



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:29 AM UTC

PDB ID : 7ELH / pdb_00007elh
EMDB ID : EMD-31183
Title : In situ structure of transcriptional enzyme complex and capsid shell protein of mammalian reovirus at initiation state
Authors : Zhou, Z.H.; Pan, M.
Deposited on : 2021-04-11
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

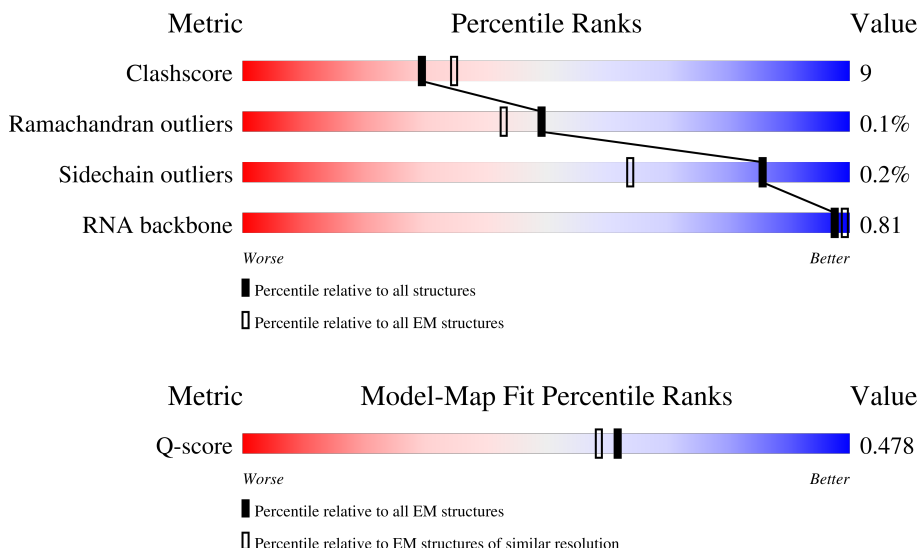
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



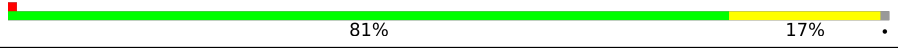
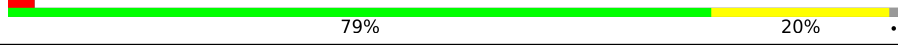
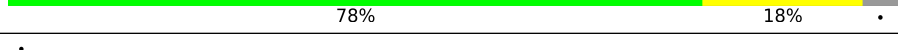
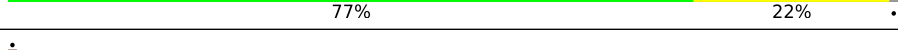
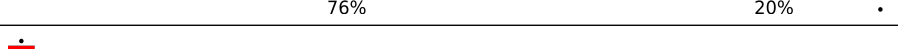
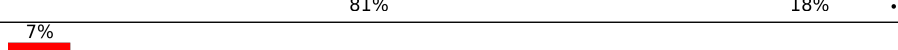
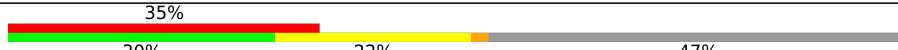
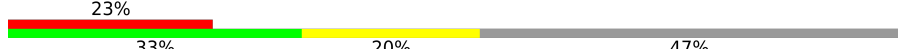
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	736	5% 64% 28% 7%
2	B	1267	74% 25%
3	C	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	D	1095	
4	E	1095	
4	F	1095	
4	G	1095	
4	H	1095	
4	I	1095	
4	J	1095	
4	K	1095	
4	L	1095	
4	M	1095	
5	e	180	
5	g	180	
5	i	180	
5	k	180	
5	m	180	
6	N	60	
6	O	60	
6	P	60	
6	Q	60	
6	R	60	
6	S	60	
6	T	60	
6	U	60	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	A	800	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 114995 atoms, of which 3098 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 Minor core protein mu2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	681	Total	C	N	O	S	0	0
			5418	3479	920	987	32		

- Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1264	Total	C	N	O	S	0	0
			9987	6374	1712	1836	65		

- Molecule 3 is a RNA chain called transcript RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	4	Total	C	N	O	P	0	0
			87	39	18	26	4		

- Molecule 4 is a protein called Lambda 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1054	Total	C	N	O	S	0	0
			8326	5322	1405	1550	49		
4	E	1088	Total	C	N	O	S	0	0
			8587	5486	1455	1595	51		
4	F	1082	Total	C	N	O	S	0	0
			8538	5450	1446	1592	50		
4	G	1088	Total	C	N	O	S	0	0
			8587	5486	1455	1595	51		
4	H	1055	Total	C	N	O	S	0	0
			8330	5320	1409	1552	49		
4	I	1088	Total	C	N	O	S	0	0
			8587	5486	1455	1595	51		
4	J	1050	Total	C	N	O	S	0	0
			8289	5296	1401	1543	49		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	1089	Total	C	N	O	S	0	0
			8595	5490	1456	1598	51		
4	L	1048	Total	C	N	O	S	0	0
			8279	5290	1399	1541	49		
4	M	1089	Total	C	N	O	S	0	0
			8595	5490	1456	1598	51		

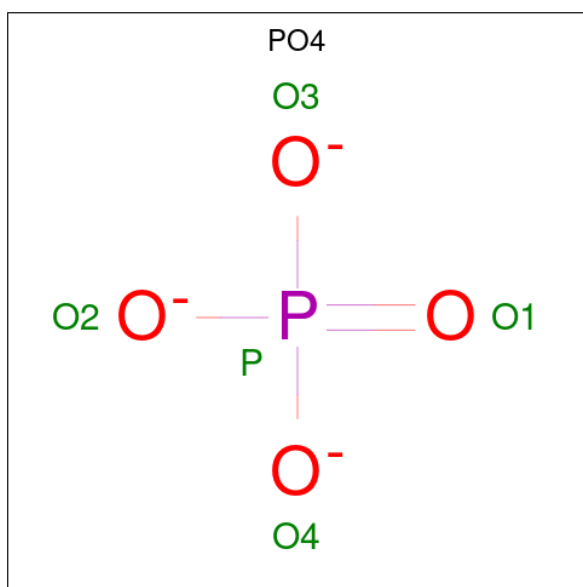
- Molecule 5 is a protein called Lambda 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	140	Total	C	N	O	S	0	0
			1050	622	198	226	4		
5	g	141	Total	C	N	O	S	0	0
			1055	625	199	227	4		
5	i	140	Total	C	N	O	S	0	0
			1050	622	198	226	4		
5	k	140	Total	C	N	O	S	0	0
			1050	622	198	226	4		
5	m	141	Total	C	N	O	S	0	0
			1056	625	199	228	4		

- Molecule 6 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	N	32	Total	C	H	N	O	P	0	0
			1008	304	336	112	224	32		
6	O	32	Total	C	H	N	O	P	0	0
			1008	304	336	112	224	32		
6	P	30	Total	C	H	N	O	P	0	0
			945	285	315	105	210	30		
6	Q	30	Total	C	H	N	O	P	0	0
			945	285	315	105	210	30		
6	R	60	Total	C	H	N	O	P	0	0
			1890	570	630	210	420	60		
6	S	60	Total	C	H	N	O	P	0	0
			1890	570	630	210	420	60		
6	T	31	Total	C	H	N	O	P	0	0
			920	295	268	110	216	31		
6	U	31	Total	C	H	N	O	P	0	0
			918	294	268	107	218	31		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).

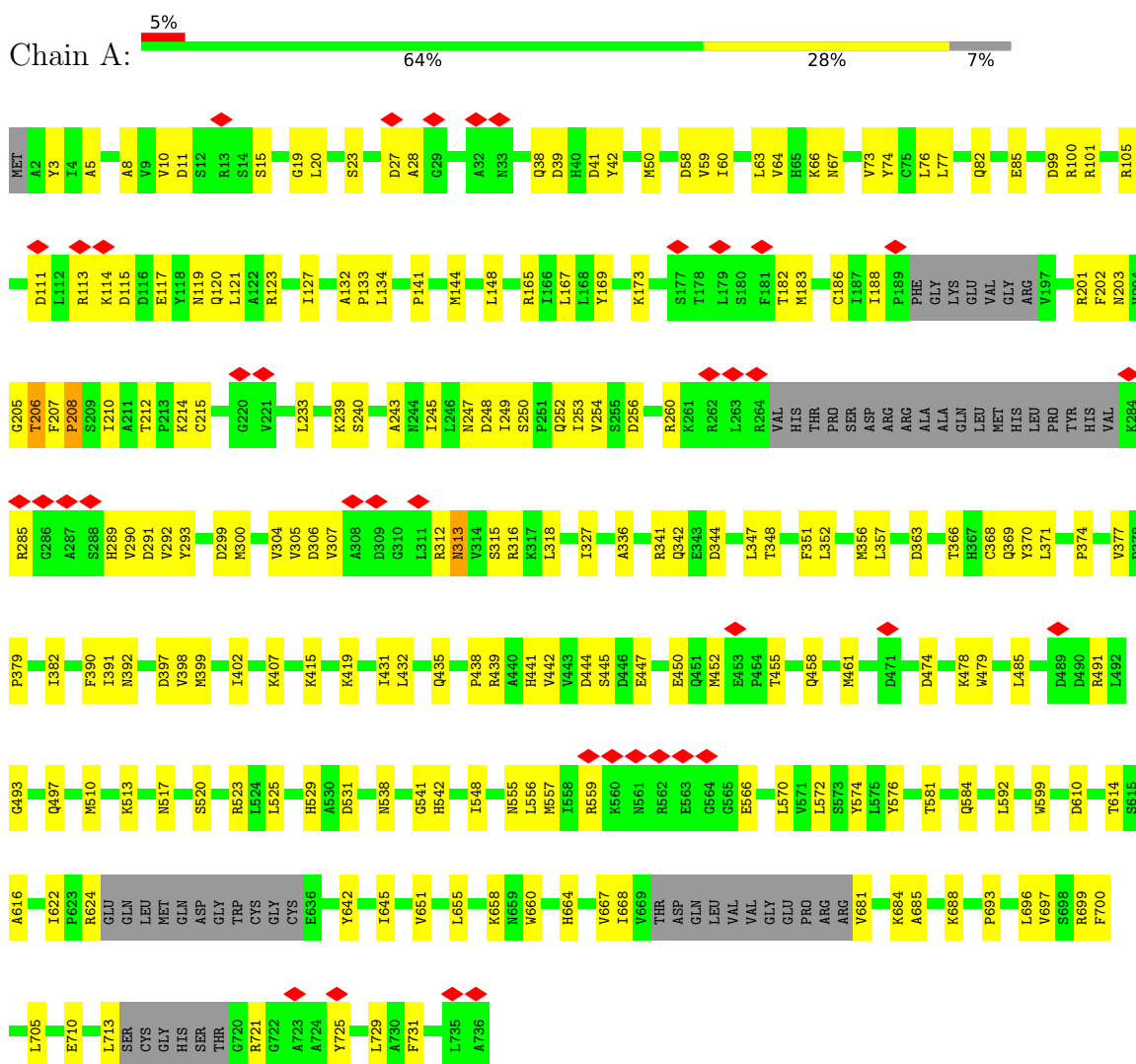


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
7	A	1	5	4	1	0

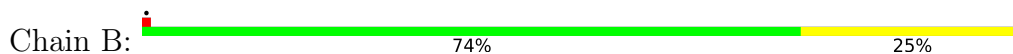
3 Residue-property plots

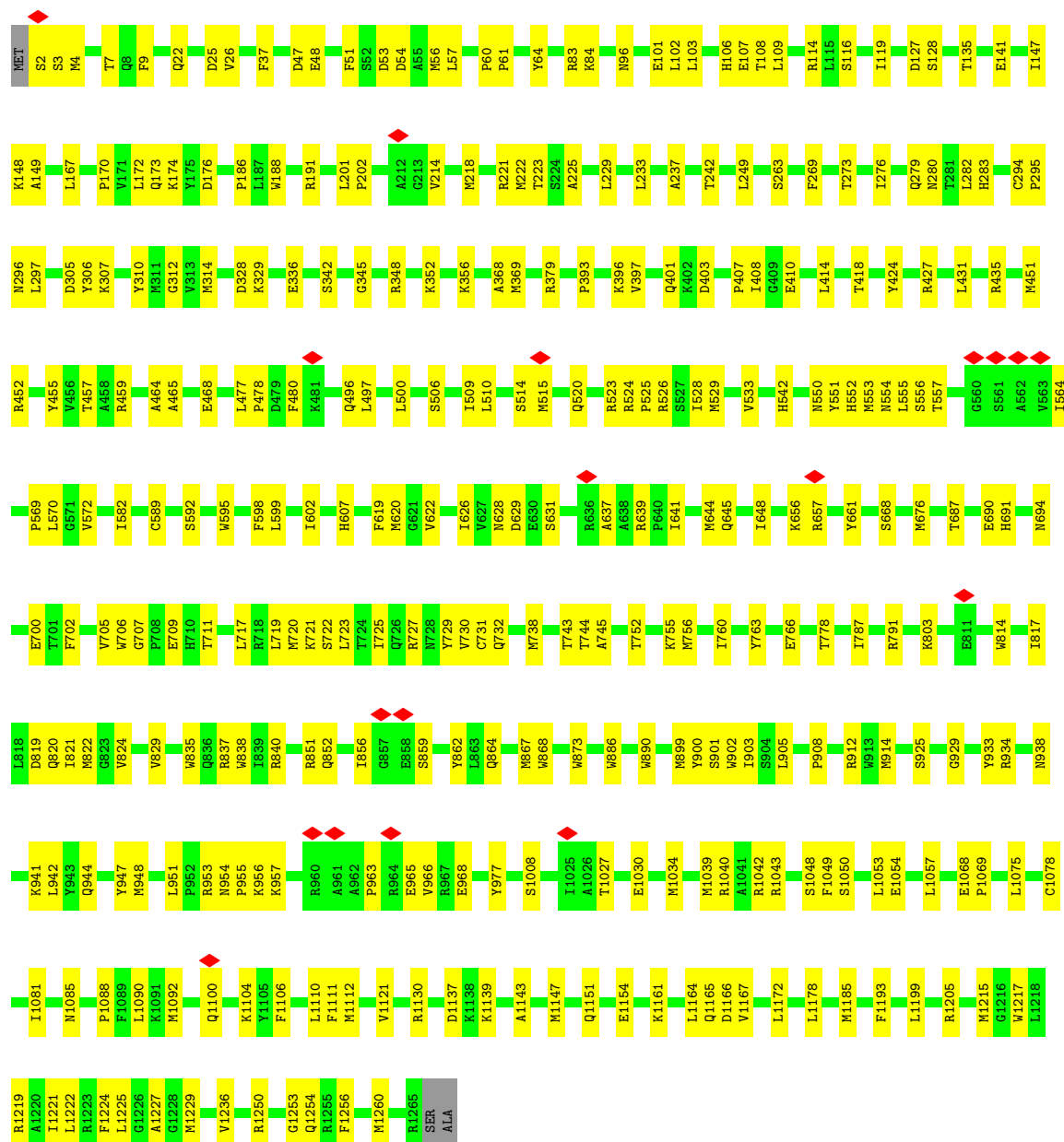
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Minor core protein mu2



- Molecule 2: RNA-directed RNA polymerase





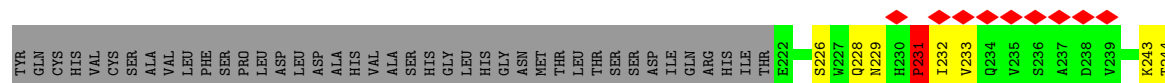
• Molecule 3: transcript RNA

Chain C: 75% 25%



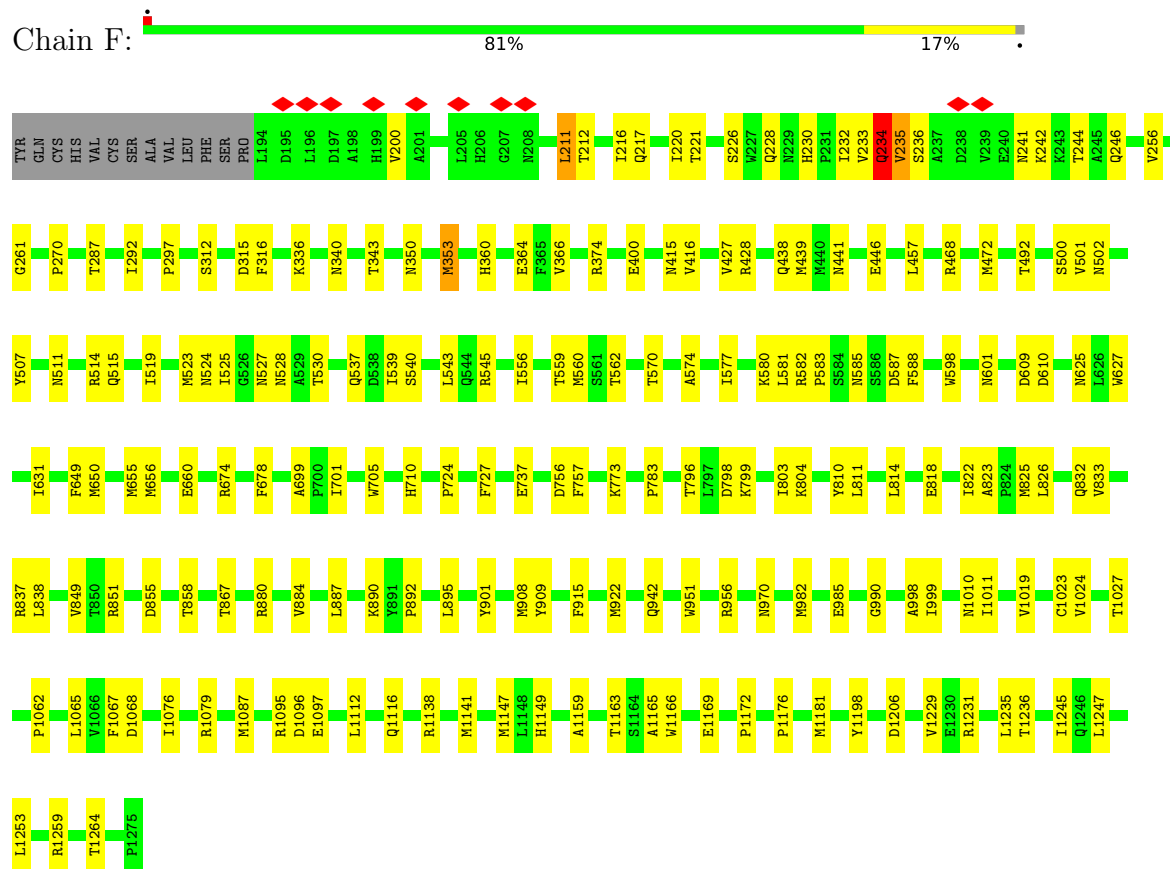
• Molecule 4: Lambda 1

Chain D: 78% 18%



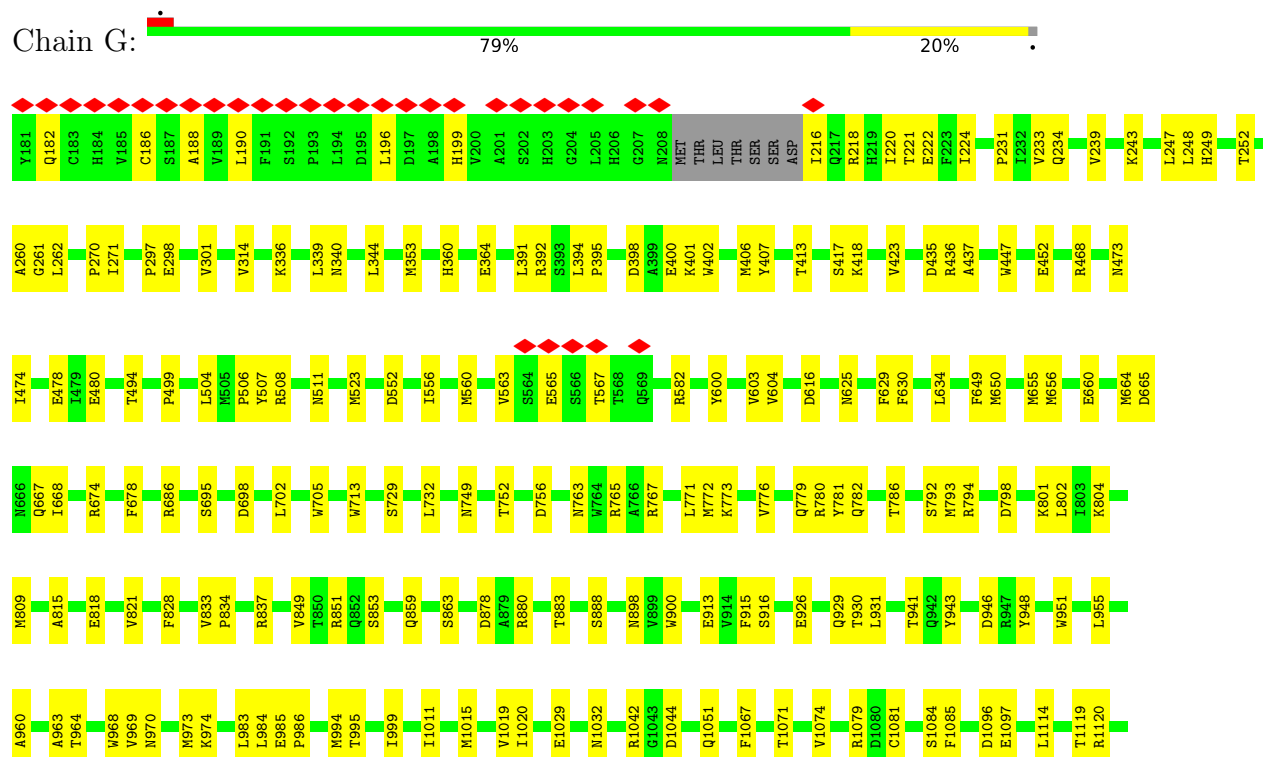
- Molecule 4: Lambda 1

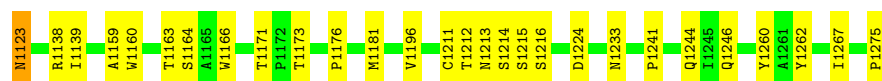
Chain F:



- Molecule 4: Lambda 1

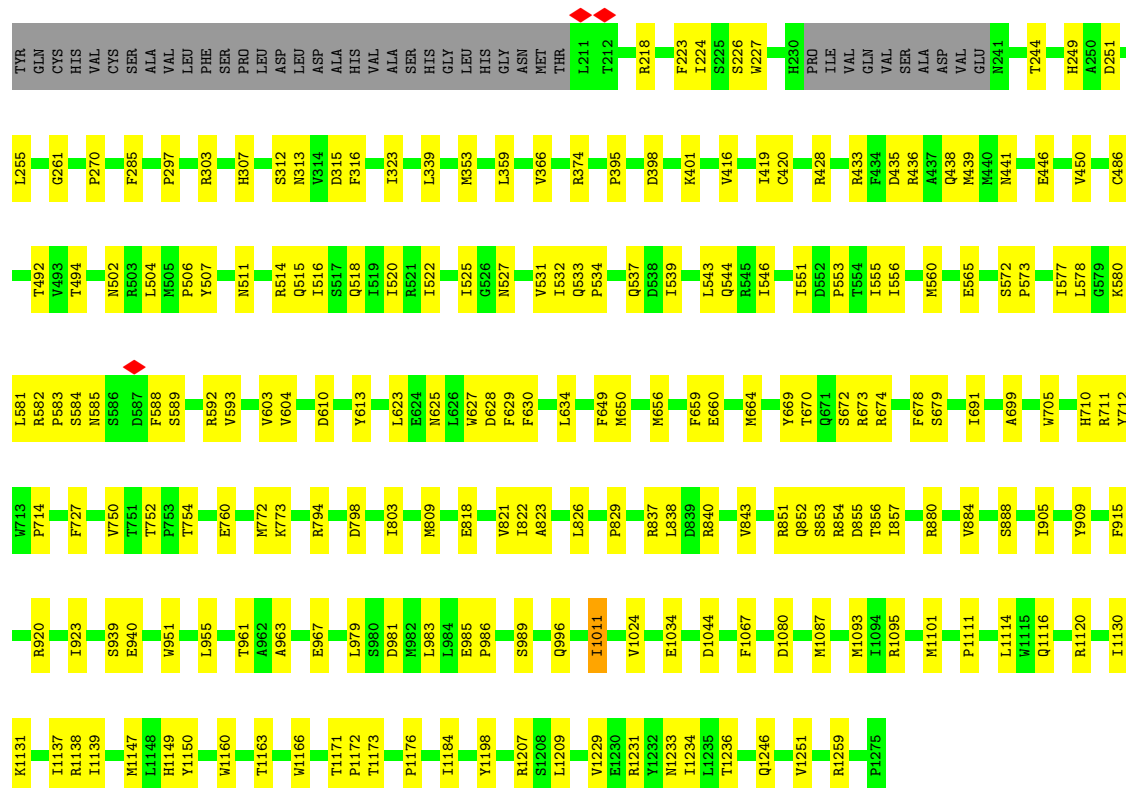
Chain G:





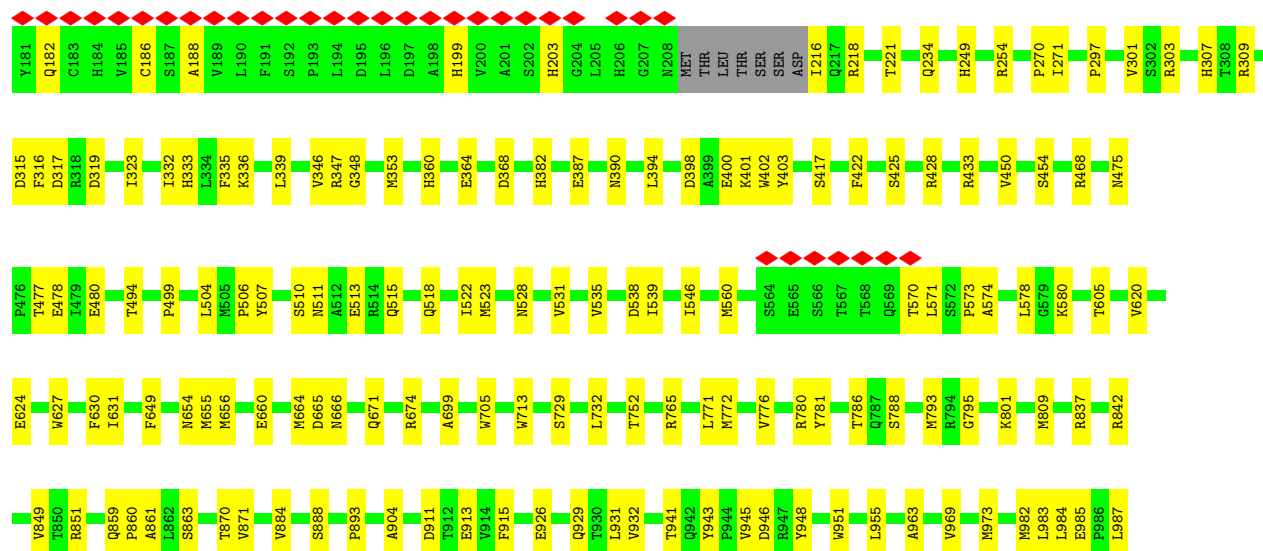
• Molecule 4: Lambda 1

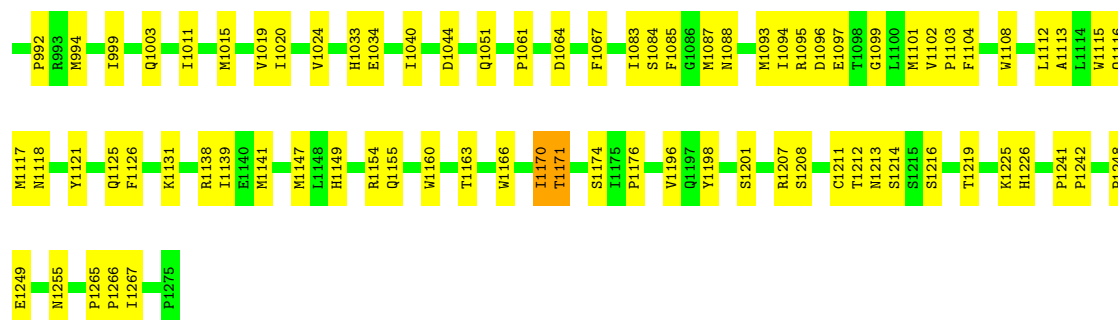
Chain H: 77% 19%



• Molecule 4: Lambda 1

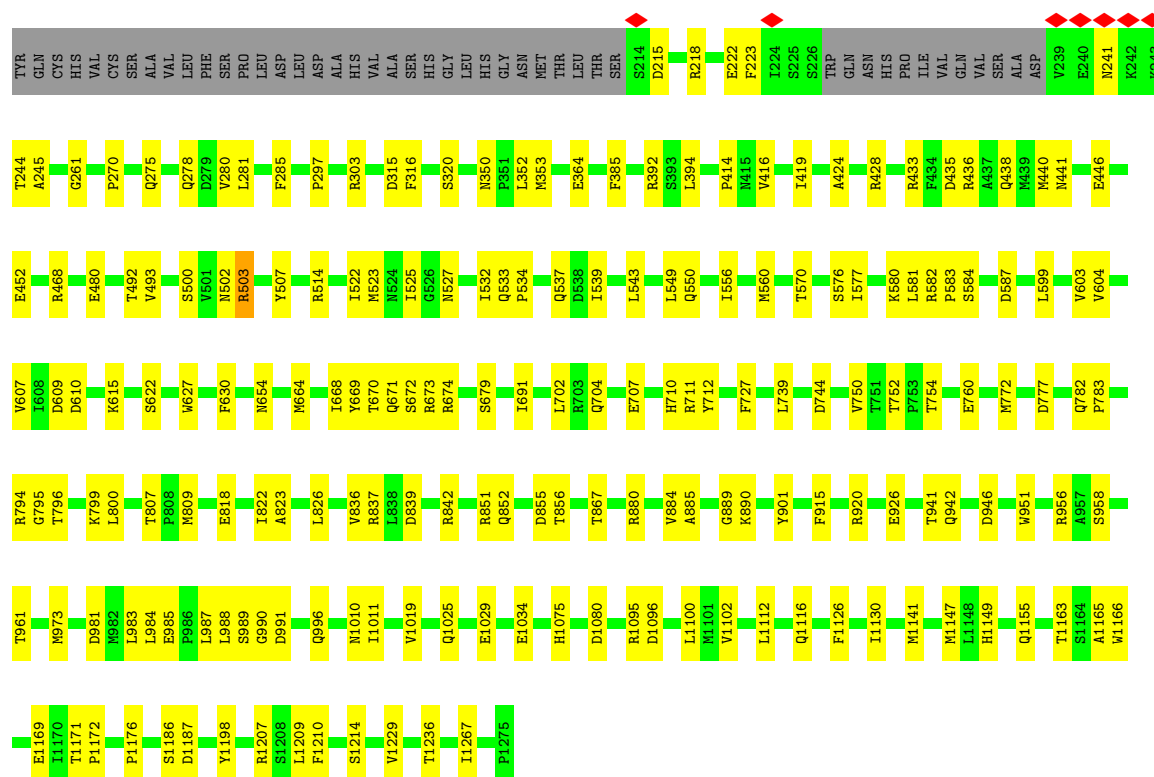
Chain I: 78% 21%





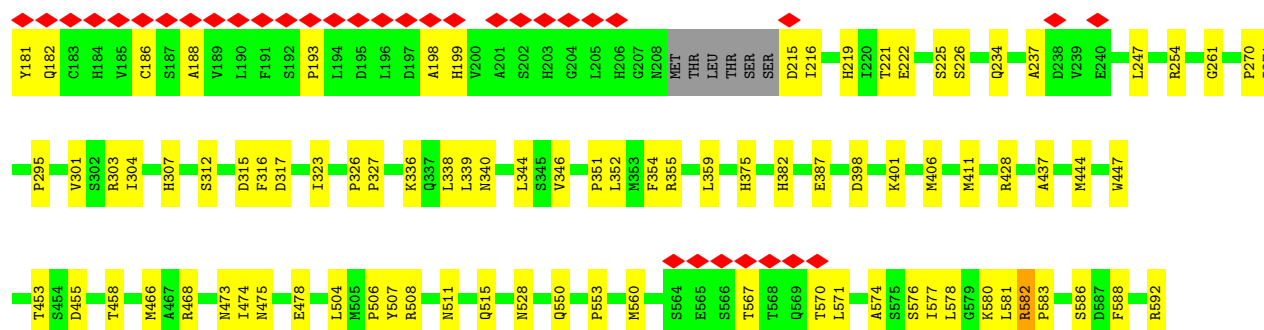
• Molecule 4: Lambda 1

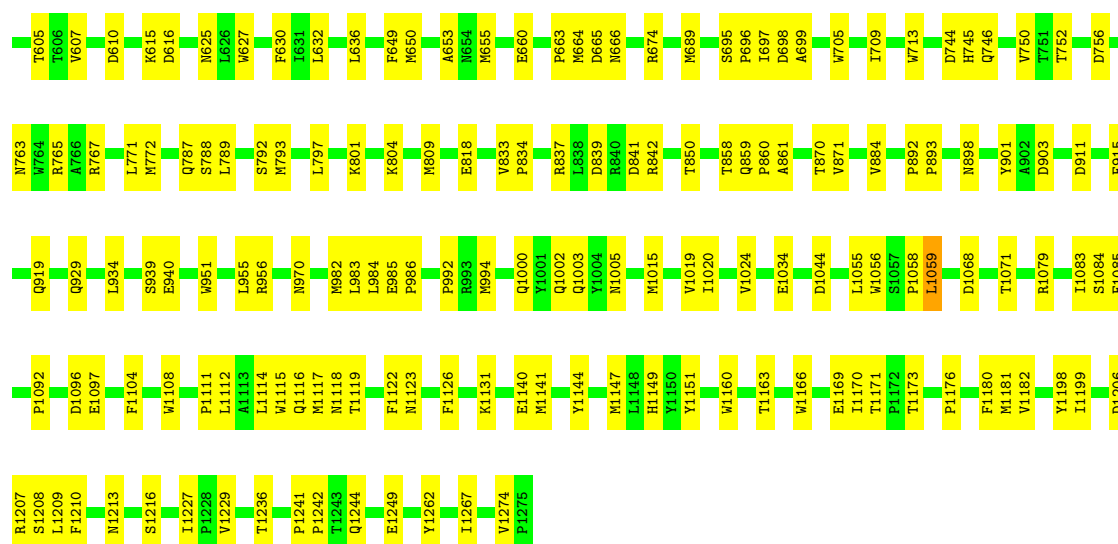
Chain J: 78% 18% .



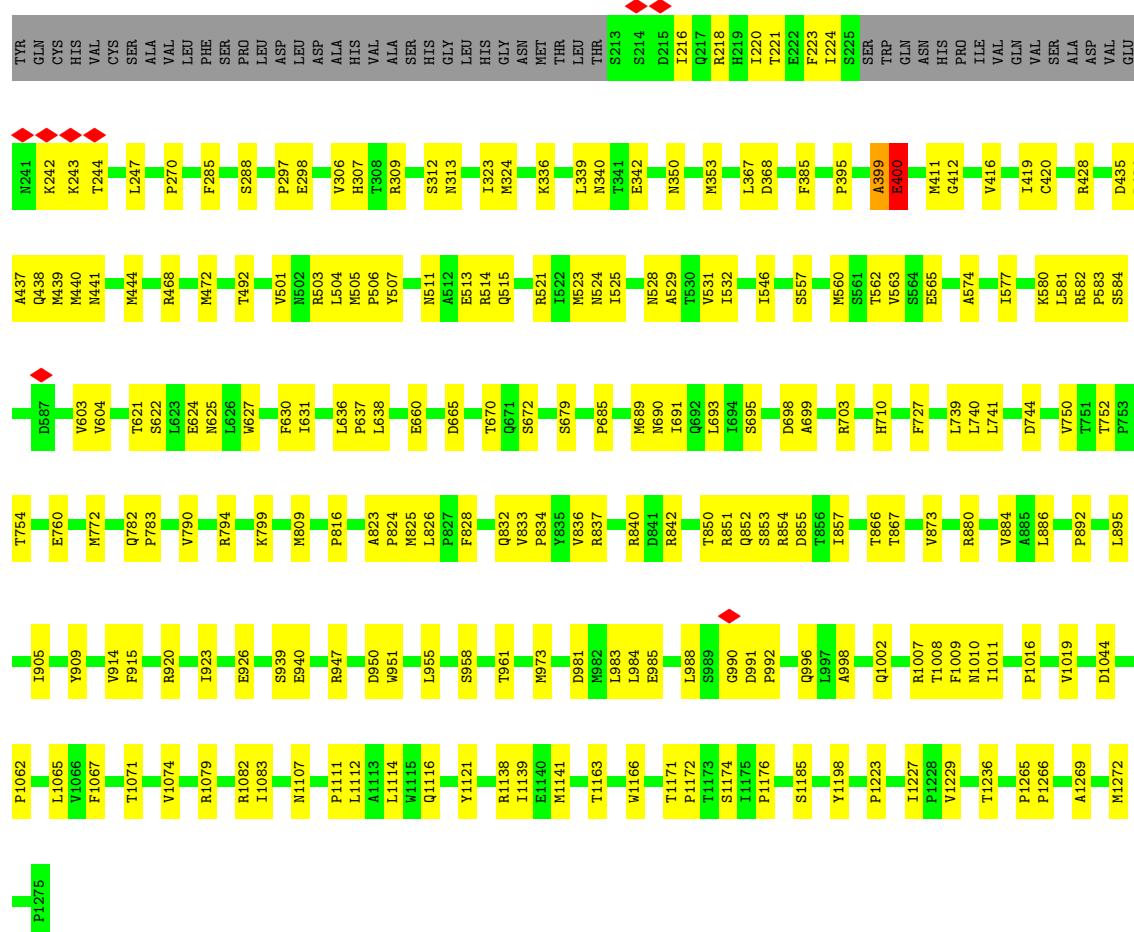
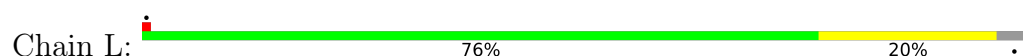
• Molecule 4: Lambda 1

Chain K: 77% 22% .



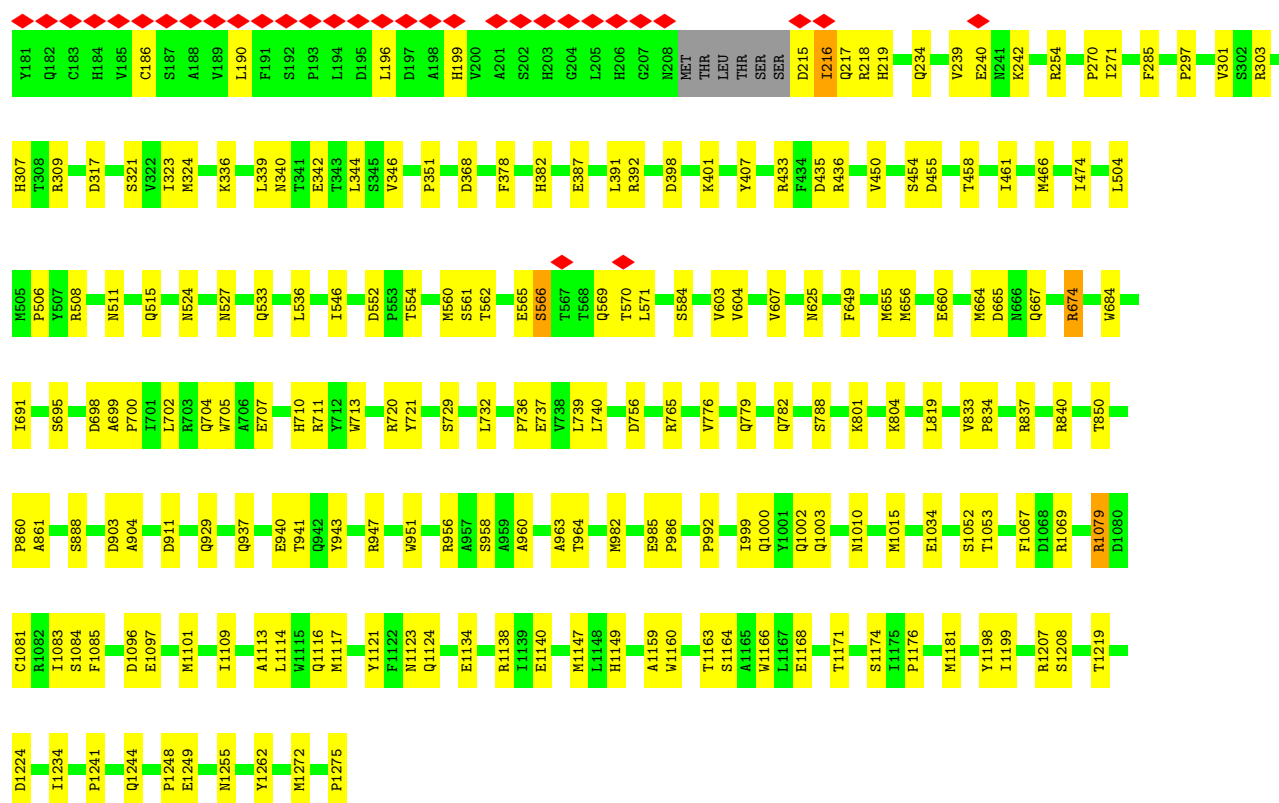


• Molecule 4: Lambda 1



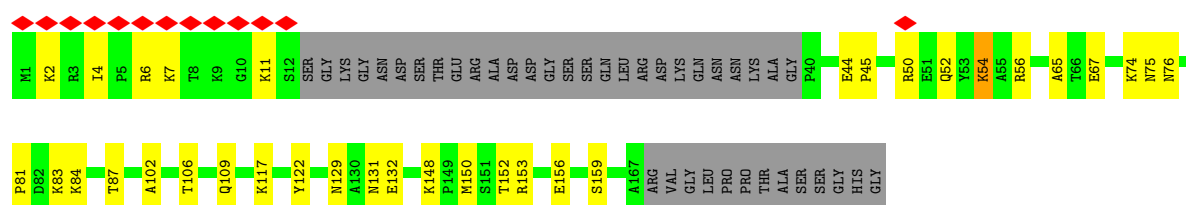
• Molecule 4: Lambda 1

Chain M: 



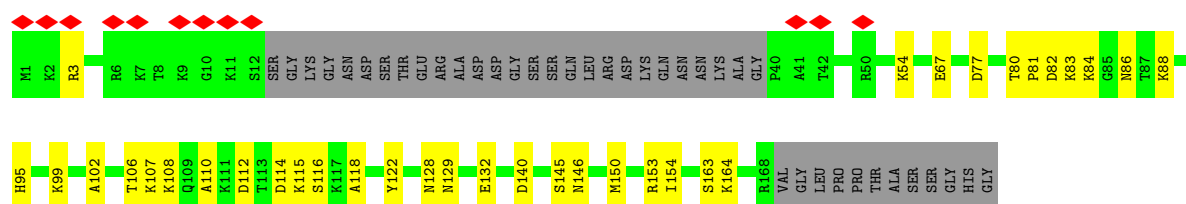
• Molecule 5: Lambda 1

Chain e: 



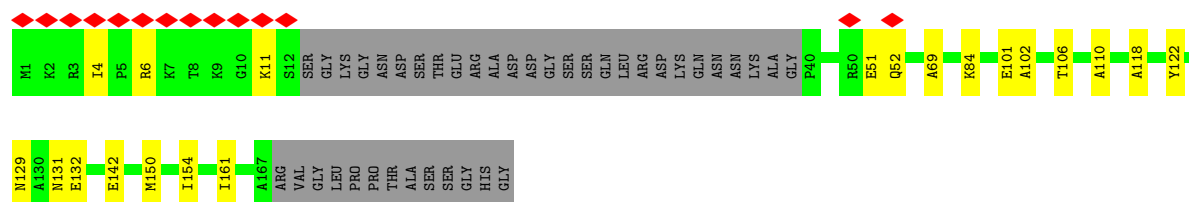
• Molecule 5: Lambda 1

Chain g: 

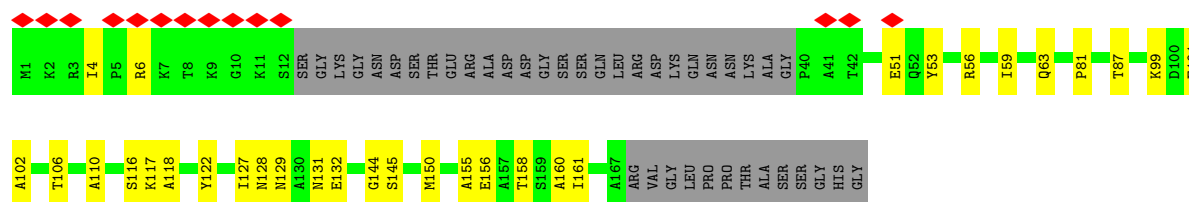


• Molecule 5: Lambda 1

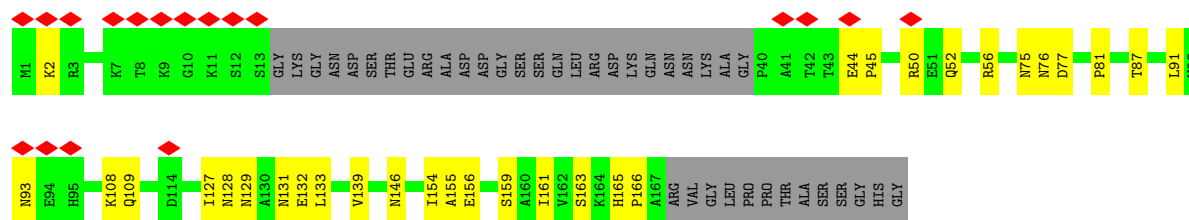
Chain i: 



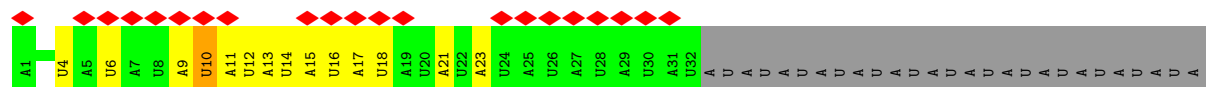
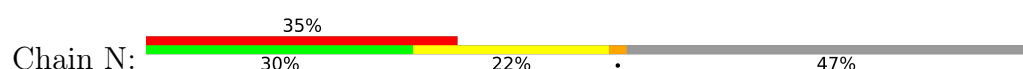
• Molecule 5: Lambda 1



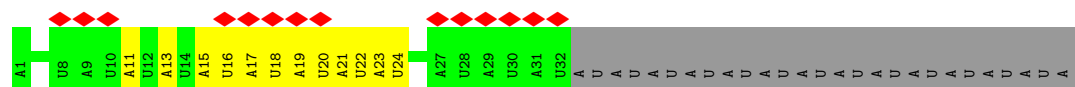
• Molecule 5: Lambda 1



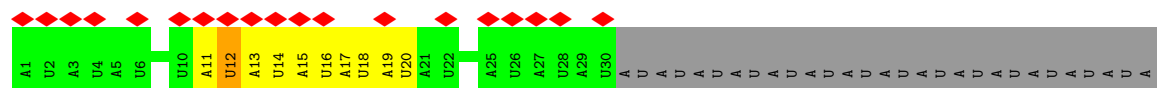
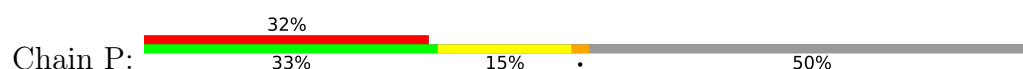
• Molecule 6: RNA (60-MER)

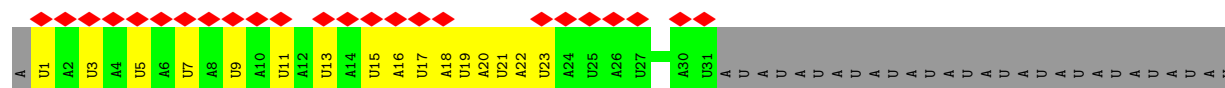


• Molecule 6: RNA (60-MER)



• Molecule 6: RNA (60-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102966	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.23	0/5534	0.45	0/7502
2	B	0.23	0/10241	0.40	0/13907
3	C	0.71	1/97 (1.0%)	0.58	0/149
4	D	0.29	0/8552	0.41	1/11716 (0.0%)
4	E	0.28	0/8820	0.38	0/12082
4	F	0.28	0/8768	0.39	0/12010
4	G	0.28	0/8820	0.37	0/12082
4	H	0.29	0/8553	0.38	0/11714
4	I	0.27	0/8820	0.37	2/12082 (0.0%)
4	J	0.28	0/8511	0.37	0/11655
4	K	0.29	1/8828 (0.0%)	0.40	2/12093 (0.0%)
4	L	0.33	2/8501 (0.0%)	0.47	4/11641 (0.0%)
4	M	0.26	1/8828 (0.0%)	0.45	1/12093 (0.0%)
5	e	0.24	0/1060	0.38	0/1420
5	g	0.24	0/1065	0.42	0/1427
5	i	0.23	0/1060	0.35	0/1420
5	k	0.24	0/1060	0.38	0/1420
5	m	0.20	0/1066	0.44	0/1428
6	N	0.68	5/751 (0.7%)	1.08	9/1164 (0.8%)
6	O	0.67	5/751 (0.7%)	1.08	9/1164 (0.8%)
6	P	0.70	5/704 (0.7%)	1.11	9/1091 (0.8%)
6	Q	0.70	5/704 (0.7%)	1.11	9/1091 (0.8%)
6	R	0.50	5/1409 (0.4%)	0.81	9/2186 (0.4%)
6	S	0.50	5/1409 (0.4%)	0.80	9/2186 (0.4%)
6	T	1.00	11/729 (1.5%)	1.04	8/1130 (0.7%)
6	U	1.04	12/726 (1.7%)	1.04	8/1125 (0.7%)
All	All	0.32	58/115367 (0.1%)	0.47	80/158978 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	1
4	F	0	2
4	L	0	1
4	M	0	1
All	All	0	6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	400	GLU	CA-C	-17.22	1.29	1.52
4	K	270	PRO	N-CD	10.11	1.61	1.47
4	L	400	GLU	N-CA	9.10	1.58	1.46
4	M	674	ARG	CA-C	-7.64	1.42	1.52
6	Q	20	U	C1'-N1	7.24	1.59	1.48
6	S	22	U	C1'-N1	7.19	1.59	1.48
6	N	10	U	C1'-N1	7.18	1.59	1.48
6	U	17	U	C1'-N1	7.18	1.59	1.48
6	T	10	U	C1'-N1	7.18	1.59	1.48
6	P	14	U	C1'-N1	7.17	1.59	1.48
6	Q	14	U	C1'-N1	7.17	1.59	1.48
6	R	36	U	C1'-N1	7.17	1.59	1.48
6	S	30	U	C1'-N1	7.16	1.59	1.48
6	N	16	U	C1'-N1	7.15	1.59	1.48
6	R	34	U	C1'-N1	7.15	1.59	1.48
6	U	19	U	C1'-N1	7.14	1.59	1.48
6	N	14	U	C1'-N1	7.14	1.59	1.48
6	Q	12	U	C1'-N1	7.13	1.59	1.48
6	N	12	U	C1'-N1	7.13	1.59	1.48
6	T	16	U	C1'-N1	7.12	1.59	1.48
6	P	16	U	C1'-N1	7.12	1.59	1.48
6	U	15	U	C1'-N1	7.10	1.59	1.48
6	O	24	U	C1'-N1	7.09	1.59	1.48
6	R	32	U	C1'-N1	7.09	1.59	1.48
6	U	23	U	C1'-N1	7.08	1.59	1.48
6	Q	18	U	C1'-N1	7.07	1.59	1.48
6	S	28	U	C1'-N1	7.06	1.59	1.48
6	U	21	U	C1'-N1	7.06	1.59	1.48
6	O	16	U	C1'-N1	7.06	1.59	1.48
6	O	20	U	C1'-N1	7.05	1.59	1.48
6	T	14	U	C1'-N1	7.04	1.59	1.48
6	O	18	U	C1'-N1	7.04	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	12	U	C1'-N1	7.03	1.58	1.48
6	S	26	U	C1'-N1	7.03	1.59	1.48
6	Q	16	U	C1'-N1	7.03	1.58	1.48
6	R	38	U	C1'-N1	7.03	1.58	1.48
6	R	40	U	C1'-N1	7.03	1.58	1.48
6	P	18	U	C1'-N1	7.03	1.58	1.48
6	S	24	U	C1'-N1	7.00	1.58	1.48
6	N	18	U	C1'-N1	7.00	1.58	1.48
6	O	22	U	C1'-N1	6.98	1.58	1.48
6	T	12	U	C1'-N1	6.97	1.58	1.48
6	P	20	U	C1'-N1	6.92	1.58	1.48
6	T	26	U	C1'-N1	6.31	1.57	1.48
6	U	1	U	C1'-N1	6.29	1.57	1.48
6	T	30	U	C1'-N1	6.27	1.57	1.48
6	T	28	U	C1'-N1	6.25	1.57	1.48
6	U	11	U	C1'-N1	6.22	1.57	1.48
6	T	24	U	C1'-N1	6.21	1.57	1.48
6	U	5	U	C1'-N1	6.21	1.57	1.48
6	U	13	U	C1'-N1	6.20	1.57	1.48
6	T	20	U	C1'-N1	6.19	1.57	1.48
3	C	1283	A	C1'-N9	-6.17	1.38	1.48
6	T	22	U	C1'-N1	6.17	1.57	1.48
6	U	3	U	C1'-N1	6.17	1.57	1.48
6	U	7	U	C1'-N1	6.16	1.57	1.48
6	T	18	U	C1'-N1	6.14	1.57	1.48
6	U	9	U	C1'-N1	6.12	1.57	1.48

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	399	ALA	O-C-N	-9.72	108.01	122.39
4	L	400	GLU	CA-C-N	-9.23	106.28	120.31
4	L	400	GLU	C-N-CA	-9.23	106.28	120.31
4	M	566	SER	N-CA-C	9.07	122.85	111.69
6	U	17	U	O3'-P-O5'	-8.69	90.96	104.00
6	P	12	U	O3'-P-O5'	-8.67	90.99	104.00
6	N	13	A	O3'-P-O5'	-8.66	91.00	104.00
6	N	17	A	O3'-P-O5'	-8.66	91.01	104.00
6	T	9	A	O3'-P-O5'	-8.65	91.02	104.00
6	O	18	U	O3'-P-O5'	-8.65	91.02	104.00
6	T	16	U	O3'-P-O5'	-8.65	91.03	104.00
6	N	16	U	O3'-P-O5'	-8.64	91.04	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	20	A	O3'-P-O5'	-8.64	91.04	104.00
6	R	31	A	O3'-P-O5'	-8.63	91.05	104.00
6	O	17	A	O3'-P-O5'	-8.63	91.05	104.00
6	P	14	U	O3'-P-O5'	-8.63	91.06	104.00
6	P	19	A	O3'-P-O5'	-8.63	91.06	104.00
6	N	9	A	O3'-P-O5'	-8.62	91.06	104.00
6	O	20	U	O3'-P-O5'	-8.62	91.07	104.00
4	K	582	ARG	CA-C-N	8.62	128.62	119.05
4	K	582	ARG	C-N-CA	8.62	128.62	119.05
6	N	14	U	O3'-P-O5'	-8.62	91.07	104.00
6	R	39	A	O3'-P-O5'	-8.62	91.07	104.00
6	T	14	U	O3'-P-O5'	-8.62	91.07	104.00
6	T	15	A	O3'-P-O5'	-8.62	91.07	104.00
6	O	23	A	O3'-P-O5'	-8.62	91.08	104.00
6	O	15	A	O3'-P-O5'	-8.61	91.08	104.00
6	R	38	U	O3'-P-O5'	-8.61	91.08	104.00
6	Q	17	A	O3'-P-O5'	-8.61	91.08	104.00
6	Q	15	A	O3'-P-O5'	-8.61	91.09	104.00
6	S	25	A	O3'-P-O5'	-8.61	91.09	104.00
6	P	16	U	O3'-P-O5'	-8.60	91.10	104.00
6	R	33	A	O3'-P-O5'	-8.60	91.10	104.00
6	Q	13	A	O3'-P-O5'	-8.60	91.10	104.00
6	R	34	U	O3'-P-O5'	-8.60	91.10	104.00
6	S	24	U	O3'-P-O5'	-8.60	91.10	104.00
6	O	19	A	O3'-P-O5'	-8.60	91.11	104.00
6	S	26	U	O3'-P-O5'	-8.59	91.12	104.00
6	P	17	A	O3'-P-O5'	-8.58	91.12	104.00
6	R	32	U	O3'-P-O5'	-8.58	91.13	104.00
6	R	37	A	O3'-P-O5'	-8.58	91.13	104.00
6	R	36	U	O3'-P-O5'	-8.58	91.13	104.00
6	T	10	U	O3'-P-O5'	-8.58	91.13	104.00
6	S	27	A	O3'-P-O5'	-8.58	91.13	104.00
6	N	12	U	O3'-P-O5'	-8.58	91.14	104.00
6	R	35	A	O3'-P-O5'	-8.57	91.14	104.00
6	P	13	A	O3'-P-O5'	-8.57	91.15	104.00
6	S	22	U	O3'-P-O5'	-8.56	91.16	104.00
6	P	18	U	O3'-P-O5'	-8.56	91.16	104.00
6	P	11	A	O3'-P-O5'	-8.56	91.16	104.00
6	Q	14	U	O3'-P-O5'	-8.56	91.16	104.00
6	Q	19	A	O3'-P-O5'	-8.55	91.17	104.00
6	S	28	U	O3'-P-O5'	-8.55	91.17	104.00
6	U	15	U	O3'-P-O5'	-8.55	91.17	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	19	U	O3'-P-O5'	-8.55	91.17	104.00
6	P	15	A	O3'-P-O5'	-8.55	91.18	104.00
6	S	23	A	O3'-P-O5'	-8.55	91.18	104.00
6	U	18	A	O3'-P-O5'	-8.55	91.18	104.00
6	Q	16	U	O3'-P-O5'	-8.54	91.18	104.00
6	T	11	A	O3'-P-O5'	-8.54	91.19	104.00
6	Q	11	A	O3'-P-O5'	-8.54	91.19	104.00
6	U	21	U	O3'-P-O5'	-8.54	91.19	104.00
6	S	21	A	O3'-P-O5'	-8.54	91.20	104.00
6	T	13	A	O3'-P-O5'	-8.53	91.20	104.00
6	N	11	A	O3'-P-O5'	-8.53	91.20	104.00
6	N	10	U	O3'-P-O5'	-8.53	91.21	104.00
6	Q	12	U	O3'-P-O5'	-8.53	91.21	104.00
6	O	21	A	O3'-P-O5'	-8.52	91.22	104.00
6	U	16	A	O3'-P-O5'	-8.52	91.22	104.00
6	O	22	U	O3'-P-O5'	-8.51	91.23	104.00
6	T	12	U	O3'-P-O5'	-8.50	91.25	104.00
6	S	29	A	O3'-P-O5'	-8.50	91.25	104.00
6	O	16	U	O3'-P-O5'	-8.50	91.25	104.00
6	Q	18	U	O3'-P-O5'	-8.49	91.27	104.00
6	N	15	A	O3'-P-O5'	-8.46	91.31	104.00
6	U	22	A	O3'-P-O5'	-8.46	91.31	104.00
4	L	400	GLU	O-C-N	6.41	131.24	122.46
4	D	428	ARG	N-CA-C	5.12	119.68	113.38
4	I	1171	THR	CA-C-N	5.08	126.18	119.84
4	I	1171	THR	C-N-CA	5.08	126.18	119.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ALA	Peptide
4	D	231	PRO	Peptide
4	F	211	LEU	Peptide
4	F	234	GLN	Peptide
4	L	399	ALA	Mainchain
4	M	285	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5418	0	5476	185	0
2	B	9987	0	9917	222	0
3	C	87	0	45	5	0
4	D	8326	0	8227	193	0
4	E	8587	0	8476	179	0
4	F	8538	0	8431	157	0
4	G	8587	0	8476	165	0
4	H	8330	0	8231	141	0
4	I	8587	0	8476	163	0
4	J	8289	0	8193	141	0
4	K	8595	0	8479	199	0
4	L	8279	0	8188	185	0
4	M	8595	0	8479	184	0
5	e	1050	0	1035	30	0
5	g	1055	0	1037	31	0
5	i	1050	0	1035	15	0
5	k	1050	0	1035	34	0
5	m	1056	0	1039	64	0
6	N	672	336	337	22	0
6	O	672	336	337	2	0
6	P	630	315	316	1	0
6	Q	630	315	316	0	0
6	R	1260	630	631	11	0
6	S	1260	630	630	3	0
6	T	652	268	327	5	0
6	U	650	268	326	0	0
7	A	5	0	0	11	0
All	All	111897	3098	107495	2024	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 9.

All (2024) 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)
4:D:285:PHE:HB2	4:M:1085:PHE:CE2	1.35	1.56
4:M:216:ILE:CD1	4:M:218:ARG:HD3	1.38	1.51
4:D:400:GLU:N	5:m:156:GLU:OE2	1.56	1.34
4:M:216:ILE:HD11	4:M:218:ARG:CD	1.55	1.33
4:M:216:ILE:CD1	4:M:218:ARG:CD	2.07	1.30
4:F:519:ILE:HG12	4:F:999:ILE:CD1	1.63	1.27
5:k:116:SER:HB3	6:R:16:U:OP1	1.10	1.25
4:D:400:GLU:OE1	5:m:159:SER:OG	1.56	1.24
4:D:285:PHE:CB	4:M:1085:PHE:HE2	1.51	1.23
4:D:400:GLU:CA	5:m:156:GLU:OE2	1.87	1.22
4:D:285:PHE:CB	4:M:1085:PHE:CE2	2.22	1.22
4:G:582:ARG:HD2	6:N:6:U:C5'	1.71	1.19
1:A:214:LYS:NZ	5:m:93:ASN:CG	2.02	1.16
1:A:100:ARG:NH1	4:M:562:THR:O	1.77	1.15
1:A:121:LEU:HD23	4:M:570:THR:HG22	1.16	1.15
1:A:529:HIS:NE2	7:A:800:PO4:O4	1.79	1.12
1:A:121:LEU:HD23	4:M:570:THR:CG2	1.80	1.12
4:E:1112:LEU:HD11	4:E:1116:GLN:HE21	1.09	1.11
1:A:214:LYS:HZ3	5:m:93:ASN:ND2	1.47	1.11
4:D:399:ALA:C	5:m:156:GLU:OE2	1.93	1.10
4:E:1112:LEU:CD1	4:E:1116:GLN:HE21	1.66	1.08
4:F:519:ILE:HG12	4:F:999:ILE:HD12	1.09	1.07
4:D:400:GLU:HA	5:m:156:GLU:OE2	1.53	1.07
4:F:519:ILE:HG23	4:F:999:ILE:HD11	1.34	1.05
1:A:415:LYS:NZ	7:A:800:PO4:O4	1.90	1.03
1:A:99:ASP:OD2	1:A:101:ARG:NH1	1.93	1.02
5:k:116:SER:CB	6:R:16:U:OP1	2.06	1.02
4:D:285:PHE:HB2	4:M:1085:PHE:CD2	1.94	1.02
4:D:496:PRO:HD3	5:m:128:ASN:HD21	1.21	1.01
1:A:214:LYS:HZ3	5:m:93:ASN:CG	1.65	1.00
1:A:101:ARG:HH22	1:A:121:LEU:HD22	1.26	1.00
1:A:214:LYS:HE2	5:m:93:ASN:HB2	1.42	0.99
4:G:582:ARG:HD2	6:N:6:U:C4'	1.93	0.99
4:G:582:ARG:HD2	6:N:6:U:H4'	1.42	0.98
4:F:560:MET:HE1	4:F:796:THR:HG23	1.46	0.98
1:A:415:LYS:NZ	7:A:800:PO4:P	2.37	0.97
4:D:382:HIS:CD2	4:M:340:ASN:HB3	1.98	0.97
4:D:503:ARG:HH12	5:m:131:ASN:HD21	1.14	0.95
1:A:121:LEU:CD2	4:M:570:THR:HG22	1.96	0.95
4:G:582:ARG:HD2	6:N:6:U:H5''	1.49	0.95
4:M:216:ILE:CD1	4:M:218:ARG:CG	2.46	0.94
4:K:586:SER:O	4:K:588:PHE:CD1	2.21	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:216:ILE:HD13	4:M:218:ARG:CD	1.95	0.94
4:F:519:ILE:CG1	4:F:999:ILE:HD12	1.98	0.93
4:F:849:VAL:HG12	4:F:999:ILE:HG12	1.50	0.93
1:A:415:LYS:NZ	7:A:800:PO4:O3	2.00	0.93
4:D:1274:VAL:CG1	4:M:674:ARG:HD2	1.99	0.92
5:g:116:SER:CB	6:N:4:U:H4'	2.01	0.90
1:A:415:LYS:HZ3	7:A:800:PO4:P	1.95	0.90
1:A:214:LYS:HZ1	5:m:93:ASN:CG	1.72	0.90
4:E:1112:LEU:C	4:E:1112:LEU:HD13	1.96	0.90
1:A:555:ASN:ND2	1:A:559:ARG:NH2	2.20	0.89
4:E:1112:LEU:HD11	4:E:1116:GLN:NE2	1.88	0.89
4:K:674:ARG:H	4:L:492:THR:HG21	1.37	0.89
4:M:1079:ARG:HD3	4:M:1079:ARG:H	1.38	0.88
4:E:1112:LEU:HD13	4:E:1112:LEU:O	1.74	0.88
4:G:929:GLN:NE2	4:G:1015:MET:SD	2.46	0.87
4:D:243:LYS:NZ	4:D:982:MET:SD	2.47	0.87
4:D:385:PHE:CE2	5:m:161:ILE:HD11	2.09	0.87
4:K:553:PRO:HG2	4:K:583:PRO:O	1.75	0.86
1:A:214:LYS:NZ	5:m:93:ASN:ND2	2.21	0.85
1:A:111:ASP:OD1	6:T:8:U:O2'	1.93	0.85
4:F:519:ILE:CG2	4:F:999:ILE:HD11	2.07	0.85
4:F:519:ILE:CG1	4:F:999:ILE:CD1	2.53	0.83
4:K:858:THR:HG22	4:K:859:GLN:H	1.43	0.83
1:A:342:GLN:HE21	1:A:344:ASP:HB2	1.44	0.83
4:K:582:ARG:HD3	6:R:14:U:OP1	1.79	0.82
4:D:495:SER:C	5:m:128:ASN:HD22	1.87	0.82
4:G:582:ARG:CD	6:N:6:U:H4'	2.09	0.82
4:K:858:THR:HG22	4:K:859:GLN:N	1.93	0.82
4:M:929:GLN:NE2	4:M:1015:MET:SD	2.51	0.82
4:H:218:ARG:NH1	6:N:10:U:O2'	2.12	0.82
5:i:129:ASN:ND2	5:i:132:GLU:OE1	2.12	0.82
1:A:101:ARG:HH22	1:A:121:LEU:CD2	1.93	0.82
4:D:496:PRO:CD	5:m:128:ASN:HD21	1.91	0.82
4:L:242:LYS:HE3	6:R:33:A:H5''	1.62	0.81
4:F:560:MET:HE1	4:F:796:THR:CG2	2.10	0.81
4:K:1206:ASP:OD1	4:K:1209:LEU:CB	2.28	0.81
1:A:111:ASP:CG	6:T:8:U:H1'	2.06	0.80
4:H:580:LYS:NZ	4:H:628:ASP:OD1	2.14	0.80
4:K:1083:ILE:O	4:L:416:VAL:HG23	1.81	0.80
1:A:214:LYS:CE	5:m:93:ASN:HB2	2.11	0.80
4:D:382:HIS:CE1	5:m:154:ILE:HD13	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:519:ILE:HG12	4:F:999:ILE:HD11	1.59	0.79
4:K:1206:ASP:OD1	4:K:1209:LEU:HB2	1.83	0.79
1:A:8:ALA:O	1:A:206:THR:OG1	2.01	0.79
2:B:452:ARG:NH2	2:B:977:TYR:O	2.15	0.79
1:A:38:GLN:HE22	1:A:203:ASN:HB3	1.48	0.78
1:A:555:ASN:HD21	1:A:559:ARG:NH2	1.81	0.78
4:K:198:ALA:CB	4:K:215:ASP:N	2.47	0.77
1:A:356:MET:HE1	1:A:548:ILE:HD11	1.67	0.77
4:D:306:VAL:HG12	4:D:324:MET:HE2	1.65	0.77
4:K:1058:PRO:HG2	4:K:1181:MET:O	1.84	0.77
4:D:416:VAL:HG21	4:M:1084:SER:HB2	1.67	0.77
4:G:582:ARG:CD	6:N:6:U:C5'	2.59	0.77
5:g:106:THR:HG22	5:g:122:TYR:H	1.49	0.76
4:G:336:LYS:CB	4:G:340:ASN:HD22	1.98	0.76
4:F:582:ARG:O	4:F:880:ARG:NH1	2.19	0.76
1:A:415:LYS:CE	7:A:800:PO4:O4	2.33	0.76
4:I:1117:MET:HE1	4:J:385:PHE:HA	1.68	0.76
4:K:198:ALA:HB1	4:K:215:ASP:N	2.00	0.76
4:F:773:LYS:NZ	4:F:798:ASP:OD1	2.19	0.75
4:J:560:MET:HE1	4:J:796:THR:HG23	1.67	0.75
1:A:64:VAL:HG12	1:A:210:ILE:HG12	1.68	0.75
1:A:664:HIS:HB2	1:A:688:LYS:HE3	1.69	0.75
5:g:116:SER:OG	6:N:4:U:H5''	1.87	0.75
4:L:580:LYS:NZ	4:L:624:GLU:OE1	2.16	0.75
4:F:610:ASP:HB2	4:G:786:THR:HG21	1.67	0.75
4:E:186:CYS:SG	4:E:199:HIS:NE2	2.57	0.74
4:J:990:GLY:HA3	4:K:804:LYS:HE2	1.68	0.74
2:B:305:ASP:O	2:B:1104:LYS:NZ	2.19	0.74
4:D:496:PRO:HD3	5:m:128:ASN:ND2	1.99	0.74
4:E:1058:PRO:HD2	4:E:1182:VAL:HG12	1.69	0.74
4:M:270:PRO:HG3	4:M:297:PRO:HB3	1.70	0.73
4:H:630:PHE:HB2	4:H:772:MET:HE1	1.70	0.73
4:L:824:PRO:HB2	4:L:825:MET:HE2	1.68	0.73
5:i:106:THR:HG22	5:i:122:TYR:H	1.54	0.73
4:D:1124:GLN:HE22	4:E:187:SER:HA	1.54	0.73
4:M:1163:THR:HG21	4:M:1198:TYR:HB2	1.71	0.73
4:F:982:MET:HG2	4:F:985:GLU:HG3	1.70	0.73
5:k:144:GLY:C	4:L:444:MET:HE3	2.14	0.73
4:M:234:GLN:NE2	4:M:911:ASP:OD1	2.21	0.72
1:A:415:LYS:HZ2	7:A:800:PO4:P	2.08	0.72
4:L:892:PRO:HD2	4:L:895:LEU:HD12	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1163:THR:HG21	4:F:1198:TYR:HB2	1.71	0.72
4:G:926:GLU:HG2	4:G:1020:ILE:HD12	1.72	0.72
4:M:1079:ARG:HD3	4:M:1079:ARG:N	2.04	0.72
5:e:11:LYS:N	4:E:319:ASP:OD2	2.21	0.72
4:I:1093:MET:CE	4:I:1102:VAL:C	2.63	0.71
4:L:242:LYS:CE	6:R:33:A:H5"	2.20	0.71
2:B:690:GLU:OE2	2:B:694:ASN:ND2	2.23	0.71
4:D:416:VAL:HG23	4:M:1083:ILE:O	1.90	0.71
4:D:580:LYS:NZ	4:D:628:ASP:OD2	2.23	0.71
5:e:65:ALA:HB2	4:E:545:ARG:HD2	1.72	0.71
5:g:129:ASN:ND2	5:g:132:GLU:OE1	2.23	0.71
4:L:523:MET:HE1	4:L:851:ARG:HD3	1.73	0.71
4:H:750:VAL:HG12	4:H:752:THR:H	1.53	0.71
1:A:450:GLU:HA	1:A:455:THR:HG22	1.72	0.71
4:D:270:PRO:HG3	4:D:297:PRO:HB3	1.73	0.71
4:K:271:ILE:HB	4:K:301:VAL:HG23	1.73	0.71
2:B:899:MET:O	2:B:903:ILE:HG12	1.91	0.71
5:e:106:THR:HG22	5:e:122:TYR:H	1.55	0.71
4:I:1163:THR:HG21	4:I:1198:TYR:HB2	1.73	0.70
5:k:131:ASN:OD1	4:L:503:ARG:NH2	2.24	0.70
1:A:616:ALA:HB3	1:A:645:ILE:HB	1.72	0.70
4:D:503:ARG:NH1	5:m:131:ASN:HD21	1.88	0.70
4:D:400:GLU:CA	5:m:156:GLU:CD	2.64	0.70
4:D:285:PHE:CA	4:M:1085:PHE:HE2	2.03	0.70
1:A:513:LYS:O	1:A:517:ASN:ND2	2.23	0.70
4:D:496:PRO:N	5:m:128:ASN:ND2	2.40	0.70
4:J:270:PRO:HG3	4:J:297:PRO:HB3	1.72	0.70
2:B:948:MET:HA	2:B:951:LEU:HD23	1.74	0.70
4:D:285:PHE:CA	4:M:1085:PHE:CE2	2.74	0.70
4:I:929:GLN:NE2	4:I:1015:MET:SD	2.64	0.70
4:K:789:LEU:O	4:K:793:MET:HG2	1.91	0.70
2:B:431:LEU:HB3	2:B:435:ARG:HH12	1.55	0.70
4:D:400:GLU:N	5:m:156:GLU:CD	2.49	0.70
4:E:186:CYS:HG	4:E:199:HIS:HE2	1.37	0.70
4:L:504:LEU:HD23	4:L:506:PRO:HD3	1.72	0.70
4:J:673:ARG:HD2	4:L:754:THR:HG21	1.73	0.70
4:K:336:LYS:NZ	4:K:346:VAL:O	2.24	0.69
4:K:382:HIS:ND1	4:K:387:GLU:OE2	2.25	0.69
4:F:232:ILE:O	4:F:236:SER:OG	2.10	0.69
4:I:382:HIS:ND1	4:I:387:GLU:OE2	2.25	0.69
4:K:858:THR:CG2	4:K:859:GLN:H	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:1163:THR:HG21	4:K:1198:TYR:HB2	1.73	0.69
4:L:990:GLY:HA3	4:M:804:LYS:HE2	1.72	0.69
4:D:382:HIS:CD2	4:M:340:ASN:CB	2.72	0.69
4:D:441:ASN:HB2	4:M:861:ALA:HB1	1.74	0.69
4:M:455:ASP:OD1	4:M:458:THR:OG1	2.06	0.69
4:M:1079:ARG:H	4:M:1079:ARG:CD	2.04	0.69
4:D:400:GLU:CD	5:m:159:SER:OG	2.35	0.69
4:I:454:SER:OG	4:I:1255:ASN:OD1	2.10	0.69
5:k:128:ASN:ND2	4:L:1272:MET:HG2	2.06	0.69
5:m:109:GLN:OE1	4:M:533:GLN:NE2	2.21	0.69
2:B:707:GLY:HA3	2:B:720:MET:HE1	1.74	0.69
4:E:560:MET:HG3	4:E:578:LEU:HD21	1.75	0.69
4:E:1112:LEU:CD1	4:E:1112:LEU:C	2.66	0.69
4:G:1159:ALA:HB2	4:G:1181:MET:HE2	1.75	0.69
4:L:223:PHE:HE2	4:L:583:PRO:HD2	1.57	0.69
4:D:1274:VAL:HG11	4:M:674:ARG:HD2	1.75	0.68
4:D:858:THR:HG23	4:D:942:GLN:HB2	1.76	0.68
5:i:101:GLU:OE2	4:I:528:ASN:ND2	2.27	0.68
4:M:571:LEU:HD23	4:M:571:LEU:O	1.93	0.68
4:J:549:LEU:HD21	4:J:807:THR:HG22	1.74	0.68
4:D:415:ASN:ND2	4:M:1121:TYR:OH	2.26	0.68
4:E:765:ARG:NH1	4:E:801:LYS:O	2.27	0.68
4:F:660:GLU:OE1	4:F:699:ALA:HA	1.93	0.68
4:D:496:PRO:CD	5:m:128:ASN:ND2	2.55	0.68
4:G:186:CYS:SG	4:G:199:HIS:NE2	2.65	0.68
4:K:1206:ASP:OD1	4:K:1209:LEU:HB3	1.94	0.68
4:L:1082:ARG:HA	4:M:1272:MET:HE1	1.76	0.68
4:E:859:GLN:HG2	4:F:438:GLN:HB3	1.75	0.68
4:K:1171:THR:HG22	4:K:1173:THR:H	1.57	0.68
4:L:270:PRO:HG3	4:L:297:PRO:HB3	1.75	0.68
4:M:937:GLN:HA	4:M:947:ARG:HH21	1.58	0.68
4:F:216:ILE:O	4:F:220:ILE:HG12	1.94	0.67
4:F:581:LEU:O	4:F:583:PRO:HD3	1.94	0.67
4:M:1034:GLU:OE2	4:M:1207:ARG:NH2	2.27	0.67
2:B:1151:GLN:HE22	4:D:585:ASN:CG	2.02	0.67
4:K:586:SER:O	4:K:588:PHE:CE1	2.46	0.67
1:A:555:ASN:HD21	1:A:559:ARG:HH21	1.40	0.67
4:K:351:PRO:HA	4:K:354:PHE:CE2	2.29	0.67
1:A:121:LEU:HA	4:M:570:THR:HG21	1.75	0.67
4:I:1095:ARG:HE	4:I:1099:GLY:HA2	1.59	0.67
5:g:116:SER:OG	6:N:4:U:C5'	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:851:ARG:HH21	2:B:862:TYR:HD2	1.43	0.67
4:E:674:ARG:H	4:F:492:THR:HG21	1.58	0.67
4:H:603:VAL:HG13	4:H:604:VAL:HG23	1.77	0.67
4:J:664:MET:HE2	4:J:671:GLN:HA	1.76	0.67
4:K:553:PRO:CG	4:K:583:PRO:O	2.41	0.67
4:E:1163:THR:HG21	4:E:1198:TYR:HB2	1.75	0.67
4:K:234:GLN:NE2	4:K:911:ASP:OD1	2.28	0.67
4:L:750:VAL:HG12	4:L:752:THR:H	1.59	0.67
4:M:216:ILE:HD13	4:M:218:ARG:CG	2.20	0.67
4:E:382:HIS:ND1	4:E:387:GLU:OE2	2.28	0.67
4:F:472:MET:HE1	4:F:922:MET:HE2	1.76	0.67
4:K:765:ARG:NH1	4:K:801:LYS:O	2.28	0.67
4:M:940:GLU:OE1	4:M:956:ARG:NH1	2.27	0.67
2:B:459:ARG:HB3	3:C:1285:G:H5"	1.77	0.67
4:I:182:GLN:NE2	4:I:188:ALA:O	2.28	0.67
1:A:101:ARG:NH2	1:A:121:LEU:CD2	2.57	0.66
4:K:466:MET:HE1	4:K:1262:TYR:HE2	1.60	0.66
4:M:344:LEU:HB2	4:M:1171:THR:HG21	1.77	0.66
4:M:271:ILE:HB	4:M:301:VAL:HG23	1.76	0.66
4:D:385:PHE:CD2	5:m:161:ILE:HD11	2.29	0.66
4:G:270:PRO:HG3	4:G:297:PRO:HB3	1.77	0.66
4:G:983:LEU:N	4:G:985:GLU:OE1	2.27	0.66
4:F:270:PRO:HG3	4:F:297:PRO:HB3	1.78	0.66
4:K:182:GLN:NE2	4:K:188:ALA:O	2.28	0.66
1:A:120:GLN:OE1	1:A:120:GLN:N	2.28	0.66
4:F:825:MET:HE3	4:F:909:TYR:CE2	2.30	0.66
4:D:400:GLU:OE2	5:m:156:GLU:HA	1.96	0.66
4:K:186:CYS:SG	4:K:199:HIS:NE2	2.65	0.66
1:A:27:ASP:OD1	1:A:28:ALA:N	2.29	0.66
4:G:630:PHE:HB2	4:G:772:MET:HE1	1.76	0.66
4:J:1075:HIS:CE1	4:J:1102:VAL:HG11	2.31	0.66
4:K:1084:SER:HB2	4:L:416:VAL:HG21	1.77	0.66
4:E:1079:ARG:HA	4:E:1114:LEU:HD21	1.76	0.66
4:F:627:TRP:O	4:F:631:ILE:HG12	1.96	0.66
4:D:439:MET:O	4:M:860:PRO:O	2.13	0.65
4:K:674:ARG:N	4:L:492:THR:HG21	2.10	0.65
4:D:495:SER:C	5:m:128:ASN:ND2	2.53	0.65
4:E:234:GLN:NE2	4:E:911:ASP:OD1	2.29	0.65
5:i:51:GLU:O	5:i:52:GLN:NE2	2.28	0.65
4:I:186:CYS:SG	4:I:199:HIS:NE2	2.67	0.65
4:G:674:ARG:H	4:H:492:THR:HG21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:776:VAL:HG21	4:G:793:MET:HG2	1.78	0.65
4:J:1116:GLN:NE2	4:J:1171:THR:O	2.28	0.65
4:M:336:LYS:HG3	4:M:339:LEU:HD22	1.77	0.65
1:A:252:GLN:NE2	1:A:256:ASP:OD2	2.29	0.65
4:D:1163:THR:HG21	4:D:1198:TYR:HB2	1.79	0.65
5:e:6:ARG:NH1	4:E:317:ASP:O	2.29	0.65
4:K:474:ILE:HD11	4:K:508:ARG:HB2	1.77	0.65
4:D:618:GLY:O	4:F:804:LYS:NZ	2.30	0.65
4:I:1093:MET:HE1	4:I:1102:VAL:C	2.21	0.65
4:J:320:SER:HB3	4:J:364:GLU:HB2	1.78	0.65
2:B:1199:LEU:HD22	2:B:1219:ARG:HG3	1.77	0.65
4:D:231:PRO:O	4:D:233:VAL:N	2.30	0.65
2:B:83:ARG:NH1	2:B:84:LYS:O	2.30	0.65
4:F:990:GLY:HA2	4:G:804:LYS:HD3	1.79	0.65
4:M:216:ILE:HD13	4:M:218:ARG:HG3	1.79	0.65
1:A:419:LYS:HD2	7:A:800:PO4:O1	1.97	0.65
2:B:595:TRP:HA	2:B:599:LEU:HB2	1.79	0.65
4:D:400:GLU:HA	5:m:156:GLU:CD	2.23	0.64
4:I:1093:MET:HE1	4:I:1102:VAL:CA	2.27	0.64
4:L:339:LEU:HB2	4:L:353:MET:HG2	1.77	0.64
4:M:524:ASN:HB2	4:M:982:MET:HE1	1.78	0.64
2:B:452:ARG:HG3	2:B:620:MET:HE3	1.78	0.64
4:G:1096:ASP:OD1	4:G:1097:GLU:N	2.30	0.64
4:K:858:THR:CG2	4:K:859:GLN:N	2.60	0.64
4:I:1067:PHE:O	4:I:1138:ARG:NH1	2.31	0.64
5:k:117:LYS:HD2	6:S:40:U:OP1	1.96	0.64
5:m:87:THR:OG1	5:m:146:ASN:ND2	2.30	0.64
1:A:121:LEU:HD23	4:M:570:THR:HG21	1.79	0.64
5:g:81:PRO:HG3	4:G:963:ALA:HB1	1.80	0.64
4:G:818:GLU:HA	4:G:821:VAL:HG22	1.80	0.64
4:J:503:ARG:H	4:J:503:ARG:HD2	1.63	0.64
4:J:750:VAL:HG12	4:J:752:THR:H	1.61	0.64
4:J:1080:ASP:HB2	4:J:1095:ARG:HH21	1.60	0.64
4:J:1112:LEU:HD12	4:J:1141:MET:HG2	1.80	0.64
5:k:101:GLU:OE2	4:K:528:ASN:ND2	2.30	0.64
4:D:503:ARG:HH12	5:m:131:ASN:ND2	1.93	0.64
4:E:435:ASP:OD1	4:E:436:ARG:N	2.31	0.64
4:J:582:ARG:O	4:J:880:ARG:NH1	2.31	0.64
4:J:782:GLN:HG3	4:J:783:PRO:HD3	1.80	0.64
4:K:1118:ASN:HB2	4:K:1122:PHE:CE2	2.32	0.64
4:G:336:LYS:HA	4:G:340:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:859:GLN:HE21	4:H:438:GLN:H	1.44	0.64
4:L:852:GLN:NE2	4:L:991:ASP:O	2.31	0.64
4:M:474:ILE:HD11	4:M:508:ARG:HB2	1.79	0.64
1:A:572:LEU:HG	1:A:576:TYR:HE2	1.62	0.64
4:J:1163:THR:HG21	4:J:1198:TYR:HB2	1.80	0.64
4:F:1067:PHE:O	4:F:1138:ARG:NH1	2.30	0.63
4:K:850:THR:OG1	4:K:1000:GLN:NE2	2.31	0.63
4:M:1159:ALA:HB2	4:M:1181:MET:HE2	1.80	0.63
1:A:111:ASP:OD1	6:T:8:U:H1'	1.98	0.63
2:B:711:THR:O	5:e:117:LYS:NZ	2.28	0.63
2:B:1205:ARG:HH21	4:H:572:SER:HB2	1.63	0.63
4:H:1163:THR:HG21	4:H:1198:TYR:HB2	1.79	0.63
4:K:1112:LEU:HD12	4:K:1141:MET:HG2	1.80	0.63
4:G:182:GLN:NE2	4:G:188:ALA:O	2.31	0.63
4:M:216:ILE:CD1	4:M:218:ARG:HG3	2.28	0.63
2:B:628:ASN:OD1	2:B:629:ASP:N	2.32	0.63
4:H:773:LYS:NZ	4:H:798:ASP:OD1	2.23	0.63
2:B:414:LEU:HD11	2:B:418:THR:HG21	1.81	0.63
2:B:756:MET:O	2:B:760:ILE:HD12	1.98	0.63
4:E:334:LEU:HA	4:E:337:GLN:HE22	1.63	0.63
4:H:983:LEU:N	4:H:985:GLU:OE1	2.31	0.63
4:J:1166:TRP:CD1	4:J:1176:PRO:HG2	2.34	0.63
1:A:352:LEU:O	1:A:356:MET:HB2	1.98	0.63
5:e:150:MET:HA	5:e:153:ARG:HE	1.64	0.63
4:K:234:GLN:NE2	4:K:247:LEU:O	2.31	0.63
4:K:859:GLN:NE2	4:L:438:GLN:H	1.97	0.63
4:E:271:ILE:HB	4:E:301:VAL:HG23	1.80	0.63
4:G:1241:PRO:HG2	4:G:1244:GLN:HB2	1.81	0.63
2:B:552:HIS:HB3	2:B:553:MET:HE2	1.81	0.62
4:H:660:GLU:OE2	4:H:699:ALA:HA	1.99	0.62
4:M:186:CYS:SG	4:M:199:HIS:NE2	2.66	0.62
4:F:858:THR:HG23	4:F:942:GLN:HB2	1.80	0.62
5:k:106:THR:HG22	5:k:122:TYR:H	1.64	0.62
4:M:351:PRO:HG3	4:M:1116:GLN:HE22	1.63	0.62
4:M:1067:PHE:O	4:M:1138:ARG:NH1	2.32	0.62
4:H:659:PHE:HD2	4:H:660:GLU:HG2	1.65	0.62
4:L:739:LEU:HD12	4:L:832:GLN:HE22	1.63	0.62
4:L:1166:TRP:CD1	4:L:1176:PRO:HG2	2.35	0.62
4:G:468:ARG:HB2	4:G:1019:VAL:HG11	1.79	0.62
5:m:2:LYS:HZ1	4:M:217:GLN:HG3	1.65	0.62
4:M:336:LYS:NZ	4:M:346:VAL:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:870:THR:HG22	4:I:871:VAL:H	1.64	0.62
4:K:839:ASP:OD2	4:K:842:ARG:NH1	2.32	0.62
4:F:601:ASN:HD21	4:F:833:VAL:H	1.48	0.62
4:L:1163:THR:HG21	4:L:1198:TYR:HB2	1.80	0.62
4:M:691:ILE:HD11	4:M:710:HIS:CE1	2.34	0.62
4:D:292:ILE:HG12	5:m:163:SER:HB3	1.82	0.62
4:F:519:ILE:HG23	4:F:999:ILE:CD1	2.19	0.62
4:K:455:ASP:OD1	4:K:458:THR:OG1	2.15	0.62
4:K:841:ASP:HB2	4:K:1005:ASN:HB3	1.82	0.62
1:A:305:VAL:HG21	1:A:312:ARG:HE	1.65	0.62
4:I:1096:ASP:OD1	4:I:1097:GLU:N	2.33	0.62
4:L:336:LYS:HA	4:L:340:ASN:HD22	1.64	0.62
4:M:1069:ARG:NH1	4:M:1140:GLU:OE2	2.32	0.62
2:B:778:THR:HG22	2:B:787:ILE:HD13	1.82	0.62
5:k:144:GLY:C	4:L:444:MET:CE	2.72	0.62
1:A:114:LYS:HA	1:A:114:LYS:HE3	1.82	0.61
1:A:214:LYS:NZ	5:m:93:ASN:CB	2.62	0.61
2:B:963:PRO:HB2	2:B:966:VAL:HG22	1.80	0.61
5:e:4:ILE:HG21	4:E:254:ARG:HH22	1.63	0.61
4:E:1245:ILE:HD12	4:E:1247:LEU:HD23	1.80	0.61
4:I:605:THR:HG21	4:I:870:THR:HG21	1.82	0.61
4:K:859:GLN:HE21	4:L:438:GLN:H	1.44	0.61
1:A:3:TYR:OH	1:A:207:PHE:O	2.07	0.61
4:J:855:ASP:HB3	4:K:756:ASP:HA	1.81	0.61
4:K:983:LEU:N	4:K:985:GLU:OE1	2.28	0.61
4:E:1119:THR:O	4:E:1123:ASN:HB2	2.00	0.61
4:G:336:LYS:HA	4:G:340:ASN:HD22	1.66	0.61
5:k:161:ILE:HD11	4:L:385:PHE:CD2	2.35	0.61
1:A:66:LYS:NZ	1:A:67:ASN:O	2.31	0.61
4:D:339:LEU:HB2	4:D:353:MET:HG2	1.82	0.61
4:D:1274:VAL:HG12	4:M:674:ARG:HD2	1.79	0.61
4:M:720:ARG:NH1	4:M:721:TYR:O	2.33	0.61
4:J:419:ILE:HD11	4:J:1214:SER:HB2	1.81	0.61
5:m:155:ALA:HA	4:M:342:GLU:OE1	1.99	0.61
2:B:1090:LEU:HD21	4:H:227:TRP:CH2	2.35	0.61
4:D:823:ALA:HA	4:D:826:LEU:HD23	1.82	0.61
4:D:855:ASP:OD1	4:D:856:THR:N	2.31	0.61
5:i:11:LYS:N	4:I:319:ASP:OD1	2.29	0.61
4:I:271:ILE:HB	4:I:301:VAL:HG23	1.82	0.61
1:A:201:ARG:HG3	1:A:202:PHE:CD2	2.34	0.61
4:D:622:SER:HA	4:F:562:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:50:ARG:O	5:e:52:GLN:NE2	2.33	0.61
4:H:851:ARG:NH1	4:H:989:SER:O	2.32	0.61
4:I:1104:PHE:HD1	4:I:1108:TRP:HH2	1.49	0.61
4:J:533:GLN:NE2	4:J:537:GLN:OE1	2.33	0.61
4:L:1067:PHE:O	4:L:1138:ARG:NH1	2.32	0.61
4:I:656:MET:HE2	4:I:660:GLU:OE1	2.00	0.61
4:I:842:ARG:HG3	4:I:1003:GLN:NE2	2.16	0.61
4:K:1096:ASP:OD1	4:K:1097:GLU:N	2.34	0.61
4:M:850:THR:HG23	4:M:1000:GLN:HE22	1.65	0.61
4:D:807:THR:HG23	4:D:889:GLY:HA3	1.82	0.60
4:G:625:ASN:HB3	4:G:655:MET:HE3	1.83	0.60
1:A:245:ILE:HD12	4:D:1266:PRO:HB3	1.81	0.60
4:D:527:ASN:HD21	4:E:792:SER:HA	1.66	0.60
4:F:560:MET:CE	4:F:796:THR:HG23	2.26	0.60
4:H:339:LEU:HB2	4:H:353:MET:HG2	1.82	0.60
4:H:1166:TRP:CD1	4:H:1176:PRO:HG2	2.36	0.60
4:I:1093:MET:HE1	4:I:1102:VAL:HA	1.82	0.60
4:G:773:LYS:NZ	4:G:798:ASP:OD1	2.31	0.60
1:A:304:VAL:HG23	1:A:382:ILE:HG23	1.81	0.60
1:A:327:ILE:HG13	1:A:357:LEU:HD13	1.84	0.60
2:B:306:TYR:HE1	2:B:555:LEU:HD22	1.66	0.60
4:L:472:MET:HE2	4:L:506:PRO:HB2	1.84	0.60
4:D:492:THR:HG21	4:M:674:ARG:N	2.16	0.60
4:J:630:PHE:HB2	4:J:772:MET:HE1	1.82	0.60
4:L:852:GLN:O	4:L:996:GLN:NE2	2.34	0.60
1:A:214:LYS:CE	5:m:93:ASN:CB	2.79	0.60
2:B:396:LYS:HB3	2:B:766:GLU:HA	1.83	0.60
4:K:970:ASN:ND2	4:K:983:LEU:O	2.35	0.60
4:L:854:ARG:NH1	4:L:866:THR:OG1	2.35	0.60
2:B:641:ILE:HB	2:B:645:GLN:HB2	1.84	0.60
4:E:970:ASN:ND2	4:E:985:GLU:OE2	2.33	0.60
4:F:1010:ASN:O	4:F:1011:ILE:HD13	2.02	0.60
4:F:350:ASN:CG	4:F:353:MET:HE2	2.26	0.60
4:G:271:ILE:HB	4:G:301:VAL:HG23	1.83	0.60
4:I:234:GLN:NE2	4:I:911:ASP:OD1	2.35	0.60
4:H:1131:LYS:HD2	4:H:1160:TRP:CE2	2.36	0.59
4:I:1093:MET:CE	4:I:1102:VAL:CA	2.80	0.59
4:K:1180:PHE:CE1	4:K:1199:ILE:HG22	2.37	0.59
4:M:398:ASP:O	4:M:401:LYS:NZ	2.30	0.59
2:B:1205:ARG:NE	4:H:565:GLU:OE1	2.35	0.59
4:D:503:ARG:HH22	5:m:131:ASN:ND2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1228:PRO:HB2	4:E:1231:ARG:HG3	1.83	0.59
4:F:246:GLN:HE22	4:F:982:MET:HB2	1.67	0.59
4:E:181:TYR:N	4:E:190:LEU:O	2.35	0.59
4:E:1166:TRP:CD1	4:E:1176:PRO:HG2	2.37	0.59
4:F:855:ASP:HB3	4:G:756:ASP:HA	1.83	0.59
4:F:1062:PRO:HG2	4:F:1065:LEU:HD23	1.84	0.59
4:M:216:ILE:HD12	4:M:218:ARG:CB	2.32	0.59
2:B:1250:ARG:O	2:B:1254:GLN:HG2	2.03	0.59
4:M:665:ASP:O	4:M:667:GLN:NE2	2.34	0.59
4:G:336:LYS:CA	4:G:340:ASN:HD22	2.14	0.59
4:J:855:ASP:OD1	4:J:856:THR:N	2.35	0.59
2:B:542:HIS:CE1	2:B:690:GLU:HG3	2.38	0.59
4:I:776:VAL:HG21	4:I:793:MET:HG3	1.85	0.59
2:B:135:THR:HG22	2:B:668:SER:HA	1.84	0.59
5:g:145:SER:O	5:g:153:ARG:NH2	2.36	0.59
4:H:691:ILE:HD11	4:H:710:HIS:CE1	2.37	0.59
4:I:315:ASP:OD1	4:I:316:PHE:N	2.36	0.59
1:A:693:PRO:HB2	1:A:696:LEU:HD23	1.83	0.59
4:D:562:THR:HG21	4:L:622:SER:HA	1.85	0.59
4:E:870:THR:HG22	4:E:871:VAL:H	1.68	0.59
5:g:108:LYS:NZ	5:g:112:ASP:OD1	2.36	0.59
4:J:983:LEU:N	4:J:985:GLU:OE1	2.36	0.59
1:A:397:ASP:OD1	1:A:398:VAL:N	2.36	0.59
2:B:173:GLN:OE1	4:F:217:GLN:NE2	2.36	0.59
2:B:348:ARG:O	2:B:352:LYS:HG2	2.03	0.59
4:G:801:LYS:HG2	4:G:802:LEU:HD12	1.85	0.59
4:I:360:HIS:NE2	4:I:364:GLU:OE2	2.35	0.59
4:L:242:LYS:HE3	6:R:34:U:P	2.43	0.59
2:B:176:ASP:OD2	2:B:837:ARG:NH1	2.35	0.59
4:E:566:SER:OG	4:E:569:GLN:O	2.16	0.59
4:I:546:ILE:HG13	4:I:904:ALA:HB1	1.85	0.59
4:M:254:ARG:HH11	4:M:254:ARG:HB2	1.68	0.59
4:E:344:LEU:HB2	4:E:1171:THR:HG21	1.84	0.58
4:G:780:ARG:NH2	4:G:781:TYR:OH	2.36	0.58
4:H:1034:GLU:OE2	4:H:1207:ARG:NH2	2.28	0.58
4:M:216:ILE:HD12	4:M:218:ARG:CG	2.33	0.58
1:A:293:TYR:HB2	1:A:699:ARG:HH21	1.68	0.58
4:F:246:GLN:NE2	4:F:982:MET:H	2.00	0.58
4:G:634:LEU:HD23	4:G:883:THR:HG23	1.84	0.58
4:J:584:SER:HB2	4:J:587:ASP:HB2	1.84	0.58
1:A:444:ASP:OD1	1:A:445:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:679:SER:HB3	4:E:788:SER:HB2	1.85	0.58
5:e:75:ASN:OD1	5:e:76:ASN:N	2.36	0.58
2:B:908:PRO:O	2:B:912:ARG:HG3	2.04	0.58
4:F:519:ILE:CG1	4:F:999:ILE:HD11	2.27	0.58
4:H:851:ARG:NH1	4:H:986:PRO:O	2.36	0.58
4:K:315:ASP:OD1	4:K:316:PHE:N	2.36	0.58
4:M:242:LYS:NZ	6:S:8:U:H5'	2.19	0.58
1:A:11:ASP:O	1:A:15:SER:OG	2.17	0.58
4:G:582:ARG:HD2	6:N:6:U:H5'	1.76	0.58
4:K:504:LEU:HG	4:K:506:PRO:HD3	1.86	0.58
2:B:607:HIS:HB2	2:B:648:ILE:HG21	1.86	0.58
4:D:1166:TRP:CD1	4:D:1176:PRO:HG2	2.38	0.58
5:m:129:ASN:ND2	5:m:132:GLU:OE1	2.37	0.58
2:B:2:SER:N	2:B:48:GLU:OE1	2.36	0.58
2:B:477:LEU:HD13	2:B:496:GLN:HB3	1.86	0.58
2:B:1143:ALA:O	2:B:1147:MET:HG2	2.03	0.58
4:D:382:HIS:NE2	4:M:340:ASN:HB3	2.17	0.58
4:L:1010:ASN:O	4:L:1011:ILE:HD13	2.04	0.58
4:E:1110:PHE:O	4:E:1139:ILE:HA	2.03	0.58
4:F:1079:ARG:NH1	4:G:1275:PRO:O	2.36	0.58
4:K:560:MET:HG3	4:K:578:LEU:HD21	1.85	0.58
4:D:315:ASP:OD1	4:D:316:PHE:N	2.36	0.58
4:D:385:PHE:CE1	5:m:161:ILE:HG12	2.39	0.58
4:K:186:CYS:HG	4:K:199:HIS:HE2	1.50	0.58
2:B:700:GLU:HB2	2:B:725:ILE:HD13	1.85	0.57
2:B:791:ARG:NH1	2:B:1078:CYS:SG	2.77	0.57
4:F:527:ASN:HD21	4:G:792:SER:HA	1.68	0.57
4:K:352:LEU:HB3	4:K:955:LEU:HD23	1.85	0.57
4:D:546:ILE:HD11	4:D:905:ILE:HG12	1.86	0.57
5:e:67:GLU:OE2	4:E:249:HIS:NE2	2.33	0.57
4:K:1119:THR:O	4:K:1123:ASN:HB2	2.03	0.57
4:H:1011:ILE:O	4:H:1011:ILE:HG22	2.03	0.57
4:G:660:GLU:HG2	4:G:702:LEU:HD13	1.87	0.57
4:L:581:LEU:O	4:L:880:ARG:NH1	2.34	0.57
4:L:823:ALA:HA	4:L:826:LEU:HD23	1.86	0.57
1:A:121:LEU:CD2	4:M:570:THR:CG2	2.67	0.57
2:B:25:ASP:OD1	2:B:26:VAL:N	2.37	0.57
4:H:920:ARG:NH2	4:H:981:ASP:OD1	2.38	0.57
4:H:1130:ILE:HD11	4:H:1137:ILE:HD12	1.86	0.57
4:J:1010:ASN:O	4:J:1011:ILE:HD13	2.05	0.57
2:B:582:ILE:HB	2:B:738:MET:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:303:ARG:NH1	4:M:1208:SER:OG	2.38	0.57
4:M:1081:CYS:SG	4:M:1114:LEU:HD11	2.45	0.57
4:H:1093:MET:HE2	4:H:1101:MET:HB3	1.87	0.57
4:J:507:TYR:CD2	4:J:915:PHE:HB3	2.39	0.57
4:L:583:PRO:HG3	4:L:884:VAL:HG11	1.85	0.57
4:M:242:LYS:NZ	6:S:7:A:O3'	2.38	0.57
2:B:1217:TRP:O	2:B:1221:ILE:HD12	2.04	0.57
4:F:1112:LEU:HD22	4:F:1141:MET:HG2	1.86	0.57
4:G:344:LEU:HB2	4:G:1171:THR:HG21	1.86	0.57
4:I:620:VAL:HG11	4:I:656:MET:SD	2.44	0.57
2:B:116:SER:HB3	2:B:119:ILE:HD12	1.87	0.57
4:E:182:GLN:NE2	4:E:188:ALA:O	2.37	0.57
4:E:351:PRO:HA	4:E:354:PHE:CD2	2.39	0.57
4:F:374:ARG:O	4:F:1259:ARG:NH1	2.37	0.57
4:F:528:ASN:HD21	4:G:563:VAL:HG12	1.69	0.57
4:H:223:PHE:O	4:H:226:SER:OG	2.16	0.57
4:I:765:ARG:NH1	4:I:801:LYS:O	2.38	0.57
1:A:39:ASP:OD2	1:A:165:ARG:NH2	2.38	0.57
4:E:901:TYR:O	4:E:905:ILE:HG13	2.04	0.57
4:M:695:SER:HB3	4:M:698:ASP:HB2	1.86	0.57
4:D:492:THR:HG21	4:M:674:ARG:H	1.69	0.56
4:G:1081:CYS:SG	4:G:1114:LEU:HD11	2.44	0.56
4:I:417:SER:OG	4:I:1214:SER:O	2.22	0.56
1:A:581:THR:O	2:B:401:GLN:NE2	2.33	0.56
2:B:1039:MET:HA	2:B:1039:MET:HE3	1.86	0.56
4:D:852:GLN:O	4:D:996:GLN:NE2	2.38	0.56
4:K:581:LEU:HD12	4:K:884:VAL:HG22	1.87	0.56
4:L:855:ASP:HB3	4:M:756:ASP:HA	1.87	0.56
4:L:1116:GLN:HB3	4:L:1172:PRO:HA	1.86	0.56
1:A:111:ASP:OD1	6:T:8:U:C2'	2.52	0.56
1:A:444:ASP:HB3	1:A:447:GLU:HG2	1.87	0.56
2:B:403:ASP:HB3	2:B:418:THR:HG22	1.88	0.56
2:B:925:SER:N	2:B:929:GLY:O	2.33	0.56
2:B:1151:GLN:NE2	4:D:585:ASN:CG	2.63	0.56
4:F:970:ASN:ND2	4:F:985:GLU:OE1	2.38	0.56
4:G:849:VAL:O	4:G:863:SER:OG	2.23	0.56
4:H:584:SER:O	4:H:585:ASN:OD1	2.23	0.56
4:I:186:CYS:HG	4:I:199:HIS:HE2	1.50	0.56
4:D:382:HIS:CE1	5:m:154:ILE:CD1	2.88	0.56
4:E:630:PHE:HD1	4:E:772:MET:HE1	1.70	0.56
4:F:956:ARG:NH2	4:G:749:ASN:OD1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:627:TRP:O	4:I:631:ILE:HD12	2.05	0.56
4:J:523:MET:HE1	4:J:987:LEU:HD23	1.86	0.56
4:K:898:ASN:ND2	4:K:1274:VAL:O	2.35	0.56
2:B:294:CYS:SG	2:B:314:MET:HE3	2.46	0.56
4:E:605:THR:HG21	4:E:870:THR:HG21	1.88	0.56
4:E:1112:LEU:CD1	4:E:1116:GLN:NE2	2.52	0.56
4:J:241:ASN:OD1	4:J:245:ALA:N	2.32	0.56
4:E:200:VAL:HA	4:E:203:HIS:CD2	2.41	0.56
4:E:457:LEU:HD13	4:E:1030:VAL:HG21	1.87	0.56
4:M:216:ILE:HD11	4:M:218:ARG:HD3	0.61	0.56
4:M:1241:PRO:HG2	4:M:1244:GLN:HB2	1.86	0.56
1:A:523:ARG:NH2	1:A:642:TYR:O	2.38	0.56
4:E:704:GLN:O	4:E:708:ILE:HG12	2.05	0.56
2:B:570:LEU:HD21	2:B:730:VAL:HG21	1.87	0.56
4:E:1121:TYR:OH	4:F:415:ASN:ND2	2.39	0.56
4:G:664:MET:HA	4:G:664:MET:HE3	1.87	0.56
4:G:1166:TRP:CD1	4:G:1176:PRO:HG2	2.41	0.56
4:K:1104:PHE:HD1	4:K:1108:TRP:HH2	1.54	0.56
1:A:182:THR:OG1	1:A:183:MET:N	2.39	0.56
2:B:719:LEU:O	2:B:723:LEU:HD23	2.05	0.56
4:G:336:LYS:HB2	4:G:340:ASN:HD22	1.68	0.56
4:J:711:ARG:HD2	4:J:712:TYR:CE1	2.40	0.56
4:D:507:TYR:CD2	4:D:915:PHE:HB3	2.41	0.56
4:E:625:ASN:HB3	4:E:655:MET:HE3	1.87	0.56
4:E:861:ALA:HB1	4:F:441:ASN:HB2	1.88	0.56
4:I:390:ASN:OD1	4:I:433:ARG:NH2	2.39	0.56
4:J:1096:ASP:N	4:J:1100:LEU:O	2.30	0.56
4:K:338:LEU:O	4:K:340:ASN:N	2.38	0.56
4:L:603:VAL:HG23	4:L:604:VAL:HG23	1.87	0.56
4:L:836:VAL:HG11	4:L:842:ARG:HB2	1.88	0.56
4:H:939:SER:OG	4:H:940:GLU:N	2.37	0.55
4:I:339:LEU:HB2	4:I:353:MET:HG2	1.87	0.55
4:I:573:PRO:HB3	4:I:793:MET:HE1	1.88	0.55
4:K:1147:MET:HE3	4:K:1149:HIS:NE2	2.20	0.55
4:D:433:ARG:HA	4:D:450:VAL:HG12	1.89	0.55
4:H:307:HIS:CE1	4:H:323:ILE:HD12	2.41	0.55
4:J:603:VAL:HG23	4:J:604:VAL:HG13	1.88	0.55
4:K:303:ARG:NH1	4:K:1208:SER:OG	2.39	0.55
4:K:398:ASP:O	4:K:401:LYS:NZ	2.39	0.55
4:D:252:THR:HG22	4:D:916:SER:HB2	1.87	0.55
4:F:519:ILE:CB	4:F:999:ILE:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:510:SER:OG	4:I:513:GLU:OE2	2.21	0.55
4:K:198:ALA:HB2	4:K:215:ASP:OD1	2.06	0.55
1:A:391:ILE:HG13	1:A:392:ASN:N	2.21	0.55
2:B:523:ARG:NH1	2:B:524:ARG:O	2.39	0.55
4:F:235:VAL:HG11	4:F:530:THR:HA	1.88	0.55
4:H:852:GLN:O	4:H:996:GLN:NE2	2.40	0.55
4:I:504:LEU:HG	4:I:506:PRO:HD3	1.89	0.55
4:K:1079:ARG:HD3	4:L:428:ARG:NH1	2.21	0.55
4:E:948:TYR:HD2	4:E:1028:ALA:HB3	1.71	0.55
4:I:477:THR:O	4:I:480:GLU:HB2	2.07	0.55
4:I:1085:PHE:HD2	4:J:285:PHE:HD1	1.54	0.55
4:I:1213:ASN:HB2	4:I:1219:THR:HG22	1.87	0.55
4:J:956:ARG:HH11	4:J:956:ARG:HG3	1.71	0.55
4:K:1241:PRO:HG2	4:K:1244:GLN:HB2	1.88	0.55
1:A:77:LEU:HD23	1:A:169:TYR:HB2	1.88	0.55
1:A:493:GLY:O	1:A:497:GLN:HG2	2.07	0.55
4:G:941:THR:HG22	4:G:943:TYR:H	1.71	0.55
4:H:446:GLU:OE2	4:H:502:ASN:HB2	2.07	0.55
4:I:1093:MET:HE3	4:I:1102:VAL:N	2.22	0.55
4:J:514:ARG:NH1	4:J:727:PHE:O	2.40	0.55
4:K:689:MET:HA	4:K:689:MET:HE3	1.89	0.55
1:A:377:VAL:HG12	1:A:379:PRO:HD2	1.89	0.55
4:G:859:GLN:NE2	4:H:438:GLN:H	2.05	0.55
4:I:468:ARG:HB2	4:I:1019:VAL:HG11	1.88	0.55
4:L:1111:PRO:HG2	4:L:1114:LEU:HB2	1.89	0.55
4:M:1124:GLN:NE2	4:M:1124:GLN:O	2.40	0.55
1:A:248:ASP:OD2	4:D:254:ARG:NH2	2.40	0.55
4:D:576:SER:O	4:D:580:LYS:HG2	2.06	0.55
5:g:114:ASP:O	5:g:115:LYS:NZ	2.31	0.55
4:G:298:GLU:HG3	4:G:1215:SER:HB2	1.89	0.55
4:I:1112:LEU:HD22	4:I:1141:MET:HG2	1.88	0.55
5:k:160:ALA:HB2	4:L:400:GLU:HB2	1.89	0.55
4:K:468:ARG:HB2	4:K:1019:VAL:HG11	1.89	0.55
2:B:457:THR:OG1	3:C:1286:C:OP1	2.18	0.55
4:F:1245:ILE:HD12	4:F:1247:LEU:HD12	1.89	0.55
4:I:1115:TRP:HD1	4:I:1170:ILE:HG21	1.70	0.55
4:J:480:GLU:HG3	4:J:493:VAL:HG23	1.87	0.55
4:L:503:ARG:HD3	4:L:1265:PRO:HG3	1.89	0.55
4:L:524:ASN:OD1	4:L:525:ILE:N	2.40	0.55
1:A:368:CYS:SG	1:A:369:GLN:N	2.80	0.54
4:D:810:TYR:OH	4:D:818:GLU:OE1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:159:SER:OG	4:F:400:GLU:OE1	2.25	0.54
4:E:929:GLN:HG3	4:E:1015:MET:HE2	1.88	0.54
4:G:582:ARG:CD	6:N:6:U:H5"	2.31	0.54
4:I:433:ARG:HA	4:I:450:VAL:HG12	1.88	0.54
4:D:444:MET:HG2	5:m:139:VAL:HG11	1.89	0.54
4:G:523:MET:HG2	4:G:986:PRO:HB2	1.89	0.54
4:I:216:ILE:HB	4:I:218:ARG:HH11	1.71	0.54
4:J:435:ASP:OD1	4:J:436:ARG:N	2.40	0.54
4:J:670:THR:HG23	4:J:672:SER:H	1.71	0.54
4:K:553:PRO:CB	4:K:583:PRO:O	2.55	0.54
4:L:582:ARG:NH1	4:L:582:ARG:O	2.40	0.54
4:M:216:ILE:HD12	4:M:218:ARG:HB2	1.87	0.54
1:A:141:PRO:HA	1:A:144:MET:SD	2.48	0.54
4:K:860:PRO:O	4:L:439:MET:O	2.24	0.54
1:A:60:ILE:O	1:A:64:VAL:HG23	2.08	0.54
1:A:212:THR:HB	1:A:215:CYS:SG	2.48	0.54
1:A:555:ASN:ND2	1:A:559:ARG:HH21	1.97	0.54
2:B:96:ASN:ND2	2:B:263:SER:O	2.30	0.54
4:F:468:ARG:HB2	4:F:1019:VAL:HG11	1.89	0.54
4:I:664:MET:HA	4:I:664:MET:HE3	1.89	0.54
4:I:1147:MET:HE3	4:I:1149:HIS:NE2	2.23	0.54
4:L:224:ILE:O	4:L:584:SER:OG	2.24	0.54
4:M:941:THR:HG22	4:M:943:TYR:H	1.72	0.54
1:A:341:ARG:NH2	1:A:374:PRO:O	2.41	0.54
4:G:1084:SER:HB2	4:H:416:VAL:HG21	1.89	0.54
4:K:577:ILE:HD13	4:K:627:TRP:CE3	2.42	0.54
2:B:101:GLU:HG2	2:B:102:LEU:HD12	1.88	0.54
4:E:569:GLN:NE2	4:E:571:LEU:O	2.39	0.54
4:F:560:MET:HE2	4:F:577:ILE:HG21	1.90	0.54
4:I:1171:THR:OG1	4:I:1174:SER:HB3	2.08	0.54
5:k:129:ASN:ND2	5:k:132:GLU:OE1	2.40	0.54
4:K:1058:PRO:CG	4:K:1181:MET:O	2.52	0.54
4:M:454:SER:OG	4:M:1255:ASN:OD1	2.26	0.54
2:B:106:HIS:ND1	2:B:109:LEU:HB2	2.23	0.54
2:B:393:PRO:HG3	2:B:592:SER:HA	1.88	0.54
2:B:557:THR:OG1	2:B:732:GLN:OE1	2.20	0.54
2:B:914:MET:HE1	2:B:933:TYR:HA	1.90	0.54
4:G:665:ASP:OD2	4:G:686:ARG:NH1	2.37	0.54
4:I:309:ARG:NE	4:I:368:ASP:OD1	2.36	0.54
4:J:468:ARG:HB2	4:J:1019:VAL:HG11	1.90	0.54
4:J:581:LEU:HD12	4:J:884:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:852:GLN:O	4:J:996:GLN:NE2	2.40	0.54
4:K:295:PRO:HD3	4:K:411:MET:HE3	1.90	0.54
4:K:665:ASP:OD1	4:K:666:ASN:N	2.40	0.54
4:M:664:MET:HA	4:M:664:MET:HE3	1.90	0.54
1:A:99:ASP:OD2	1:A:101:ARG:CZ	2.54	0.54
4:D:428:ARG:O	4:D:428:ARG:HG2	2.07	0.54
4:E:656:MET:HE3	4:E:660:GLU:HB2	1.90	0.54
4:E:1147:MET:HE3	4:E:1149:HIS:NE2	2.21	0.54
4:F:446:GLU:OE2	4:F:502:ASN:HB2	2.07	0.54
4:K:1058:PRO:HD2	4:K:1182:VAL:HG22	1.90	0.54
4:J:222:GLU:HG3	4:J:582:ARG:HH22	1.73	0.54
4:J:522:ILE:O	4:J:525:ILE:HG22	2.08	0.54
4:M:1096:ASP:OD1	4:M:1097:GLU:N	2.40	0.54
4:E:749:ASN:OD1	4:E:750:VAL:N	2.41	0.53
4:G:765:ARG:NH1	4:G:801:LYS:O	2.40	0.53
4:H:439:MET:HA	4:H:439:MET:HE2	1.89	0.53
4:H:854:ARG:HB2	4:H:857:ILE:HD12	1.90	0.53
4:I:932:VAL:HG12	4:I:994:MET:HG3	1.90	0.53
4:J:920:ARG:NH2	4:J:981:ASP:OD1	2.42	0.53
4:M:216:ILE:HD13	4:M:218:ARG:HD2	1.87	0.53
1:A:300:MET:HG3	1:A:390:PHE:CE1	2.43	0.53
2:B:410:GLU:HB3	2:B:656:LYS:HZ1	1.73	0.53
2:B:1049:PHE:N	2:B:1054:GLU:OE1	2.40	0.53
4:F:581:LEU:HD12	4:F:884:VAL:HG22	1.89	0.53
4:I:732:LEU:HD13	4:I:999:ILE:HG21	1.89	0.53
4:D:855:ASP:HB3	4:E:756:ASP:HA	1.89	0.53
4:F:562:THR:HB	4:F:799:LYS:HZ1	1.73	0.53
4:H:504:LEU:HD23	4:H:506:PRO:HD3	1.89	0.53
4:H:664:MET:HE2	4:H:664:MET:HA	1.90	0.53
4:I:307:HIS:CE1	4:I:323:ILE:HD12	2.44	0.53
4:M:254:ARG:HB2	4:M:254:ARG:NH1	2.24	0.53
4:G:221:THR:HG22	4:G:1267:ILE:HB	1.91	0.53
4:G:391:LEU:HB3	4:G:407:TYR:HE2	1.72	0.53
4:I:674:ARG:H	4:J:492:THR:HG21	1.73	0.53
4:I:713:TRP:O	4:I:837:ARG:NH2	2.39	0.53
4:L:529:ALA:HB1	4:M:565:GLU:HB3	1.90	0.53
4:L:983:LEU:HG	4:L:984:LEU:HG	1.89	0.53
2:B:1151:GLN:HE22	4:D:585:ASN:ND2	2.06	0.53
4:K:577:ILE:HD13	4:K:627:TRP:CD2	2.44	0.53
4:M:625:ASN:HB3	4:M:655:MET:HE3	1.90	0.53
1:A:431:ILE:HG13	1:A:432:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:HIS:HE2	7:A:800:PO4:P	2.26	0.53
4:G:474:ILE:HD11	4:G:508:ARG:HB2	1.91	0.53
4:G:508:ARG:HH11	4:G:508:ARG:HG3	1.73	0.53
4:H:435:ASP:OD1	4:H:436:ARG:N	2.41	0.53
4:I:665:ASP:OD2	4:I:666:ASN:N	2.42	0.53
4:L:218:ARG:O	4:L:221:THR:OG1	2.23	0.53
4:L:242:LYS:CE	6:R:34:U:P	2.97	0.53
1:A:101:ARG:NH2	1:A:101:ARG:HB2	2.24	0.53
2:B:528:ILE:HD13	3:C:1285:G:C5	2.44	0.53
4:D:518:GLN:NE2	4:D:829:PRO:HG2	2.23	0.53
4:G:946:ASP:OD1	4:G:946:ASP:N	2.38	0.53
4:H:649:PHE:HA	4:H:705:TRP:HE1	1.73	0.53
4:I:630:PHE:HD2	4:I:772:MET:HE1	1.73	0.53
4:L:529:ALA:HB2	4:L:873:VAL:HG21	1.90	0.53
2:B:743:THR:HG23	2:B:745:ALA:H	1.74	0.53
4:E:949:LEU:HD12	4:E:952:ILE:HG13	1.90	0.53
4:F:439:MET:HE3	4:F:439:MET:HA	1.91	0.53
4:G:650:MET:HG2	4:G:678:PHE:CE1	2.44	0.53
4:H:224:ILE:HA	4:H:227:TRP:HD1	1.74	0.53
4:K:355:ARG:O	4:K:359:LEU:HD23	2.09	0.53
1:A:299:ASP:OD1	1:A:392:ASN:ND2	2.27	0.53
1:A:442:VAL:HG12	1:A:525:LEU:HB3	1.91	0.53
2:B:1085:ASN:O	2:B:1088:PRO:HD2	2.09	0.53
4:D:435:ASP:OD1	4:D:436:ARG:N	2.41	0.53
4:E:1112:LEU:HD21	4:E:1175:ILE:HD12	1.90	0.53
4:G:360:HIS:NE2	4:G:364:GLU:OE2	2.42	0.53
4:G:667:GLN:HG3	4:G:668:ILE:HD12	1.90	0.53
4:G:732:LEU:HD13	4:G:999:ILE:HG21	1.90	0.53
4:J:1025:GLN:NE2	4:J:1029:GLU:OE2	2.42	0.53
4:K:870:THR:HG22	4:K:871:VAL:H	1.73	0.53
4:L:243:LYS:NZ	4:M:561:SER:O	2.37	0.53
4:M:458:THR:HA	4:M:461:ILE:HD12	1.91	0.53
1:A:419:LYS:HD2	7:A:800:PO4:P	2.50	0.52
4:E:398:ASP:O	4:E:401:LYS:NZ	2.26	0.52
4:G:763:ASN:OD1	4:G:767:ARG:NH1	2.42	0.52
4:H:251:ASP:HB2	4:H:979:LEU:HD13	1.90	0.52
4:J:710:HIS:O	4:J:837:ARG:NH2	2.33	0.52
4:F:560:MET:HE2	4:F:577:ILE:CG2	2.40	0.52
4:J:223:PHE:CE2	4:J:583:PRO:HG3	2.44	0.52
4:K:1085:PHE:CD2	4:L:285:PHE:HD1	2.27	0.52
2:B:856:ILE:HB	2:B:859:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1027:THR:OG1	2:B:1030:GLU:OE1	2.18	0.52
5:g:116:SER:HB3	6:N:4:U:H4'	1.90	0.52
4:J:679:SER:HB3	4:K:788:SER:HB2	1.90	0.52
4:K:1111:PRO:HD2	4:K:1114:LEU:HD12	1.92	0.52
4:L:782:GLN:HG3	4:L:783:PRO:HD3	1.92	0.52
2:B:307:LYS:NZ	2:B:1100:GLN:OE1	2.39	0.52
4:E:849:VAL:O	4:E:863:SER:OG	2.27	0.52
4:F:855:ASP:N	4:F:855:ASP:OD1	2.41	0.52
4:H:1120:ARG:HG2	4:H:1120:ARG:HH11	1.75	0.52
4:I:518:GLN:O	4:I:522:ILE:HG12	2.09	0.52
4:J:577:ILE:HD13	4:J:627:TRP:CE3	2.43	0.52
4:J:1116:GLN:HB3	4:J:1172:PRO:HA	1.90	0.52
4:L:419:ILE:HG13	4:L:420:CYS:N	2.24	0.52
4:L:638:LEU:HD11	4:L:886:LEU:HD21	1.90	0.52
4:M:569:GLN:HA	4:M:569:GLN:OE1	2.09	0.52
4:E:510:SER:OG	4:E:513:GLU:OE2	2.25	0.52
4:E:523:MET:HG2	4:E:986:PRO:HB2	1.92	0.52
5:g:116:SER:HB2	6:N:4:U:H4'	1.87	0.52
4:G:224:ILE:HG22	4:G:231:PRO:HB3	1.92	0.52
4:H:823:ALA:HA	4:H:826:LEU:HD23	1.91	0.52
4:J:1147:MET:HE3	4:J:1149:HIS:NE2	2.24	0.52
5:k:127:ILE:HD11	4:K:607:VAL:HG11	1.91	0.52
4:K:237:ALA:HA	4:K:247:LEU:HD12	1.92	0.52
1:A:538:ASN:ND2	2:B:676:MET:O	2.37	0.52
2:B:702:PHE:HB2	2:B:763:TYR:CE2	2.45	0.52
2:B:1081:ILE:HG23	2:B:1088:PRO:HB2	1.91	0.52
4:D:1168:GLU:HB3	5:e:50:ARG:HG3	1.91	0.52
4:F:823:ALA:HA	4:F:826:LEU:HD23	1.91	0.52
4:F:1166:TRP:CD1	4:F:1176:PRO:HG2	2.45	0.52
5:g:82:ASP:OD2	5:g:86:ASN:N	2.37	0.52
4:H:855:ASP:OD1	4:H:856:THR:N	2.43	0.52
4:I:859:GLN:OE1	4:I:860:PRO:HD2	2.10	0.52
4:J:275:GLN:O	4:J:278:GLN:NE2	2.36	0.52
4:J:946:ASP:OD2	4:J:1025:GLN:NE2	2.34	0.52
4:L:242:LYS:HE3	6:R:33:A:O3'	2.09	0.52
1:A:101:ARG:NH2	1:A:121:LEU:HD21	2.25	0.52
4:E:1084:SER:HB2	4:F:416:VAL:HG21	1.91	0.52
4:H:270:PRO:HG3	4:H:297:PRO:HB3	1.92	0.52
4:K:605:THR:HG21	4:K:870:THR:HG21	1.92	0.52
4:M:1163:THR:HG22	4:M:1199:ILE:HD12	1.91	0.52
4:D:851:ARG:NH1	4:D:986:PRO:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:511:ASN:OD1	4:E:729:SER:N	2.40	0.52
4:G:480:GLU:OE1	4:G:494:THR:HA	2.09	0.52
4:H:711:ARG:HD2	4:H:712:TYR:CE1	2.45	0.52
4:I:1085:PHE:CD2	4:J:285:PHE:HD1	2.27	0.52
4:J:823:ALA:HA	4:J:826:LEU:HD23	1.91	0.52
4:K:219:HIS:ND1	4:K:222:GLU:OE2	2.32	0.52
1:A:113:ARG:HG3	1:A:114:LYS:HD2	1.91	0.52
1:A:660:TRP:CD1	1:A:731:PHE:HB2	2.45	0.52
2:B:186:PRO:HB2	2:B:237:ALA:HB2	1.92	0.52
2:B:814:TRP:O	2:B:817:ILE:HG22	2.10	0.52
4:D:472:MET:HE2	4:D:506:PRO:HB2	1.91	0.52
4:E:724:PRO:HG3	4:E:737:GLU:HG3	1.92	0.52
4:E:805:SER:OG	4:E:886:LEU:O	2.19	0.52
4:E:1079:ARG:HH11	4:F:428:ARG:NH1	2.08	0.52
4:F:598:TRP:O	4:F:832:GLN:NE2	2.43	0.52
4:H:544:GLN:CD	4:H:592:ARG:HE	2.18	0.52
4:H:679:SER:HB3	4:I:788:SER:HB2	1.92	0.52
4:H:821:VAL:HG11	4:H:905:ILE:HD12	1.91	0.52
4:I:1051:GLN:HG3	4:I:1196:VAL:HG22	1.92	0.52
2:B:514:SER:OG	2:B:515:MET:N	2.43	0.52
1:A:557:MET:HA	1:A:566:GLU:HB3	1.92	0.51
2:B:1090:LEU:HD12	2:B:1236:VAL:HG12	1.92	0.51
2:B:1222:LEU:HA	2:B:1225:LEU:HD13	1.92	0.51
4:D:360:HIS:NE2	4:D:364:GLU:OE2	2.44	0.51
4:E:667:GLN:HG3	4:E:668:ILE:HD12	1.91	0.51
4:E:694:ILE:O	4:E:703:ARG:NH1	2.43	0.51
4:F:560:MET:HE2	4:F:574:ALA:HA	1.91	0.51
4:L:691:ILE:O	4:L:703:ARG:NH1	2.43	0.51
4:E:992:PRO:O	4:E:994:MET:HG2	2.10	0.51
4:H:1147:MET:HE3	4:H:1149:HIS:NE2	2.25	0.51
4:I:1034:GLU:OE2	4:I:1207:ARG:NH2	2.39	0.51
4:K:1085:PHE:CD2	4:L:285:PHE:CD1	2.98	0.51
4:K:1085:PHE:HD2	4:L:285:PHE:CD1	2.27	0.51
4:E:1096:ASP:OD1	4:E:1097:GLU:N	2.36	0.51
4:G:1233:ASN:HB2	4:G:1246:GLN:HE22	1.76	0.51
4:D:1079:ARG:HG2	4:E:1275:PRO:HG2	1.92	0.51
4:D:1116:GLN:HB3	4:D:1172:PRO:HA	1.92	0.51
4:I:535:VAL:O	4:I:539:ILE:HG12	2.11	0.51
4:K:344:LEU:HB2	4:K:1171:THR:HG21	1.91	0.51
1:A:391:ILE:HG13	1:A:392:ASN:H	1.75	0.51
4:D:518:GLN:O	4:D:522:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:549:LEU:HD21	4:D:807:THR:HG22	1.91	0.51
4:H:255:LEU:HD21	4:H:923:ILE:HD11	1.93	0.51
4:H:543:LEU:HA	4:H:546:ILE:HG22	1.92	0.51
4:J:570:THR:OG1	4:L:565:GLU:O	2.16	0.51
4:M:1052:SER:OG	4:M:1053:THR:N	2.43	0.51
4:G:815:ALA:HA	4:G:818:GLU:OE2	2.11	0.51
4:H:398:ASP:OD2	4:H:401:LYS:NZ	2.31	0.51
4:H:589:SER:O	4:H:593:VAL:HG23	2.11	0.51
4:J:691:ILE:HD11	4:J:710:HIS:CD2	2.45	0.51
4:J:1112:LEU:HD23	4:J:1116:GLN:HG3	1.92	0.51
4:L:435:ASP:OD1	4:L:436:ARG:N	2.43	0.51
4:M:218:ARG:HH21	4:M:239:VAL:HG21	1.75	0.51
1:A:610:ASP:O	1:A:614:THR:HG22	2.11	0.51
2:B:427:ARG:O	2:B:431:LEU:HG	2.10	0.51
2:B:822:MET:HE2	2:B:873:TRP:HB3	1.93	0.51
4:E:818:GLU:OE1	4:E:901:TYR:OH	2.26	0.51
4:H:582:ARG:O	4:H:880:ARG:NH1	2.44	0.51
4:I:346:VAL:HG23	4:I:347:ARG:HD3	1.92	0.51
4:I:1116:GLN:NE2	4:I:1171:THR:O	2.43	0.51
2:B:53:ASP:OD1	2:B:54:ASP:N	2.43	0.51
4:F:256:VAL:HG11	4:F:1264:THR:HG21	1.93	0.51
4:H:1067:PHE:O	4:H:1138:ARG:NH1	2.43	0.51
4:I:1093:MET:HE1	4:I:1103:PRO:HD3	1.91	0.51
4:K:466:MET:HE1	4:K:1262:TYR:CE2	2.43	0.51
4:L:525:ILE:HD11	4:L:532:ILE:HD13	1.93	0.51
4:M:216:ILE:HD12	4:M:218:ARG:H	1.76	0.51
2:B:744:THR:HA	4:F:545:ARG:HG2	1.92	0.51
4:D:262:LEU:HD21	4:D:406:MET:SD	2.51	0.51
4:E:338:LEU:O	4:E:340:ASN:N	2.44	0.51
4:H:656:MET:HB3	4:H:660:GLU:HB2	1.93	0.51
4:K:1151:TYR:CD2	4:K:1181:MET:HG2	2.46	0.51
4:K:1213:ASN:HB3	4:K:1216:SER:OG	2.10	0.51
4:L:563:VAL:HG11	4:L:574:ALA:HB2	1.93	0.51
1:A:306:ASP:HB3	1:A:313:ASN:HB2	1.93	0.51
1:A:531:ASP:OD1	1:A:581:THR:OG1	2.27	0.51
4:D:638:LEU:HD11	4:D:886:LEU:HD21	1.93	0.51
4:I:649:PHE:HA	4:I:705:TRP:HE1	1.75	0.51
4:J:1229:VAL:HG13	4:J:1236:THR:HG21	1.93	0.51
4:L:1062:PRO:HG2	4:L:1065:LEU:HD12	1.92	0.51
1:A:5:ALA:HA	1:A:205:GLY:O	2.11	0.50
1:A:260:ARG:CZ	5:m:91:LEU:HD11	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:HH12	1:A:721:ARG:NH2	2.10	0.50
4:D:380:GLN:OE1	4:M:958:SER:HB3	2.11	0.50
4:E:1233:ASN:HB2	4:E:1246:GLN:HE22	1.76	0.50
4:F:998:ALA:O	4:F:999:ILE:HG13	2.11	0.50
4:J:392:ARG:NH1	4:J:452:GLU:OE2	2.44	0.50
4:J:1034:GLU:OE2	4:J:1207:ARG:NH1	2.43	0.50
4:L:689:MET:HE1	4:L:840:ARG:NE	2.25	0.50
2:B:297:LEU:HD23	2:B:310:TYR:HA	1.93	0.50
2:B:524:ARG:HG2	2:B:524:ARG:HH11	1.75	0.50
2:B:554:ASN:ND2	2:B:556:SER:OG	2.44	0.50
2:B:629:ASP:OD1	2:B:639:ARG:NH1	2.44	0.50
4:D:669:TYR:HA	4:D:673:ARG:HG3	1.94	0.50
4:F:656:MET:HE1	4:F:701:ILE:HB	1.93	0.50
4:G:582:ARG:CD	6:N:6:U:H5'	2.37	0.50
4:J:577:ILE:HD13	4:J:627:TRP:CD2	2.46	0.50
4:K:929:GLN:HB2	4:K:1015:MET:HE2	1.93	0.50
4:M:660:GLU:HG3	4:M:699:ALA:HA	1.92	0.50
1:A:397:ASP:OD1	1:A:399:MET:N	2.44	0.50
2:B:336:GLU:OE1	6:P:12:U:H5'	2.11	0.50
2:B:589:CYS:SG	2:B:691:HIS:HD2	2.34	0.50
4:D:660:GLU:OE1	4:D:699:ALA:HA	2.11	0.50
4:H:514:ARG:NH1	4:H:727:PHE:O	2.44	0.50
4:I:511:ASN:OD1	4:I:729:SER:N	2.45	0.50
4:J:711:ARG:HH11	4:J:711:ARG:HG3	1.76	0.50
4:K:352:LEU:HD23	4:K:955:LEU:HB3	1.92	0.50
2:B:397:VAL:HB	2:B:766:GLU:HB2	1.93	0.50
2:B:706:TRP:CZ3	2:B:763:TYR:HB2	2.46	0.50
4:D:285:PHE:HB2	4:M:1085:PHE:HE2	0.76	0.50
4:E:858:THR:OG1	4:E:859:GLN:N	2.44	0.50
5:g:77:ASP:OD1	5:g:80:THR:OG1	2.29	0.50
4:G:656:MET:O	4:G:656:MET:HG3	2.11	0.50
5:k:156:GLU:OE2	4:L:400:GLU:N	2.44	0.50
4:M:656:MET:HG3	4:M:660:GLU:HB3	1.94	0.50
4:M:1160:TRP:CE2	4:M:1164:SER:HB2	2.46	0.50
4:G:507:TYR:CE2	4:G:915:PHE:HB3	2.46	0.50
4:I:303:ARG:NH1	4:I:1208:SER:OG	2.45	0.50
4:K:576:SER:O	4:K:580:LYS:HG2	2.12	0.50
4:K:859:GLN:NE2	4:L:437:ALA:HA	2.26	0.50
4:D:495:SER:CA	5:m:128:ASN:ND2	2.74	0.50
4:D:854:ARG:NH1	4:D:866:THR:OG1	2.44	0.50
4:F:756:ASP:OD1	4:F:757:PHE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:584:SER:O	4:H:585:ASN:CG	2.54	0.50
4:I:1095:ARG:HB2	4:I:1101:MET:HE1	1.94	0.50
4:I:1166:TRP:CD1	4:I:1176:PRO:HG2	2.47	0.50
4:M:391:LEU:HB3	4:M:407:TYR:HE2	1.76	0.50
4:M:721:TYR:CD1	4:M:739:LEU:HB2	2.46	0.50
4:M:1166:TRP:CD1	4:M:1176:PRO:HG2	2.47	0.50
1:A:285:ARG:HD2	1:A:290:VAL:HG22	1.92	0.50
2:B:54:ASP:N	2:B:54:ASP:OD1	2.43	0.50
4:E:518:GLN:HE21	4:E:831:PHE:HB2	1.76	0.50
4:F:1068:ASP:N	4:F:1068:ASP:OD1	2.41	0.50
4:G:955:LEU:HD23	4:G:955:LEU:H	1.76	0.50
4:H:629:PHE:CD2	4:H:772:MET:HE2	2.47	0.50
4:J:446:GLU:OE1	4:J:502:ASN:ND2	2.42	0.50
4:K:1059:LEU:N	4:K:1059:LEU:HD23	2.27	0.50
4:M:511:ASN:OD1	4:M:729:SER:N	2.44	0.50
2:B:569:PRO:HA	2:B:572:VAL:HG12	1.94	0.50
2:B:934:ARG:O	2:B:938:ASN:ND2	2.45	0.50
4:D:913:GLU:O	4:D:916:SER:OG	2.27	0.50
5:g:116:SER:OG	6:N:4:U:H4'	2.10	0.50
4:L:740:LEU:H	4:L:832:GLN:NE2	2.10	0.50
4:L:920:ARG:NH1	4:L:981:ASP:OD2	2.35	0.50
5:m:56:ARG:N	4:M:903:ASP:OD1	2.39	0.50
4:G:260:ALA:O	4:G:392:ARG:NH2	2.45	0.50
1:A:73:VAL:HG21	1:A:167:LEU:HD23	1.94	0.49
1:A:655:LEU:HA	1:A:658:LYS:HD2	1.94	0.49
4:D:577:ILE:HD13	4:D:627:TRP:CE3	2.46	0.49
4:D:939:SER:OG	4:D:940:GLU:N	2.45	0.49
4:E:323:ILE:O	4:E:334:LEU:HD21	2.12	0.49
4:I:884:VAL:O	4:I:888:SER:OG	2.28	0.49
4:K:1085:PHE:CE2	4:L:285:PHE:HB2	2.47	0.49
4:L:521:ARG:HD2	4:L:828:PHE:CD1	2.47	0.49
4:L:660:GLU:OE2	4:L:699:ALA:HA	2.12	0.49
1:A:132:ALA:HB3	1:A:133:PRO:HD3	1.93	0.49
1:A:474:ASP:HB3	1:A:478:LYS:NZ	2.27	0.49
2:B:148:LYS:HG2	2:B:803:LYS:HB2	1.94	0.49
4:E:1093:MET:HB3	4:E:1101:MET:HB3	1.93	0.49
4:G:413:THR:HG22	4:G:423:VAL:HG13	1.92	0.49
4:H:525:ILE:HD11	4:H:532:ILE:HD13	1.93	0.49
4:I:1093:MET:HE3	4:I:1102:VAL:C	2.36	0.49
4:J:350:ASN:HB3	4:J:353:MET:HG2	1.94	0.49
2:B:1049:PHE:CG	2:B:1053:LEU:HD23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:385:PHE:CD1	5:m:161:ILE:HG12	2.47	0.49
4:F:234:GLN:O	4:F:236:SER:N	2.45	0.49
4:F:560:MET:CE	4:F:574:ALA:HA	2.42	0.49
1:A:249:ILE:HD12	1:A:254:VAL:HG22	1.95	0.49
2:B:107:GLU:O	2:B:108:THR:OG1	2.29	0.49
5:g:140:ASP:HB3	5:g:146:ASN:HD21	1.78	0.49
4:M:216:ILE:CD1	4:M:218:ARG:CB	2.90	0.49
1:A:419:LYS:HD2	7:A:800:PO4:O2	2.12	0.49
1:A:557:MET:HE3	1:A:570:LEU:HD21	1.95	0.49
4:E:752:THR:HB	4:E:809:MET:HE2	1.94	0.49
4:G:234:GLN:NE2	4:G:247:LEU:O	2.42	0.49
4:G:392:ARG:NH1	4:G:452:GLU:OE1	2.45	0.49
4:G:582:ARG:NE	6:N:6:U:H5'	2.27	0.49
4:G:851:ARG:HB3	4:G:994:MET:HE3	1.93	0.49
4:I:931:LEU:HD22	4:I:984:LEU:HD23	1.93	0.49
4:L:630:PHE:HB2	4:L:772:MET:HE1	1.94	0.49
5:m:75:ASN:ND2	5:m:77:ASP:OD1	2.44	0.49
1:A:556:LEU:HD12	1:A:570:LEU:HD13	1.94	0.49
1:A:655:LEU:HD11	1:A:697:VAL:O	2.12	0.49
4:D:691:ILE:HD11	4:D:710:HIS:CD2	2.48	0.49
5:g:102:ALA:O	5:g:106:THR:HG23	2.13	0.49
4:J:991:ASP:H	4:K:804:LYS:CE	2.25	0.49
1:A:41:ASP:OD1	1:A:42:TYR:N	2.45	0.49
2:B:141:GLU:HG3	2:B:214:VAL:HG12	1.94	0.49
2:B:1106:PHE:CZ	2:B:1185:MET:HE1	2.48	0.49
4:E:560:MET:HE1	4:E:796:THR:HG23	1.93	0.49
4:F:524:ASN:OD1	4:F:525:ILE:N	2.45	0.49
4:G:713:TRP:HB3	4:G:837:ARG:NH2	2.27	0.49
4:H:244:THR:HG22	4:H:531:VAL:HA	1.95	0.49
4:J:670:THR:HG21	4:L:754:THR:OG1	2.13	0.49
4:K:571:LEU:O	4:K:571:LEU:HD23	2.12	0.49
4:L:307:HIS:CE1	4:L:323:ILE:HD12	2.48	0.49
4:E:392:ARG:NH1	4:E:452:GLU:OE2	2.45	0.49
4:I:475:ASN:ND2	4:I:478:GLU:OE1	2.45	0.49
4:L:577:ILE:HD13	4:L:627:TRP:CD2	2.48	0.49
5:i:69:ALA:HA	4:I:538:ASP:OD2	2.13	0.49
4:K:1166:TRP:CD1	4:K:1176:PRO:HG2	2.48	0.49
4:L:958:SER:H	4:L:961:THR:HG22	1.78	0.49
4:M:776:VAL:HA	4:M:782:GLN:HE22	1.78	0.49
1:A:402:ILE:HG13	1:A:402:ILE:O	2.13	0.49
2:B:56:MET:HE1	2:B:188:TRP:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:687:THR:O	2:B:691:HIS:ND1	2.25	0.49
4:E:665:ASP:OD1	4:E:665:ASP:N	2.44	0.49
4:E:1169:GLU:HB2	4:E:1176:PRO:HG3	1.95	0.49
5:g:110:ALA:HB2	5:g:118:ALA:HB2	1.95	0.49
4:H:486:CYS:SG	4:H:909:TYR:OH	2.59	0.49
4:H:650:MET:HG2	4:H:678:PHE:CE1	2.47	0.49
4:H:1150:TYR:HB3	4:H:1184:ILE:HD11	1.95	0.49
4:I:752:THR:HB	4:I:809:MET:HE2	1.95	0.49
4:K:507:TYR:CD2	4:K:915:PHE:HB3	2.48	0.49
4:M:1101:MET:HA	4:M:1101:MET:HE3	1.95	0.49
1:A:307:VAL:O	1:A:307:VAL:HG12	2.12	0.48
2:B:57:LEU:HD23	2:B:188:TRP:HZ3	1.78	0.48
2:B:408:ILE:HD11	2:B:631:SER:OG	2.13	0.48
4:F:577:ILE:O	4:F:581:LEU:HD23	2.12	0.48
5:i:142:GLU:HG3	4:J:433:ARG:HH12	1.78	0.48
1:A:173:LYS:O	1:A:173:LYS:HD3	2.13	0.48
4:D:1068:ASP:N	4:D:1068:ASP:OD1	2.45	0.48
4:H:951:TRP:CD1	4:H:951:TRP:H	2.30	0.48
5:i:150:MET:O	5:i:154:ILE:HG12	2.12	0.48
4:K:1068:ASP:OD1	4:K:1071:THR:OG1	2.24	0.48
4:M:649:PHE:HA	4:M:705:TRP:HE1	1.77	0.48
1:A:342:GLN:HG2	1:A:344:ASP:H	1.78	0.48
2:B:890:TRP:H	2:B:890:TRP:HE3	1.58	0.48
4:G:190:LEU:HD13	4:G:196:LEU:HA	1.94	0.48
2:B:269:PHE:O	2:B:273:THR:HG22	2.13	0.48
2:B:1167:VAL:HG23	2:B:1172:LEU:HB2	1.96	0.48
4:D:951:TRP:CD1	4:D:951:TRP:H	2.31	0.48
5:e:131:ASN:OD1	4:F:500:SER:HA	2.13	0.48
4:E:354:PHE:HE1	4:E:1145:PRO:HD3	1.77	0.48
4:I:528:ASN:OD1	4:I:531:VAL:N	2.47	0.48
4:J:807:THR:HG23	4:J:889:GLY:HA3	1.95	0.48
4:K:398:ASP:O	4:K:401:LYS:HG2	2.13	0.48
2:B:890:TRP:CH2	2:B:1088:PRO:HG3	2.48	0.48
2:B:1069:PRO:HB2	4:F:585:ASN:OD1	2.13	0.48
4:K:752:THR:HB	4:K:809:MET:HE2	1.94	0.48
4:K:1229:VAL:HG13	4:K:1236:THR:HG21	1.95	0.48
4:L:223:PHE:CE2	4:L:583:PRO:HD2	2.44	0.48
4:F:570:THR:OG1	4:H:565:GLU:O	2.27	0.48
4:I:861:ALA:HB1	4:J:441:ASN:HB2	1.95	0.48
4:J:622:SER:HB2	4:L:562:THR:HG21	1.96	0.48
4:J:961:THR:HG22	4:K:893:PRO:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1126:PHE:O	4:J:1130:ILE:HG12	2.13	0.48
4:M:321:SER:HA	4:M:368:ASP:OD2	2.14	0.48
4:D:510:SER:OG	4:D:513:GLU:OE1	2.29	0.48
4:F:287:THR:HG22	4:F:292:ILE:HB	1.95	0.48
5:k:53:TYR:OH	4:K:903:ASP:OD2	2.31	0.48
4:K:351:PRO:HA	4:K:354:PHE:CD2	2.49	0.48
4:K:859:GLN:HG2	4:L:438:GLN:HB3	1.96	0.48
4:M:707:GLU:OE2	4:M:711:ARG:NH2	2.47	0.48
2:B:598:PHE:O	2:B:602:ILE:HD12	2.14	0.48
5:e:56:ARG:NH2	4:E:894:ASP:OD2	2.45	0.48
4:H:507:TYR:CD2	4:H:915:PHE:HB3	2.49	0.48
4:D:495:SER:HA	5:m:128:ASN:ND2	2.29	0.48
4:D:576:SER:OG	4:D:627:TRP:NE1	2.46	0.48
4:E:951:TRP:CD1	4:E:951:TRP:H	2.31	0.48
4:G:511:ASN:OD1	4:G:729:SER:N	2.47	0.48
4:H:853:SER:OG	4:H:857:ILE:O	2.31	0.48
4:K:1131:LYS:HD2	4:K:1160:TRP:CE2	2.49	0.48
1:A:438:PRO:HG2	1:A:441:HIS:CG	2.49	0.48
2:B:282:LEU:HD22	2:B:369:MET:HE1	1.95	0.48
2:B:551:TYR:HD1	2:B:552:HIS:CD2	2.32	0.48
4:D:1266:PRO:HG2	4:D:1269:ALA:HB2	1.96	0.48
4:E:598:TRP:O	4:E:832:GLN:NE2	2.37	0.48
4:F:241:ASN:HD22	4:G:563:VAL:HG11	1.79	0.48
4:F:609:ASP:OD2	4:F:610:ASP:N	2.46	0.48
4:H:1233:ASN:HB2	4:H:1246:GLN:HE22	1.78	0.48
4:I:926:GLU:HG2	4:I:1020:ILE:HD12	1.96	0.48
4:J:261:GLY:HA2	4:J:394:LEU:HD11	1.96	0.48
4:J:560:MET:HE2	4:J:577:ILE:HG21	1.94	0.48
4:J:951:TRP:CD1	4:J:951:TRP:H	2.32	0.48
4:K:570:THR:OG1	4:K:571:LEU:N	2.47	0.48
4:L:247:LEU:HD11	4:L:525:ILE:HD12	1.95	0.48
4:L:560:MET:HE2	4:L:560:MET:HA	1.96	0.48
4:M:382:HIS:ND1	4:M:387:GLU:OE2	2.46	0.48
4:M:504:LEU:HG	4:M:506:PRO:HD3	1.96	0.48
4:M:511:ASN:O	4:M:515:GLN:HG3	2.14	0.48
1:A:214:LYS:HA	1:A:247:ASN:ND2	2.29	0.47
4:D:1112:LEU:HD23	4:D:1116:GLN:HG3	1.96	0.47
4:E:1036:ASN:HB2	4:E:1207:ARG:HB2	1.96	0.47
4:F:951:TRP:H	4:F:951:TRP:CD1	2.31	0.47
4:G:508:ARG:HG3	4:G:508:ARG:NH1	2.29	0.47
4:I:1093:MET:HE1	4:I:1103:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1131:LYS:HD2	4:I:1160:TRP:CE2	2.49	0.47
4:K:859:GLN:HE21	4:L:438:GLN:N	2.11	0.47
4:L:825:MET:HE3	4:L:909:TYR:OH	2.13	0.47
2:B:497:LEU:HA	2:B:500:LEU:HD12	1.96	0.47
4:F:822:ILE:HG22	4:F:826:LEU:HD21	1.96	0.47
5:g:3:ARG:NH1	4:G:314:VAL:O	2.47	0.47
5:g:128:ASN:HD22	4:H:494:THR:C	2.22	0.47
4:H:1111:PRO:HG2	4:H:1114:LEU:HB2	1.95	0.47
4:I:983:LEU:HD23	4:I:984:LEU:HD13	1.96	0.47
4:J:609:ASP:OD1	4:J:610:ASP:N	2.47	0.47
4:M:435:ASP:OD1	4:M:436:ARG:N	2.46	0.47
4:M:960:ALA:O	4:M:964:THR:HG23	2.14	0.47
2:B:890:TRP:HH2	2:B:1088:PRO:HD3	1.80	0.47
4:E:566:SER:OG	4:E:569:GLN:NE2	2.47	0.47
4:E:650:MET:HG2	4:E:678:PHE:CE1	2.50	0.47
4:F:1229:VAL:HG13	4:F:1236:THR:HG21	1.96	0.47
4:H:560:MET:HG3	4:H:578:LEU:HD21	1.95	0.47
4:I:1211:CYS:SG	4:I:1212:THR:N	2.88	0.47
5:k:145:SER:N	4:L:444:MET:CE	2.77	0.47
5:k:161:ILE:HD11	4:L:385:PHE:CG	2.49	0.47
4:K:473:ASN:OD1	4:K:474:ILE:N	2.48	0.47
4:K:1002:GLN:HG2	4:K:1003:GLN:O	2.14	0.47
4:K:1034:GLU:OE2	4:K:1207:ARG:NH2	2.34	0.47
4:K:1117:MET:CE	4:L:385:PHE:HA	2.44	0.47
5:m:50:ARG:O	5:m:52:GLN:NE2	2.47	0.47
2:B:947:TYR:OH	2:B:1048:SER:O	2.28	0.47
4:E:518:GLN:OE1	4:E:829:PRO:HG2	2.14	0.47
4:F:340:ASN:OD1	4:F:343:THR:OG1	2.32	0.47
4:F:650:MET:HG2	4:F:678:PHE:CE1	2.49	0.47
4:H:555:ILE:HG22	4:H:803:ILE:HD11	1.96	0.47
2:B:410:GLU:HB3	2:B:656:LYS:NZ	2.29	0.47
2:B:509:ILE:HG13	2:B:510:LEU:HD22	1.97	0.47
2:B:956:LYS:HA	2:B:956:LYS:HE3	1.95	0.47
5:e:84:LYS:HB3	5:e:84:LYS:HE2	1.69	0.47
5:e:129:ASN:ND2	5:e:132:GLU:OE1	2.48	0.47
4:G:473:ASN:OD1	4:G:474:ILE:N	2.48	0.47
4:H:556:ILE:HD11	4:H:888:SER:HB3	1.95	0.47
4:J:783:PRO:HB3	4:L:794:ARG:HH21	1.78	0.47
4:K:983:LEU:HG	4:K:984:LEU:HD13	1.96	0.47
5:m:75:ASN:OD1	5:m:76:ASN:N	2.48	0.47
1:A:668:ILE:HD11	1:A:684:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:PHE:CD2	2:B:620:MET:HG2	2.50	0.47
4:D:261:GLY:O	4:D:1259:ARG:NH2	2.48	0.47
4:D:530:THR:HG22	4:E:567:THR:HG22	1.96	0.47
4:F:315:ASP:OD1	4:F:316:PHE:N	2.47	0.47
4:G:1079:ARG:HG2	4:H:428:ARG:NH1	2.29	0.47
4:H:518:GLN:NE2	4:H:829:PRO:HG2	2.29	0.47
4:I:1093:MET:HE1	4:I:1103:PRO:N	2.29	0.47
4:K:649:PHE:HA	4:K:705:TRP:HE1	1.80	0.47
1:A:10:VAL:HG11	1:A:205:GLY:HA2	1.97	0.47
4:D:252:THR:CG2	4:D:916:SER:HB2	2.45	0.47
5:e:152:THR:O	5:e:156:GLU:HG3	2.14	0.47
4:F:1116:GLN:HB3	4:F:1172:PRO:HA	1.97	0.47
4:G:220:ILE:HG22	4:G:221:THR:HG23	1.97	0.47
4:G:948:TYR:CE1	4:G:1029:GLU:HB2	2.50	0.47
4:H:551:ILE:HD13	4:H:588:PHE:CD1	2.50	0.47
4:I:955:LEU:H	4:I:955:LEU:HD23	1.79	0.47
4:I:1104:PHE:CE1	4:I:1126:PHE:HE1	2.31	0.47
4:J:599:LEU:HD22	4:J:739:LEU:HD11	1.96	0.47
4:J:1165:ALA:O	4:J:1169:GLU:HG3	2.15	0.47
5:k:161:ILE:HD11	4:L:385:PHE:CE2	2.49	0.47
4:K:861:ALA:HA	4:L:439:MET:O	2.15	0.47
4:M:215:ASP:HB3	4:M:219:HIS:NE2	2.29	0.47
4:M:656:MET:CG	4:M:660:GLU:HB3	2.45	0.47
2:B:172:LEU:HB3	2:B:174:LYS:HG2	1.96	0.47
4:D:285:PHE:HA	4:M:1085:PHE:CE2	2.50	0.47
4:D:374:ARG:HD3	4:D:375:HIS:H	1.79	0.47
4:E:732:LEU:HD13	4:E:999:ILE:HG21	1.97	0.47
4:E:763:ASN:OD1	4:E:767:ARG:NH1	2.48	0.47
4:G:398:ASP:O	4:G:401:LYS:HG2	2.15	0.47
4:G:565:GLU:OE1	4:G:567:THR:OG1	2.21	0.47
4:G:878:ASP:OD1	4:G:880:ARG:N	2.47	0.47
4:I:870:THR:HG22	4:I:871:VAL:N	2.28	0.47
4:I:1061:PRO:HG3	4:I:1201:SER:O	2.15	0.47
4:K:181:TYR:CZ	4:K:193:PRO:HD3	2.50	0.47
4:K:870:THR:HG22	4:K:871:VAL:N	2.29	0.47
4:L:523:MET:HE2	4:L:523:MET:HB3	1.70	0.47
4:M:324:MET:HE2	4:M:324:MET:HB2	1.74	0.47
1:A:111:ASP:OD1	6:T:8:U:C1'	2.62	0.47
4:F:500:SER:OG	4:F:501:VAL:N	2.47	0.47
4:F:649:PHE:HA	4:F:705:TRP:HE1	1.79	0.47
4:F:724:PRO:HG3	4:F:737:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1118:ASN:ND2	4:J:414:PRO:HB3	2.30	0.47
4:K:763:ASN:OD1	4:K:767:ARG:NH1	2.48	0.47
2:B:455:TYR:HE2	2:B:533:VAL:HG13	1.80	0.47
2:B:1008:SER:HB2	2:B:1147:MET:HE3	1.97	0.47
4:D:527:ASN:ND2	4:E:792:SER:HA	2.30	0.47
4:D:1002:GLN:HG3	4:D:1008:THR:HG22	1.97	0.47
4:D:1067:PHE:CZ	4:D:1107:ASN:HB3	2.50	0.47
4:E:320:SER:HB3	4:E:364:GLU:HG3	1.96	0.47
4:E:507:TYR:CD2	4:E:915:PHE:HB3	2.49	0.47
4:F:228:GLN:HA	4:F:233:VAL:HG11	1.97	0.47
4:G:435:ASP:OD1	4:G:436:ARG:N	2.48	0.47
4:G:1085:PHE:CE2	4:H:285:PHE:HB2	2.50	0.47
4:I:1064:ASP:OD1	4:I:1064:ASP:N	2.47	0.47
4:L:342:GLU:CD	5:m:56:ARG:HD2	2.40	0.47
5:m:165:HIS:ND1	5:m:166:PRO:HD2	2.29	0.47
1:A:570:LEU:O	1:A:574:TYR:HD2	1.98	0.46
4:D:539:ILE:HG12	4:D:826:LEU:HD11	1.96	0.46
4:D:807:THR:HG21	4:D:885:ALA:O	2.15	0.46
5:e:54:LYS:HE3	5:e:54:LYS:HB3	1.58	0.46
4:E:1126:PHE:O	4:E:1130:ILE:HD12	2.14	0.46
4:F:539:ILE:HG12	4:F:826:LEU:HD11	1.96	0.46
4:F:990:GLY:CA	4:G:804:LYS:HD3	2.45	0.46
4:H:1087:MET:HE1	4:I:499:PRO:HD3	1.98	0.46
4:H:1116:GLN:HB3	4:H:1172:PRO:HA	1.97	0.46
4:I:511:ASN:O	4:I:515:GLN:HG3	2.15	0.46
4:L:411:MET:HG2	4:L:412:GLY:O	2.16	0.46
5:m:108:LYS:NZ	4:M:533:GLN:OE1	2.24	0.46
1:A:20:LEU:O	1:A:23:SER:OG	2.25	0.46
1:A:431:ILE:HG13	1:A:432:LEU:H	1.80	0.46
2:B:103:LEU:HB3	2:B:218:MET:HE1	1.96	0.46
2:B:229:LEU:O	2:B:233:LEU:HD23	2.15	0.46
4:G:853:SER:N	4:G:995:THR:OG1	2.49	0.46
4:I:1044:ASP:HB3	4:I:1139:ILE:O	2.15	0.46
4:K:304:ILE:HD11	4:K:1210:PHE:HD1	1.79	0.46
4:L:309:ARG:NE	4:L:368:ASP:OD1	2.30	0.46
4:E:839:ASP:OD2	4:E:842:ARG:HD3	2.15	0.46
4:F:810:TYR:OH	4:F:818:GLU:OE1	2.28	0.46
4:G:649:PHE:HA	4:G:705:TRP:HE1	1.81	0.46
4:H:670:THR:HG23	4:H:672:SER:H	1.79	0.46
4:H:714:PRO:HA	4:H:760:GLU:OE1	2.16	0.46
4:K:696:PRO:HG2	4:K:697:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:244:THR:HA	4:L:531:VAL:HG23	1.98	0.46
4:M:1248:PRO:HD2	4:M:1249:GLU:OE1	2.15	0.46
2:B:127:ASP:OD1	2:B:128:SER:N	2.48	0.46
2:B:342:SER:O	2:B:345:GLY:N	2.48	0.46
2:B:1078:CYS:SG	2:B:1092:MET:HE1	2.55	0.46
2:B:1256:PHE:O	2:B:1260:MET:HG3	2.15	0.46
4:D:374:ARG:O	4:D:1259:ARG:NH1	2.47	0.46
4:D:1235:LEU:HD21	4:D:1254:TYR:CE2	2.50	0.46
4:E:1044:ASP:CG	4:E:1140:GLU:HA	2.41	0.46
4:F:242:LYS:HE2	4:F:242:LYS:HB2	1.77	0.46
4:H:669:TYR:HA	4:H:673:ARG:HG3	1.97	0.46
4:H:1229:VAL:HG13	4:H:1236:THR:HG21	1.97	0.46
4:K:261:GLY:HA3	4:K:312:SER:HA	1.97	0.46
4:L:947:ARG:HB3	4:L:950:ASP:OD2	2.16	0.46
1:A:50:MET:HE2	1:A:50:MET:HB2	1.80	0.46
1:A:82:GLN:HA	1:A:85:GLU:HG2	1.97	0.46
2:B:515:MET:SD	3:C:1283:A:O2'	2.71	0.46
2:B:864:GLN:O	2:B:1042:ARG:NH1	2.48	0.46
2:B:899:MET:HA	2:B:902:TRP:CD1	2.50	0.46
4:E:779:GLN:HG2	4:E:779:GLN:O	2.16	0.46
4:H:416:VAL:O	4:H:416:VAL:HG12	2.15	0.46
4:I:480:GLU:OE2	4:I:494:THR:HA	2.16	0.46
4:K:951:TRP:CD1	4:K:951:TRP:H	2.33	0.46
4:L:1185:SER:OG	4:L:1223:PRO:O	2.27	0.46
2:B:1161:LYS:O	2:B:1165:GLN:HB2	2.15	0.46
2:B:1165:GLN:HG2	2:B:1166:ASP:N	2.31	0.46
4:E:354:PHE:CE1	4:E:1145:PRO:HD3	2.50	0.46
4:H:532:ILE:HG12	4:H:604:VAL:HG21	1.98	0.46
4:I:963:ALA:HA	4:I:992:PRO:HG3	1.95	0.46
4:M:684:TRP:CE3	4:M:840:ARG:HG3	2.51	0.46
4:M:956:ARG:HH11	4:M:956:ARG:HG3	1.79	0.46
4:M:1234:ILE:HD13	4:M:1255:ASN:HA	1.98	0.46
4:D:288:SER:HB3	4:D:298:GLU:OE1	2.15	0.46
4:E:473:ASN:OD1	4:E:474:ILE:N	2.49	0.46
4:E:695:SER:HB3	4:E:698:ASP:HB2	1.97	0.46
5:g:67:GLU:OE1	4:G:249:HIS:NE2	2.44	0.46
4:H:955:LEU:HD23	4:H:955:LEU:H	1.80	0.46
4:I:982:MET:HG2	4:I:985:GLU:HG2	1.98	0.46
4:K:992:PRO:O	4:K:994:MET:HG2	2.16	0.46
4:L:411:MET:HE1	4:L:419:ILE:HD12	1.98	0.46
1:A:117:GLU:HG3	4:M:566:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:666:ASN:ND2	4:E:669:TYR:H	2.13	0.46
4:E:1079:ARG:HG2	4:F:428:ARG:HH12	1.80	0.46
4:G:951:TRP:CD1	4:G:951:TRP:H	2.34	0.46
4:I:859:GLN:HG2	4:J:438:GLN:HB3	1.97	0.46
4:J:668:ILE:O	4:J:673:ARG:HD3	2.16	0.46
4:J:807:THR:HG21	4:J:885:ALA:O	2.16	0.46
4:K:744:ASP:OD1	4:K:745:HIS:N	2.49	0.46
4:M:307:HIS:CE1	4:M:323:ILE:HG12	2.51	0.46
1:A:729:LEU:HD23	1:A:729:LEU:H	1.81	0.46
2:B:64:TYR:HB3	2:B:221:ARG:HB3	1.97	0.46
4:D:255:LEU:HD21	4:D:923:ILE:HD11	1.97	0.46
4:E:603:VAL:HG23	4:E:604:VAL:HG23	1.98	0.46
4:G:417:SER:OG	4:G:1214:SER:O	2.33	0.46
4:G:859:GLN:HG2	4:H:438:GLN:HB3	1.98	0.46
4:H:837:ARG:HG2	4:H:838:LEU:H	1.81	0.46
4:J:416:VAL:O	4:J:416:VAL:HG12	2.16	0.46
4:J:615:LYS:O	4:J:674:ARG:NH1	2.47	0.46
4:K:406:MET:O	4:K:453:THR:OG1	2.32	0.46
4:K:615:LYS:HD3	4:K:616:ASP:CG	2.41	0.46
4:K:982:MET:HE2	4:K:982:MET:HB3	1.75	0.46
4:K:1180:PHE:HE1	4:K:1199:ILE:HG22	1.81	0.46
4:M:546:ILE:HG13	4:M:904:ALA:HB1	1.98	0.46
1:A:651:VAL:O	1:A:655:LEU:HD23	2.16	0.46
2:B:727:ARG:HG2	2:B:727:ARG:HH11	1.80	0.46
4:E:285:PHE:CD2	4:E:286:PHE:HD1	2.34	0.46
4:F:514:ARG:NH1	4:F:727:PHE:O	2.49	0.46
4:I:1113:ALA:O	4:I:1117:MET:HG2	2.17	0.46
4:J:822:ILE:HG22	4:J:826:LEU:HD21	1.98	0.46
4:K:940:GLU:OE2	4:K:956:ARG:HD3	2.16	0.46
4:M:466:MET:HE1	4:M:1262:TYR:CE2	2.51	0.46
4:M:1147:MET:HE3	4:M:1149:HIS:NE2	2.31	0.46
4:D:313:ASN:HD22	4:D:395:PRO:HG2	1.81	0.45
4:D:615:LYS:O	4:D:674:ARG:NH1	2.46	0.45
4:G:1032:ASN:OD1	4:G:1042:ARG:NH2	2.49	0.45
4:G:1079:ARG:HG2	4:H:428:ARG:HH12	1.81	0.45
4:H:533:GLN:HE22	4:H:537:GLN:NE2	2.14	0.45
4:H:822:ILE:HG22	4:H:826:LEU:HD21	1.98	0.45
4:H:1120:ARG:HG2	4:H:1120:ARG:NH1	2.30	0.45
4:I:523:MET:HE2	4:I:523:MET:HB3	1.76	0.45
4:J:777:ASP:OD1	4:J:794:ARG:NH2	2.38	0.45
4:K:592:ARG:N	4:K:592:ARG:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:507:TYR:CD2	4:L:915:PHE:HB3	2.51	0.45
4:L:583:PRO:HG3	4:L:884:VAL:HG21	1.97	0.45
4:L:739:LEU:HD12	4:L:832:GLN:NE2	2.27	0.45
1:A:485:LEU:HD13	4:D:226:SER:HB2	1.98	0.45
5:g:163:SER:OG	5:g:164:LYS:N	2.47	0.45
4:J:818:GLU:OE2	4:J:901:TYR:OH	2.31	0.45
4:L:220:ILE:HG23	4:L:557:SER:HB2	1.98	0.45
2:B:901:SER:O	2:B:905:LEU:HD23	2.16	0.45
4:D:392:ARG:NH1	4:D:452:GLU:OE2	2.49	0.45
5:e:81:PRO:HA	5:e:87:THR:HA	1.97	0.45
5:e:109:GLN:NE2	4:E:537:GLN:OE1	2.48	0.45
4:H:560:MET:HA	4:H:560:MET:HE2	1.98	0.45
4:H:1234:ILE:H	4:H:1234:ILE:HD12	1.80	0.45
4:K:586:SER:HA	4:K:588:PHE:CE1	2.51	0.45
4:K:745:HIS:O	4:K:746:GLN:NE2	2.49	0.45
4:M:684:TRP:HB2	4:M:840:ARG:HD2	1.99	0.45
4:M:765:ARG:NH1	4:M:801:LYS:O	2.49	0.45
2:B:829:VAL:HG13	2:B:890:TRP:HE1	1.81	0.45
4:D:444:MET:HG2	5:m:139:VAL:CG1	2.46	0.45
4:D:1131:LYS:HG2	4:D:1132:THR:HG23	1.98	0.45
4:F:1095:ARG:HG2	4:F:1096:ASP:O	2.17	0.45
4:G:1119:THR:O	4:G:1123:ASN:HB2	2.16	0.45
4:H:851:ARG:HH12	4:H:989:SER:HB3	1.81	0.45
4:I:1213:ASN:HB3	4:I:1216:SER:OG	2.16	0.45
4:I:1248:PRO:HD2	4:I:1249:GLU:OE1	2.17	0.45
4:J:539:ILE:HG12	4:J:826:LEU:HD11	1.98	0.45
4:K:198:ALA:CB	4:K:215:ASP:OD1	2.64	0.45
4:K:861:ALA:HB1	4:L:441:ASN:HB2	1.99	0.45
4:K:939:SER:OG	4:K:940:GLU:N	2.49	0.45
4:L:242:LYS:HE2	6:R:34:U:OP1	2.15	0.45
4:L:313:ASN:HD22	4:L:395:PRO:HG2	1.82	0.45
5:m:133:LEU:O	4:M:527:ASN:ND2	2.43	0.45
4:M:309:ARG:NH2	4:M:317:ASP:OD1	2.49	0.45
4:M:1109:ILE:HD13	4:M:1138:ARG:HB3	1.97	0.45
2:B:369:MET:HE3	2:B:369:MET:HB2	1.82	0.45
2:B:1111:PHE:O	2:B:1112:MET:HE2	2.16	0.45
4:E:518:GLN:NE2	4:E:831:PHE:HB2	2.31	0.45
4:H:818:GLU:O	4:H:822:ILE:HG12	2.16	0.45
4:I:428:ARG:HA	4:I:428:ARG:HD3	1.79	0.45
4:I:1083:ILE:O	4:J:416:VAL:HG23	2.16	0.45
4:J:795:GLY:O	4:J:799:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:851:ARG:HH12	4:J:989:SER:HB3	1.81	0.45
4:J:958:SER:HB3	4:K:750:VAL:HG12	1.99	0.45
4:L:546:ILE:HD11	4:L:905:ILE:HG12	1.97	0.45
4:M:186:CYS:HG	4:M:199:HIS:HE2	1.59	0.45
1:A:105:ARG:HD3	1:A:115:ASP:OD2	2.17	0.45
1:A:117:GLU:CG	4:M:566:SER:HB2	2.46	0.45
2:B:242:THR:HG21	2:B:838:TRP:CE3	2.52	0.45
4:D:244:THR:HG22	4:D:531:VAL:HA	1.98	0.45
4:D:415:ASN:ND2	4:M:1121:TYR:CZ	2.85	0.45
4:D:439:MET:O	4:M:861:ALA:HA	2.16	0.45
4:G:560:MET:HE2	4:G:560:MET:HA	1.97	0.45
4:G:603:VAL:HG23	4:G:604:VAL:HG23	1.98	0.45
4:G:1212:THR:HG21	4:G:1224:ASP:HA	1.99	0.45
4:I:422:PHE:O	4:I:425:SER:OG	2.34	0.45
4:M:398:ASP:HB3	4:M:401:LYS:NZ	2.31	0.45
1:A:127:ILE:HG22	1:A:134:LEU:HD11	1.99	0.45
2:B:242:THR:HG21	2:B:838:TRP:HE3	1.81	0.45
2:B:407:PRO:O	2:B:408:ILE:HD13	2.17	0.45
2:B:520:GLN:HE22	2:B:526:ARG:HB2	1.82	0.45
2:B:528:ILE:HG21	3:C:1285:G:C4	2.52	0.45
2:B:819:ASP:OD1	2:B:953:ARG:HD2	2.17	0.45
4:E:955:LEU:HD23	4:E:955:LEU:H	1.81	0.45
4:H:374:ARG:O	4:H:1259:ARG:NH1	2.50	0.45
4:I:570:THR:O	4:I:571:LEU:HD22	2.16	0.45
4:I:951:TRP:H	4:I:951:TRP:CD1	2.34	0.45
4:J:984:LEU:O	4:J:988:LEU:HG	2.17	0.45
4:K:507:TYR:CE2	4:K:915:PHE:HB3	2.52	0.45
4:K:576:SER:OG	4:K:627:TRP:NE1	2.50	0.45
4:K:625:ASN:HB3	4:K:655:MET:HE3	1.97	0.45
4:L:740:LEU:H	4:L:832:GLN:HE22	1.63	0.45
1:A:101:ARG:CZ	1:A:101:ARG:HB2	2.47	0.45
1:A:435:GLN:HE22	1:A:438:PRO:HA	1.80	0.45
2:B:307:LYS:HD2	2:B:307:LYS:HA	1.79	0.45
4:E:334:LEU:HA	4:E:337:GLN:NE2	2.31	0.45
4:H:754:THR:O	4:H:809:MET:HE1	2.16	0.45
4:H:961:THR:HG22	4:I:893:PRO:O	2.16	0.45
4:J:419:ILE:H	4:J:419:ILE:HD12	1.81	0.45
4:K:636:LEU:HA	4:K:636:LEU:HD23	1.79	0.45
4:L:353:MET:SD	4:L:955:LEU:HD23	2.57	0.45
4:L:790:VAL:O	4:L:794:ARG:HG3	2.17	0.45
4:M:215:ASP:CB	4:M:219:HIS:NE2	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:SER:HG	1:A:253:ILE:HG12	1.82	0.45
1:A:379:PRO:HB2	4:D:228:GLN:HG2	1.97	0.45
1:A:447:GLU:HA	1:A:450:GLU:OE1	2.17	0.45
1:A:622:ILE:HD11	1:A:725:TYR:HB3	1.99	0.45
2:B:4:MET:N	2:B:4:MET:SD	2.89	0.45
2:B:478:PRO:HB2	2:B:480:PHE:CE1	2.52	0.45
4:D:285:PHE:CD1	4:M:1085:PHE:CD2	3.05	0.45
4:F:556:ILE:H	4:F:556:ILE:HD12	1.82	0.45
4:F:818:GLU:O	4:F:822:ILE:HG12	2.17	0.45
4:I:1033:HIS:O	4:I:1207:ARG:NH1	2.49	0.45
4:J:215:ASP:O	4:J:218:ARG:HG2	2.16	0.45
4:J:669:TYR:HA	4:J:673:ARG:HG3	1.99	0.45
4:L:690:ASN:HB3	4:L:693:LEU:HD23	1.99	0.45
5:m:81:PRO:HA	5:m:87:THR:HA	1.99	0.45
4:M:713:TRP:HB3	4:M:837:ARG:NH2	2.32	0.45
1:A:347:LEU:HD23	1:A:351:PHE:HD2	1.82	0.45
1:A:555:ASN:O	1:A:559:ARG:HG3	2.17	0.45
2:B:9:PHE:HZ	2:B:37:PHE:HE2	1.65	0.45
2:B:106:HIS:HB2	2:B:114:ARG:HH12	1.81	0.45
2:B:900:TYR:CZ	2:B:1225:LEU:HD23	2.51	0.45
4:D:229:ASN:N	4:D:231:PRO:HD2	2.32	0.45
4:E:822:ILE:HG22	4:E:826:LEU:HD11	1.99	0.45
4:G:616:ASP:HA	4:G:674:ARG:NH2	2.32	0.45
4:G:629:PHE:HD2	4:G:772:MET:HE2	1.81	0.45
4:I:249:HIS:N	4:I:913:GLU:OE2	2.48	0.45
4:I:654:ASN:ND2	4:I:671:GLN:O	2.50	0.45
5:k:51:GLU:H	5:k:51:GLU:CD	2.24	0.45
5:k:81:PRO:HA	5:k:87:THR:HA	1.99	0.45
4:K:1227:ILE:HD12	4:K:1227:ILE:H	1.82	0.45
1:A:101:ARG:HH12	4:M:570:THR:HB	1.82	0.44
2:B:1130:ARG:HG2	2:B:1260:MET:HE2	2.00	0.44
4:D:1274:VAL:CB	4:M:674:ARG:HD2	2.45	0.44
4:E:398:ASP:HB3	4:E:401:LYS:NZ	2.32	0.44
4:H:303:ARG:HG2	4:H:1209:LEU:HA	1.99	0.44
4:H:553:PRO:HB2	4:H:583:PRO:HB2	1.98	0.44
4:H:1171:THR:HG22	4:H:1173:THR:H	1.83	0.44
4:I:630:PHE:CD2	4:I:772:MET:HE1	2.52	0.44
4:K:650:MET:HE3	4:K:653:ALA:HB3	1.98	0.44
4:L:1229:VAL:HG13	4:L:1236:THR:HG21	1.99	0.44
1:A:300:MET:HG3	1:A:390:PHE:HE1	1.83	0.44
4:E:691:ILE:H	4:E:691:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:577:ILE:HD13	4:F:627:TRP:CD2	2.52	0.44
4:G:556:ILE:H	4:G:556:ILE:HD12	1.81	0.44
4:H:539:ILE:HG12	4:H:826:LEU:HD11	1.99	0.44
4:I:1087:MET:HE3	4:I:1088:ASN:H	1.82	0.44
4:J:1209:LEU:HD23	4:J:1210:PHE:N	2.33	0.44
5:k:110:ALA:HB2	5:k:118:ALA:HB2	1.98	0.44
4:L:981:ASP:OD1	4:L:981:ASP:N	2.51	0.44
5:m:127:ILE:HD11	4:M:607:VAL:HG11	1.98	0.44
4:M:951:TRP:CD1	4:M:951:TRP:H	2.35	0.44
1:A:19:GLY:O	1:A:23:SER:N	2.50	0.44
1:A:304:VAL:HG13	1:A:315:SER:HB3	2.00	0.44
2:B:1137:ASP:OD2	2:B:1139:LYS:HG2	2.17	0.44
4:D:516:ILE:HD11	4:D:1013:PRO:HB2	1.99	0.44
4:D:961:THR:HG22	4:E:893:PRO:O	2.17	0.44
4:D:1233:ASN:HA	4:D:1236:THR:HG22	1.99	0.44
4:G:339:LEU:HB2	4:G:353:MET:HG2	1.98	0.44
5:k:161:ILE:HD13	4:L:385:PHE:CD1	2.52	0.44
4:M:833:VAL:HG13	4:M:834:PRO:HD2	1.99	0.44
2:B:296:ASN:N	2:B:312:GLY:O	2.40	0.44
2:B:629:ASP:N	2:B:637:ALA:O	2.41	0.44
2:B:905:LEU:HD12	4:F:211:LEU:HD22	2.00	0.44
4:E:1112:LEU:HD13	4:E:1116:GLN:HG3	1.99	0.44
4:F:610:ASP:OD2	4:F:674:ARG:NH2	2.48	0.44
4:F:998:ALA:C	4:F:999:ILE:HG13	2.42	0.44
4:G:216:ILE:HG22	4:G:218:ARG:H	1.83	0.44
4:H:580:LYS:HA	4:H:580:LYS:HD2	1.70	0.44
4:I:580:LYS:HD3	4:I:624:GLU:HG3	2.00	0.44
4:K:1112:LEU:HD23	4:K:1116:GLN:HG3	2.00	0.44
4:L:416:VAL:O	4:L:416:VAL:HG12	2.17	0.44
4:L:985:GLU:HA	4:L:988:LEU:HD12	1.98	0.44
4:L:1007:ARG:HH21	4:L:1009:PHE:HE1	1.66	0.44
1:A:435:GLN:OE1	1:A:438:PRO:HB3	2.17	0.44
1:A:584:GLN:HG2	2:B:407:PRO:HG3	1.98	0.44
2:B:965:GLU:O	2:B:968:GLU:HG3	2.18	0.44
4:D:382:HIS:HE1	5:m:154:ILE:CD1	2.29	0.44
4:D:446:GLU:OE2	4:D:502:ASN:HB2	2.17	0.44
4:E:707:GLU:HB3	4:E:711:ARG:HH12	1.82	0.44
4:G:752:THR:HB	4:G:809:MET:HE2	2.00	0.44
4:J:352:LEU:HB2	4:J:353:MET:HE2	1.98	0.44
4:J:754:THR:O	4:J:809:MET:HE1	2.17	0.44
1:A:439:ARG:NH1	1:A:439:ARG:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:TRP:CD1	1:A:491:ARG:HH11	2.35	0.44
4:D:990:GLY:H	4:E:804:LYS:HE3	1.81	0.44
4:E:511:ASN:O	4:E:515:GLN:HG3	2.17	0.44
4:F:537:GLN:O	4:F:540:SER:OG	2.24	0.44
4:G:1213:ASN:HB3	4:G:1216:SER:OG	2.17	0.44
4:H:851:ARG:HA	4:H:996:GLN:O	2.18	0.44
4:I:1155:GLN:OE1	4:I:1155:GLN:HA	2.18	0.44
4:K:225:SER:OG	4:K:226:SER:N	2.50	0.44
4:K:630:PHE:HB2	4:K:772:MET:SD	2.57	0.44
4:K:632:LEU:HD23	4:K:636:LEU:HG	1.99	0.44
4:K:663:PRO:O	4:K:664:MET:HE2	2.17	0.44
4:K:1169:GLU:HB2	4:K:1176:PRO:HG3	1.99	0.44
4:L:1227:ILE:H	4:L:1227:ILE:HD12	1.82	0.44
4:L:1266:PRO:HG2	4:L:1269:ALA:HB2	2.00	0.44
1:A:667:VAL:HG22	1:A:685:ALA:HB2	1.98	0.44
2:B:465:ALA:HA	2:B:468:GLU:CD	2.43	0.44
2:B:1053:LEU:O	2:B:1057:LEU:HD23	2.18	0.44
4:D:324:MET:HE3	4:D:324:MET:HB2	1.75	0.44
4:F:416:VAL:O	4:F:416:VAL:HG12	2.18	0.44
4:G:1051:GLN:HB2	4:G:1196:VAL:HG22	1.99	0.44
4:H:218:ARG:NH2	6:N:10:U:H1'	2.33	0.44
4:J:607:VAL:HG21	4:K:787:GLN:OE1	2.17	0.44
5:k:155:ALA:HA	5:k:158:THR:HG22	1.99	0.44
4:K:818:GLU:OE1	4:K:901:TYR:OH	2.28	0.44
4:M:1134:GLU:N	4:M:1134:GLU:OE1	2.51	0.44
6:N:21:A:C2	6:O:13:A:C2	3.05	0.44
2:B:3:SER:O	2:B:7:THR:OG1	2.26	0.44
4:D:385:PHE:CE1	5:m:161:ILE:CG1	3.00	0.44
4:D:656:MET:HE1	4:D:660:GLU:OE2	2.18	0.44
4:E:190:LEU:HD13	4:E:196:LEU:HA	1.99	0.44
4:E:1115:TRP:CD1	4:E:1115:TRP:O	2.71	0.44
4:F:235:VAL:CG1	4:F:530:THR:HA	2.47	0.44
5:i:84:LYS:HE3	5:i:84:LYS:HB2	1.85	0.44
4:I:1084:SER:HB2	4:J:416:VAL:HG21	2.00	0.44
4:L:627:TRP:O	4:L:631:ILE:HG12	2.17	0.44
4:L:853:SER:OG	4:L:857:ILE:O	2.35	0.44
4:M:560:MET:HE2	4:M:560:MET:HA	1.99	0.44
4:M:732:LEU:HD13	4:M:999:ILE:HG21	2.00	0.44
4:M:779:GLN:O	4:M:779:GLN:HG2	2.18	0.44
2:B:506:SER:O	2:B:509:ILE:HG12	2.18	0.44
4:D:338:LEU:HD12	4:D:338:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:398:ASP:HB3	4:E:401:LYS:HZ2	1.83	0.44
4:F:287:THR:OG1	4:F:415:ASN:OD1	2.34	0.44
4:F:577:ILE:HD13	4:F:627:TRP:CE3	2.53	0.44
4:G:563:VAL:HG13	4:G:563:VAL:O	2.17	0.44
5:i:131:ASN:ND2	4:J:500:SER:HA	2.33	0.44
4:I:573:PRO:HB3	4:I:793:MET:CE	2.48	0.44
4:I:1212:THR:HG23	4:I:1219:THR:HG21	2.00	0.44
4:K:375:HIS:HE1	4:K:444:MET:HG2	1.82	0.44
4:K:610:ASP:OD2	4:K:610:ASP:N	2.50	0.44
4:K:1085:PHE:HE2	4:L:285:PHE:HA	1.83	0.44
4:L:216:ILE:O	4:L:220:ILE:HD12	2.18	0.44
4:L:1079:ARG:HG3	4:M:1275:PRO:HG2	1.99	0.44
1:A:318:LEU:HD23	1:A:363:ASP:HA	1.99	0.43
4:D:480:GLU:HB2	4:D:493:VAL:HG23	1.99	0.43
4:D:908:MET:HE1	4:D:909:TYR:HE1	1.83	0.43
4:E:649:PHE:HA	4:E:705:TRP:HE1	1.81	0.43
4:E:948:TYR:CZ	4:E:1029:GLU:OE2	2.70	0.43
4:E:1229:VAL:HG13	4:E:1236:THR:HG21	1.98	0.43
4:F:241:ASN:ND2	4:G:563:VAL:HG11	2.33	0.43
4:F:1087:MET:HE1	4:G:499:PRO:HD2	2.00	0.43
4:G:262:LEU:HD21	4:G:406:MET:SD	2.58	0.43
4:I:851:ARG:CZ	4:J:441:ASN:HD21	2.31	0.43
4:J:503:ARG:H	4:J:503:ARG:CD	2.27	0.43
4:K:307:HIS:CE1	4:K:323:ILE:HG12	2.53	0.43
4:M:433:ARG:HA	4:M:450:VAL:HG12	1.99	0.43
4:M:700:PRO:O	4:M:704:GLN:HG3	2.17	0.43
1:A:572:LEU:HG	1:A:576:TYR:CE2	2.48	0.43
2:B:356:LYS:HE2	2:B:356:LYS:HB2	1.75	0.43
2:B:955:PRO:HG2	2:B:957:LYS:NZ	2.33	0.43
4:D:580:LYS:HD3	4:D:624:GLU:OE1	2.17	0.43
4:E:398:ASP:O	4:E:401:LYS:HG2	2.18	0.43
4:E:840:ARG:O	4:E:843:VAL:HG22	2.18	0.43
5:g:84:LYS:HE3	5:g:84:LYS:HB2	1.83	0.43
5:g:95:HIS:CE1	5:g:99:LYS:HE3	2.53	0.43
4:G:504:LEU:HG	4:G:506:PRO:HD3	2.00	0.43
4:G:833:VAL:HG13	4:G:834:PRO:HD2	2.00	0.43
4:J:532:ILE:HG12	4:J:604:VAL:HG11	2.00	0.43
4:K:340:ASN:N	4:K:340:ASN:HD22	2.15	0.43
4:M:1002:GLN:HG2	4:M:1003:GLN:O	2.18	0.43
1:A:624:ARG:HH12	1:A:721:ARG:NH1	2.16	0.43
4:E:251:ASP:OD1	4:E:981:ASP:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:898:ASN:ND2	4:G:1275:PRO:O	2.52	0.43
4:G:931:LEU:HD13	4:G:984:LEU:HD23	2.00	0.43
4:I:649:PHE:HA	4:I:705:TRP:NE1	2.32	0.43
4:K:221:THR:HG22	4:K:1267:ILE:HB	2.00	0.43
4:K:359:LEU:HD12	4:K:934:LEU:HD22	1.99	0.43
4:M:737:GLU:N	4:M:737:GLU:OE2	2.51	0.43
1:A:58:ASP:OD1	1:A:59:VAL:N	2.51	0.43
2:B:223:THR:HG22	2:B:225:ALA:H	1.82	0.43
2:B:941:LYS:NZ	2:B:944:GLN:HG2	2.33	0.43
4:D:384:PRO:HB2	4:M:1113:ALA:HB1	1.99	0.43
4:D:799:LYS:HZ3	4:L:621:THR:HB	1.83	0.43
4:E:686:ARG:HA	4:E:689:MET:HE3	1.99	0.43
4:F:1023:CYS:O	4:F:1027:THR:HG23	2.19	0.43
4:G:851:ARG:CZ	4:H:441:ASN:HD21	2.31	0.43
4:H:261:GLY:HA3	4:H:312:SER:HA	2.01	0.43
4:H:581:LEU:HD12	4:H:884:VAL:HG22	2.00	0.43
5:k:6:ARG:NH1	4:K:317:ASP:O	2.51	0.43
4:L:514:ARG:NH1	4:L:727:PHE:O	2.48	0.43
4:L:920:ARG:HH12	4:L:981:ASP:CG	2.24	0.43
2:B:752:THR:HA	2:B:755:LYS:HZ2	1.83	0.43
4:D:416:VAL:O	4:D:416:VAL:HG12	2.18	0.43
4:D:511:ASN:O	4:D:515:GLN:HG3	2.19	0.43
5:e:2:LYS:NZ	4:E:217:GLN:HG3	2.34	0.43
4:E:630:PHE:HD1	4:E:772:MET:CE	2.30	0.43
4:E:926:GLU:OE2	4:E:1019:VAL:N	2.52	0.43
4:E:1241:PRO:HG2	4:E:1244:GLN:HB2	2.01	0.43
4:F:511:ASN:O	4:F:515:GLN:HG3	2.18	0.43
4:F:559:THR:HG21	4:F:803:ILE:HD13	2.00	0.43
5:g:83:LYS:HD2	4:G:968:TRP:CZ2	2.53	0.43
4:G:1120:ARG:HD3	4:G:1120:ARG:HA	1.72	0.43
5:i:4:ILE:HG21	4:I:254:ARG:HH12	1.83	0.43
5:i:102:ALA:O	5:i:106:THR:HG23	2.18	0.43
4:I:270:PRO:HG3	4:I:297:PRO:HB2	2.01	0.43
4:I:705:TRP:CE3	4:I:771:LEU:HD22	2.52	0.43
4:J:424:ALA:HA	4:J:428:ARG:HH22	1.84	0.43
4:J:507:TYR:CE1	4:J:1267:ILE:HD11	2.53	0.43
4:J:627:TRP:CE3	4:J:627:TRP:HA	2.54	0.43
5:k:144:GLY:O	4:L:444:MET:HE3	2.18	0.43
4:L:468:ARG:HB2	4:L:1019:VAL:HG11	1.99	0.43
1:A:431:ILE:CD1	1:A:599:TRP:HB3	2.49	0.43
1:A:432:LEU:HD23	1:A:432:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:SD	1:A:510:MET:HE2	2.58	0.43
2:B:201:LEU:HA	2:B:202:PRO:HD3	1.91	0.43
2:B:719:LEU:O	2:B:722:SER:OG	2.32	0.43
4:E:537:GLN:HE21	4:E:541:VAL:HG23	1.83	0.43
4:F:890:LYS:HE3	4:F:890:LYS:HB3	1.84	0.43
4:F:892:PRO:HD2	4:F:895:LEU:HD22	2.01	0.43
4:G:776:VAL:HG23	4:G:782:GLN:NE2	2.33	0.43
4:H:313:ASN:HD22	4:H:395:PRO:HG2	1.83	0.43
4:I:660:GLU:CG	4:I:699:ALA:HA	2.48	0.43
4:I:849:VAL:O	4:I:863:SER:OG	2.36	0.43
4:J:303:ARG:HG2	4:J:1209:LEU:HA	2.01	0.43
5:k:150:MET:HE2	5:k:150:MET:HA	2.00	0.43
4:K:705:TRP:CE3	4:K:771:LEU:HD22	2.54	0.43
4:K:1141:MET:HE2	4:K:1144:TYR:HB3	2.01	0.43
4:L:306:VAL:HB	4:L:324:MET:HG3	2.00	0.43
1:A:289:HIS:HB3	1:A:700:PHE:CZ	2.53	0.43
1:A:356:MET:HG3	1:A:592:LEU:HD12	2.01	0.43
2:B:51:PHE:CD1	2:B:188:TRP:HB2	2.54	0.43
4:E:674:ARG:HA	4:E:674:ARG:HD2	1.68	0.43
4:E:704:GLN:HA	4:E:707:GLU:OE2	2.19	0.43
4:E:1159:ALA:O	4:E:1163:THR:HG23	2.18	0.43
5:g:150:MET:O	5:g:154:ILE:HD12	2.19	0.43
4:G:1163:THR:HG23	4:G:1164:SER:N	2.33	0.43
4:G:1171:THR:HG22	4:G:1173:THR:H	1.82	0.43
4:I:332:ILE:HG12	4:I:348:GLY:HA2	2.01	0.43
4:K:375:HIS:CE1	4:K:444:MET:HE2	2.53	0.43
4:K:695:SER:HB3	4:K:698:ASP:HB2	2.01	0.43
4:L:309:ARG:HB3	4:L:312:SER:OG	2.18	0.43
4:L:939:SER:OG	4:L:940:GLU:N	2.49	0.43
4:M:216:ILE:CD1	4:M:218:ARG:HB2	2.48	0.43
4:M:309:ARG:NE	4:M:368:ASP:OD1	2.35	0.43
2:B:814:TRP:CD1	2:B:852:GLN:HE21	2.37	0.43
2:B:817:ILE:O	2:B:821:ILE:HG12	2.19	0.43
2:B:941:LYS:HZ1	2:B:944:GLN:HG2	1.83	0.43
4:E:370:LEU:HD23	4:E:370:LEU:HA	1.82	0.43
4:F:625:ASN:HB3	4:F:655:MET:SD	2.58	0.43
4:H:634:LEU:HD23	4:H:634:LEU:HA	1.89	0.43
4:J:438:GLN:NE2	4:J:440:MET:O	2.52	0.43
4:L:710:HIS:O	4:L:837:ARG:NH2	2.47	0.43
4:L:850:THR:HG22	4:L:998:ALA:HB3	2.01	0.43
1:A:186:CYS:HB2	1:A:188:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:SER:O	4:D:252:THR:HG23	2.19	0.43
2:B:170:PRO:HG3	2:B:886:TRP:HB2	2.00	0.43
2:B:644:MET:O	2:B:648:ILE:HG12	2.19	0.43
4:D:533:GLN:HE21	4:D:533:GLN:HB3	1.62	0.43
4:E:833:VAL:HG13	4:E:834:PRO:HD2	2.00	0.43
4:F:1147:MET:HE3	4:F:1149:HIS:NE2	2.34	0.43
4:G:222:GLU:HG2	4:G:233:VAL:HG12	2.01	0.43
4:I:1154:ARG:HB3	4:I:1154:ARG:HH11	1.84	0.43
4:J:315:ASP:OD2	4:J:316:PHE:N	2.51	0.43
1:A:407:LYS:HE3	1:A:541:GLY:HA2	2.01	0.43
4:G:705:TRP:CE3	4:G:771:LEU:HD22	2.53	0.43
4:H:315:ASP:OD1	4:H:316:PHE:N	2.52	0.43
4:I:560:MET:HG3	4:I:578:LEU:HD21	2.00	0.43
4:K:475:ASN:O	4:K:478:GLU:HG2	2.18	0.43
4:K:713:TRP:HB3	4:K:837:ARG:NH2	2.33	0.43
1:A:233:LEU:HD22	2:B:626:ILE:HD12	2.01	0.42
2:B:222:MET:HA	2:B:222:MET:HE2	2.01	0.42
2:B:1151:GLN:HB3	2:B:1154:GLU:OE2	2.18	0.42
4:E:1114:LEU:HD22	4:E:1114:LEU:HA	1.76	0.42
4:H:433:ARG:HA	4:H:450:VAL:HG12	2.01	0.42
4:I:780:ARG:NH2	4:I:781:TYR:OH	2.52	0.42
4:I:992:PRO:O	4:I:994:MET:HG2	2.19	0.42
5:k:56:ARG:HH22	4:K:892:PRO:HB3	1.84	0.42
4:K:1044:ASP:CG	4:K:1140:GLU:HA	2.43	0.42
1:A:74:TYR:CZ	1:A:148:LEU:HD11	2.54	0.42
1:A:348:THR:O	1:A:352:LEU:HD23	2.19	0.42
1:A:356:MET:HE2	1:A:356:MET:HA	2.01	0.42
2:B:22:GLN:HB3	2:B:867:MET:HE1	2.01	0.42
4:D:385:PHE:HA	4:M:1117:MET:HE3	1.46	0.42
4:D:744:ASP:HB3	4:D:760:GLU:OE2	2.18	0.42
4:E:454:SER:OG	4:E:1255:ASN:OD1	2.34	0.42
4:F:360:HIS:CE1	4:F:364:GLU:OE2	2.72	0.42
4:F:601:ASN:ND2	4:F:833:VAL:H	2.14	0.42
4:G:600:TYR:OH	4:G:828:PHE:O	2.30	0.42
4:H:1044:ASP:HB3	4:H:1139:ILE:O	2.19	0.42
4:L:501:VAL:O	4:L:501:VAL:HG12	2.18	0.42
4:L:622:SER:OG	4:L:625:ASN:OD1	2.33	0.42
2:B:60:PRO:HA	2:B:61:PRO:HD3	1.93	0.42
4:D:305:VAL:HG13	4:D:324:MET:HE3	2.01	0.42
4:D:724:PRO:HG3	4:D:737:GLU:OE2	2.19	0.42
4:D:1272:MET:HE3	5:m:128:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:587:ASP:OD1	4:F:588:PHE:N	2.53	0.42
4:G:1211:CYS:SG	4:G:1212:THR:N	2.93	0.42
4:K:797:LEU:HD23	4:K:797:LEU:HA	1.89	0.42
4:L:577:ILE:HD13	4:L:627:TRP:CE3	2.54	0.42
4:L:695:SER:HB3	4:L:698:ASP:HB2	2.01	0.42
4:M:190:LEU:HD13	4:M:196:LEU:HA	2.00	0.42
1:A:304:VAL:HG12	1:A:316:ARG:H	1.85	0.42
1:A:713:LEU:H	1:A:713:LEU:HD12	1.85	0.42
4:D:825:MET:HE3	4:D:909:TYR:CE2	2.53	0.42
4:F:523:MET:CE	4:F:851:ARG:HH11	2.33	0.42
4:G:252:THR:HB	4:G:916:SER:HB3	2.00	0.42
4:I:507:TYR:CD2	4:I:915:PHE:HB3	2.54	0.42
4:I:941:THR:HG22	4:I:943:TYR:H	1.83	0.42
4:I:1121:TYR:O	4:I:1125:GLN:HG2	2.18	0.42
4:J:839:ASP:OD2	4:J:842:ARG:HD3	2.19	0.42
4:K:705:TRP:CE2	4:K:709:ILE:HD11	2.54	0.42
4:K:940:GLU:OE2	4:K:956:ARG:NH1	2.52	0.42
4:L:562:THR:HB	4:L:799:LYS:NZ	2.34	0.42
4:L:1171:THR:HB	4:L:1174:SER:H	1.84	0.42
4:M:1159:ALA:HB2	4:M:1181:MET:CE	2.49	0.42
1:A:363:ASP:HB3	1:A:366:THR:O	2.20	0.42
1:A:624:ARG:HH12	1:A:721:ARG:CZ	2.33	0.42
2:B:464:ALA:O	2:B:468:GLU:OE1	2.38	0.42
5:g:54:LYS:HA	5:g:54:LYS:HD2	1.85	0.42
4:G:552:ASP:O	4:G:888:SER:HB2	2.20	0.42
4:G:1260:TYR:HB3	4:G:1262:TYR:CE1	2.54	0.42
4:J:704:GLN:HA	4:J:707:GLU:OE2	2.20	0.42
4:L:741:LEU:HD11	4:L:816:PRO:HB3	2.00	0.42
4:L:1044:ASP:HB3	4:L:1139:ILE:O	2.19	0.42
4:L:1067:PHE:CZ	4:L:1107:ASN:HB3	2.55	0.42
4:M:240:GLU:OE1	4:M:240:GLU:N	2.48	0.42
1:A:681:VAL:N	1:A:710:GLU:OE2	2.52	0.42
4:D:330:ASN:OD1	4:D:331:ASN:N	2.53	0.42
4:D:1067:PHE:O	4:D:1138:ARG:NH1	2.53	0.42
4:D:1093:MET:HE3	4:D:1093:MET:HB2	1.87	0.42
5:e:148:LYS:HB3	5:e:153:ARG:HD2	2.00	0.42
4:H:419:ILE:HG13	4:H:420:CYS:N	2.35	0.42
4:H:527:ASN:HD21	4:I:795:GLY:HA3	1.85	0.42
4:H:1080:ASP:OD2	4:H:1095:ARG:NH2	2.49	0.42
5:k:127:ILE:H	5:k:127:ILE:HD12	1.85	0.42
4:L:973:MET:HE3	4:L:973:MET:HB3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:LEU:HD23	2:B:368:ALA:HA	2.01	0.42
2:B:510:LEU:HD12	2:B:657:ARG:HD3	2.01	0.42
4:D:1264:THR:O	4:D:1264:THR:OG1	2.32	0.42
4:E:474:ILE:HD11	4:E:508:ARG:HB2	2.02	0.42
4:F:246:GLN:NE2	4:F:982:MET:HB2	2.33	0.42
4:G:218:ARG:HH21	4:G:239:VAL:HG21	1.84	0.42
4:H:522:ILE:HA	4:H:525:ILE:HG22	2.00	0.42
4:H:1011:ILE:HD13	4:H:1011:ILE:HA	1.74	0.42
4:I:1020:ILE:O	4:I:1024:VAL:HG23	2.20	0.42
4:L:665:ASP:OD2	4:L:685:PRO:HA	2.20	0.42
6:N:23:A:C2	6:O:11:A:C2	3.07	0.42
2:B:329:LYS:HE3	2:B:329:LYS:HB3	1.82	0.42
2:B:954:ASN:C	2:B:1034:MET:HE2	2.45	0.42
2:B:1151:GLN:NE2	4:D:585:ASN:ND2	2.68	0.42
4:D:756:ASP:OD1	4:D:757:PHE:N	2.52	0.42
4:E:599:LEU:HD21	4:E:819:LEU:HD22	2.01	0.42
4:E:1115:TRP:CD1	4:E:1115:TRP:C	2.98	0.42
4:F:217:GLN:O	4:F:221:THR:HG23	2.19	0.42
4:F:427:VAL:HG23	4:F:1235:LEU:O	2.20	0.42
4:F:543:LEU:HD23	4:F:543:LEU:HA	1.84	0.42
4:I:987:LEU:HD13	4:I:994:MET:SD	2.60	0.42
4:K:1115:TRP:HD1	4:K:1170:ILE:HG21	1.83	0.42
4:L:670:THR:HG23	4:L:672:SER:H	1.83	0.42
4:L:744:ASP:HB3	4:L:760:GLU:OE1	2.20	0.42
5:m:44:GLU:HA	5:m:45:PRO:HD3	1.92	0.42
4:M:736:PRO:HG2	4:M:737:GLU:OE2	2.19	0.42
1:A:291:ASP:OD1	1:A:292:VAL:N	2.53	0.42
2:B:279:GLN:OE1	2:B:283:HIS:ND1	2.43	0.42
2:B:295:PRO:HG3	2:B:1075:LEU:HD21	2.01	0.42
4:D:477:THR:O	4:D:480:GLU:HG2	2.20	0.42
4:E:582:ARG:HB2	4:E:582:ARG:NH1	2.35	0.42
4:E:853:SER:N	4:E:995:THR:OG1	2.53	0.42
4:F:507:TYR:CD2	4:F:915:PHE:HB3	2.55	0.42
4:F:811:LEU:HD23	4:F:811:LEU:HA	1.86	0.42
4:H:511:ASN:O	4:H:515:GLN:HG3	2.20	0.42
4:H:625:ASN:HA	4:H:628:ASP:OD2	2.19	0.42
4:K:326:PRO:HA	4:K:327:PRO:HD3	1.95	0.42
4:K:956:ARG:CZ	4:K:956:ARG:HB2	2.48	0.42
4:L:990:GLY:O	4:L:992:PRO:HD3	2.20	0.42
4:M:963:ALA:HA	4:M:992:PRO:HG3	2.01	0.42
4:D:926:GLU:HG2	4:D:1020:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1113:ALA:O	4:D:1117:MET:HG2	2.20	0.42
4:E:705:TRP:CE2	4:E:709:ILE:HD11	2.55	0.42
4:E:940:GLU:OE2	4:E:956:ARG:HD3	2.20	0.42
4:E:1112:LEU:CD1	4:E:1116:GLN:HG3	2.50	0.42
4:F:200:VAL:O	4:F:200:VAL:HG12	2.20	0.42
4:F:336:LYS:HA	4:F:340:ASN:HD22	1.84	0.42
4:F:580:LYS:O	4:F:880:ARG:NE	2.53	0.42
4:G:969:VAL:O	4:G:973:MET:HG3	2.20	0.42
4:K:550:GLN:HE21	4:K:892:PRO:HG3	1.85	0.42
4:L:1007:ARG:NH2	4:L:1009:PHE:HE1	2.18	0.42
5:m:127:ILE:H	5:m:127:ILE:HD12	1.85	0.42
4:M:740:LEU:HD13	4:M:834:PRO:HA	2.01	0.42
4:D:631:ILE:HD13	4:D:883:THR:HG21	2.02	0.41
4:D:799:LYS:HE2	4:L:621:THR:HG22	2.02	0.41
4:E:203:HIS:HB2	4:E:205:LEU:HD23	2.02	0.41
4:E:430:ARG:HH21	4:E:1242:PRO:HG3	1.85	0.41
4:G:926:GLU:O	4:G:930:THR:HG23	2.20	0.41
4:G:948:TYR:CD1	4:G:1029:GLU:HB2	2.55	0.41
4:H:577:ILE:HD13	4:H:627:TRP:CE3	2.55	0.41
4:H:610:ASP:OD2	4:I:786:THR:HG21	2.20	0.41
4:H:613:TYR:HB2	4:H:674:ARG:NH2	2.35	0.41
4:H:649:PHE:HA	4:H:705:TRP:NE1	2.35	0.41
4:I:221:THR:HG22	4:I:1267:ILE:HB	2.02	0.41
4:I:400:GLU:HA	4:I:403:TYR:CD2	2.54	0.41
4:I:1083:ILE:HG12	4:I:1094:ILE:HD13	2.01	0.41
5:k:59:ILE:O	5:k:63:GLN:HG3	2.19	0.41
4:L:505:MET:HE3	4:L:505:MET:HB2	1.85	0.41
2:B:47:ASP:HA	2:B:191:ARG:HD2	2.02	0.41
2:B:167:LEU:HD21	2:B:840:ARG:CZ	2.50	0.41
2:B:379:ARG:HG2	2:B:525:PRO:HG2	2.02	0.41
2:B:744:THR:HG23	4:F:908:MET:HB2	2.02	0.41
2:B:1040:ARG:HD2	2:B:1043:ARG:HH21	1.86	0.41
4:E:504:LEU:HG	4:E:506:PRO:HD3	2.02	0.41
4:F:457:LEU:HD11	4:F:1027:THR:HG22	2.01	0.41
4:H:218:ARG:CZ	6:N:10:U:O2'	2.68	0.41
4:H:963:ALA:O	4:H:967:GLU:HG3	2.19	0.41
4:I:398:ASP:O	4:I:401:LYS:NZ	2.33	0.41
4:I:1093:MET:HE3	4:I:1102:VAL:CA	2.50	0.41
4:I:1095:ARG:HD3	4:I:1101:MET:HE2	2.01	0.41
4:J:576:SER:OG	4:J:627:TRP:NE1	2.46	0.41
4:J:1186:SER:OG	4:J:1187:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:511:ASN:O	4:K:515:GLN:HG3	2.19	0.41
4:L:242:LYS:HG3	6:R:33:A:O3'	2.20	0.41
2:B:106:HIS:CB	2:B:114:ARG:HH12	2.33	0.41
4:E:190:LEU:HD22	4:E:195:ASP:HB3	2.01	0.41
4:E:337:GLN:H	4:E:337:GLN:CD	2.27	0.41
4:E:993:ARG:H	4:E:993:ARG:HG2	1.54	0.41
4:F:814:LEU:HD12	4:F:901:TYR:CE1	2.55	0.41
5:g:77:ASP:O	5:g:80:THR:OG1	2.27	0.41
4:G:960:ALA:O	4:G:964:THR:HG23	2.20	0.41
4:G:1160:TRP:O	4:G:1163:THR:HG22	2.20	0.41
4:J:556:ILE:O	4:J:560:MET:HG2	2.21	0.41
4:J:1155:GLN:OE1	4:J:1155:GLN:N	2.54	0.41
4:K:567:THR:OG1	4:K:570:THR:HG22	2.21	0.41
4:L:307:HIS:CD2	4:L:323:ILE:HG23	2.55	0.41
4:L:951:TRP:CD1	4:L:951:TRP:H	2.36	0.41
4:M:603:VAL:HG23	4:M:604:VAL:HG23	2.02	0.41
1:A:119:ASN:HB3	1:A:123:ARG:NH1	2.35	0.41
2:B:452:ARG:HG3	2:B:620:MET:CE	2.49	0.41
4:D:306:VAL:HG12	4:D:324:MET:CE	2.42	0.41
4:D:811:LEU:HD23	4:D:811:LEU:HA	1.85	0.41
4:F:1165:ALA:O	4:F:1169:GLU:HG3	2.20	0.41
5:g:150:MET:O	5:g:153:ARG:N	2.54	0.41
4:I:221:THR:OG1	4:I:234:GLN:HB2	2.21	0.41
4:I:394:LEU:HD12	4:I:402:TRP:CG	2.56	0.41
4:I:969:VAL:O	4:I:973:MET:HG3	2.21	0.41
4:J:973:MET:HE2	4:J:973:MET:HB2	1.90	0.41
1:A:407:LYS:HD3	1:A:542:HIS:CE1	2.56	0.41
1:A:458:GLN:HA	1:A:461:MET:SD	2.60	0.41
2:B:328:ASP:OD2	2:B:348:ARG:NH2	2.53	0.41
4:D:720:ARG:HA	4:D:737:GLU:O	2.20	0.41
4:E:338:LEU:HB3	4:E:339:LEU:H	1.69	0.41
4:E:585:ASN:OD1	4:E:586:SER:N	2.52	0.41
4:G:478:GLU:OE2	4:G:508:ARG:NH2	2.53	0.41
4:G:695:SER:HB3	4:G:698:ASP:HB3	2.02	0.41
4:J:241:ASN:OD1	4:J:244:THR:N	2.53	0.41
4:K:833:VAL:HG13	4:K:834:PRO:HD2	2.03	0.41
4:K:915:PHE:O	4:K:919:GLN:HG3	2.20	0.41
4:L:926:GLU:OE2	4:L:926:GLU:HA	2.19	0.41
4:M:819:LEU:HD23	4:M:819:LEU:HA	1.87	0.41
4:M:1000:GLN:HB3	4:M:1010:ASN:HA	2.02	0.41
2:B:424:TYR:CZ	2:B:705:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:287:THR:HG22	4:D:292:ILE:HB	2.03	0.41
4:F:261:GLY:HA3	4:F:312:SER:HA	2.03	0.41
4:F:783:PRO:HB3	4:H:794:ARG:HH11	1.85	0.41
4:G:900:TRP:CD1	4:G:900:TRP:C	2.98	0.41
4:G:970:ASN:O	4:G:974:LYS:HG3	2.21	0.41
4:H:366:VAL:HG21	4:H:1024:VAL:HA	2.03	0.41
4:H:840:ARG:HA	4:H:843:VAL:HG23	2.01	0.41
4:I:333:HIS:HA	4:I:336:LYS:HG2	2.03	0.41
4:I:335:PHE:CZ	4:I:1040:ILE:HD11	2.56	0.41
4:J:223:PHE:CZ	4:J:583:PRO:HG3	2.55	0.41
4:J:800:LEU:HD23	4:J:800:LEU:HA	1.82	0.41
5:k:145:SER:N	4:L:444:MET:HE3	2.36	0.41
4:K:660:GLU:HG3	4:K:699:ALA:HA	2.02	0.41
4:L:350:ASN:HB3	4:L:353:MET:HE2	2.02	0.41
1:A:127:ILE:HD12	1:A:127:ILE:H	1.85	0.41
1:A:182:THR:O	1:A:183:MET:HE2	2.21	0.41
2:B:276:ILE:O	2:B:280:ASN:ND2	2.42	0.41
2:B:707:GLY:CA	2:B:720:MET:HE1	2.48	0.41
2:B:709:GLU:O	5:e:117:LYS:HE3	2.20	0.41
2:B:729:TYR:CE2	2:B:731:CYS:HB3	2.56	0.41
2:B:835:TRP:H	2:B:835:TRP:CD1	2.38	0.41
2:B:856:ILE:O	2:B:856:ILE:HG22	2.20	0.41
2:B:1178:LEU:HD23	2:B:1178:LEU:HA	1.95	0.41
4:D:512:ALA:O	4:D:516:ILE:HG12	2.20	0.41
4:D:610:ASP:OD2	4:E:786:THR:HG21	2.20	0.41
4:E:703:ARG:HG3	4:E:707:GLU:OE1	2.20	0.41
4:F:230:HIS:NE2	4:F:233:VAL:HG23	2.35	0.41
4:F:1076:ILE:HB	4:F:1097:GLU:CD	2.46	0.41
4:G:243:LYS:HG3	4:G:243:LYS:O	2.21	0.41
4:G:261:GLY:HA2	4:G:394:LEU:HD11	2.03	0.41
4:G:394:LEU:HD13	4:G:395:PRO:HD2	2.03	0.41
4:G:417:SER:OG	4:G:418:LYS:N	2.53	0.41
4:G:556:ILE:HD11	4:G:888:SER:HB3	2.02	0.41
4:H:249:HIS:O	4:H:249:HIS:ND1	2.52	0.41
5:i:6:ARG:NH1	4:I:317:ASP:O	2.53	0.41
4:J:744:ASP:HB3	4:J:760:GLU:OE1	2.21	0.41
4:K:338:LEU:C	4:K:340:ASN:H	2.28	0.41
4:K:437:ALA:HB2	4:K:447:TRP:CD1	2.55	0.41
4:K:574:ALA:O	4:K:578:LEU:HD23	2.20	0.41
4:L:367:LEU:HD23	4:L:367:LEU:HA	1.82	0.41
4:L:528:ASN:O	4:L:531:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:740:LEU:O	4:L:741:LEU:HD23	2.21	0.41
4:L:990:GLY:HA3	4:M:804:LYS:CE	2.46	0.41
4:M:536:LEU:HD23	4:M:536:LEU:HA	1.86	0.41
4:M:776:VAL:HG23	4:M:782:GLN:NE2	2.35	0.41
4:M:1164:SER:O	4:M:1168:GLU:HG2	2.20	0.41
1:A:101:ARG:NH2	1:A:101:ARG:CB	2.83	0.41
2:B:529:MET:HG2	2:B:661:TYR:CE2	2.55	0.41
2:B:550:ASN:HA	2:B:554:ASN:OD1	2.20	0.41
2:B:711:THR:HG23	2:B:717:LEU:HD22	2.03	0.41
2:B:868:TRP:CD1	2:B:942:LEU:HA	2.56	0.41
4:D:1044:ASP:HB3	4:D:1139:ILE:O	2.20	0.41
5:e:44:GLU:HA	5:e:45:PRO:HD3	1.91	0.41
4:E:983:LEU:H	4:E:985:GLU:HG2	1.86	0.41
4:G:649:PHE:HA	4:G:705:TRP:NE1	2.36	0.41
4:I:620:VAL:HG12	4:I:655:MET:HE2	2.03	0.41
4:I:1093:MET:HE3	4:I:1101:MET:C	2.46	0.41
4:J:926:GLU:OE1	4:J:1019:VAL:N	2.54	0.41
5:k:4:ILE:HD12	4:K:254:ARG:HH22	1.85	0.41
4:K:1056:TRP:CE3	4:K:1056:TRP:O	2.73	0.41
4:K:1241:PRO:HA	4:K:1242:PRO:HD3	1.97	0.41
4:L:1071:THR:HB	4:L:1074:VAL:HG21	2.03	0.41
4:M:1171:THR:HB	4:M:1174:SER:H	1.85	0.41
1:A:572:LEU:O	1:A:576:TYR:HD2	2.04	0.41
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.93	0.41
2:B:295:PRO:HG3	2:B:1075:LEU:HD11	2.02	0.41
2:B:820:GLN:O	2:B:824:VAL:HG23	2.21	0.41
2:B:1050:SER:O	2:B:1054:GLU:HG2	2.21	0.41
2:B:1110:LEU:HD13	2:B:1121:VAL:HG11	2.03	0.41
4:D:402:TRP:O	4:D:406:MET:HG3	2.21	0.41
4:D:406:MET:HE3	4:D:407:TYR:CZ	2.56	0.41
4:E:351:PRO:HA	4:E:354:PHE:CE2	2.56	0.41
4:E:506:PRO:O	4:E:919:GLN:NE2	2.52	0.41
4:E:562:THR:OG1	4:E:565:GLU:HG3	2.20	0.41
4:E:963:ALA:HA	4:E:992:PRO:HG3	2.02	0.41
4:E:1051:GLN:HB2	4:E:1196:VAL:HG22	2.03	0.41
4:F:241:ASN:OD1	4:F:244:THR:HG22	2.20	0.41
4:G:400:GLU:OE2	4:G:400:GLU:N	2.49	0.41
4:G:402:TRP:O	4:G:406:MET:HG3	2.21	0.41
4:G:1067:PHE:O	4:G:1138:ARG:NH1	2.51	0.41
4:G:1071:THR:HB	4:G:1074:VAL:HG21	2.02	0.41
4:H:359:LEU:HD23	4:H:359:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:573:PRO:HA	4:H:623:LEU:HD21	2.02	0.41
5:i:161:ILE:O	5:i:161:ILE:HG13	2.20	0.41
4:I:660:GLU:HG2	4:I:699:ALA:HA	2.03	0.41
4:J:428:ARG:HD3	4:J:428:ARG:HA	1.79	0.41
4:J:702:LEU:HD23	4:J:702:LEU:HA	1.82	0.41
4:J:836:VAL:HG11	4:J:842:ARG:HB2	2.01	0.41
5:k:102:ALA:O	5:k:106:THR:HG23	2.20	0.41
4:K:428:ARG:HA	4:K:428:ARG:HD3	1.85	0.41
4:K:1020:ILE:O	4:K:1024:VAL:HG23	2.21	0.41
4:L:216:ILE:H	4:L:216:ILE:HD12	1.86	0.41
4:L:242:LYS:HE2	6:R:34:U:P	2.61	0.41
4:L:513:GLU:HG3	4:L:1016:PRO:HG3	2.02	0.41
4:L:679:SER:HB3	4:M:788:SER:HB2	2.02	0.41
4:L:867:THR:O	4:L:867:THR:HG22	2.20	0.41
5:m:165:HIS:CG	5:m:166:PRO:HD2	2.55	0.41
4:M:985:GLU:N	4:M:986:PRO:HD2	2.36	0.41
1:A:510:MET:HE3	1:A:510:MET:HB3	1.82	0.41
2:B:451:MET:HE3	2:B:451:MET:HB3	1.76	0.41
2:B:1068:GLU:OE1	4:F:226:SER:OG	2.39	0.41
2:B:1193:PHE:HE1	2:B:1227:ALA:HB2	1.85	0.41
4:D:973:MET:HE2	4:D:973:MET:HB3	1.90	0.41
5:e:50:ARG:HB3	5:e:52:GLN:HE22	1.86	0.41
4:F:246:GLN:HE22	4:F:982:MET:CB	2.32	0.41
4:F:1159:ALA:HB2	4:F:1181:MET:SD	2.61	0.41
4:G:779:GLN:O	4:G:779:GLN:HG2	2.20	0.41
4:G:794:ARG:HE	4:G:794:ARG:HB3	1.73	0.41
4:G:815:ALA:HA	4:G:818:GLU:CD	2.47	0.41
4:H:516:ILE:O	4:H:520:ILE:HG12	2.21	0.41
4:I:186:CYS:HG	4:I:203:HIS:CE1	2.39	0.41
4:I:507:TYR:CE2	4:I:915:PHE:HB3	2.56	0.41
4:J:280:VAL:HG12	4:J:281:LEU:HD22	2.02	0.41
4:M:378:PHE:HD1	4:M:392:ARG:HA	1.85	0.41
1:A:63:LEU:O	1:A:63:LEU:HD12	2.22	0.40
1:A:207:PHE:HA	1:A:208:PRO:HD3	1.81	0.40
2:B:721:LYS:HE3	2:B:721:LYS:HB3	1.90	0.40
2:B:905:LEU:HD22	2:B:1229:MET:HE3	2.02	0.40
2:B:1215:MET:SD	2:B:1253:GLY:HA3	2.61	0.40
4:D:670:THR:OG1	4:D:671:GLN:N	2.54	0.40
4:D:926:GLU:CG	4:D:1020:ILE:HD12	2.51	0.40
5:e:7:LYS:HD2	4:E:238:ASP:OD2	2.21	0.40
4:E:306:VAL:O	4:E:324:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:744:ASP:OD1	4:E:745:HIS:N	2.55	0.40
4:F:867:THR:HG22	4:F:867:THR:O	2.21	0.40
4:F:1206:ASP:OD1	4:F:1206:ASP:O	2.38	0.40
5:g:77:ASP:OD1	5:g:77:ASP:O	2.39	0.40
4:I:946:ASP:HB3	4:I:948:TYR:CE1	2.56	0.40
4:J:580:LYS:HD2	4:J:580:LYS:HA	1.84	0.40
4:J:654:ASN:ND2	4:J:673:ARG:O	2.53	0.40
4:J:1171:THR:HG23	5:k:53:TYR:HB2	2.04	0.40
4:K:351:PRO:HG3	4:K:1116:GLN:OE1	2.21	0.40
4:K:586:SER:C	4:K:588:PHE:CE1	2.98	0.40
4:K:1085:PHE:CD2	4:L:285:PHE:HB2	2.56	0.40
4:L:288:SER:HB3	4:L:298:GLU:OE1	2.21	0.40
4:M:552:ASP:O	4:M:888:SER:HB2	2.21	0.40
2:B:619:PHE:O	2:B:622:VAL:N	2.50	0.40
4:D:1001:TYR:CZ	4:D:1009:PHE:HD2	2.39	0.40
5:e:74:LYS:NZ	5:e:75:ASN:O	2.54	0.40
5:e:102:ALA:O	5:e:106:THR:HG23	2.20	0.40
5:e:109:GLN:OE1	4:E:533:GLN:NE2	2.49	0.40
4:E:1189:ASP:N	4:E:1189:ASP:OD1	2.52	0.40
4:E:1265:PRO:HA	4:E:1266:PRO:HD3	1.98	0.40
4:F:649:PHE:HA	4:F:705:TRP:NE1	2.36	0.40
4:F:837:ARG:C	4:F:838:LEU:HD22	2.47	0.40
4:I:1265:PRO:HA	4:I:1266:PRO:HD3	1.99	0.40
4:K:649:PHE:HA	4:K:705:TRP:NE1	2.36	0.40
4:K:985:GLU:N	4:K:986:PRO:HD2	2.37	0.40
4:K:1104:PHE:CD1	4:K:1108:TRP:HH2	2.37	0.40
4:L:440:MET:HE1	4:L:501:VAL:HG22	2.03	0.40
4:L:833:VAL:HB	4:L:834:PRO:HD2	2.03	0.40
4:M:702:LEU:HD23	4:M:702:LEU:HA	1.93	0.40
4:D:285:PHE:CG	4:M:1085:PHE:CE2	3.05	0.40
4:D:503:ARG:NH2	5:m:131:ASN:ND2	2.68	0.40
4:D:668:ILE:O	4:D:673:ARG:HD3	2.21	0.40
4:D:695:SER:HB3	4:D:698:ASP:HB2	2.02	0.40
4:E:1204:TYR:CE1	4:E:1206:ASP:HB2	2.56	0.40
5:g:128:ASN:ND2	4:H:494:THR:O	2.54	0.40
4:H:533:GLN:N	4:H:534:PRO:HD2	2.36	0.40
4:I:1225:LYS:HD2	4:I:1226:HIS:O	2.22	0.40
4:J:527:ASN:OD1	4:K:792:SER:HA	2.22	0.40
4:J:533:GLN:N	4:J:534:PRO:HD2	2.37	0.40
4:J:852:GLN:HE22	4:K:804:LYS:HD3	1.86	0.40
4:J:867:THR:HG22	4:J:867:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:99:LYS:HE2	5:k:99:LYS:HB2	1.84	0.40
4:K:1249:GLU:OE2	4:K:1249:GLU:N	2.51	0.40
4:L:511:ASN:O	4:L:515:GLN:HG3	2.21	0.40
4:L:636:LEU:N	4:L:637:PRO:HD2	2.35	0.40
4:L:754:THR:O	4:L:809:MET:HE1	2.22	0.40
4:L:825:MET:SD	4:L:914:VAL:HG21	2.62	0.40
4:L:1083:ILE:HD12	4:L:1121:TYR:CZ	2.56	0.40
4:M:649:PHE:HA	4:M:705:TRP:NE1	2.36	0.40
1:A:39:ASP:N	1:A:39:ASP:OD1	2.50	0.40
2:B:564:ILE:HD12	2:B:1185:MET:HG3	2.03	0.40
2:B:1164:LEU:HB2	4:D:575:SER:OG	2.22	0.40
2:B:1178:LEU:HB3	2:B:1224:PHE:CD2	2.56	0.40
5:e:83:LYS:H	5:e:83:LYS:HG2	1.76	0.40
4:E:370:LEU:HD22	4:E:465:TRP:CD2	2.56	0.40
4:F:1231:ARG:HB3	4:F:1253:LEU:HD23	2.04	0.40
4:G:248:LEU:HD12	4:G:913:GLU:OE2	2.21	0.40
4:G:437:ALA:HB2	4:G:447:TRP:CE2	2.57	0.40
4:H:1231:ARG:HG3	4:H:1251:VAL:O	2.22	0.40
4:I:943:TYR:HD2	4:I:945:VAL:HG23	1.87	0.40
4:I:1093:MET:CE	4:I:1101:MET:C	2.95	0.40
4:I:1241:PRO:HA	4:I:1242:PRO:HD3	1.97	0.40
4:J:539:ILE:O	4:J:543:LEU:HD23	2.21	0.40
4:K:1092:PRO:HG2	4:K:1104:PHE:CD2	2.56	0.40
4:K:1104:PHE:CE1	4:K:1126:PHE:HE1	2.39	0.40
4:L:1002:GLN:HG3	4:L:1008:THR:HG22	2.04	0.40
1:A:239:LYS:O	1:A:243:ALA:HB2	2.22	0.40
1:A:370:TYR:O	1:A:371:LEU:HD23	2.22	0.40
1:A:520:SER:HB3	1:A:684:LYS:HD2	2.02	0.40
2:B:4:MET:HE3	2:B:4:MET:HB3	1.96	0.40
2:B:147:ILE:HD12	2:B:149:ALA:O	2.21	0.40
2:B:1205:ARG:NH2	4:H:572:SER:HB2	2.34	0.40
4:D:321:SER:HA	4:D:368:ASP:OD2	2.22	0.40
4:D:584:SER:C	4:D:586:SER:H	2.29	0.40
4:E:800:LEU:HD23	4:E:800:LEU:HA	1.82	0.40
4:E:987:LEU:HD23	4:E:987:LEU:HA	1.82	0.40
4:E:1235:LEU:HA	4:E:1235:LEU:HD23	1.87	0.40
4:F:366:VAL:HG21	4:F:1024:VAL:HA	2.04	0.40
4:F:501:VAL:HG12	4:F:501:VAL:O	2.22	0.40
4:F:519:ILE:CG2	4:F:999:ILE:CD1	2.89	0.40
4:F:583:PRO:HA	4:F:880:ARG:NH1	2.37	0.40
4:F:887:LEU:HD23	4:F:887:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:116:SER:OG	6:N:4:U:C4'	2.69	0.40
4:G:234:GLN:HE21	4:G:248:LEU:HA	1.87	0.40
4:G:878:ASP:OD1	4:G:878:ASP:C	2.64	0.40
4:G:1011:ILE:HD13	4:G:1011:ILE:HA	1.85	0.40
4:G:1044:ASP:HB3	4:G:1139:ILE:O	2.21	0.40
5:i:110:ALA:HB2	5:i:118:ALA:HB2	2.03	0.40
4:I:574:ALA:O	4:I:578:LEU:HD23	2.22	0.40
4:J:550:GLN:OE1	4:J:890:LYS:NZ	2.55	0.40
4:J:577:ILE:O	4:J:581:LEU:HD23	2.21	0.40
4:J:941:THR:OG1	4:J:942:GLN:N	2.54	0.40
4:L:923:ILE:HD13	4:L:923:ILE:HA	1.97	0.40
4:L:1112:LEU:HD13	4:L:1141:MET:HE3	2.03	0.40
4:M:552:ASP:OD1	4:M:554:THR:OG1	2.21	0.40
4:M:1219:THR:HB	4:M:1224:ASP:OD1	2.22	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	669/736 (91%)	607 (91%)	61 (9%)	1 (0%)	48	75
2	B	1262/1267 (100%)	1223 (97%)	39 (3%)	0	100	100
4	D	1052/1095 (96%)	1007 (96%)	42 (4%)	3 (0%)	36	65
4	E	1084/1095 (99%)	1041 (96%)	43 (4%)	0	100	100
4	F	1080/1095 (99%)	1032 (96%)	45 (4%)	3 (0%)	36	65
4	G	1084/1095 (99%)	1040 (96%)	44 (4%)	0	100	100
4	H	1051/1095 (96%)	1014 (96%)	37 (4%)	0	100	100
4	I	1084/1095 (99%)	1041 (96%)	43 (4%)	0	100	100
4	J	1046/1095 (96%)	1011 (97%)	35 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	1085/1095 (99%)	1046 (96%)	38 (4%)	1 (0%)	48	75
4	L	1044/1095 (95%)	1018 (98%)	26 (2%)	0	100	100
4	M	1085/1095 (99%)	1048 (97%)	37 (3%)	0	100	100
5	e	136/180 (76%)	133 (98%)	3 (2%)	0	100	100
5	g	137/180 (76%)	131 (96%)	6 (4%)	0	100	100
5	i	136/180 (76%)	133 (98%)	3 (2%)	0	100	100
5	k	136/180 (76%)	128 (94%)	8 (6%)	0	100	100
5	m	137/180 (76%)	134 (98%)	3 (2%)	0	100	100
All	All	13308/13853 (96%)	12787 (96%)	513 (4%)	8 (0%)	49	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	232	ILE
4	K	339	LEU
4	D	231	PRO
4	D	585	ASN
1	A	208	PRO
4	F	212	THR
4	F	234	GLN
4	F	235	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/646 (93%)	596 (100%)	3 (0%)	81	83
2	B	1080/1082 (100%)	1080 (100%)	0	100	100
4	D	933/969 (96%)	931 (100%)	2 (0%)	87	88
4	E	962/969 (99%)	960 (100%)	2 (0%)	87	88
4	F	957/969 (99%)	955 (100%)	2 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	962/969 (99%)	961 (100%)	1 (0%)	88	90
4	H	933/969 (96%)	932 (100%)	1 (0%)	88	90
4	I	962/969 (99%)	960 (100%)	2 (0%)	87	88
4	J	928/969 (96%)	927 (100%)	1 (0%)	88	90
4	K	963/969 (99%)	960 (100%)	3 (0%)	86	86
4	L	928/969 (96%)	927 (100%)	1 (0%)	88	90
4	M	963/969 (99%)	959 (100%)	4 (0%)	84	84
5	e	115/145 (79%)	114 (99%)	1 (1%)	70	78
5	g	115/145 (79%)	113 (98%)	2 (2%)	53	71
5	i	115/145 (79%)	115 (100%)	0	100	100
5	k	115/145 (79%)	115 (100%)	0	100	100
5	m	116/145 (80%)	116 (100%)	0	100	100
All	All	11746/12143 (97%)	11721 (100%)	25 (0%)	85	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	206	THR
1	A	313	ASN
4	D	585	ASN
4	D	1011	ILE
5	e	54	LYS
4	E	1112	LEU
4	E	1114	LEU
4	F	353	MET
4	F	710	HIS
5	g	88	LYS
5	g	107	LYS
4	G	1123	ASN
4	H	1011	ILE
4	I	1011	ILE
4	I	1170	ILE
4	J	503	ARG
4	K	216	ILE
4	K	1055	LEU
4	K	1059	LEU
4	L	400	GLU

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Mol	Chain	Res	Type
4	M	216	ILE
4	M	584	SER
4	M	1079	ARG
4	M	1123	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	203	ASN
1	A	247	ASN
1	A	342	GLN
1	A	488	HIS
1	A	517	ASN
1	A	536	ASN
1	A	555	ASN
1	A	569	GLN
1	A	666	GLN
2	B	87	GLN
2	B	173	GLN
2	B	504	HIS
2	B	542	HIS
2	B	550	ASN
2	B	554	ASN
2	B	580	GLN
2	B	694	ASN
2	B	917	ASN
2	B	1151	GLN
4	D	228	GLN
4	D	229	ASN
4	D	278	GLN
4	D	307	HIS
4	D	382	HIS
4	D	415	ASN
4	D	558	ASN
4	D	585	ASN
4	D	715	ASN
4	D	774	ASN
4	D	812	GLN
4	D	917	ASN
4	D	1002	GLN
4	D	1003	GLN

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Mol	Chain	Res	Type
4	D	1075	HIS
4	D	1107	ASN
4	D	1124	GLN
4	D	1197	GLN
4	D	1213	ASN
4	D	1233	ASN
4	D	1246	GLN
5	e	52	GLN
5	e	131	ASN
4	E	208	ASN
4	E	234	GLN
4	E	307	HIS
4	E	710	HIS
4	E	718	GLN
4	E	1002	GLN
4	E	1033	HIS
4	E	1116	GLN
4	E	1226	HIS
4	F	217	GLN
4	F	246	GLN
4	F	441	ASN
4	F	511	ASN
4	F	715	ASN
4	F	917	ASN
4	F	929	GLN
4	F	1010	ASN
4	F	1025	GLN
4	F	1107	ASN
4	F	1197	GLN
5	g	146	ASN
5	g	165	HIS
4	G	234	GLN
4	G	246	GLN
4	G	340	ASN
4	G	380	GLN
4	G	390	ASN
4	G	715	ASN
4	G	731	ASN
4	G	859	GLN
4	G	898	ASN
4	G	917	ASN
4	G	929	GLN

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Mol	Chain	Res	Type
4	G	937	GLN
4	G	970	ASN
4	G	1002	GLN
4	G	1025	GLN
4	G	1116	GLN
4	G	1123	ASN
4	G	1125	GLN
4	G	1213	ASN
4	G	1246	GLN
4	H	241	ASN
4	H	307	HIS
4	H	441	ASN
4	H	533	GLN
4	H	715	ASN
4	H	787	GLN
4	H	996	GLN
4	H	1002	GLN
4	H	1107	ASN
4	H	1118	ASN
4	H	1213	ASN
4	H	1244	GLN
5	i	141	ASN
5	i	165	HIS
4	I	293	GLN
4	I	307	HIS
4	I	515	GLN
4	I	654	ASN
4	I	682	HIS
4	I	690	ASN
4	I	710	HIS
4	I	715	ASN
4	I	746	GLN
4	I	970	ASN
4	I	1107	ASN
4	I	1226	HIS
4	I	1244	GLN
4	J	333	HIS
4	J	360	HIS
4	J	441	ASN
4	J	475	ASN
4	J	511	ASN
4	J	715	ASN

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Mol	Chain	Res	Type
4	J	725	ASN
4	J	1003	GLN
4	J	1010	ASN
4	J	1033	HIS
4	J	1036	ASN
4	J	1107	ASN
4	J	1125	GLN
4	J	1213	ASN
4	J	1233	ASN
5	k	49	ASN
4	K	246	GLN
4	K	307	HIS
4	K	360	HIS
4	K	375	HIS
4	K	550	GLN
4	K	625	ASN
4	K	859	GLN
4	L	219	HIS
4	L	313	ASN
4	L	441	ASN
4	L	715	ASN
4	L	774	ASN
4	L	832	GLN
4	L	1000	GLN
4	L	1003	GLN
4	L	1036	ASN
4	L	1107	ASN
4	L	1197	GLN
5	m	63	GLN
5	m	128	ASN
5	m	131	ASN
5	m	141	ASN
5	m	146	ASN
4	M	234	GLN
4	M	307	HIS
4	M	373	ASN
4	M	438	GLN
4	M	667	GLN
4	M	731	ASN
4	M	917	ASN
4	M	1000	GLN
4	M	1025	GLN

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Mol	Chain	Res	Type
4	M	1107	ASN
4	M	1116	GLN
4	M	1118	ASN
4	M	1123	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	3/4 (75%)	1 (33%)	0
6	N	31/60 (51%)	0	0
6	O	31/60 (51%)	0	0
6	P	29/60 (48%)	0	0
6	Q	29/60 (48%)	0	0
6	R	59/60 (98%)	0	0
6	S	59/60 (98%)	0	0
6	T	30/60 (50%)	0	0
6	U	30/60 (50%)	0	0
All	All	301/484 (62%)	1 (0%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	1284	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PO4	A	800	-	4,4,4	0.96	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

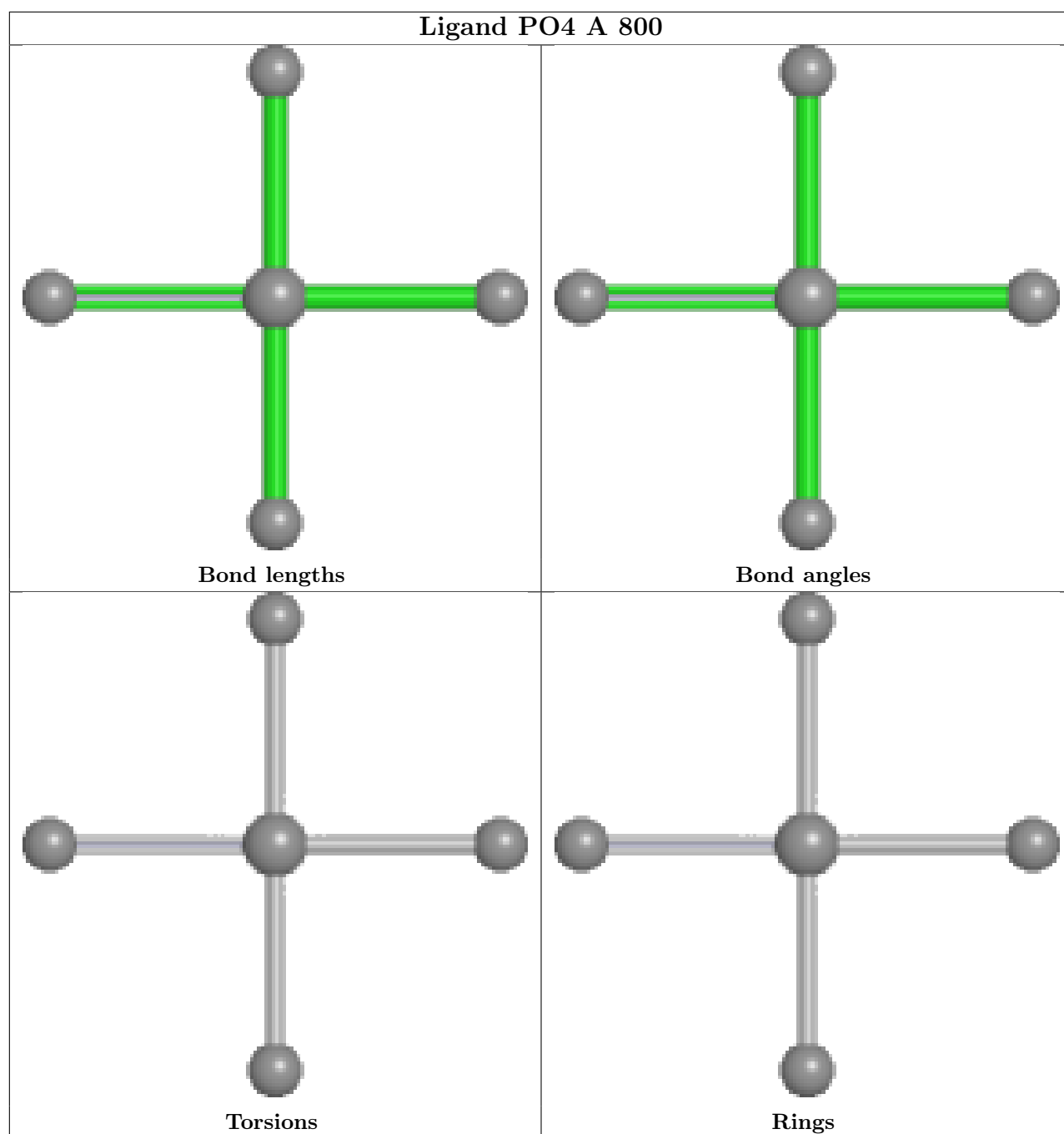
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	800	PO4	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

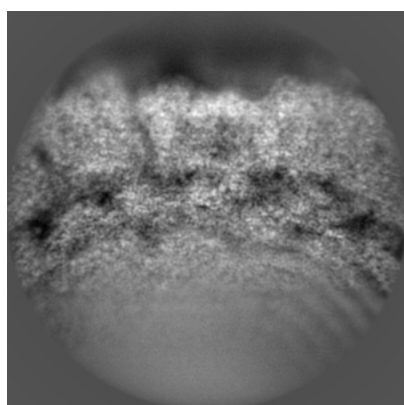
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31183. These allow visual inspection of the internal detail of the map and identification of artifacts.

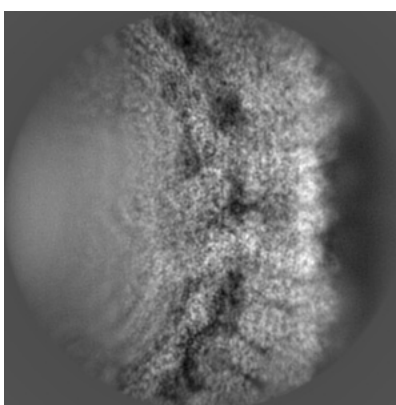
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

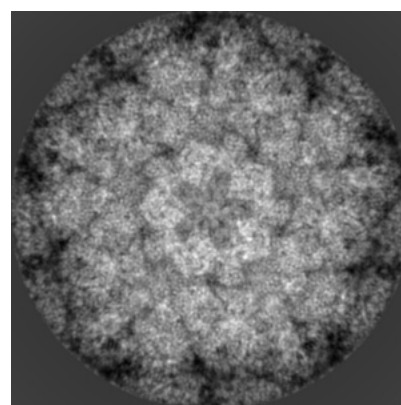
6.1.1 Primary map



X



Y

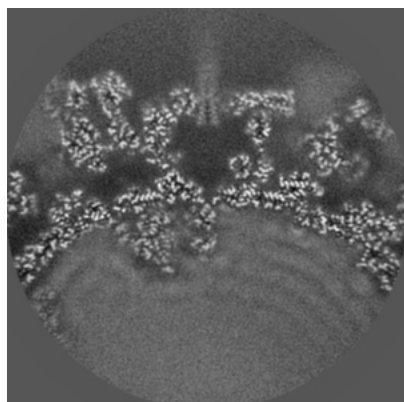


Z

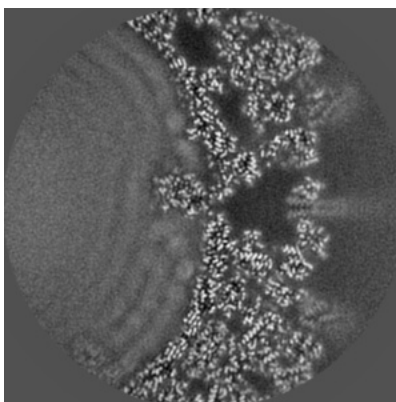
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

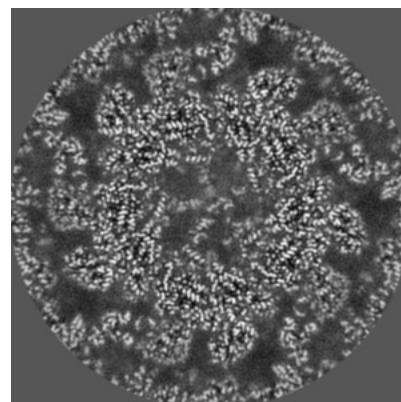
6.2.1 Primary map



X Index: 200



Y Index: 200

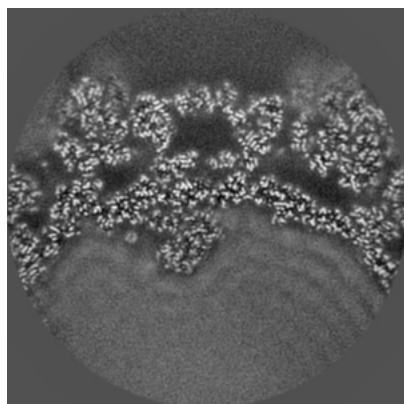


Z Index: 200

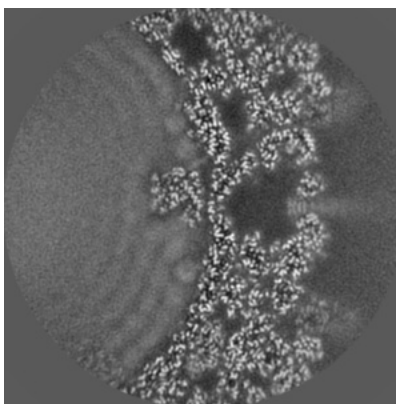
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

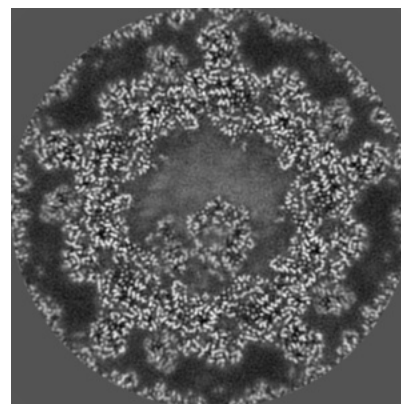
6.3.1 Primary map



X Index: 222



Y Index: 194

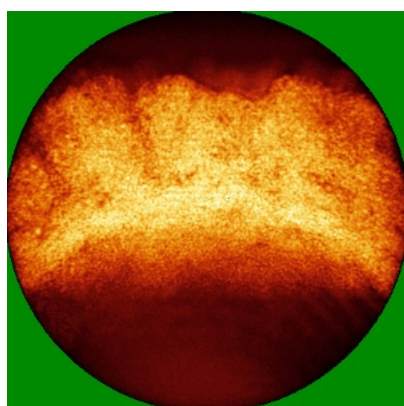


Z Index: 190

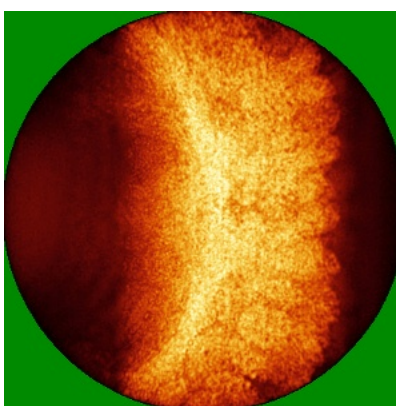
The images above show the largest variance slices of the map in three orthogonal directions.

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

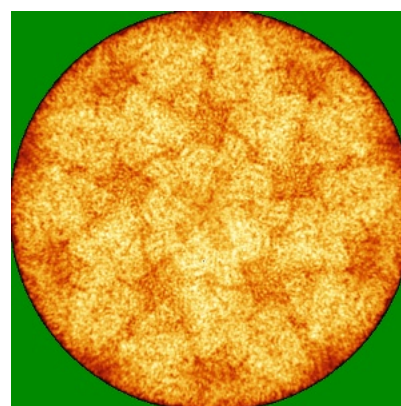
6.4.1 Primary map



X



Y

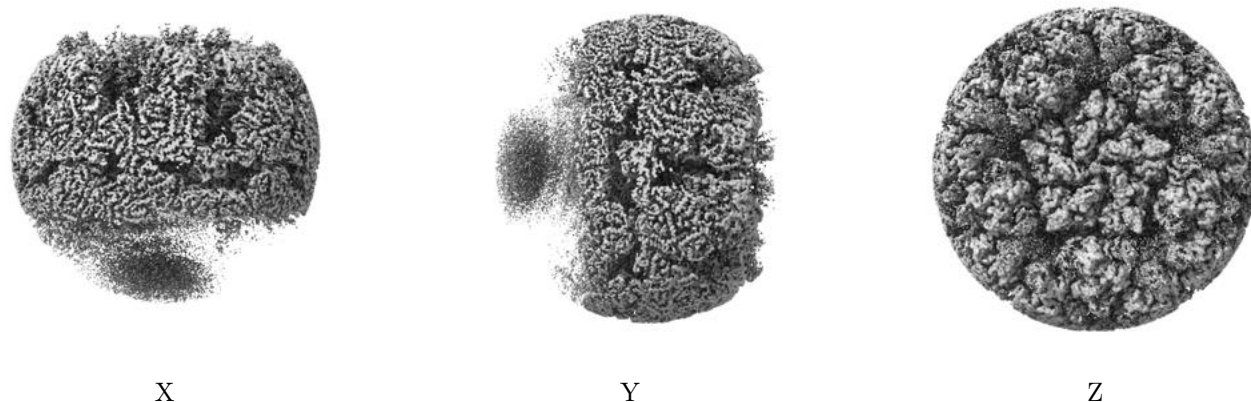


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

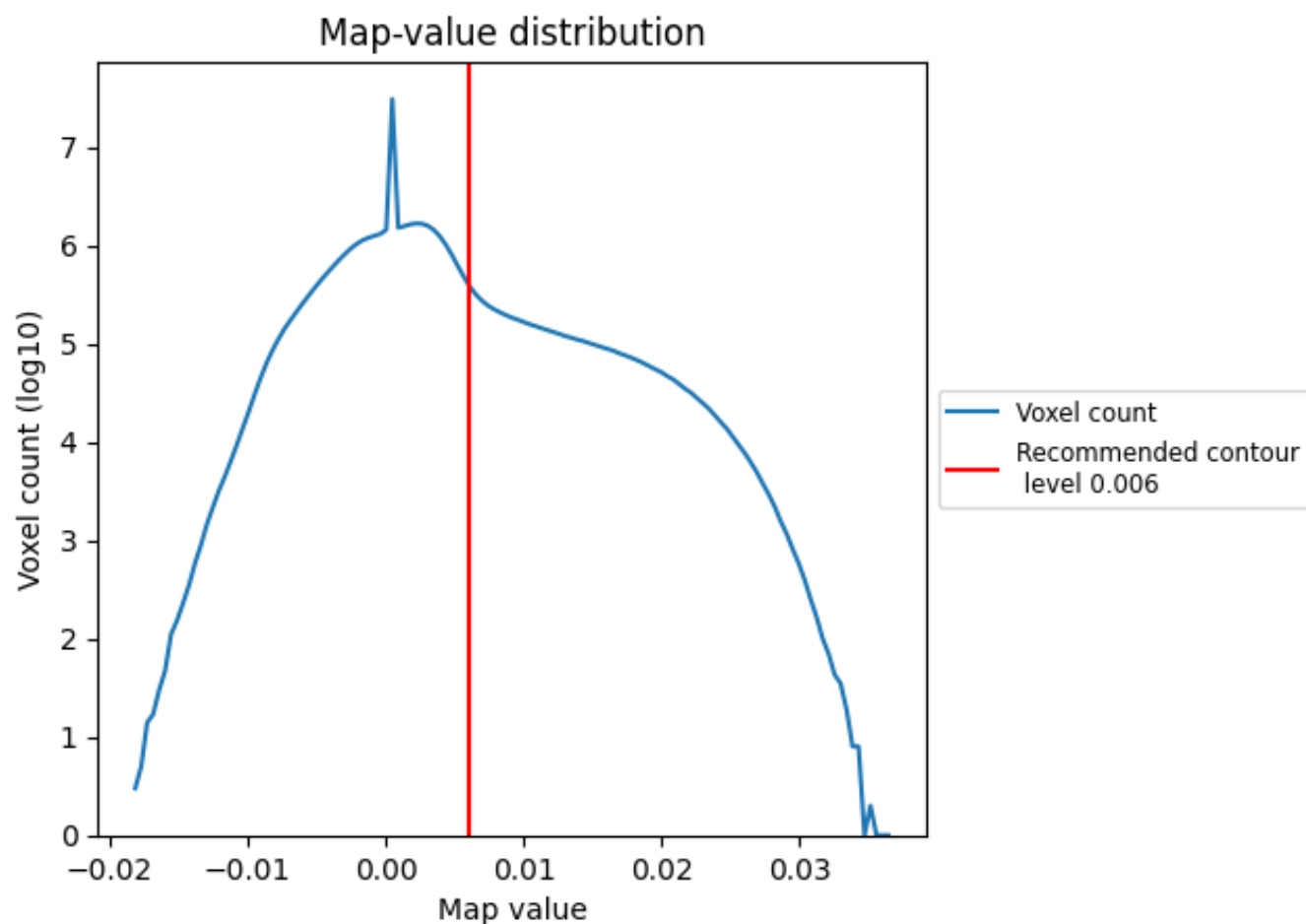
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

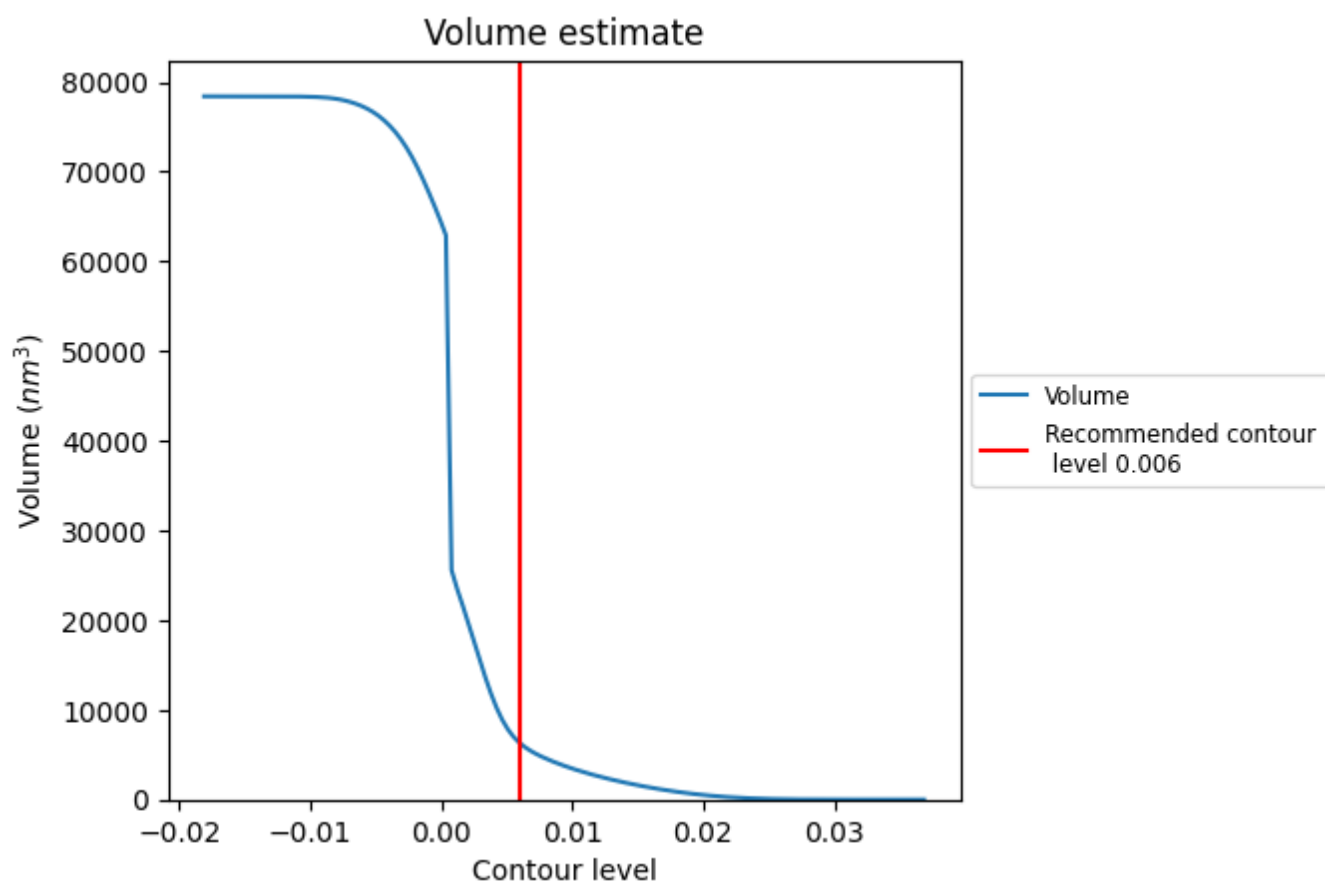
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

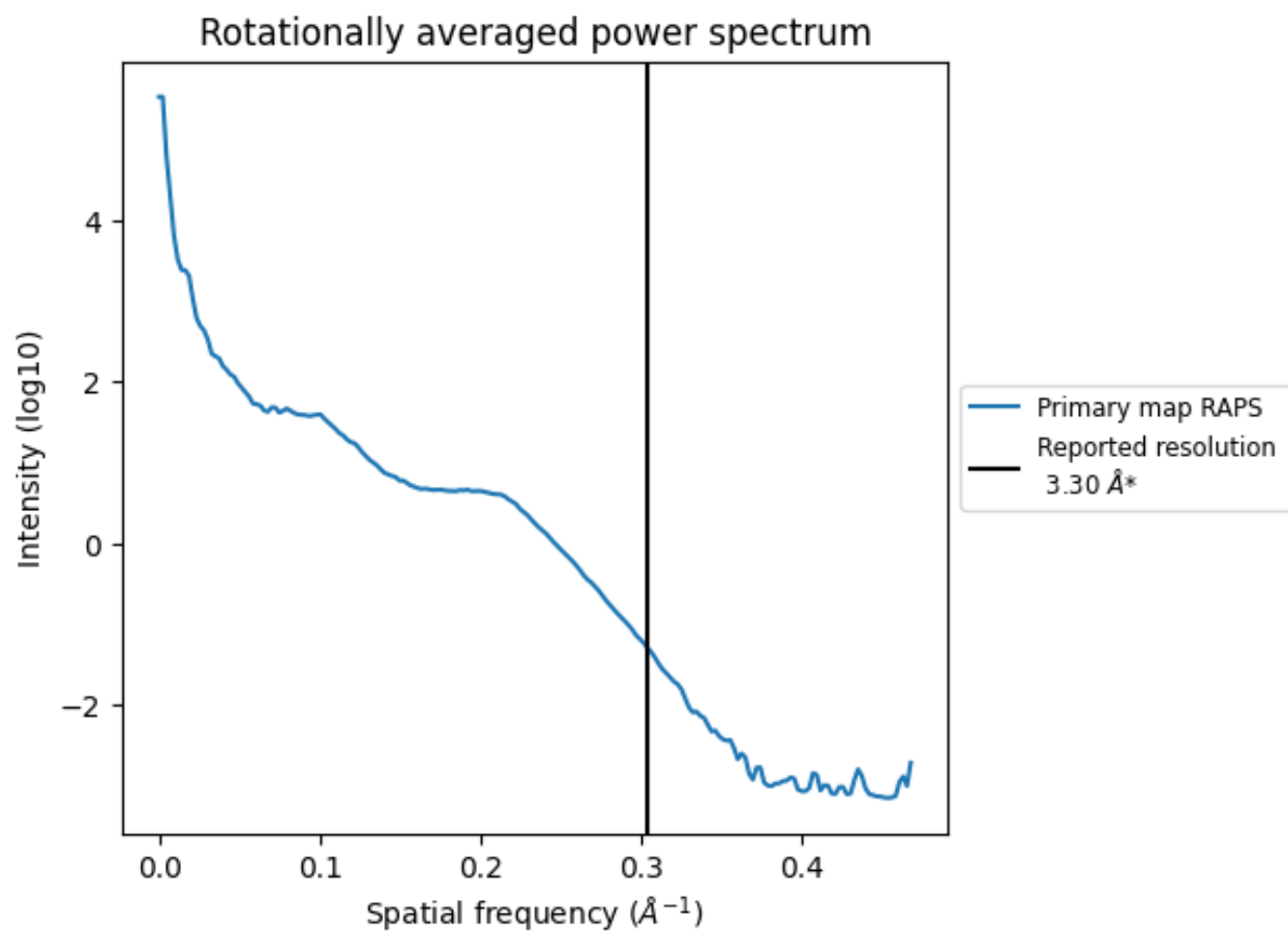
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6293 nm³; this corresponds to an approximate mass of 5684 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

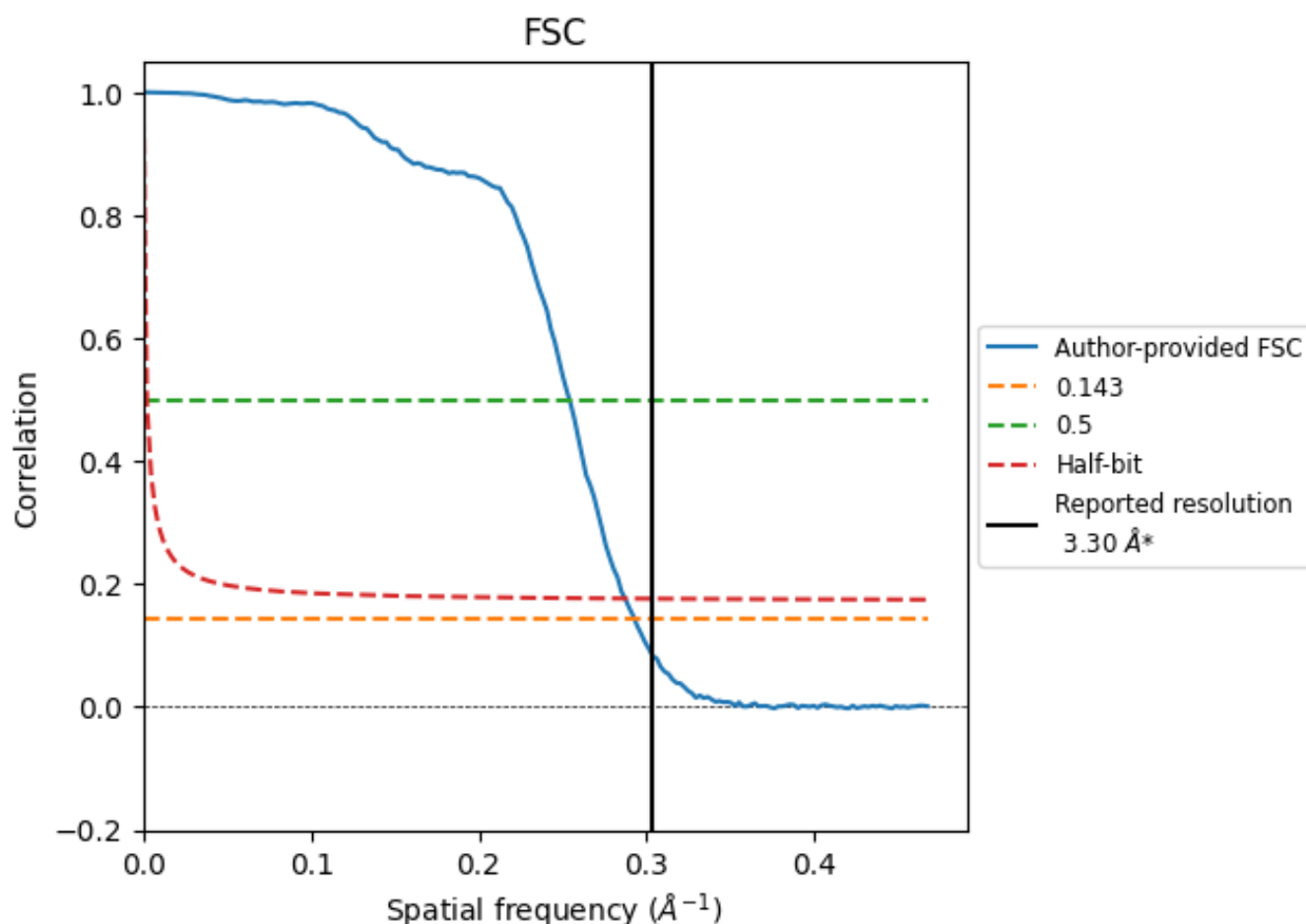


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.42	3.94	3.48
Unmasked-calculated*	-	-	-

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

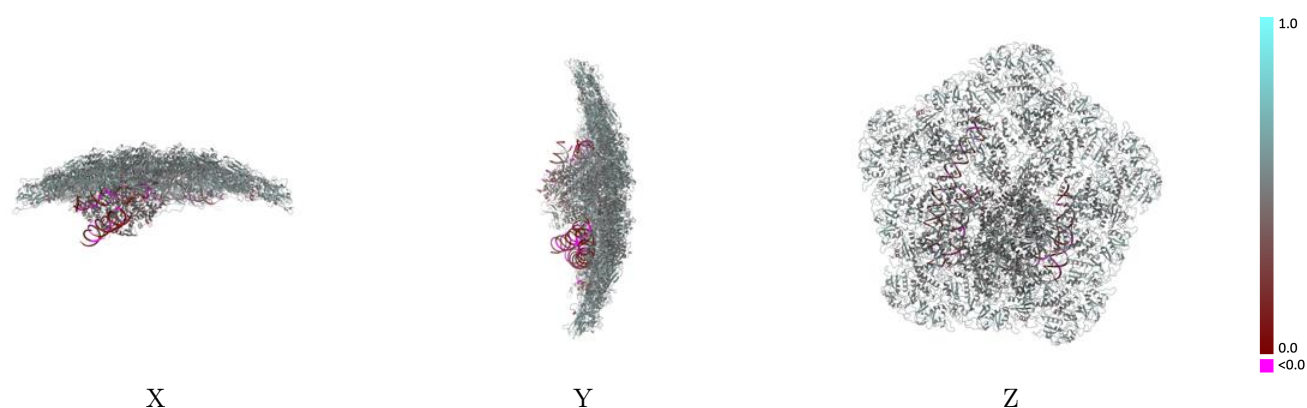
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31183 and PDB model 7ELH. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

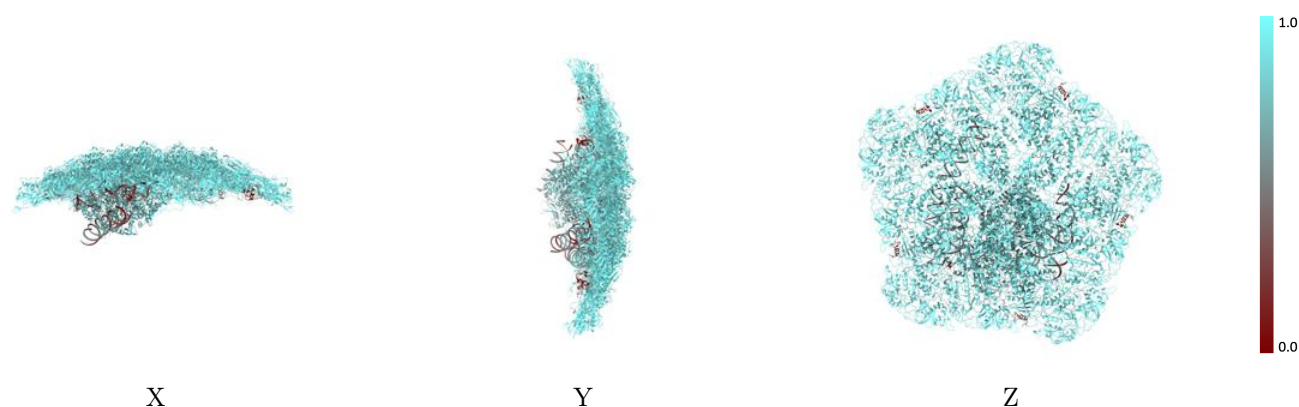
This section was not generated.

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



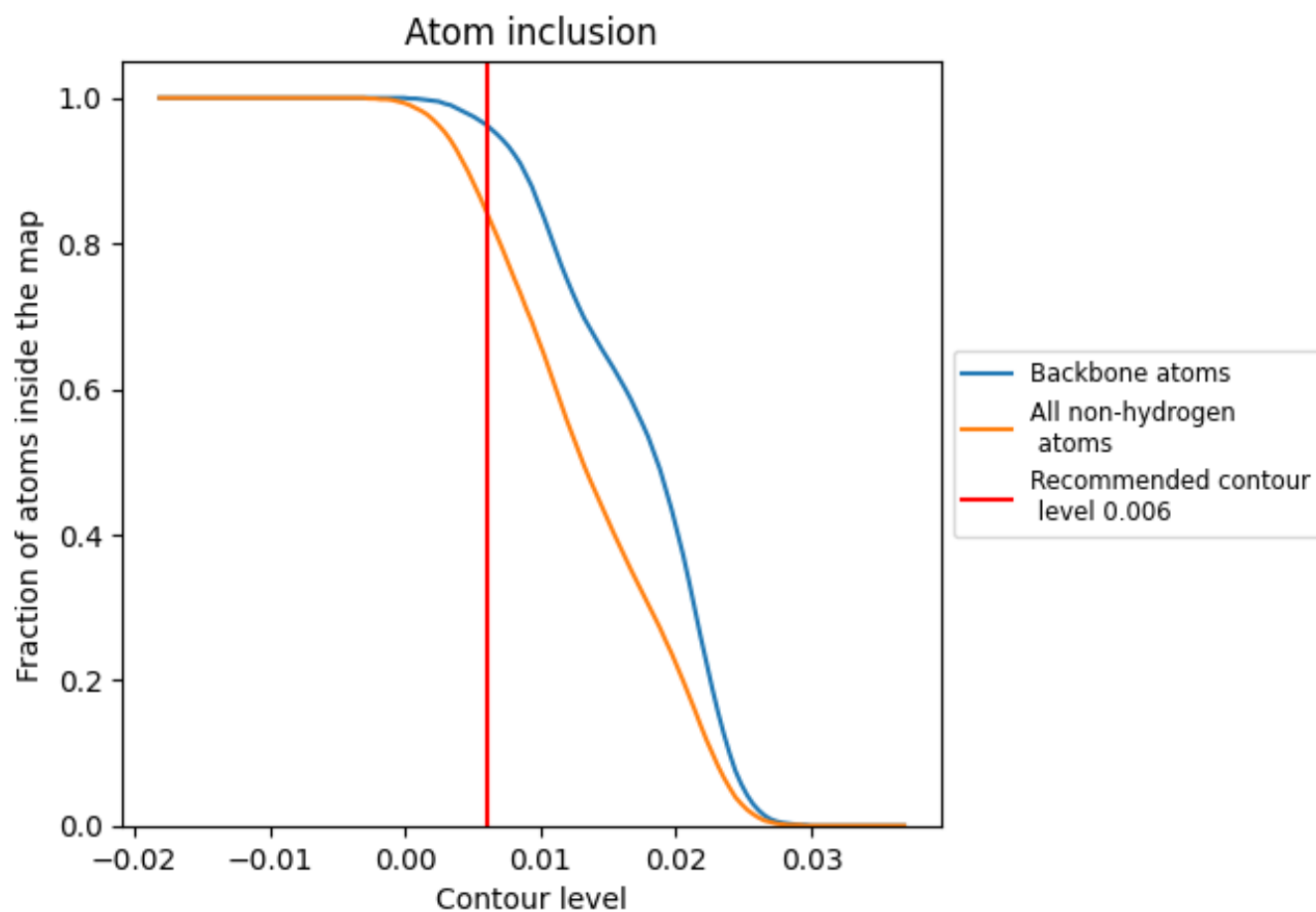
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.4780
A	 0.7560	 0.4550
B	 0.8020	 0.4730
C	 0.6550	 0.4250
D	 0.8920	 0.5130
E	 0.8760	 0.5090
F	 0.8920	 0.5120
G	 0.8740	 0.5100
H	 0.8960	 0.5140
I	 0.8730	 0.5080
J	 0.8950	 0.5140
K	 0.8680	 0.5070
L	 0.8910	 0.5110
M	 0.8710	 0.5050
N	 0.3350	 0.0380
O	 0.4520	 0.0900
P	 0.3590	 0.0900
Q	 0.3830	 0.1070
R	 0.5940	 0.1080
S	 0.4990	 0.1000
T	 0.3930	 0.0530
U	 0.2980	 0.0780
e	 0.7400	 0.4880
g	 0.7630	 0.4960
i	 0.7310	 0.4880
k	 0.7480	 0.4860
m	 0.6950	 0.4570

