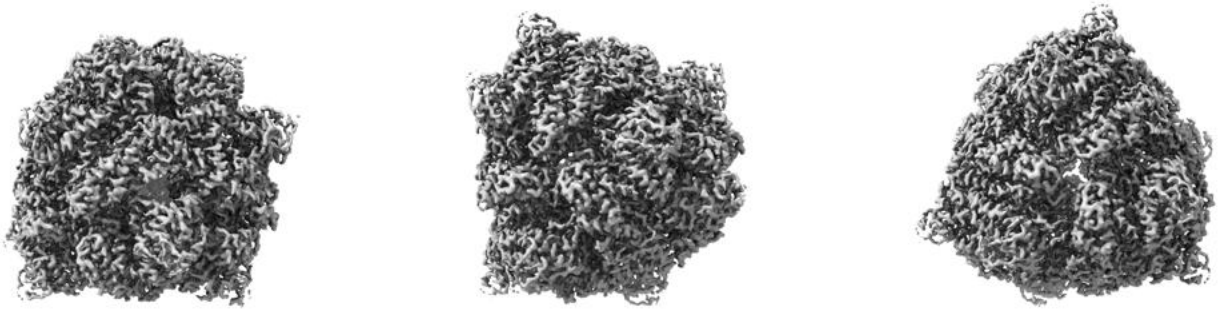
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

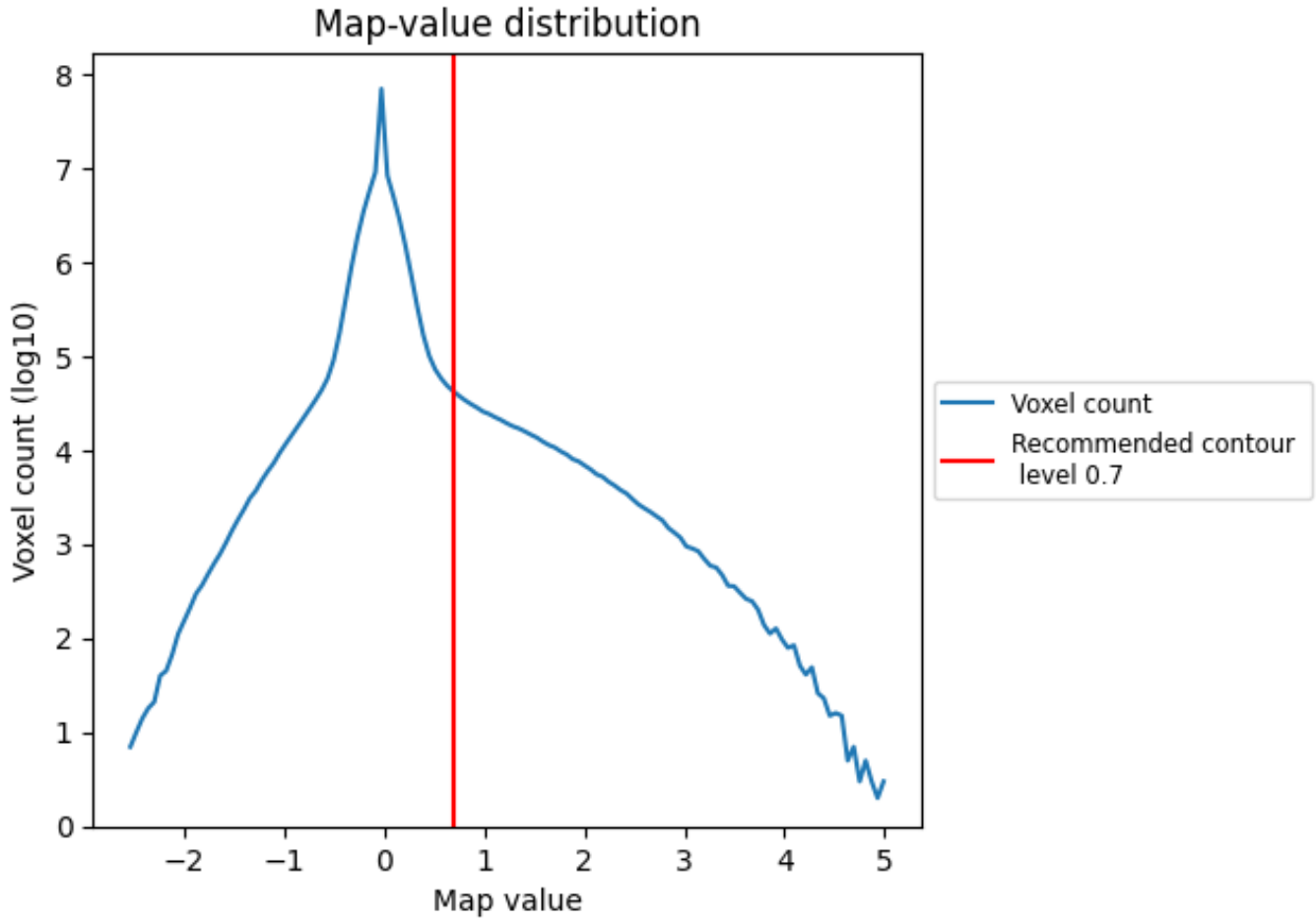
6.5 Mask visualisation (i)

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

7 Map analysis

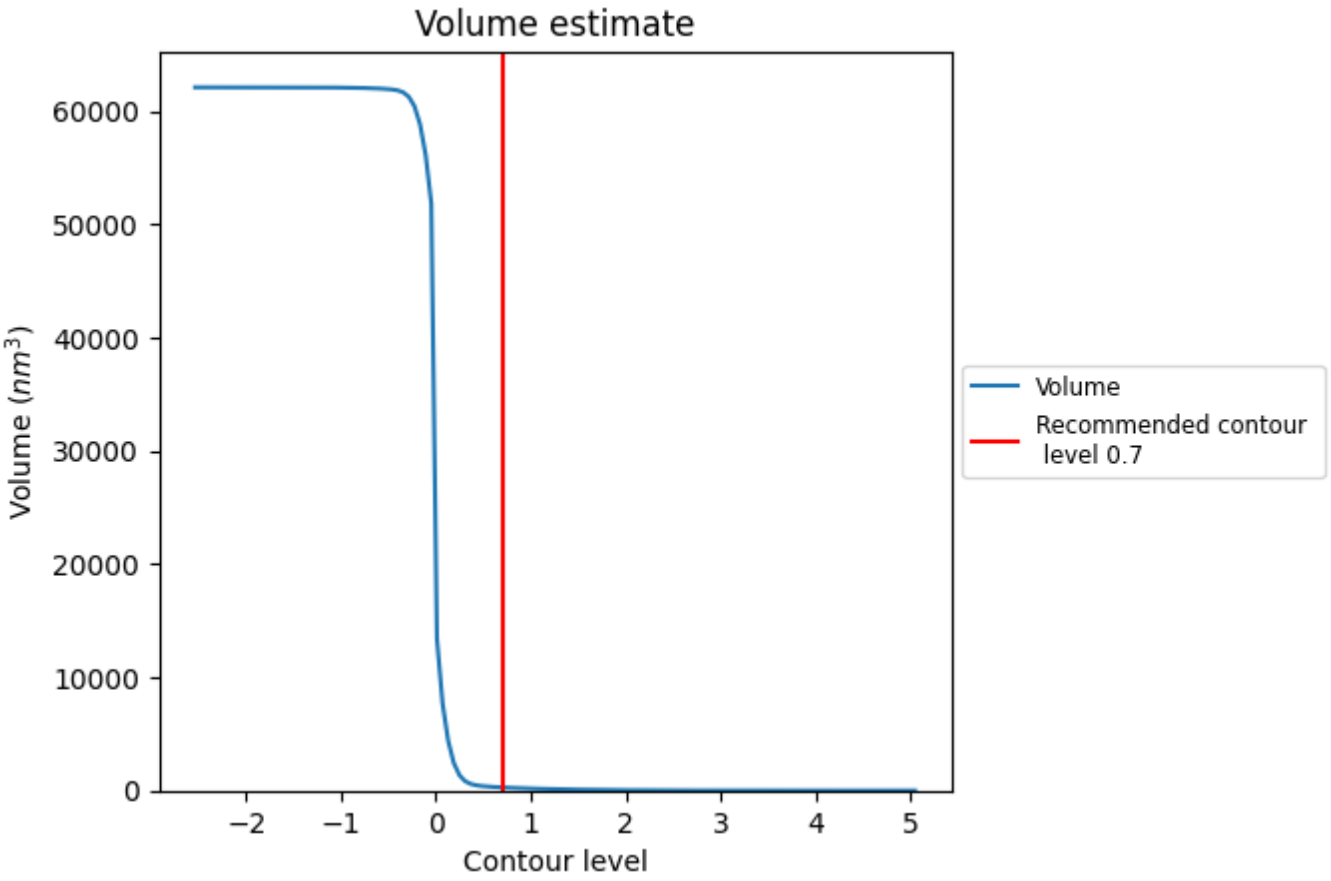
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

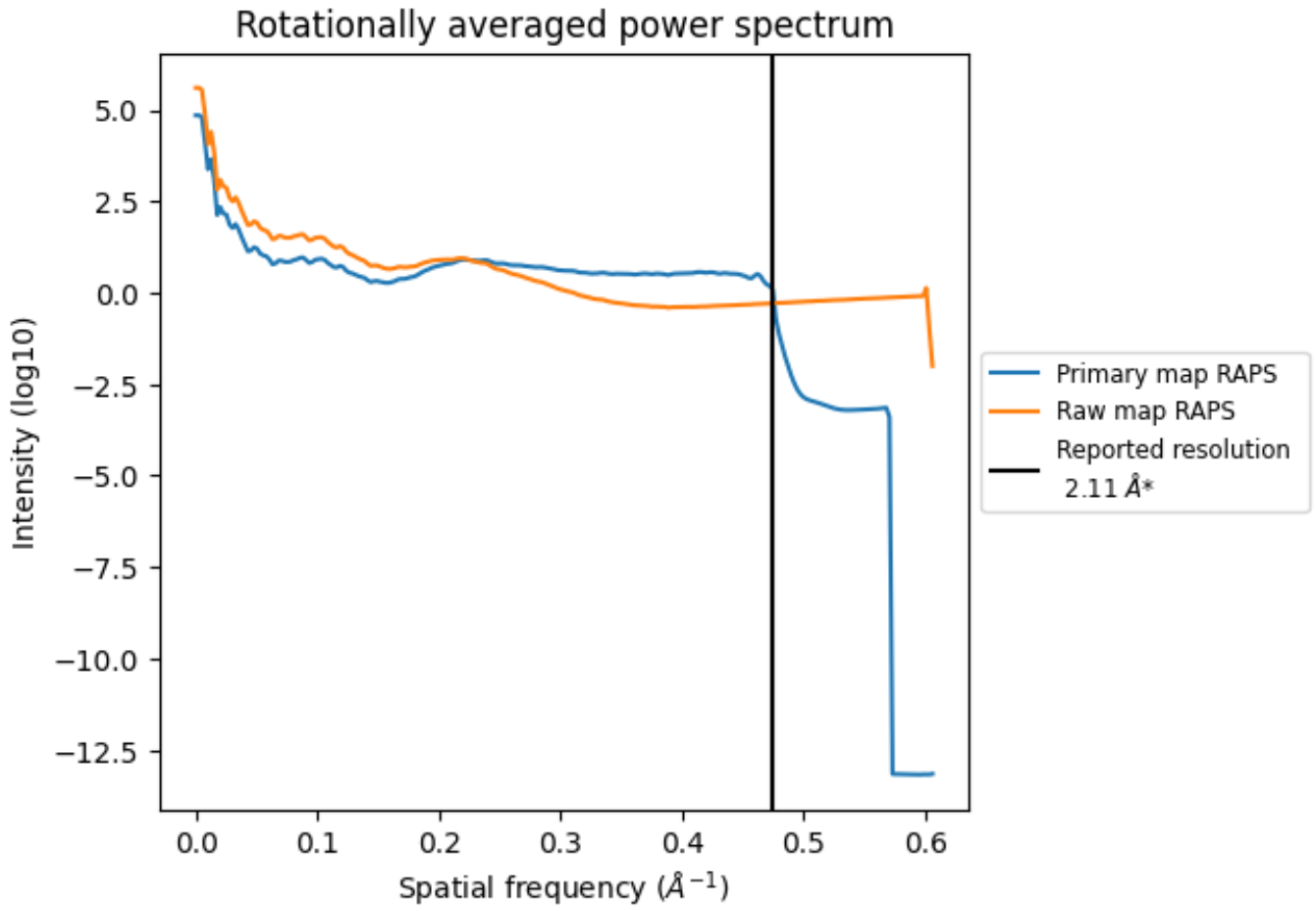
7.2 Volume estimate



The volume at the recommended contour level is 275 nm^3; this corresponds to an approximate mass of 249 kDa.

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

7.3 Rotationally averaged power spectrum (i)

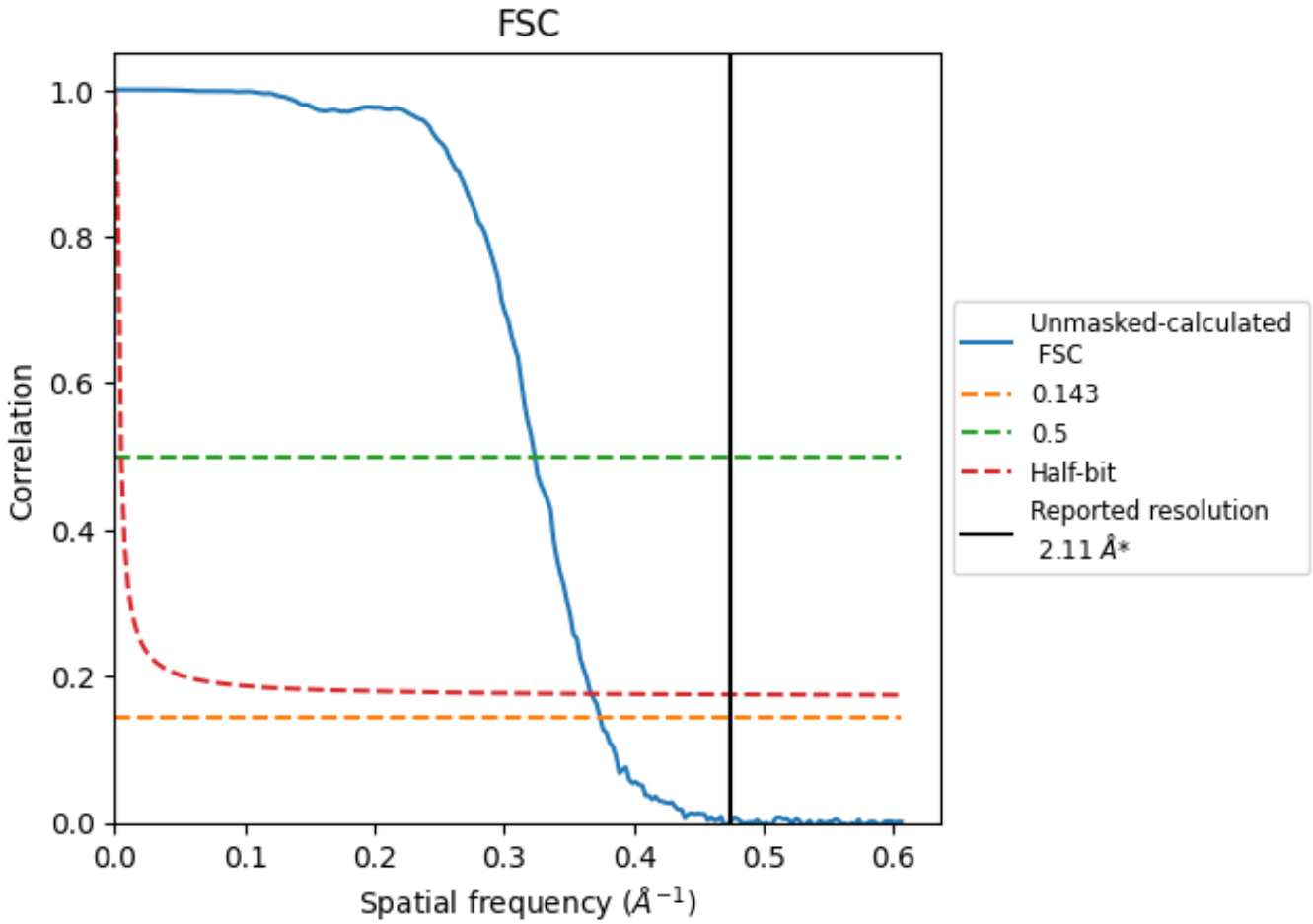


*Reported resolution corresponds to spatial frequency of 0.474 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.474 Å^{-1}

8.2 Resolution estimates (i)

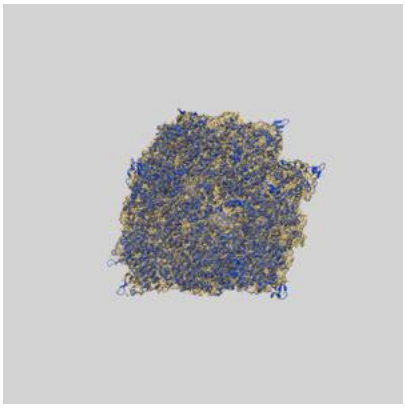
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.67	3.09	2.72

*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 2.67 differs from the reported value 2.11 by more than 10 %

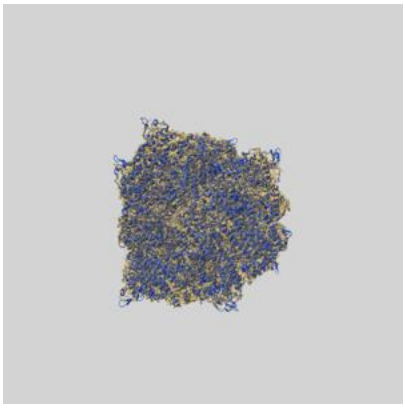
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29327 and PDB model 8FNV. Per-residue inclusion information can be found in section 3 on page 6.

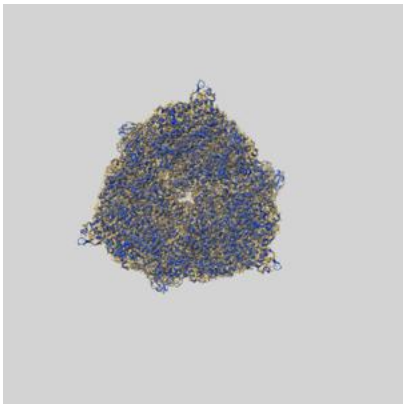
9.1 Map-model overlay



X



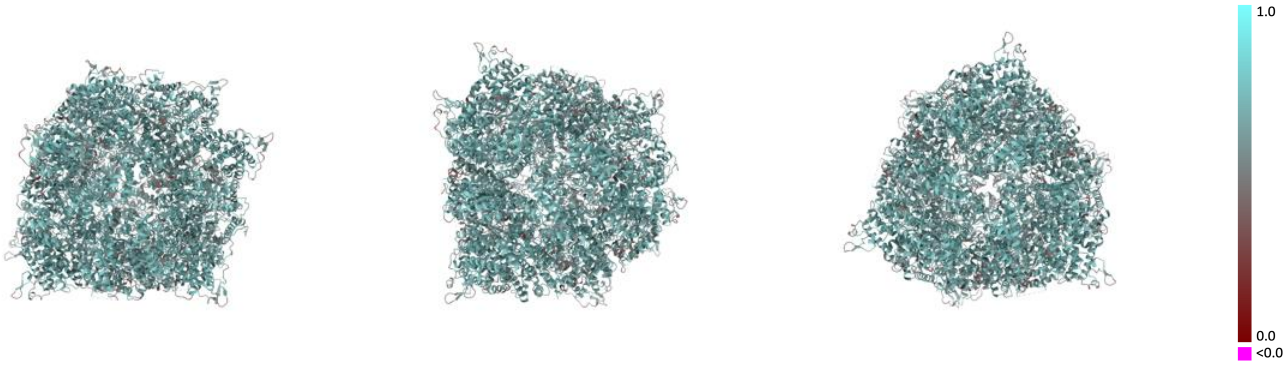
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

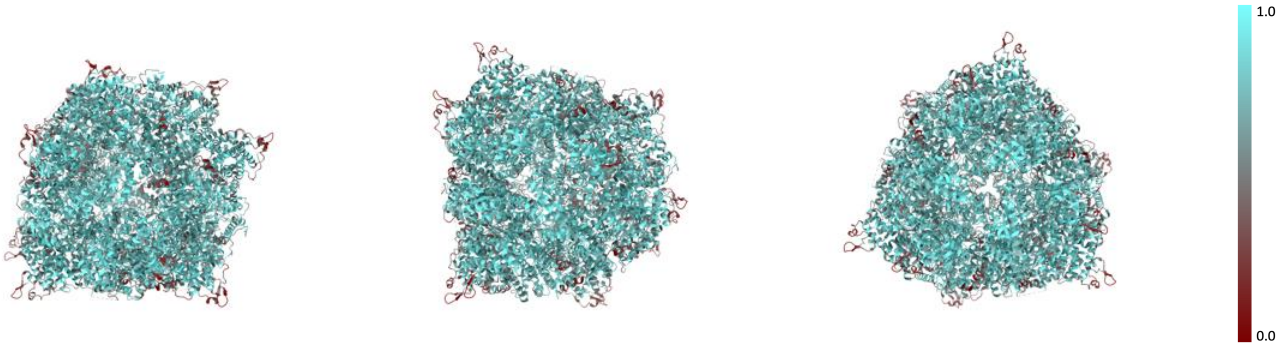
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

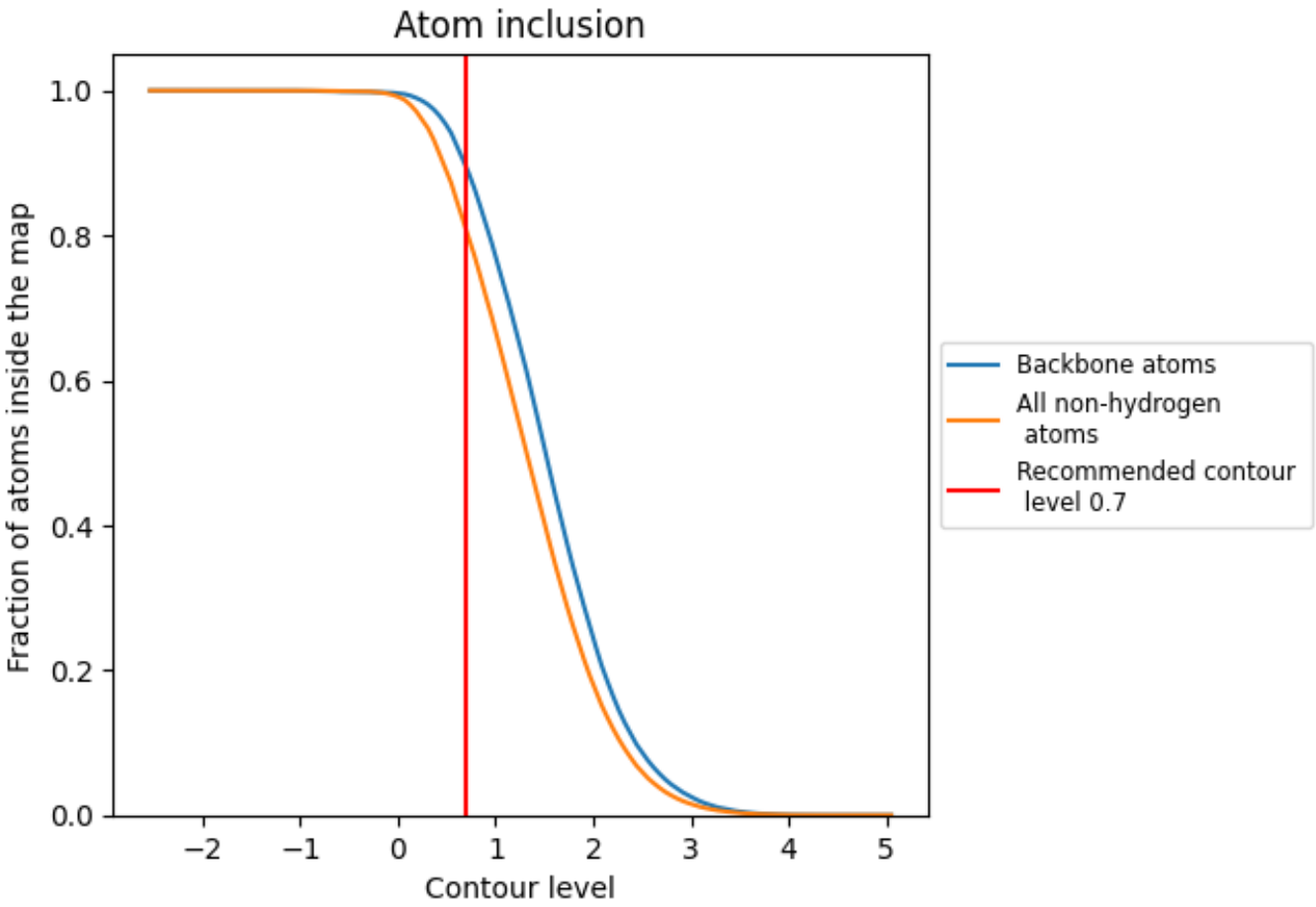
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.6640
A	0.8058	0.6630
B	0.8079	0.6630
C	0.8055	0.6640
D	0.8091	0.6650
E	0.8073	0.6640
F	0.8078	0.6640
G	0.8048	0.6630
H	0.8074	0.6630
I	0.8066	0.6630
J	0.8083	0.6630
K	0.8060	0.6630
L	0.8071	0.6640