



# Full wwPDB EM Validation Report ⓘ

Aug 11, 2025 – 03:22 PM EDT

PDB ID : 9D47 / pdb\_00009d47  
EMDB ID : EMD-46552  
Title : Atomic model of Candida albicans Fatty Acid Synthase (FAS) in complex with  
Palmitoyl-CoA (in vitro binding)  
Authors : Hasan, N.S.M.; Keszei, F.A.A.; Mazhab-Jafari, M.T.  
Deposited on : 2024-08-12  
Resolution : 2.62 Å(reported)  
Based on initial model : 6U5V

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

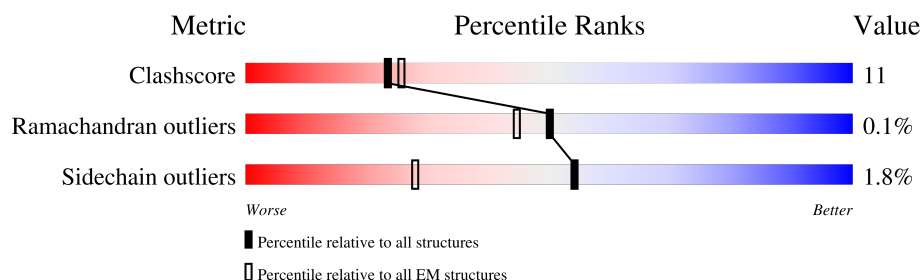
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.62 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	2037	<div> <div>12%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	E	2037	<div> <div>12%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	I	2037	<div> <div>11%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	M	2037	<div> <div>12%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	Q	2037	<div> <div>11%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	U	2037	<div> <div>12%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
2	C	1885	<div> <div>58%</div> <div>15%</div> <div>27%</div> </div>
2	G	1885	<div> <div>58%</div> <div>15%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	1885	
2	O	1885	
2	S	1885	
2	X	1885	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 160092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

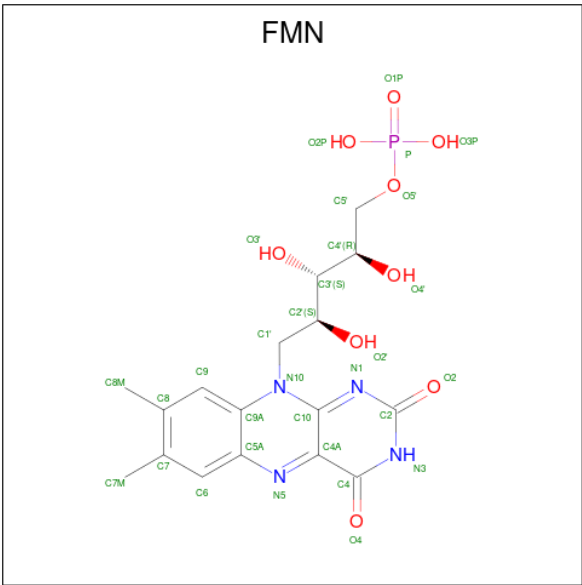
- Molecule 1 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		
1	E	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		
1	I	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		
1	M	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		
1	Q	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		
1	U	2000	Total	C	N	O	S	1	0
			15289	9831	2538	2870	50		

- Molecule 2 is a protein called Fatty acid synthase subunit alpha.

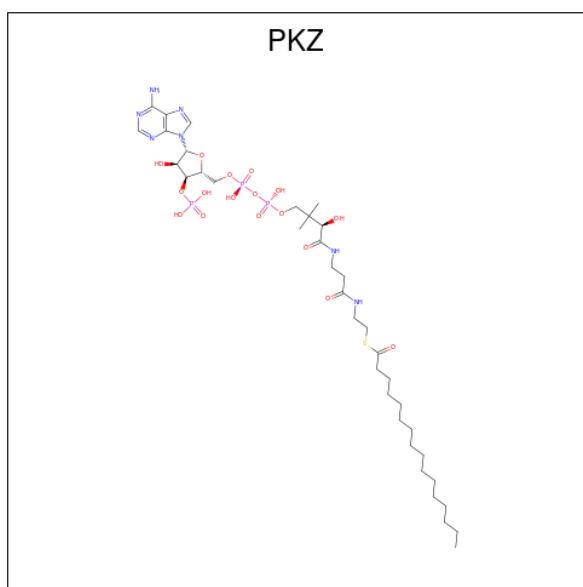
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		
2	G	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		
2	K	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		
2	O	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		
2	S	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		
2	X	1385	Total	C	N	O	S	0	0
			10790	6859	1823	2065	43		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	I	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	M	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	Q	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	U	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 4 is Palmitoyl-CoA (CCD ID: PKZ) (formula: C<sub>37</sub>H<sub>66</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	
4	G	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	
4	K	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	
4	O	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	
4	S	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	
4	X	1	Total	C	N	O	P	S	0
			39	27	2	8	1	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	235	Total	O	0
			235	235	
5	E	224	Total	O	0
			224	224	
5	I	242	Total	O	0
			242	242	
5	M	220	Total	O	0
			220	220	
5	Q	246	Total	O	0
			246	246	
5	U	227	Total	O	0
			227	227	

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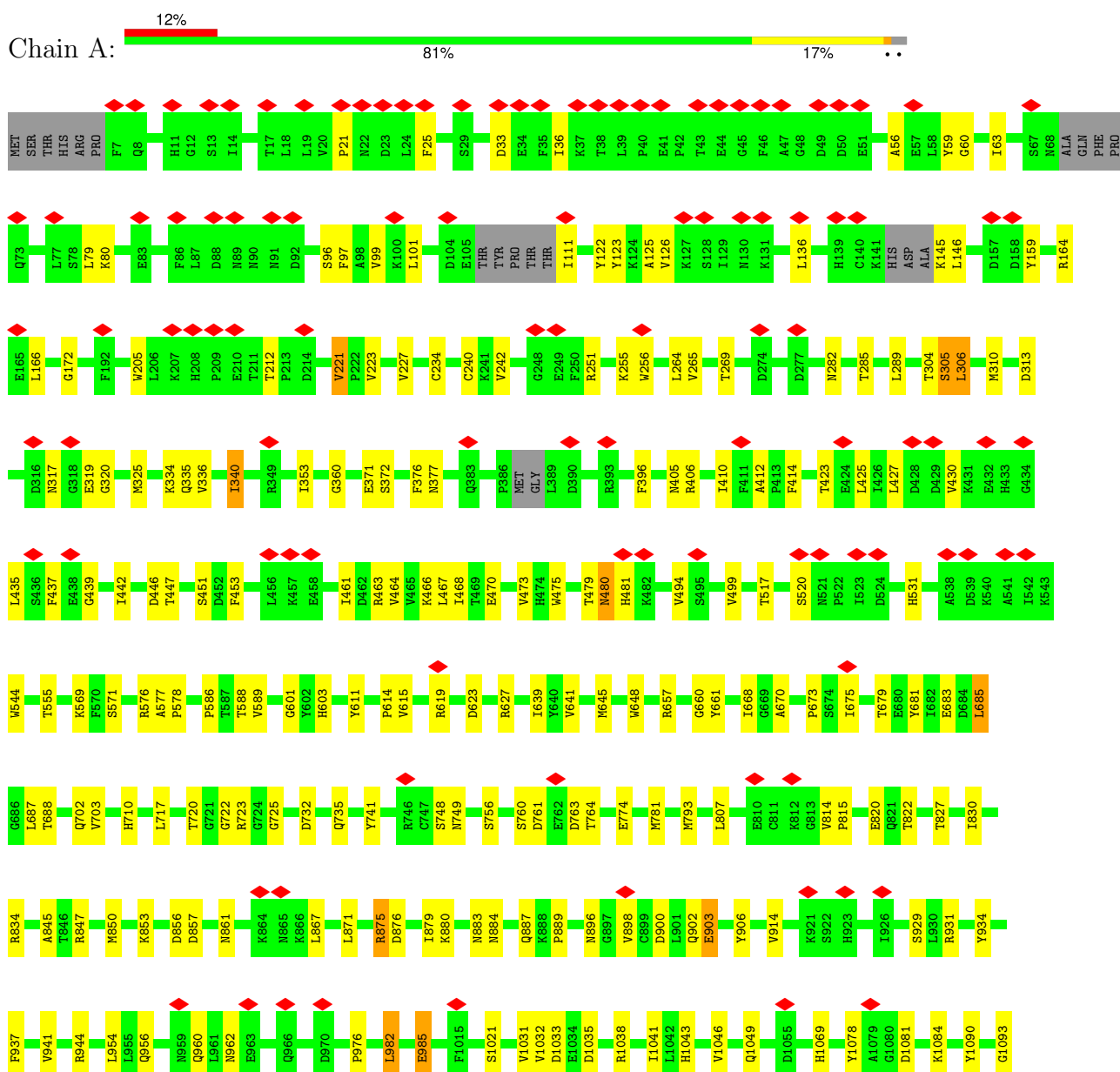
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Mol	Chain	Residues	Atoms		AltConf
5	C	290	Total 290	O 290	0
5	G	310	Total 310	O 310	0
5	K	302	Total 302	O 302	0
5	O	308	Total 308	O 308	0
5	S	302	Total 302	O 302	0
5	X	292	Total 292	O 292	0

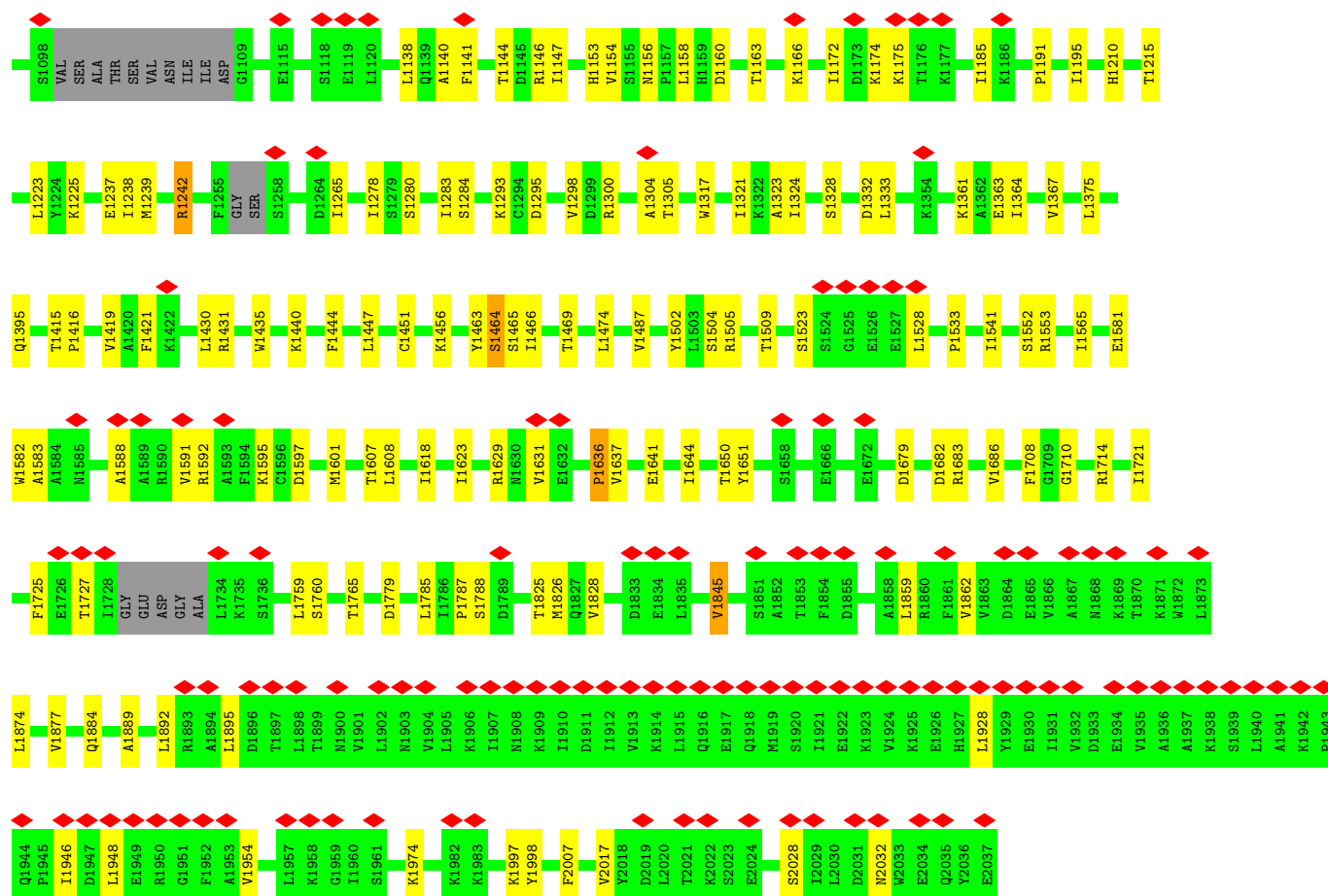
### 3 Residue-property plots

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.

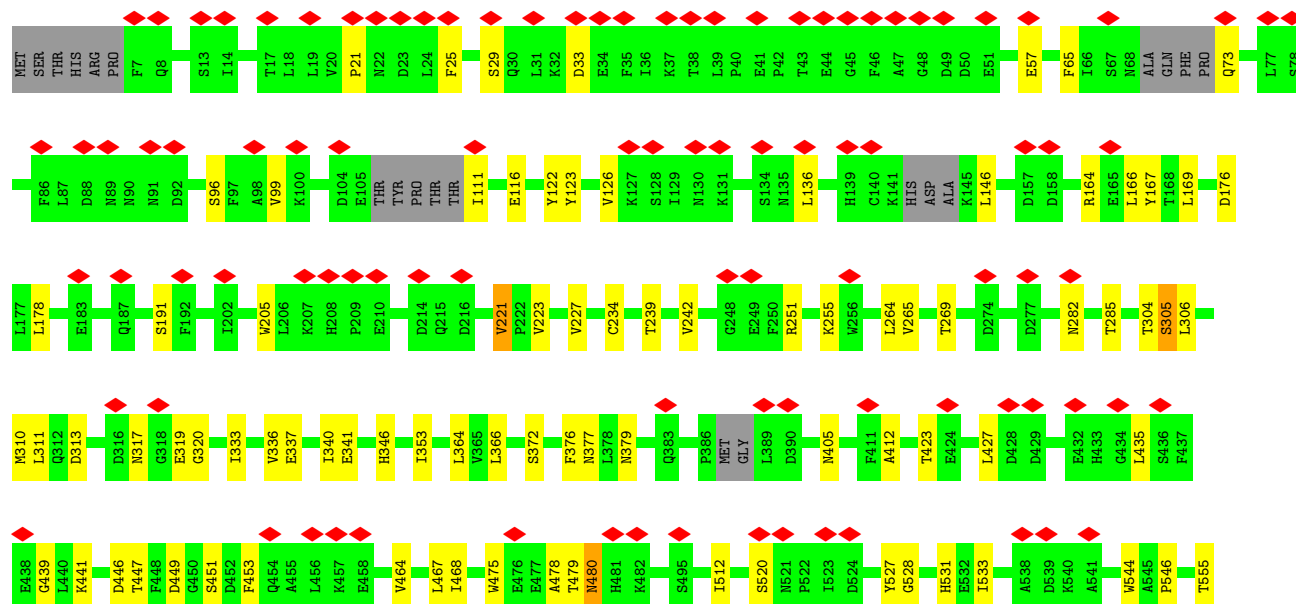
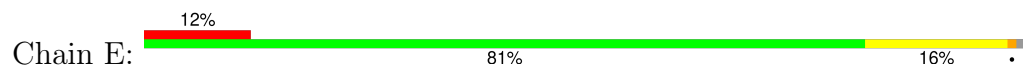
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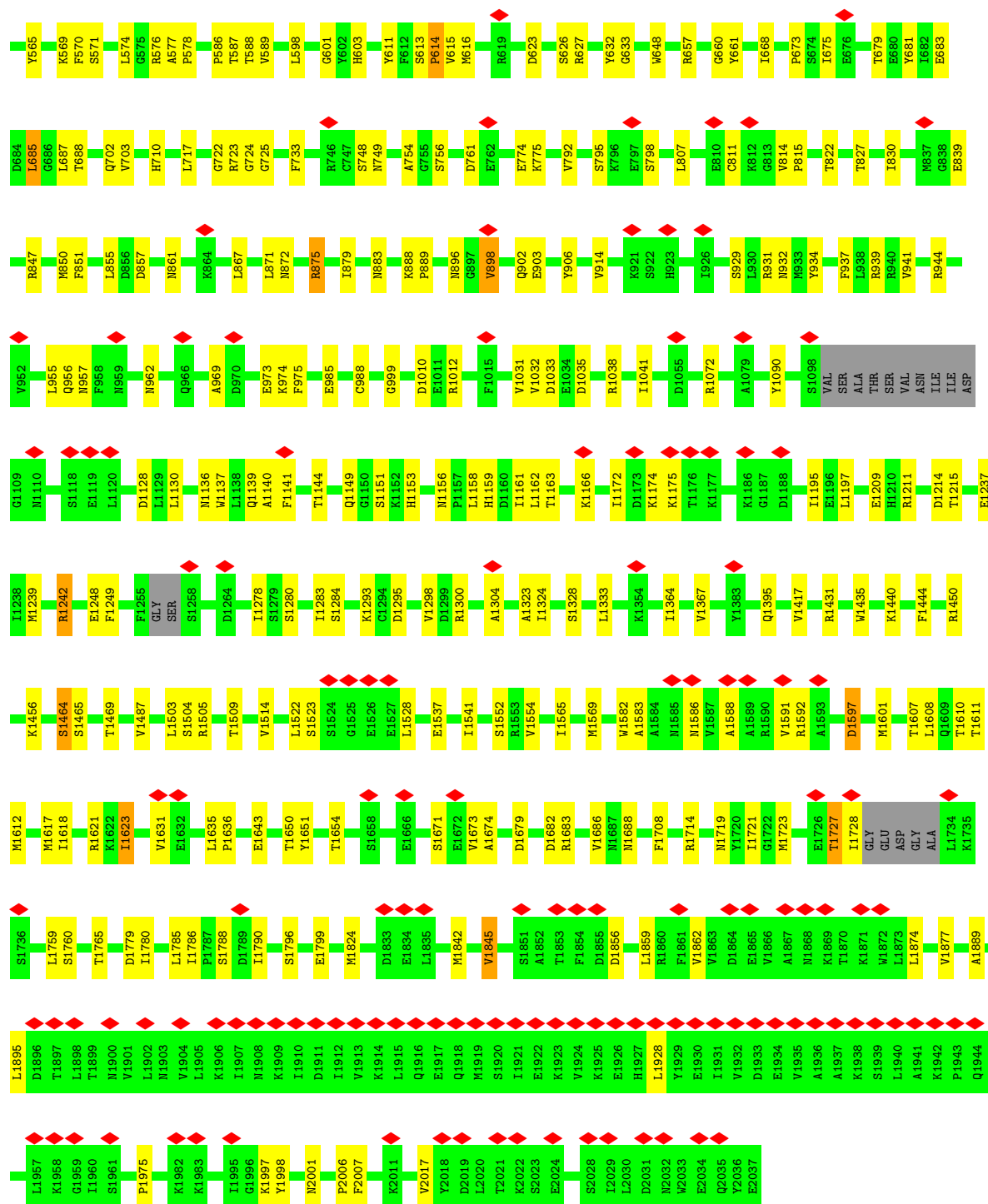




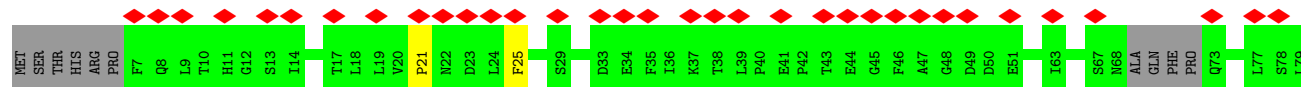
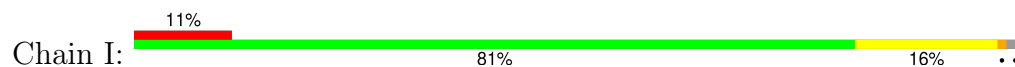


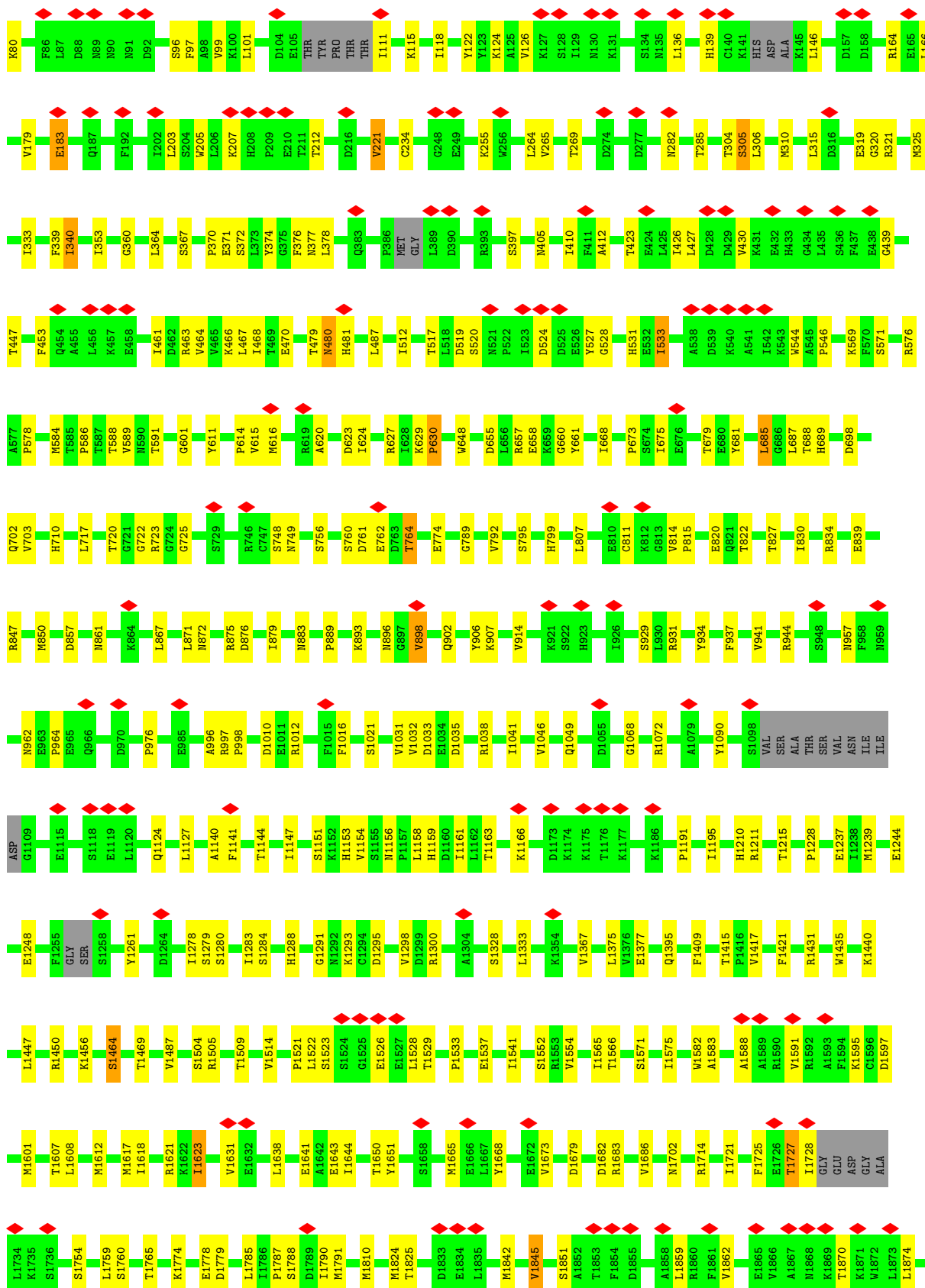
• Molecule 1: Fatty acid synthase subunit beta

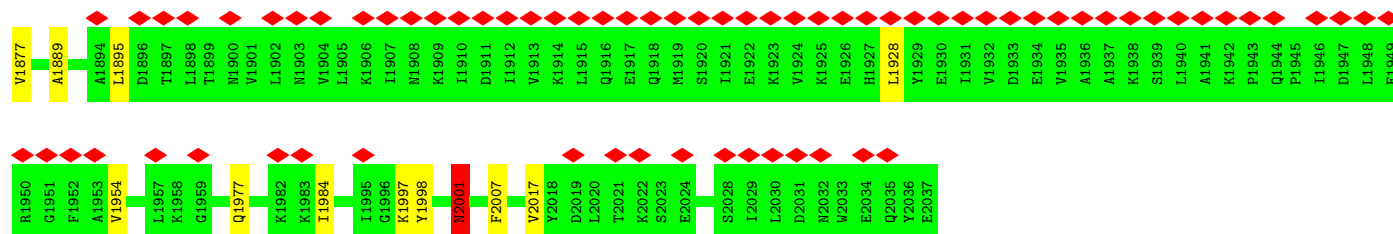




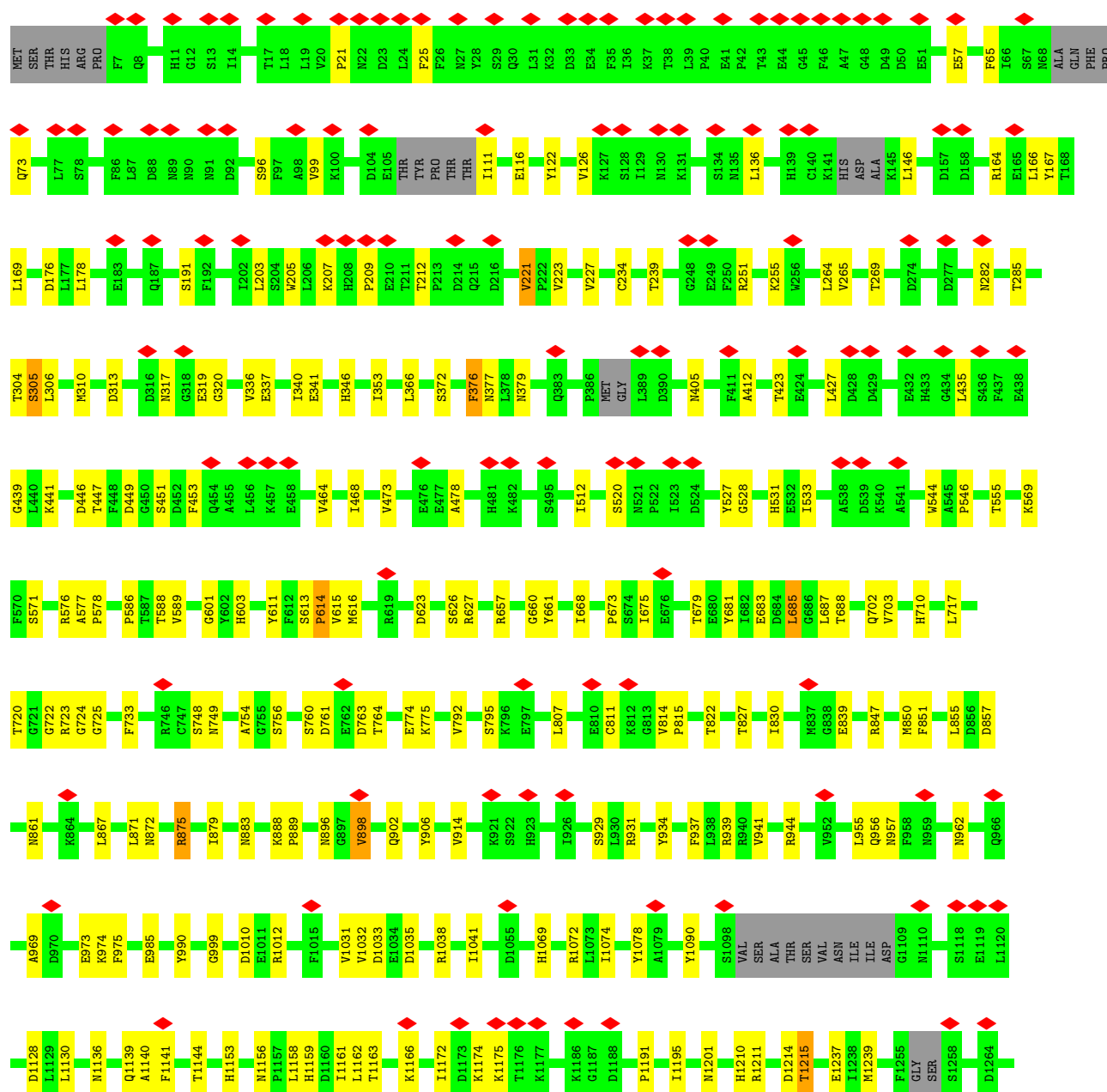
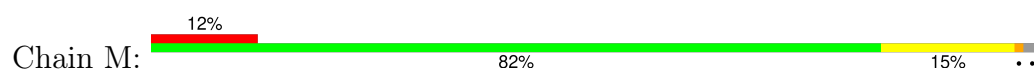
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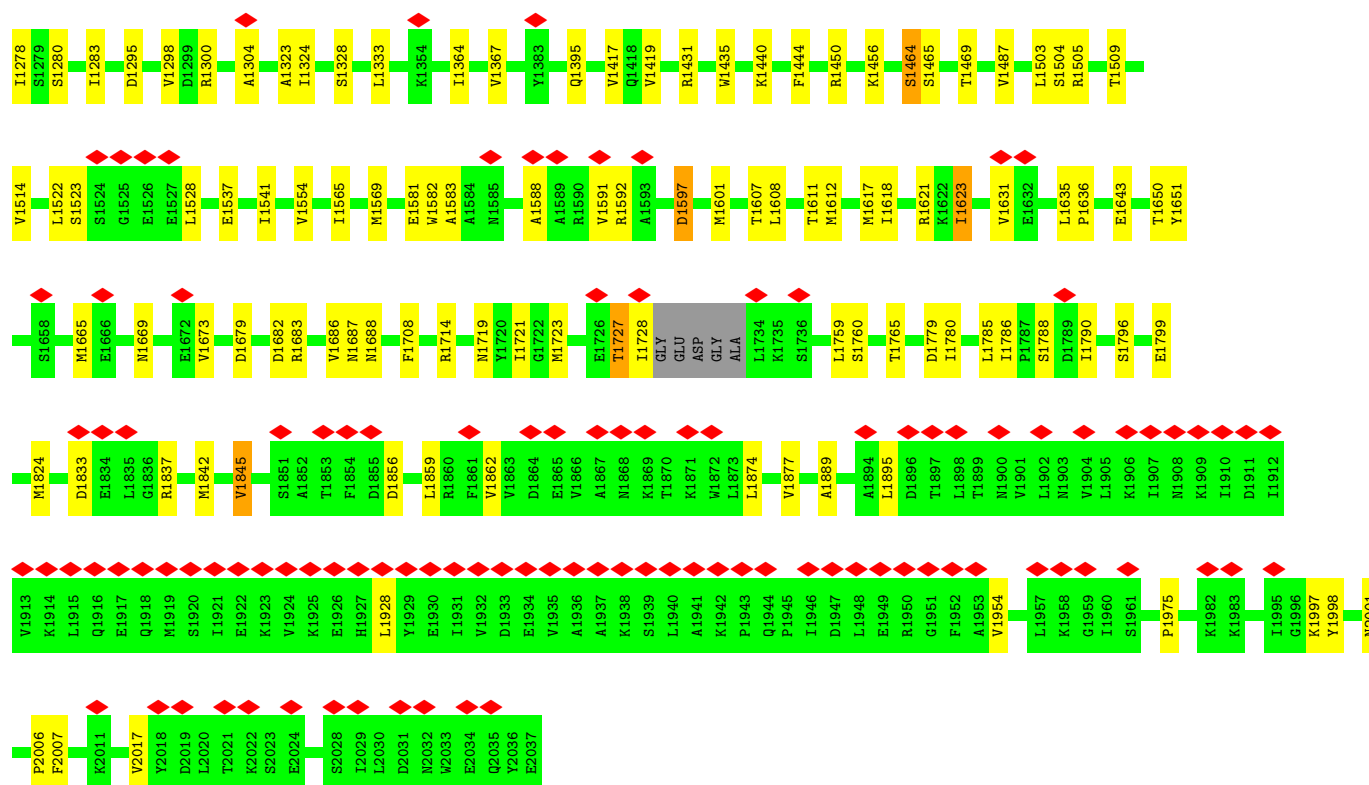




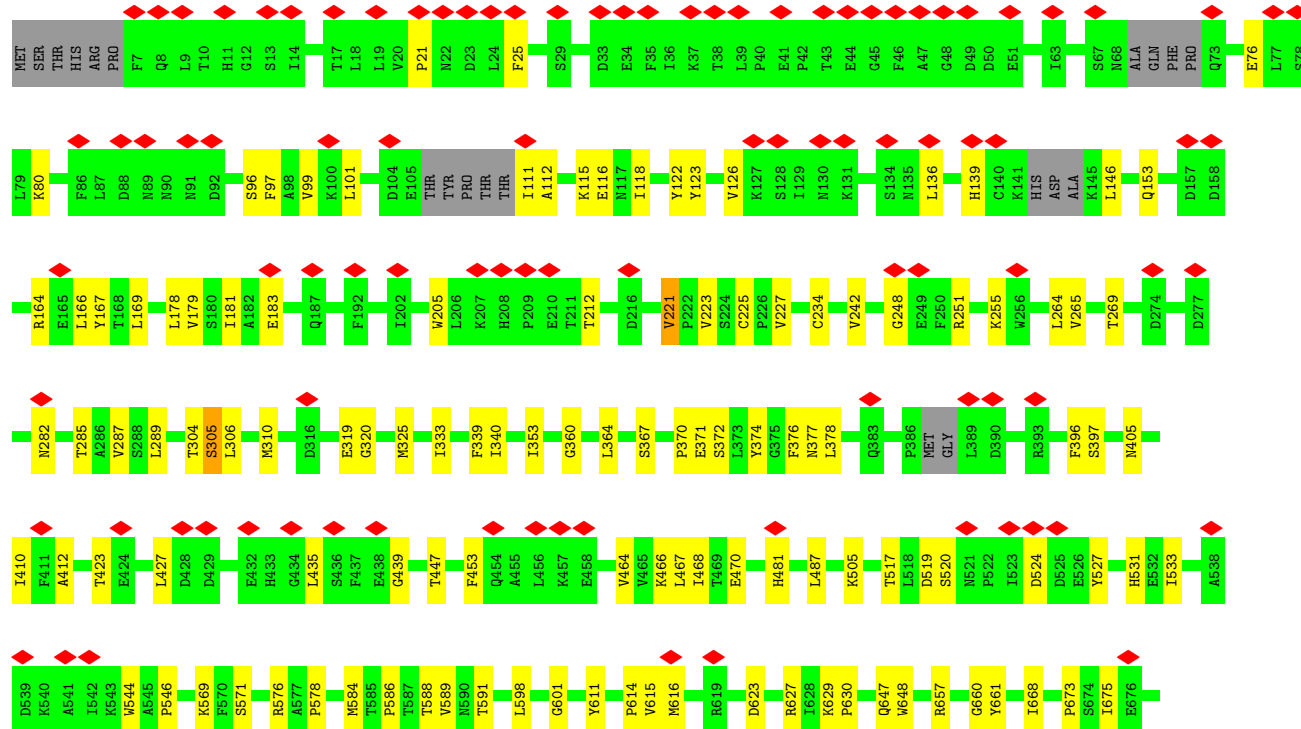
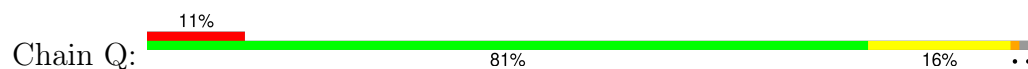


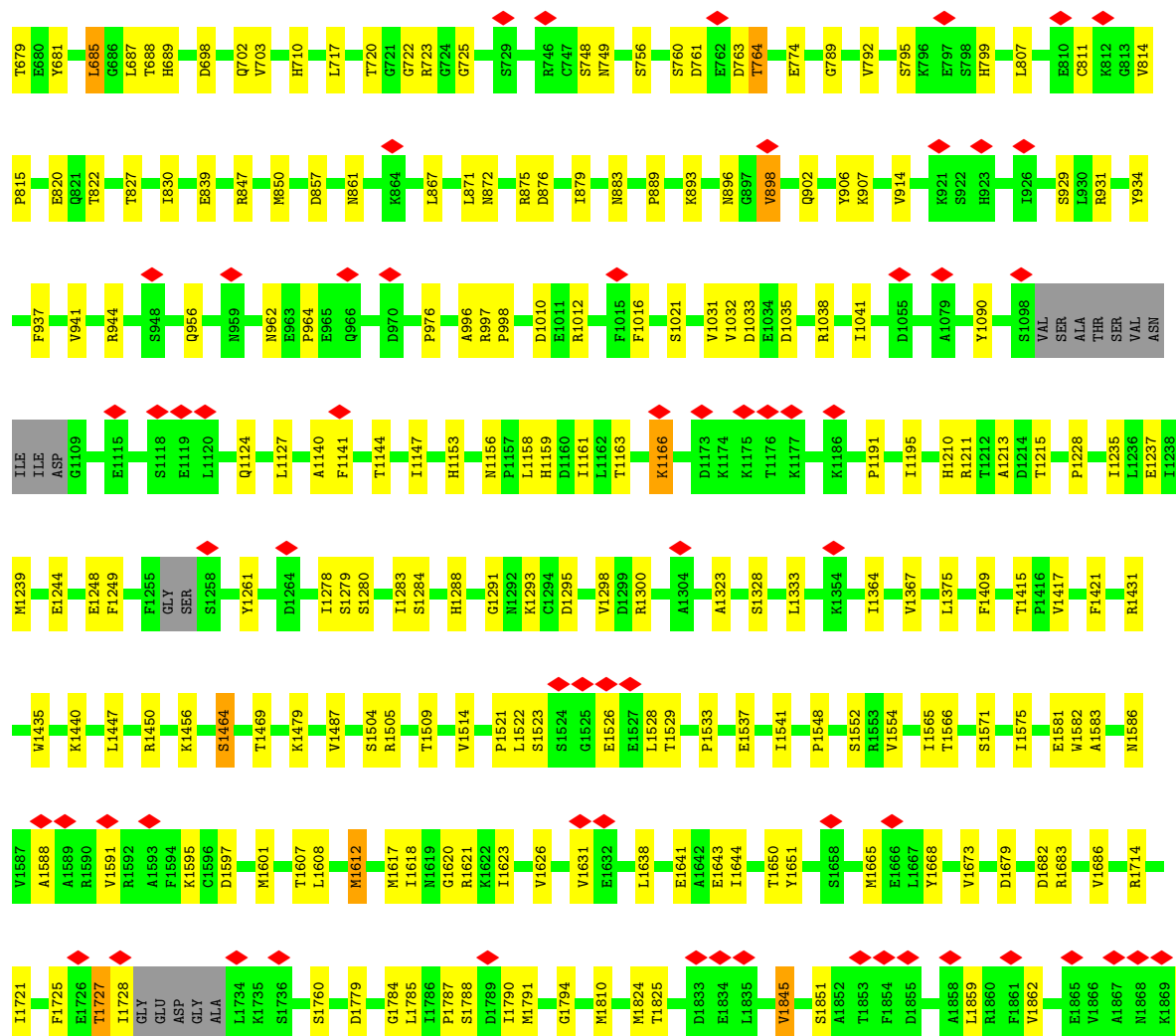
• Molecule 1: Fatty acid synthase subunit beta



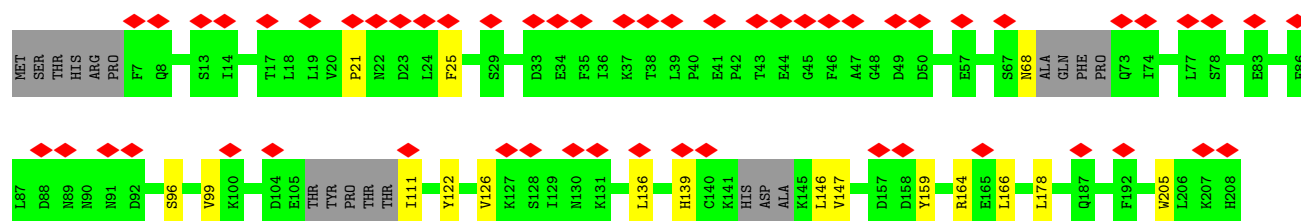
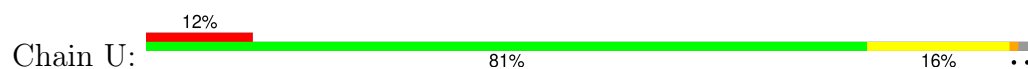


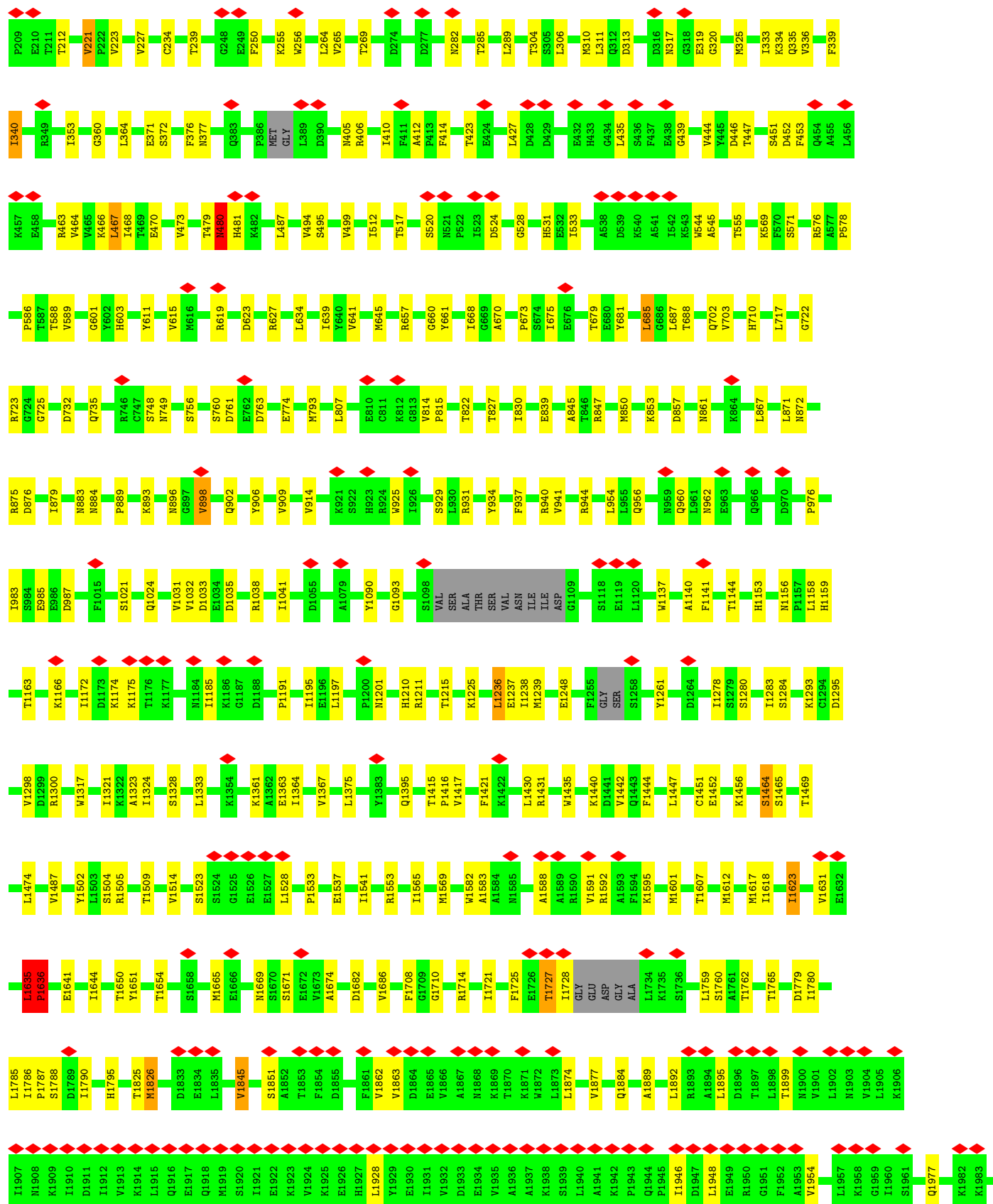
• Molecule 1: Fatty acid synthase subunit beta

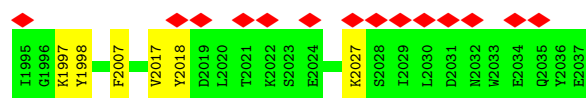




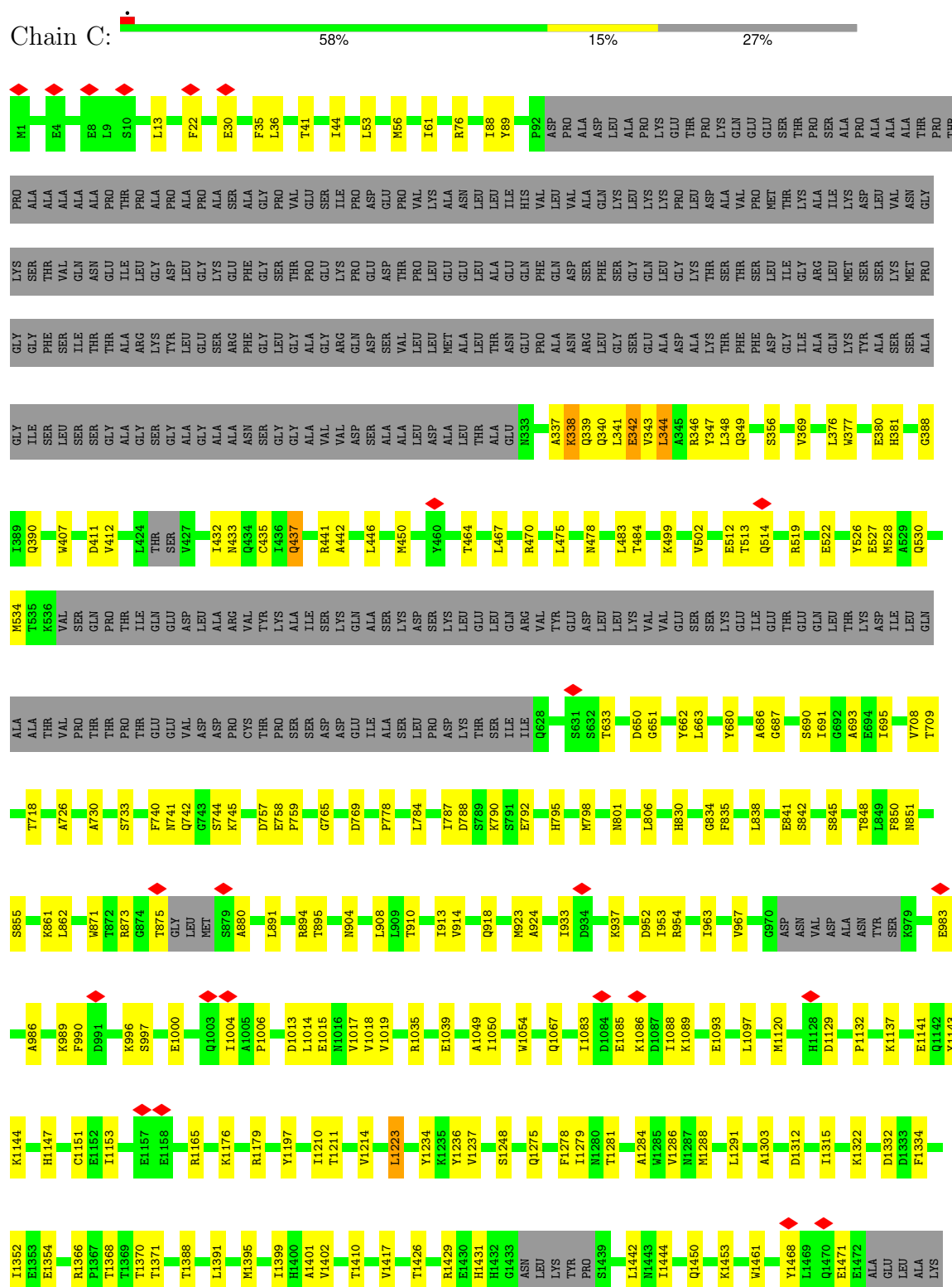
• Molecule 1: Fatty acid synthase subunit beta





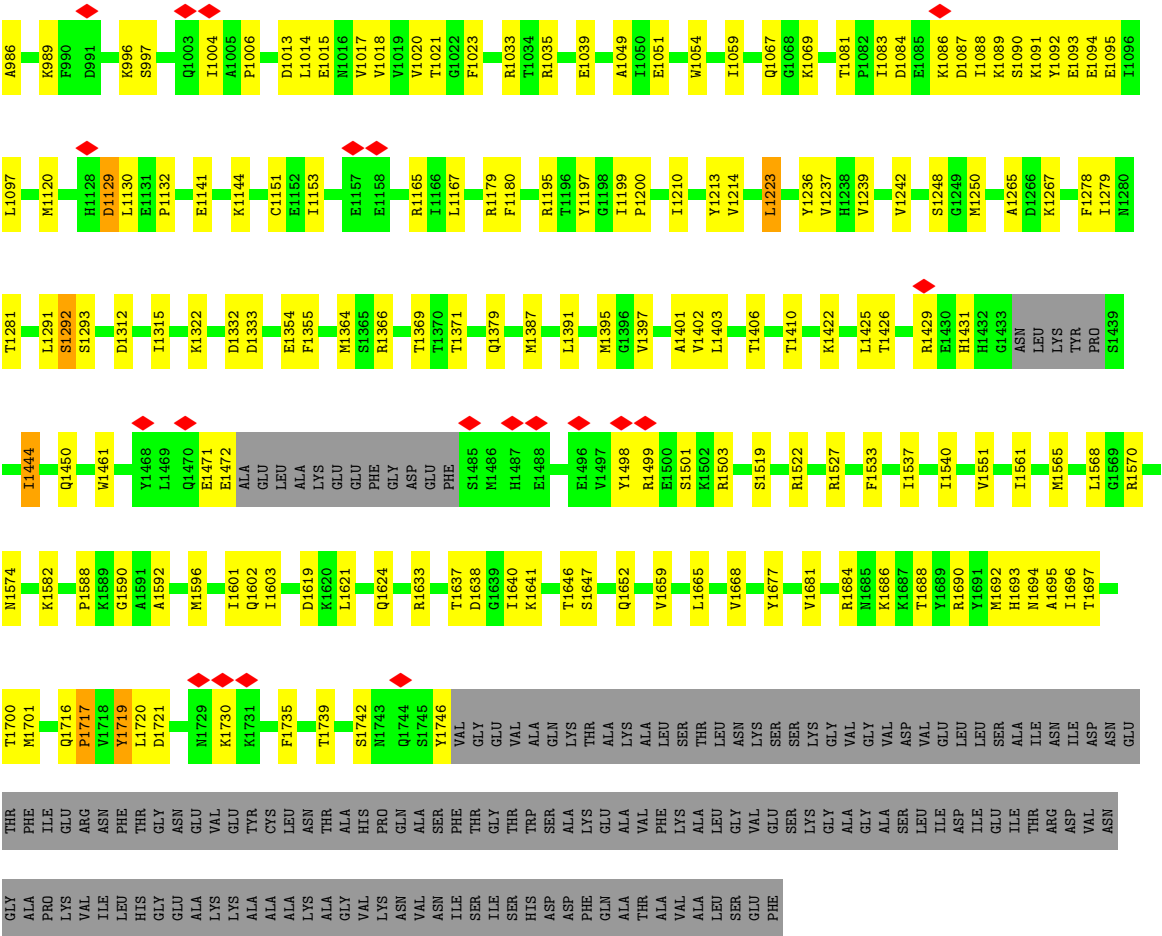


# • Molecule 2: Fatty acid synthase subunit alpha

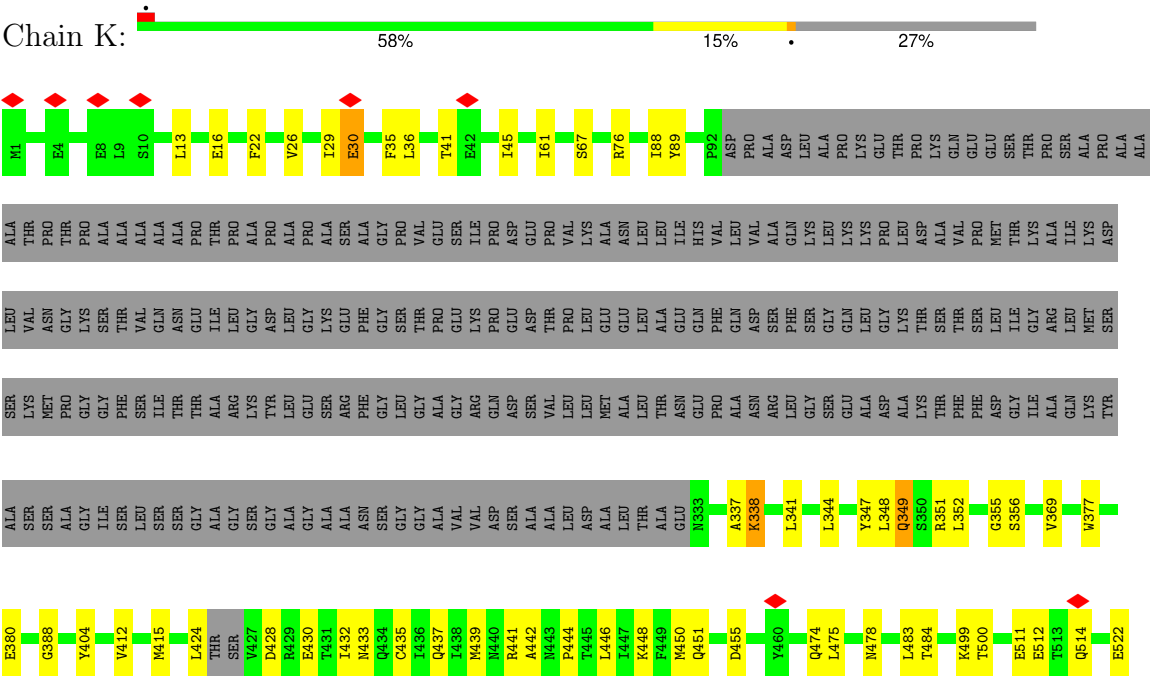








• Molecule 2: Fatty acid synthase subunit alpha

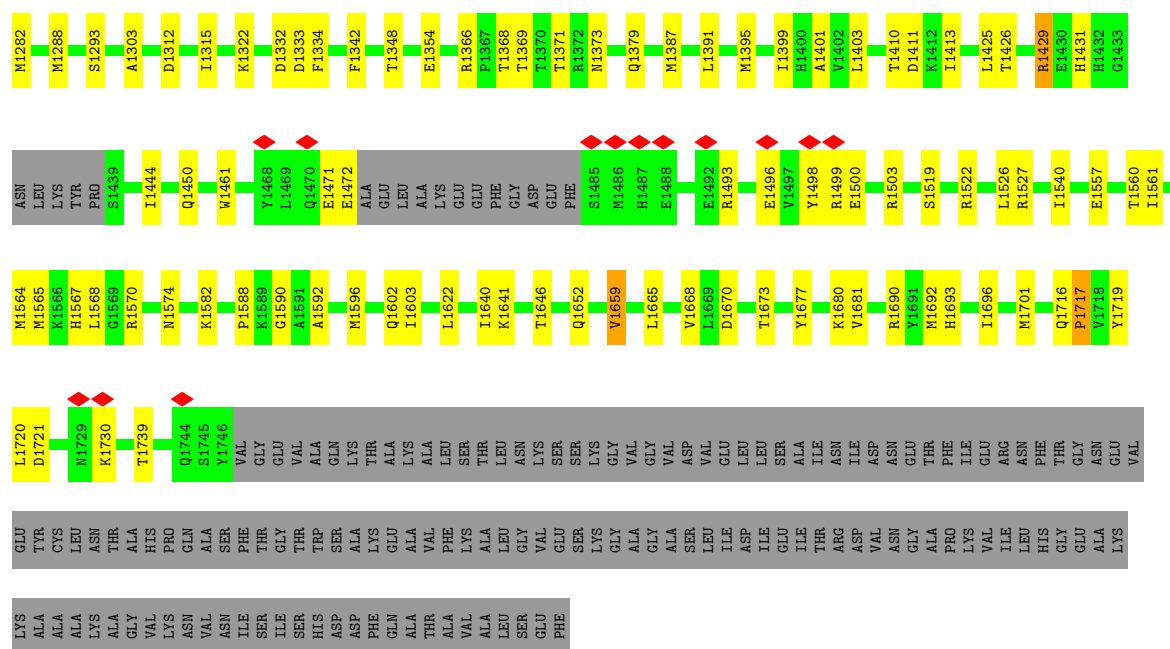




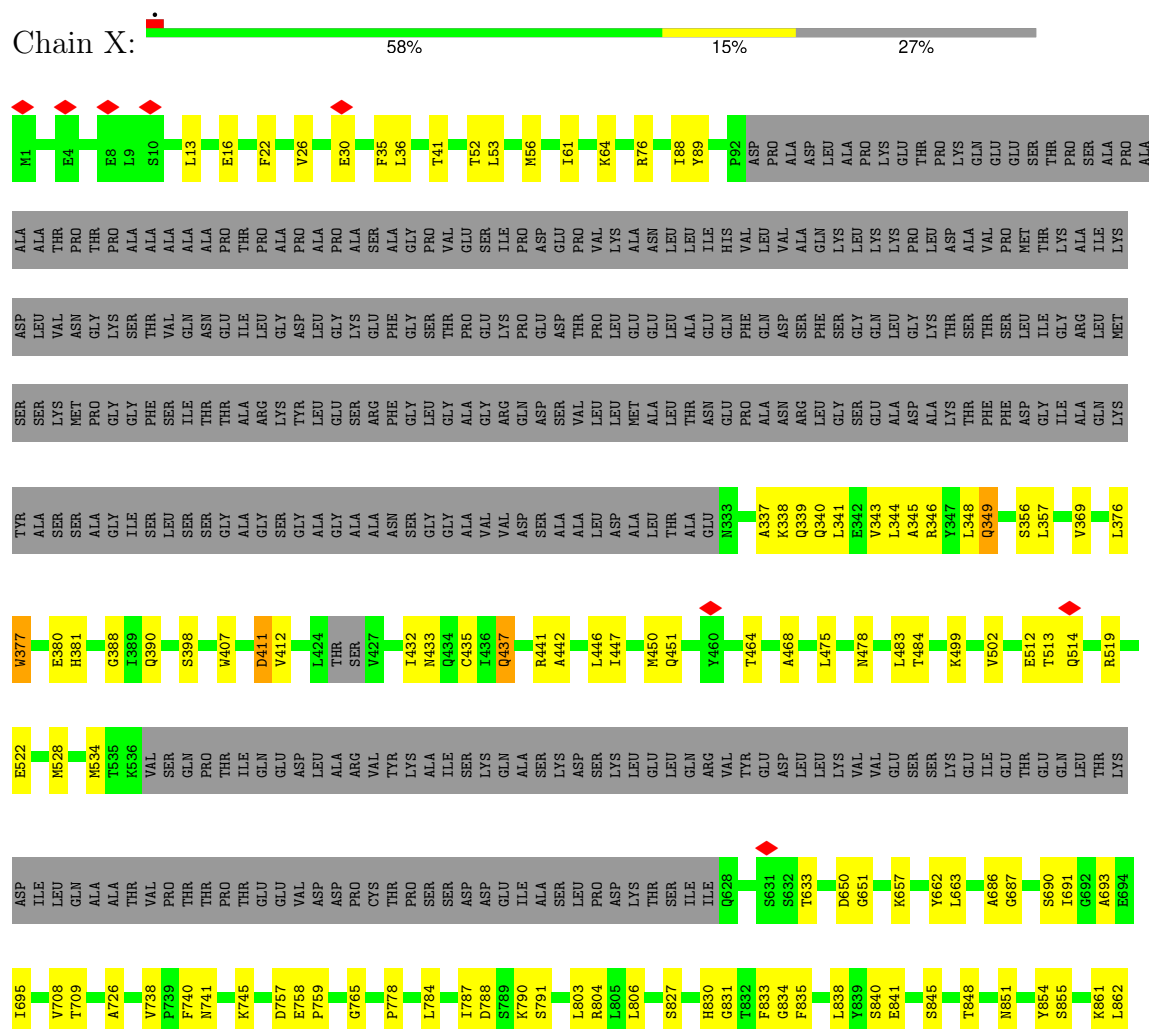


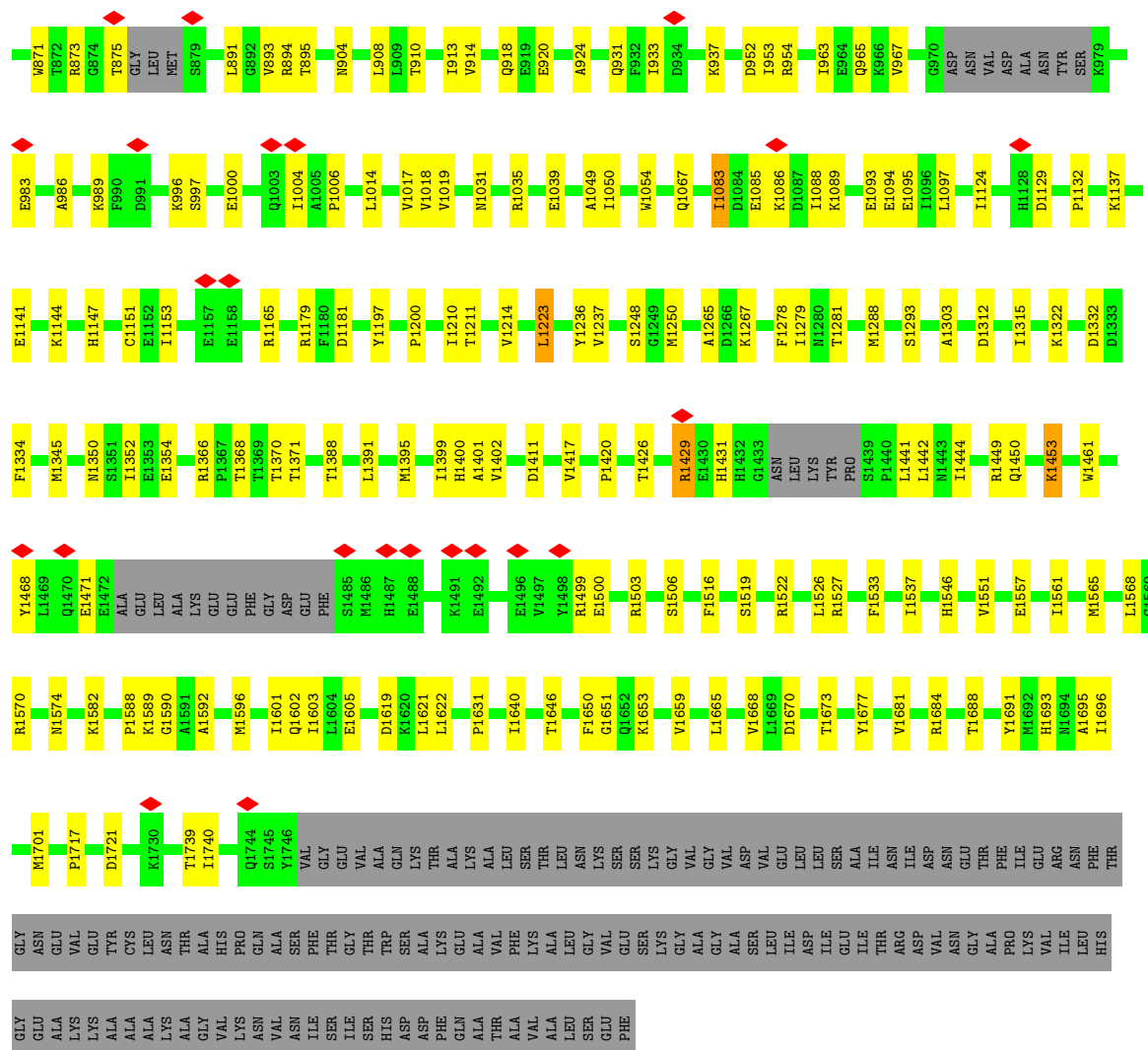
- Molecule 2: Fatty acid synthase subunit alpha





• Molecule 2: Fatty acid synthase subunit alpha





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	741610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.1	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.154	Depositor
Minimum map value	-11.606	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.630	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	346.08, 346.08, 346.08	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.24	2/15638 (0.0%)	0.47	8/21284 (0.0%)
1	E	0.37	5/15638 (0.0%)	0.51	8/21284 (0.0%)
1	I	0.44	9/15638 (0.1%)	0.57	9/21284 (0.0%)
1	M	0.36	5/15638 (0.0%)	0.50	8/21284 (0.0%)
1	Q	0.46	7/15638 (0.0%)	0.57	12/21284 (0.1%)
1	U	0.25	4/15638 (0.0%)	0.44	3/21284 (0.0%)
2	C	0.39	6/11008 (0.1%)	0.53	4/14897 (0.0%)
2	G	0.41	8/11008 (0.1%)	0.52	6/14897 (0.0%)
2	K	0.73	13/11008 (0.1%)	0.70	20/14897 (0.1%)
2	O	0.43	8/11008 (0.1%)	0.56	15/14897 (0.1%)
2	S	0.44	9/11008 (0.1%)	0.56	14/14897 (0.1%)
2	X	0.27	3/11008 (0.0%)	0.44	2/14897 (0.0%)
All	All	0.41	79/159876 (0.0%)	0.53	109/217086 (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
2	K	0	3
2	O	0	1
2	S	0	2
All	All	0	6

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	629	PRO	N-CD	49.92	2.17	1.47
1	Q	630	PRO	N-CD	37.66	2.00	1.47
2	K	1717	PRO	N-CD	33.48	1.94	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	630	PRO	CA-CB	29.24	1.94	1.53
1	Q	630	PRO	CG-CD	-26.49	0.60	1.50
2	C	1717	PRO	CB-CG	24.54	2.72	1.49
1	M	614	PRO	CB-CG	24.31	2.71	1.49
1	E	614	PRO	CB-CG	24.26	2.71	1.49
1	I	630	PRO	CB-CG	23.40	2.66	1.49
2	S	1717	PRO	CB-CG	23.21	2.65	1.49
2	O	1717	PRO	CB-CG	22.36	2.61	1.49
2	G	1717	PRO	CB-CG	21.51	2.57	1.49
2	G	1717	PRO	CG-CD	-19.96	0.82	1.50
2	K	629	PRO	CG-CD	-19.68	0.83	1.50
2	K	1717	PRO	CG-CD	-19.66	0.83	1.50
1	E	614	PRO	CG-CD	-19.05	0.85	1.50
1	M	614	PRO	CG-CD	-19.02	0.86	1.50
2	C	1717	PRO	CG-CD	-17.38	0.91	1.50
2	S	1717	PRO	CG-CD	-16.79	0.93	1.50
2	O	1717	PRO	CG-CD	-15.20	0.99	1.50
2	S	51	PRO	N-CD	15.14	1.69	1.47
1	I	2001	ASN	CG-OD1	-14.69	0.95	1.23
1	E	1635	LEU	C-N	14.69	1.50	1.33
1	I	630	PRO	CG-CD	14.38	1.99	1.50
1	Q	629	LYS	C-N	14.33	1.50	1.33
1	M	1635	LEU	C-N	13.98	1.49	1.33
2	O	1420	PRO	N-CD	13.77	1.67	1.47
2	K	1716	GLN	C-N	13.19	1.50	1.34
1	E	1636	PRO	N-CD	12.92	1.65	1.47
1	I	630	PRO	N-CD	-12.74	1.29	1.47
1	M	1636	PRO	N-CD	12.41	1.65	1.47
2	S	534	MET	CG-SD	-11.60	1.51	1.80
2	K	534	MET	CG-SD	-11.56	1.51	1.80
2	O	1717	PRO	N-CD	11.37	1.63	1.47
2	O	1419	ALA	C-N	11.13	1.47	1.33
2	K	629	PRO	CB-CG	11.03	2.04	1.49
2	K	628	GLN	CA-C	10.79	1.75	1.52
1	Q	2001	ASN	CG-OD1	-10.68	1.03	1.23
2	G	1717	PRO	N-CD	9.72	1.61	1.47
1	U	1635	LEU	C-N	9.57	1.44	1.33
1	I	630	PRO	N-CA	8.69	1.57	1.47
2	K	629	PRO	N-CA	-8.42	1.36	1.47
2	S	50	SER	C-N	8.22	1.53	1.33
2	X	377	TRP	CD2-CE3	-8.10	1.27	1.40
2	K	1717	PRO	CA-CB	-7.90	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1717	PRO	CA-CB	-7.78	1.42	1.53
2	G	377	TRP	CD2-CE3	-7.75	1.27	1.40
2	O	1420	PRO	CG-CD	-7.62	1.24	1.50
1	M	614	PRO	CA-CB	-7.53	1.43	1.53
2	G	1717	PRO	CA-CB	-7.34	1.43	1.53
2	S	1717	PRO	N-CD	7.17	1.57	1.47
2	S	1717	PRO	CA-CB	-7.04	1.43	1.53
1	E	614	PRO	CA-CB	-6.91	1.43	1.53
1	Q	629	LYS	N-CA	6.87	1.56	1.45
2	S	51	PRO	CG-CD	-6.72	1.27	1.50
2	K	629	PRO	CA-CB	-6.72	1.44	1.53
2	X	377	TRP	CZ3-CH2	-6.67	1.23	1.40
2	G	344	LEU	CG-CD1	-6.59	1.30	1.52
1	Q	630	PRO	CA-CB	-6.47	1.44	1.53
2	O	1420	PRO	CA-CB	-6.35	1.44	1.53
2	C	342	GLU	CG-CD	-6.35	1.36	1.52
1	I	630	PRO	CA-C	6.34	1.60	1.52
1	U	1636	PRO	N-CD	6.23	1.56	1.47
1	A	903	GLU	CD-OE1	-6.22	1.13	1.25
2	G	377	TRP	CZ3-CH2	-6.02	1.25	1.40
1	A	982	LEU	CG-CD1	-5.97	1.32	1.52
1	I	629	LYS	C-N	-5.81	1.25	1.33
2	C	342	GLU	CD-OE2	-5.73	1.14	1.25
2	C	1717	PRO	CA-CB	-5.60	1.45	1.53
2	G	377	TRP	CD2-CE2	-5.56	1.31	1.41
2	K	628	GLN	C-O	5.52	1.34	1.23
1	I	2001	ASN	CB-CG	-5.45	1.38	1.52
2	K	893	VAL	CB-CG1	-5.32	1.34	1.52
2	S	893	VAL	CB-CG1	-5.32	1.34	1.52
2	C	342	GLU	CB-CG	-5.20	1.36	1.52
1	Q	2001	ASN	CG-ND2	-5.19	1.22	1.33
2	X	411	ASP	CG-OD1	-5.18	1.15	1.25
1	U	467	LEU	CG-CD1	-5.15	1.35	1.52
1	U	480	ASN	CG-ND2	-5.05	1.22	1.33

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	630	PRO	N-CD-CG	-44.19	36.92	103.20
1	I	630	PRO	CA-N-CD	-43.70	50.83	112.00
2	K	1717	PRO	N-CD-CG	-33.83	52.45	103.20
2	K	629	PRO	N-CD-CG	-33.62	52.77	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	614	PRO	CB-CG-CD	-33.14	0.05	106.10
1	M	614	PRO	CB-CG-CD	-33.03	0.41	106.10
2	C	1717	PRO	CB-CG-CD	-32.15	3.22	106.10
2	S	1717	PRO	CB-CG-CD	-25.59	24.23	106.10
2	G	1717	PRO	CB-CG-CD	-22.57	33.89	106.10
1	I	630	PRO	CB-CG-CD	-22.32	34.67	106.10
2	O	1717	PRO	CB-CG-CD	-21.49	37.33	106.10
2	K	629	PRO	CB-CG-CD	-18.80	45.94	106.10
2	G	1717	PRO	N-CD-CG	-18.44	75.53	103.20
1	A	903	GLU	OE1-CD-OE2	-18.00	79.71	122.90
1	Q	630	PRO	CA-N-CD	-17.55	87.43	112.00
2	K	629	PRO	CA-N-CD	-17.06	88.12	112.00
2	O	1717	PRO	N-CD-CG	-16.28	78.79	103.20
2	O	1420	PRO	N-CD-CG	-16.12	79.01	103.20
2	O	1717	PRO	CA-CB-CG	-15.20	75.62	104.50
2	S	51	PRO	N-CD-CG	-15.02	80.67	103.20
2	O	1717	PRO	N-CA-CB	-14.51	86.72	103.26
2	K	1717	PRO	N-CA-CB	-13.67	89.03	103.52
2	S	1717	PRO	N-CA-CB	-13.41	88.58	103.33
2	K	629	PRO	N-CA-CB	-13.14	89.46	103.25
2	G	1717	PRO	N-CA-CB	-13.09	88.94	103.33
2	K	628	GLN	CA-C-O	-12.81	99.03	120.80
1	I	629	LYS	C-N-CD	12.04	174.34	125.00
2	G	1717	PRO	CA-CB-CG	-11.85	81.99	104.50
2	S	1717	PRO	CA-CB-CG	-11.75	82.18	104.50
1	Q	630	PRO	N-CA-CB	-11.63	89.38	103.45
2	S	1717	PRO	N-CD-CG	-11.62	85.77	103.20
2	K	1717	PRO	CA-N-CD	-11.61	95.74	112.00
1	I	2001	ASN	CB-CG-ND2	11.58	133.78	116.40
1	Q	630	PRO	CA-CB-CG	-11.39	82.86	104.50
2	C	1717	PRO	N-CA-CB	-11.09	91.13	103.33
2	O	1420	PRO	N-CA-CB	-10.43	90.83	103.45
2	C	1717	PRO	CA-CB-CG	-10.29	84.94	104.50
2	S	50	SER	CA-C-N	-9.97	107.38	119.84
2	S	50	SER	C-N-CA	-9.97	107.38	119.84
2	K	1716	GLN	CA-C-O	-9.96	106.52	120.16
1	Q	629	LYS	CA-C-N	-9.77	109.16	120.11
1	Q	629	LYS	C-N-CA	-9.77	109.16	120.11
1	I	630	PRO	CA-CB-CG	-9.71	86.06	104.50
1	M	614	PRO	CA-CB-CG	-9.64	86.19	104.50
2	O	1420	PRO	CA-CB-CG	-9.64	86.19	104.50
2	O	1420	PRO	CB-CG-CD	-9.59	75.41	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1716	GLN	CA-C-N	-9.59	109.03	119.19
2	K	1716	GLN	C-N-CA	-9.59	109.03	119.19
1	E	614	PRO	CA-CB-CG	-9.58	86.30	104.50
1	A	903	GLU	CG-CD-OE1	9.52	140.29	118.40
1	E	1636	PRO	N-CD-CG	-9.51	88.93	103.20
1	M	1636	PRO	N-CD-CG	-9.11	89.53	103.20
2	K	1717	PRO	CA-CB-CG	-8.69	88.00	104.50
2	O	1420	PRO	CA-N-CD	-8.62	99.93	112.00
2	K	1717	PRO	CB-CG-CD	-8.61	78.56	106.10
1	I	2001	ASN	CB-CG-OD1	-8.51	103.77	120.80
1	M	614	PRO	N-CA-CB	-8.31	93.99	103.30
1	A	903	GLU	CG-CD-OE2	7.97	136.74	118.40
1	Q	629	LYS	C-N-CD	7.95	157.60	125.00
1	E	614	PRO	N-CA-CB	-7.94	94.21	103.26
2	S	51	PRO	CA-CB-CG	-7.86	89.57	104.50
1	Q	630	PRO	CB-CG-CD	-7.69	81.50	106.10
2	K	628	GLN	C-N-CD	7.56	156.00	125.00
2	G	1719	TYR	CA-C-N	7.44	135.75	121.54
2	G	1719	TYR	C-N-CA	7.44	135.75	121.54
1	E	614	PRO	CA-N-CD	-7.42	101.61	112.00
1	Q	629	LYS	CA-C-O	-7.37	112.76	120.87
2	X	1420	PRO	CA-CB-CG	-7.32	90.59	104.50
1	M	614	PRO	CA-N-CD	-7.24	101.86	112.00
1	U	1826	MET	CG-SD-CE	7.07	116.46	100.90
2	K	1716	GLN	C-N-CD	6.98	153.63	125.00
2	X	1420	PRO	N-CD-CG	-6.98	92.73	103.20
2	K	628	GLN	CA-C-N	-6.91	111.20	119.84
2	K	628	GLN	C-N-CA	-6.91	111.20	119.84
1	A	1636	PRO	N-CD-CG	-6.90	92.85	103.20
2	C	1717	PRO	CA-N-CD	-6.78	102.50	112.00
2	K	629	PRO	N-CA-C	6.74	126.35	112.47
1	A	903	GLU	CA-CB-CG	6.70	127.49	114.10
2	S	1263	ARG	CA-C-O	-6.56	113.93	120.82
1	E	1635	LEU	CA-C-N	-6.54	112.39	119.98
1	E	1635	LEU	C-N-CA	-6.54	112.39	119.98
1	M	1635	LEU	CA-C-N	-6.24	112.74	119.98
1	M	1635	LEU	C-N-CA	-6.24	112.74	119.98
2	O	1717	PRO	CA-N-CD	-6.19	103.33	112.00
1	U	1636	PRO	N-CD-CG	-6.14	93.99	103.20
1	Q	1521	PRO	N-CD-CG	-6.14	94.00	103.20
2	K	1263	ARG	CA-C-O	-6.06	114.46	120.82
1	U	1416	PRO	N-CD-CG	-5.98	94.23	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	51	PRO	CA-N-CD	-5.96	103.65	112.00
2	O	1420	PRO	N-CA-C	5.85	119.69	111.33
2	S	51	PRO	N-CA-CB	-5.83	97.13	103.25
1	I	1521	PRO	N-CD-CG	-5.82	94.47	103.20
2	S	1717	PRO	CA-N-CD	-5.82	103.85	112.00
1	I	629	LYS	CA-C-O	5.63	129.37	121.27
1	A	1636	PRO	CA-CB-CG	-5.49	94.06	104.50
2	S	51	PRO	N-CA-C	5.40	123.60	112.47
1	A	1416	PRO	CA-N-CD	-5.38	104.47	112.00
1	Q	1521	PRO	CA-N-CD	-5.36	104.50	112.00
2	O	1419	ALA	CA-C-N	-5.16	114.33	120.11
2	O	1419	ALA	C-N-CA	-5.16	114.33	120.11
2	O	1420	PRO	CB-CA-C	5.15	119.33	111.40
2	K	629	PRO	CA-CB-CG	-5.14	94.73	104.50
1	Q	629	LYS	N-CA-CB	-5.09	102.72	110.05
1	A	903	GLU	CB-CG-CD	5.08	121.23	112.60
1	I	1521	PRO	CA-N-CD	-5.08	104.89	112.00
1	M	2006	PRO	CA-N-CD	-5.02	104.97	112.00
2	O	1419	ALA	C-N-CD	5.02	145.57	125.00
2	S	50	SER	C-N-CD	5.02	145.56	125.00
1	E	2006	PRO	CA-N-CD	-5.01	104.98	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	1263	ARG	Mainchain
2	K	1429	ARG	Sidechain
2	K	628	GLN	Peptide
2	O	1429	ARG	Sidechain
2	S	1263	ARG	Mainchain
2	S	1429	ARG	Sidechain

## 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	15289	0	14857	339	0
1	E	15289	0	14857	306	0
1	I	15289	0	14857	282	0
1	M	15289	0	14857	279	0
1	Q	15289	0	14857	288	0
1	U	15289	0	14857	301	0
2	C	10790	0	10600	321	0
2	G	10790	0	10600	302	0
2	K	10790	0	10600	310	0
2	O	10790	0	10600	310	0
2	S	10790	0	10600	307	0
2	X	10790	0	10600	284	0
3	A	31	0	19	2	0
3	E	31	0	19	1	0
3	I	31	0	19	2	0
3	M	31	0	19	3	0
3	Q	31	0	19	2	0
3	U	31	0	19	4	0
4	C	39	0	0	8	0
4	G	39	0	0	9	0
4	K	39	0	0	10	0
4	O	39	0	0	8	0
4	S	39	0	0	10	0
4	X	39	0	0	9	0
5	A	235	0	0	122	0
5	C	290	0	0	100	0
5	E	224	0	0	101	0
5	G	310	0	0	112	0
5	I	242	0	0	91	0
5	K	302	0	0	100	0
5	M	220	0	0	94	0
5	O	308	0	0	104	0
5	Q	246	0	0	98	0
5	S	302	0	0	101	0
5	U	227	0	0	98	0
5	X	292	0	0	99	0
All	All	160092	0	152856	3346	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 11.

All (3346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:628:GLN:CA	2:K:628:GLN:C	1.75	1.54
1:I:630:PRO:CG	1:I:630:PRO:CD	1.99	1.41
2:K:629:PRO:CG	2:K:629:PRO:N	1.79	1.40
2:S:1717:PRO:N	2:S:1717:PRO:CG	1.77	1.39
1:M:614:PRO:CG	1:M:614:PRO:N	1.86	1.38
1:E:614:PRO:CG	1:E:614:PRO:N	1.87	1.36
2:C:983:GLU:HG3	5:C:2014:HOH:O	1.24	1.34
2:C:1717:PRO:N	2:C:1717:PRO:CG	1.84	1.34
2:K:629:PRO:CG	2:K:629:PRO:CB	2.04	1.33
2:S:51:PRO:CD	2:S:51:PRO:N	1.68	1.32
2:O:798:MET:HE2	5:O:2001:HOH:O	1.30	1.31
1:M:754:ALA:HB3	5:M:2410:HOH:O	1.27	1.31
1:U:876:ASP:HB2	5:U:2370:HOH:O	1.15	1.30
2:G:1652:GLN:HG3	5:G:2226:HOH:O	1.32	1.29
2:S:798:MET:HE2	5:S:2059:HOH:O	1.21	1.28
2:X:983:GLU:HG3	5:X:2020:HOH:O	1.23	1.27
1:E:754:ALA:HB3	5:E:2410:HOH:O	1.26	1.25
2:G:633:THR:HG21	5:G:2091:HOH:O	1.36	1.24
1:I:439:GLY:HA2	5:I:2255:HOH:O	1.39	1.20
2:O:633:THR:HG21	5:O:2098:HOH:O	1.36	1.19
2:C:1546:HIS:HD2	5:C:2015:HOH:O	1.23	1.19
2:X:983:GLU:HB3	5:X:2004:HOH:O	1.37	1.19
2:X:1388:THR:HG21	5:X:2240:HOH:O	1.42	1.18
1:Q:439:GLY:HA2	5:Q:2268:HOH:O	1.38	1.18
1:Q:1166:LYS:HG3	5:Q:2202:HOH:O	1.42	1.18
2:X:983:GLU:CB	5:X:2004:HOH:O	1.89	1.18
2:X:1546:HIS:HD2	5:X:2012:HOH:O	1.20	1.16
2:S:1717:PRO:CD	2:S:1717:PRO:HG3	1.69	1.15
1:U:439:GLY:HA2	5:U:2290:HOH:O	1.46	1.14
1:M:1419:VAL:HG11	5:M:2204:HOH:O	1.44	1.14
1:Q:876:ASP:HB3	5:Q:2357:HOH:O	1.44	1.14
1:I:876:ASP:HB2	5:I:2273:HOH:O	1.48	1.13
1:I:1450:ARG:CB	5:I:2381:HOH:O	1.96	1.13
1:I:876:ASP:HB3	5:I:2360:HOH:O	1.45	1.13
1:M:614:PRO:CD	1:M:614:PRO:HG2	1.63	1.13
1:Q:876:ASP:HB2	5:Q:2279:HOH:O	1.48	1.12
1:Q:1450:ARG:CB	5:Q:2383:HOH:O	1.97	1.12
1:U:1851:SER:HA	5:U:2303:HOH:O	1.48	1.12
2:C:1717:PRO:CD	2:C:1717:PRO:HG2	1.68	1.11
2:S:1717:PRO:CG	2:S:1717:PRO:HD2	1.61	1.11
1:M:614:PRO:CD	1:M:614:PRO:HG3	1.63	1.11
1:U:876:ASP:HB3	5:U:2359:HOH:O	1.49	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:614:PRO:CD	1:E:614:PRO:HG2	1.63	1.09
2:S:1717:PRO:CD	2:S:1717:PRO:HG2	1.69	1.09
1:A:876:ASP:HB3	5:A:2365:HOH:O	1.51	1.09
1:A:982:LEU:HD11	5:C:2045:HOH:O	1.51	1.09
1:E:614:PRO:CD	1:E:614:PRO:HG3	1.63	1.09
2:C:1388:THR:HG21	5:C:2230:HOH:O	1.50	1.09
2:X:468:ALA:HB1	5:X:2261:HOH:O	1.52	1.09
2:G:30:GLU:HB2	5:G:2113:HOH:O	1.53	1.09
2:S:1332:ASP:HB2	5:S:2130:HOH:O	1.52	1.09
2:G:1291:LEU:HB3	5:G:2238:HOH:O	1.51	1.08
2:K:798:MET:HE2	5:K:2142:HOH:O	1.51	1.08
2:S:1717:PRO:CG	2:S:1717:PRO:HD3	1.61	1.08
2:K:1332:ASP:HB2	5:K:2124:HOH:O	1.52	1.08
1:E:439:GLY:HA2	5:E:2273:HOH:O	1.52	1.08
1:M:439:GLY:HA2	5:M:2272:HOH:O	1.52	1.07
2:K:629:PRO:CD	2:K:629:PRO:HG3	1.59	1.07
1:I:702:GLN:HB3	5:I:2344:HOH:O	1.55	1.07
2:S:983:GLU:HG3	5:S:2122:HOH:O	1.49	1.07
2:K:983:GLU:HG3	5:K:2102:HOH:O	1.53	1.07
1:A:439:GLY:HA2	5:A:2320:HOH:O	1.52	1.07
2:O:30:GLU:HB2	5:O:2116:HOH:O	1.53	1.07
2:C:1717:PRO:CD	2:C:1717:PRO:HG3	1.68	1.06
2:K:629:PRO:CG	2:K:629:PRO:HD3	1.58	1.06
2:K:629:PRO:CG	2:K:629:PRO:HD2	1.58	1.06
2:X:1083:ILE:HD13	5:X:2057:HOH:O	1.53	1.06
1:I:285:THR:HG21	5:I:2390:HOH:O	1.53	1.06
2:C:1717:PRO:CG	2:C:1717:PRO:HD3	1.57	1.06
2:S:1207:VAL:HG12	5:S:2025:HOH:O	1.54	1.05
2:K:1207:VAL:HG12	5:K:2020:HOH:O	1.53	1.05
1:I:124:LYS:HA	1:I:124:LYS:HE3	1.34	1.05
2:C:1717:PRO:CG	2:C:1717:PRO:HD2	1.57	1.05
2:C:1652:GLN:HG3	5:C:2176:HOH:O	1.54	1.04
2:G:841:GLU:OE1	2:X:848:THR:OG1	1.75	1.04
2:K:629:PRO:CD	2:K:629:PRO:HG2	1.59	1.03
1:A:1419:VAL:HG11	5:A:2304:HOH:O	1.57	1.02
1:Q:702:GLN:HB3	5:Q:2349:HOH:O	1.56	1.02
1:A:670:ALA:HB3	5:A:2226:HOH:O	1.60	1.02
1:M:614:PRO:CG	1:M:614:PRO:HD2	1.51	1.02
1:M:614:PRO:CG	1:M:614:PRO:HD3	1.51	1.02
5:U:2300:HOH:O	2:X:26:VAL:HG21	1.56	1.02
1:A:903:GLU:OE2	2:C:1690:ARG:NH2	1.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:GLU:HA	2:C:1690:ARG:NH2	1.73	1.01
2:K:30:GLU:HB2	5:K:2235:HOH:O	1.59	1.00
2:S:30:GLU:HB2	5:S:2240:HOH:O	1.60	1.00
1:E:985:GLU:OE1	2:G:1697:THR:OG1	1.79	1.00
1:U:898:VAL:HG21	5:U:2427:HOH:O	1.60	1.00
1:E:614:PRO:CG	1:E:614:PRO:HD2	1.51	1.00
2:X:464:THR:HG21	5:X:2024:HOH:O	1.59	1.00
1:U:670:ALA:HB3	5:U:2216:HOH:O	1.60	1.00
1:E:614:PRO:CG	1:E:614:PRO:HD3	1.51	1.00
2:X:519:ARG:HD2	5:X:2047:HOH:O	1.61	0.99
2:C:342:GLU:OE2	2:O:351:ARG:NH2	1.96	0.99
2:G:1180:PHE:HE2	5:G:2001:HOH:O	1.42	0.99
2:S:953:ILE:HG21	5:S:2257:HOH:O	1.63	0.98
1:Q:898:VAL:HG12	5:Q:2260:HOH:O	1.63	0.98
1:I:2001:ASN:OD1	2:K:26:VAL:HG23	1.62	0.98
2:C:519:ARG:HD2	5:C:2062:HOH:O	1.64	0.98
2:K:953:ILE:HG21	5:K:2250:HOH:O	1.64	0.98
1:M:1450:ARG:CB	5:M:2403:HOH:O	2.12	0.97
1:A:722:GLY:HA2	5:A:2305:HOH:O	1.64	0.97
2:C:347:TYR:OH	2:K:1129:ASP:OD1	1.82	0.97
2:X:1179:ARG:HG2	5:X:2107:HOH:O	1.63	0.97
2:C:1179:ARG:HG2	5:C:2133:HOH:O	1.64	0.97
1:A:702:GLN:HB3	5:A:2353:HOH:O	1.64	0.96
1:I:898:VAL:HG12	5:I:2269:HOH:O	1.63	0.96
1:A:845:ALA:HA	5:A:2377:HOH:O	1.63	0.96
1:E:1450:ARG:CB	5:E:2403:HOH:O	2.12	0.96
5:Q:2253:HOH:O	2:S:968:VAL:HG21	1.65	0.96
1:E:616:MET:HG3	5:E:2360:HOH:O	1.66	0.96
2:K:1089:LYS:HB2	5:K:2214:HOH:O	1.65	0.96
5:I:2253:HOH:O	2:K:968:VAL:HG21	1.64	0.96
2:G:1213:TYR:HD2	5:G:2244:HOH:O	1.49	0.96
1:Q:893:LYS:HD3	5:Q:2442:HOH:O	1.66	0.95
2:K:724:MET:HE3	5:K:2032:HOH:O	1.66	0.95
1:I:893:LYS:HD3	5:I:2438:HOH:O	1.66	0.94
1:U:898:VAL:HG12	5:U:2236:HOH:O	1.67	0.94
1:M:616:MET:HG3	5:M:2362:HOH:O	1.67	0.94
1:M:1444:PHE:HA	5:M:2397:HOH:O	1.65	0.94
1:U:1367:VAL:HG11	5:U:2286:HOH:O	1.65	0.94
1:M:724:GLY:HA3	5:M:2321:HOH:O	1.66	0.94
1:U:722:GLY:HA2	5:U:2309:HOH:O	1.64	0.94
2:S:1503:ARG:HD3	5:S:2009:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1444:PHE:HA	5:E:2393:HOH:O	1.65	0.94
1:M:875:ARG:HD2	5:M:2212:HOH:O	1.66	0.94
2:X:1089:LYS:HB2	5:X:2077:HOH:O	1.67	0.94
2:O:1069:LYS:HE3	5:O:2009:HOH:O	1.68	0.94
2:S:724:MET:HE3	5:S:2036:HOH:O	1.66	0.94
1:E:875:ARG:HD2	5:E:2216:HOH:O	1.66	0.94
1:E:724:GLY:HA3	5:E:2326:HOH:O	1.66	0.93
1:E:480:ASN:O	1:E:480:ASN:ND2	2.00	0.93
2:G:1120:MET:HE1	2:S:1263:ARG:O	1.68	0.93
1:A:1146:ARG:HG3	5:A:2245:HOH:O	1.67	0.93
2:S:1717:PRO:CG	2:S:1717:PRO:CD	0.93	0.93
1:U:889:PRO:HB3	5:U:2341:HOH:O	1.65	0.93
1:M:478:ALA:HB1	5:M:2401:HOH:O	1.68	0.92
1:E:1440:LYS:HB3	5:E:2309:HOH:O	1.70	0.92
1:U:702:GLN:HB3	5:U:2340:HOH:O	1.68	0.92
2:G:1069:LYS:HE3	5:G:2011:HOH:O	1.68	0.92
1:A:889:PRO:HB3	5:A:2339:HOH:O	1.70	0.92
1:Q:1714:ARG:NH2	2:K:918:GLN:OE1	2.01	0.92
2:C:1049:ALA:HB1	5:C:2056:HOH:O	1.69	0.92
1:U:845:ALA:HA	5:U:2391:HOH:O	1.69	0.92
2:G:435:CYS:SG	4:G:1901:PKZ:C5	2.58	0.91
1:A:1361:LYS:HD3	5:A:2224:HOH:O	1.68	0.91
2:C:1717:PRO:CG	2:C:1717:PRO:CD	0.91	0.91
1:A:1367:VAL:HG11	5:A:2278:HOH:O	1.70	0.91
2:X:435:CYS:SG	4:X:1901:PKZ:C5	2.59	0.91
2:C:435:CYS:SG	4:C:1901:PKZ:C5	2.59	0.91
2:X:1442:LEU:HD11	5:X:2274:HOH:O	1.71	0.91
1:E:478:ALA:HB1	5:E:2411:HOH:O	1.70	0.91
2:O:435:CYS:SG	4:O:1901:PKZ:C5	2.58	0.91
1:M:1440:LYS:HB3	5:M:2311:HOH:O	1.69	0.90
2:S:1641:LYS:HE3	5:S:2106:HOH:O	1.70	0.90
2:X:633:THR:HG21	5:X:2111:HOH:O	1.68	0.90
2:C:633:THR:HG21	5:C:2109:HOH:O	1.70	0.90
1:I:1851:SER:HA	5:I:2359:HOH:O	1.72	0.90
2:C:1442:LEU:HD11	5:C:2236:HOH:O	1.70	0.90
2:C:478:ASN:ND2	4:C:1901:PKZ:O1	2.04	0.90
2:K:435:CYS:SG	4:K:1901:PKZ:C5	2.59	0.90
2:X:478:ASN:ND2	4:X:1901:PKZ:O1	2.05	0.90
2:X:1739:THR:HG21	5:X:2148:HOH:O	1.70	0.90
2:K:1641:LYS:HE3	5:K:2103:HOH:O	1.70	0.90
2:S:435:CYS:SG	4:S:1901:PKZ:C5	2.60	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:520:SER:HA	5:U:2273:HOH:O	1.69	0.90
1:M:985:GLU:OE1	2:O:1697:THR:OG1	1.90	0.89
2:K:1635:ILE:HD12	5:K:2289:HOH:O	1.72	0.89
1:Q:1851:SER:HA	5:Q:2355:HOH:O	1.71	0.89
2:C:1089:LYS:HB2	5:C:2093:HOH:O	1.69	0.89
2:X:1049:ALA:HB1	5:X:2045:HOH:O	1.71	0.89
1:E:702:GLN:HB3	5:E:2324:HOH:O	1.72	0.89
2:G:1089:LYS:HB2	5:G:2162:HOH:O	1.71	0.89
2:K:1263:ARG:O	2:O:1120:MET:HE1	1.70	0.89
1:I:722:GLY:HA2	5:I:2345:HOH:O	1.71	0.89
2:O:1641:LYS:HE3	5:O:2140:HOH:O	1.72	0.89
1:A:1826:MET:HG3	5:A:2431:HOH:O	1.71	0.89
2:C:835:PHE:CD1	5:C:2086:HOH:O	2.26	0.89
2:G:1180:PHE:CE2	5:G:2001:HOH:O	2.19	0.89
2:G:1179:ARG:HG2	5:G:2187:HOH:O	1.73	0.89
1:Q:722:GLY:HA2	5:Q:2352:HOH:O	1.73	0.88
1:U:360:GLY:HA2	5:U:2337:HOH:O	1.73	0.88
2:G:1641:LYS:HE3	5:G:2134:HOH:O	1.72	0.88
1:A:898:VAL:HG12	5:A:2222:HOH:O	1.72	0.88
2:O:1089:LYS:HB2	5:O:2171:HOH:O	1.71	0.88
2:C:464:THR:HG21	5:C:2005:HOH:O	1.74	0.88
1:E:725:GLY:HA3	5:E:2302:HOH:O	1.73	0.88
2:C:1083:ILE:HD13	5:C:2052:HOH:O	1.71	0.88
2:S:478:ASN:ND2	4:S:1901:PKZ:O1	2.07	0.88
1:M:702:GLN:HB3	5:M:2329:HOH:O	1.71	0.88
1:M:340:ILE:HD12	1:M:376:PHE:HZ	1.38	0.88
1:M:1201:ASN:HA	5:M:2268:HOH:O	1.74	0.88
2:S:788:ASP:HA	5:S:2279:HOH:O	1.73	0.88
1:M:725:GLY:HA3	5:M:2303:HOH:O	1.73	0.87
1:U:1361:LYS:HD3	5:U:2224:HOH:O	1.74	0.87
1:A:1714:ARG:NH2	2:O:918:GLN:OE1	2.07	0.87
1:E:798:SER:HB2	5:E:2376:HOH:O	1.73	0.87
2:X:835:PHE:CD1	5:X:2079:HOH:O	2.26	0.87
1:E:340:ILE:HD12	1:E:376:PHE:HZ	1.38	0.87
1:E:898:VAL:HG12	5:E:2298:HOH:O	1.75	0.87
2:O:1179:ARG:HG2	5:O:2189:HOH:O	1.73	0.87
1:A:577:ALA:HB2	5:A:2267:HOH:O	1.73	0.87
1:M:898:VAL:HG12	5:M:2297:HOH:O	1.74	0.87
2:G:835:PHE:CD1	5:G:2098:HOH:O	2.27	0.87
1:U:1225:LYS:HD2	1:U:1238:ILE:HD11	1.57	0.87
2:S:450:MET:HG2	4:S:1901:PKZ:C13	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1211:THR:CG2	5:X:2159:HOH:O	2.22	0.87
2:K:1503:ARG:HD3	5:K:2006:HOH:O	1.72	0.87
1:A:834:ARG:HG2	5:A:2391:HOH:O	1.75	0.86
2:K:450:MET:HG2	4:K:1901:PKZ:C13	2.04	0.86
2:K:478:ASN:ND2	4:K:1901:PKZ:O1	2.07	0.86
2:K:788:ASP:HA	5:K:2277:HOH:O	1.74	0.86
2:O:835:PHE:CD1	5:O:2103:HOH:O	2.26	0.86
1:A:360:GLY:HA2	5:A:2348:HOH:O	1.75	0.86
2:O:478:ASN:ND2	4:O:1901:PKZ:O1	2.09	0.86
2:G:404:TYR:HD1	5:G:2275:HOH:O	1.59	0.86
2:S:511:GLU:N	2:S:511:GLU:OE1	2.09	0.86
1:U:1714:ARG:NH2	2:G:918:GLN:OE1	2.09	0.86
1:A:1304:ALA:HA	5:A:2205:HOH:O	1.76	0.86
1:M:614:PRO:CG	1:M:614:PRO:CD	0.86	0.85
1:E:614:PRO:CG	1:E:614:PRO:CD	0.86	0.85
2:O:404:TYR:HD1	5:O:2276:HOH:O	1.59	0.85
2:G:478:ASN:ND2	4:G:1901:PKZ:O1	2.09	0.85
1:E:688:THR:HG23	5:E:2386:HOH:O	1.77	0.85
2:C:880:ALA:HB2	5:C:2267:HOH:O	1.76	0.85
2:G:376:LEU:HD11	5:G:2188:HOH:O	1.77	0.85
2:G:983:GLU:HG3	5:G:2175:HOH:O	1.77	0.84
1:I:1554:VAL:HG11	5:I:2286:HOH:O	1.78	0.84
2:C:1211:THR:CG2	5:C:2150:HOH:O	2.25	0.84
2:X:1211:THR:HG23	5:X:2159:HOH:O	1.76	0.84
2:O:983:GLU:HG3	5:O:2184:HOH:O	1.77	0.84
1:I:976:PRO:HG3	5:I:2248:HOH:O	1.77	0.84
1:M:688:THR:HG23	5:M:2388:HOH:O	1.77	0.83
2:K:629:PRO:CG	2:K:629:PRO:CD	0.83	0.83
2:C:356:SER:OG	2:O:356:SER:OG	1.93	0.83
5:C:2169:HOH:O	2:O:376:LEU:HD11	1.77	0.83
2:S:964:GLU:HG3	5:S:2160:HOH:O	1.79	0.83
1:I:1533:PRO:HG3	5:I:2422:HOH:O	1.79	0.83
1:M:313:ASP:O	1:M:317:ASN:ND2	2.12	0.83
2:C:848:THR:OG1	2:O:841:GLU:OE1	1.96	0.83
2:G:344:LEU:HD13	2:O:344:LEU:HD11	1.60	0.83
1:M:722:GLY:HA2	5:M:2344:HOH:O	1.78	0.82
1:A:875:ARG:HG2	5:A:2251:HOH:O	1.79	0.82
1:Q:976:PRO:HG3	5:Q:2248:HOH:O	1.78	0.82
2:K:1493:ARG:HG2	5:K:2031:HOH:O	1.79	0.82
2:S:1089:LYS:HB2	5:S:2153:HOH:O	1.76	0.82
1:E:1541:ILE:CD1	5:E:2366:HOH:O	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:964:GLU:HG3	5:K:2148:HOH:O	1.78	0.82
2:X:1223:LEU:HD22	5:X:2279:HOH:O	1.79	0.82
1:I:447:THR:HG22	1:I:467:LEU:HD23	1.61	0.82
5:Q:2254:HOH:O	2:S:22:PHE:CE1	2.33	0.82
1:M:1541:ILE:CD1	5:M:2366:HOH:O	2.27	0.82
2:G:1049:ALA:HB1	5:G:2073:HOH:O	1.78	0.82
1:E:313:ASP:O	1:E:317:ASN:ND2	2.12	0.82
1:E:722:GLY:HA2	5:E:2343:HOH:O	1.78	0.82
2:K:404:TYR:CD1	5:K:2228:HOH:O	2.32	0.82
2:C:1085:GLU:HA	2:C:1088:ILE:HD12	1.62	0.82
2:C:1211:THR:HG23	5:C:2150:HOH:O	1.79	0.81
1:U:1569:MET:HA	1:U:1569:MET:HE3	1.61	0.81
2:O:1049:ALA:HB1	5:O:2079:HOH:O	1.78	0.81
2:S:1493:ARG:HG2	5:S:2037:HOH:O	1.78	0.81
2:S:404:TYR:CD1	5:S:2231:HOH:O	2.32	0.81
1:Q:591:THR:HG23	5:Q:2212:HOH:O	1.80	0.81
2:K:348:LEU:HD22	5:K:2215:HOH:O	1.80	0.81
2:G:356:SER:OG	2:X:356:SER:OG	1.92	0.81
2:C:1691:TYR:CE1	5:C:2177:HOH:O	2.34	0.81
1:Q:1554:VAL:HG11	5:Q:2276:HOH:O	1.80	0.81
1:I:2001:ASN:OD1	2:K:26:VAL:CG2	2.28	0.80
2:C:348:LEU:HG	2:S:337:ALA:HB2	1.62	0.80
2:K:819:PRO:HG3	5:K:2065:HOH:O	1.81	0.80
2:S:1716:GLN:C	2:S:1717:PRO:CG	2.54	0.80
2:C:718:THR:CG2	5:C:2205:HOH:O	2.28	0.80
2:S:1716:GLN:CB	2:S:1717:PRO:HG3	2.12	0.80
2:S:779:GLU:HG2	5:S:2071:HOH:O	1.80	0.80
2:S:1716:GLN:C	2:S:1717:PRO:HG3	2.07	0.80
5:A:2431:HOH:O	2:C:22:PHE:CZ	2.34	0.80
1:Q:1541:ILE:CD1	5:Q:2360:HOH:O	2.30	0.80
2:C:718:THR:HG22	5:C:2205:HOH:O	1.82	0.80
1:A:520:SER:HA	5:A:2280:HOH:O	1.80	0.80
1:E:447:THR:HG22	1:E:467:LEU:HD23	1.64	0.79
1:E:587:THR:CG2	5:E:2376:HOH:O	2.30	0.79
1:A:903:GLU:OE2	2:C:1690:ARG:NH1	2.15	0.79
1:M:1201:ASN:CA	5:M:2268:HOH:O	2.30	0.79
2:C:1050:ILE:HG12	2:C:1088:ILE:HD13	1.64	0.79
2:C:1086:LYS:HE3	5:C:2110:HOH:O	1.81	0.79
2:K:629:PRO:CG	2:K:629:PRO:CA	2.59	0.79
1:A:1533:PRO:HD2	5:A:2225:HOH:O	1.83	0.79
1:E:587:THR:HG22	5:E:2376:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1546:HIS:CD2	5:X:2012:HOH:O	2.07	0.79
1:E:1248:GLU:CB	5:E:2423:HOH:O	2.30	0.79
2:G:377:TRP:CE3	2:X:377:TRP:CE3	2.71	0.79
2:S:819:PRO:HG3	5:S:2070:HOH:O	1.82	0.79
1:U:710:HIS:O	1:U:749:ASN:ND2	2.16	0.79
2:X:1354:GLU:OE1	2:X:1366:ARG:NH1	2.16	0.79
5:I:2249:HOH:O	2:K:22:PHE:CE1	2.35	0.79
2:G:404:TYR:CD1	5:G:2275:HOH:O	2.34	0.79
2:S:893:VAL:HG23	5:S:2080:HOH:O	1.83	0.79
1:E:988:CYS:HB2	5:E:2416:HOH:O	1.81	0.78
1:I:1791:MET:CB	5:K:2284:HOH:O	2.31	0.78
1:Q:1533:PRO:HG3	5:Q:2434:HOH:O	1.83	0.78
1:E:710:HIS:O	1:E:749:ASN:ND2	2.16	0.78
1:Q:710:HIS:O	1:Q:749:ASN:ND2	2.16	0.78
2:C:35:PHE:O	2:C:41:THR:OG1	2.00	0.78
1:A:256:TRP:CZ2	5:A:2209:HOH:O	2.35	0.78
1:A:577:ALA:CB	5:A:2267:HOH:O	2.31	0.78
1:M:340:ILE:HD12	1:M:376:PHE:CZ	2.18	0.78
1:A:903:GLU:CD	2:C:1690:ARG:HH22	1.91	0.78
1:A:1304:ALA:CA	5:A:2205:HOH:O	2.31	0.78
1:E:520:SER:HA	5:E:2271:HOH:O	1.83	0.78
1:I:306:LEU:HG	5:I:2347:HOH:O	1.84	0.78
1:I:710:HIS:O	1:I:749:ASN:ND2	2.16	0.78
1:A:903:GLU:HA	2:C:1690:ARG:HH21	1.46	0.78
1:U:1592:ARG:CZ	5:U:2231:HOH:O	2.32	0.78
2:G:1354:GLU:OE1	2:G:1366:ARG:NH1	2.16	0.78
2:S:1717:PRO:N	2:S:1717:PRO:HG3	1.84	0.78
1:A:1845:VAL:CG2	5:A:2394:HOH:O	2.32	0.78
1:M:710:HIS:O	1:M:749:ASN:ND2	2.16	0.78
1:Q:1479:LYS:HA	5:Q:2261:HOH:O	1.84	0.78
2:C:1354:GLU:OE1	2:C:1366:ARG:NH1	2.16	0.78
2:K:628:GLN:C	2:K:628:GLN:CB	2.56	0.78
2:O:1354:GLU:OE1	2:O:1366:ARG:NH1	2.16	0.78
1:A:377:ASN:OD1	1:A:405:ASN:ND2	2.17	0.78
1:M:774:GLU:CB	5:M:2290:HOH:O	2.31	0.78
1:U:313:ASP:O	1:U:317:ASN:ND2	2.17	0.78
2:K:893:VAL:HG23	5:K:2077:HOH:O	1.84	0.78
1:A:145:LYS:CB	5:A:2223:HOH:O	2.32	0.78
1:A:710:HIS:O	1:A:749:ASN:ND2	2.16	0.77
2:K:845:SER:OG	2:S:845:SER:OG	2.02	0.77
1:E:1611:THR:HG23	5:E:2256:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:615:VAL:HG23	5:I:2401:HOH:O	1.84	0.77
2:S:1354:GLU:OE1	2:S:1366:ARG:NH1	2.16	0.77
1:I:377:ASN:OD1	1:I:405:ASN:ND2	2.18	0.77
1:M:520:SER:HA	5:M:2269:HOH:O	1.82	0.77
1:U:956:GLN:CG	5:U:2218:HOH:O	2.31	0.77
1:E:340:ILE:HD12	1:E:376:PHE:CZ	2.20	0.77
1:U:1787:PRO:HB3	5:U:2400:HOH:O	1.85	0.77
2:K:1354:GLU:OE1	2:K:1366:ARG:NH1	2.16	0.77
1:Q:1528:LEU:HD21	1:Q:1612:MET:SD	2.24	0.77
1:U:545:ALA:CB	5:U:2352:HOH:O	2.31	0.77
2:C:1527:ARG:NH2	2:C:1568:LEU:O	2.18	0.77
2:O:404:TYR:CD1	5:O:2276:HOH:O	2.34	0.77
2:K:1739:THR:HG21	5:K:2187:HOH:O	1.84	0.77
1:U:377:ASN:OD1	1:U:405:ASN:ND2	2.18	0.77
2:S:336:LEU:HD22	5:S:2178:HOH:O	1.85	0.77
1:A:985:GLU:OE2	2:C:1697:THR:OG1	2.03	0.77
1:A:1787:PRO:HB3	5:A:2406:HOH:O	1.84	0.77
1:Q:615:VAL:HG23	5:Q:2406:HOH:O	1.84	0.77
5:C:2169:HOH:O	2:O:376:LEU:HD21	1.84	0.77
2:O:35:PHE:O	2:O:41:THR:OG1	2.03	0.77
2:O:412:VAL:HG12	4:O:1901:PKZ:C16	2.15	0.77
2:S:1086:LYS:HE3	5:S:2132:HOH:O	1.85	0.77
1:M:1673:VAL:HG11	5:M:2380:HOH:O	1.84	0.77
2:X:893:VAL:HG23	5:X:2021:HOH:O	1.83	0.77
1:A:1175:LYS:HA	5:A:2202:HOH:O	1.84	0.77
1:U:956:GLN:HG2	5:U:2218:HOH:O	1.84	0.77
2:C:759:PRO:CD	5:C:2116:HOH:O	2.33	0.77
2:G:412:VAL:HG12	4:G:1901:PKZ:C16	2.15	0.77
2:K:814:PRO:HG2	5:K:2045:HOH:O	1.84	0.77
2:K:1519:SER:O	2:O:1499:ARG:NE	2.18	0.77
1:E:774:GLU:CB	5:E:2291:HOH:O	2.32	0.76
1:E:1673:VAL:HG11	5:E:2379:HOH:O	1.84	0.76
1:I:591:THR:HG23	5:I:2206:HOH:O	1.83	0.76
2:C:1281:THR:HB	5:C:2114:HOH:O	1.85	0.76
2:G:1519:SER:O	2:S:1499:ARG:NE	2.18	0.76
2:X:1527:ARG:NH2	2:X:1568:LEU:O	2.17	0.76
2:K:629:PRO:N	2:K:629:PRO:HG2	1.91	0.76
1:A:982:LEU:HD13	2:C:1690:ARG:NH2	2.00	0.76
2:G:1499:ARG:NE	2:S:1519:SER:O	2.19	0.76
2:X:390:GLN:HB2	5:X:2241:HOH:O	1.84	0.76
1:M:775:LYS:CB	5:M:2260:HOH:O	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:377:ASN:OD1	1:Q:405:ASN:ND2	2.18	0.76
1:A:615:VAL:HG23	5:A:2352:HOH:O	1.85	0.76
2:S:814:PRO:HG2	5:S:2049:HOH:O	1.84	0.76
1:I:657:ARG:NH1	1:I:661:TYR:O	2.19	0.76
1:U:956:GLN:CB	5:U:2218:HOH:O	2.32	0.76
2:C:1582:LYS:NZ	2:C:1596:MET:SD	2.59	0.76
2:S:404:TYR:HD1	5:S:2231:HOH:O	1.69	0.76
1:I:1541:ILE:CD1	5:I:2346:HOH:O	2.32	0.76
1:Q:1791:MET:CB	5:S:2288:HOH:O	2.32	0.76
1:E:377:ASN:OD1	1:E:405:ASN:ND2	2.19	0.76
1:E:839:GLU:CB	5:E:2223:HOH:O	2.33	0.76
5:I:2249:HOH:O	2:K:22:PHE:HE1	1.69	0.76
1:U:615:VAL:HG23	5:U:2345:HOH:O	1.84	0.76
2:K:404:TYR:HD1	5:K:2228:HOH:O	1.69	0.76
1:E:577:ALA:HB2	5:E:2317:HOH:O	1.85	0.76
2:K:1086:LYS:HE3	5:K:2125:HOH:O	1.85	0.75
1:A:313:ASP:O	1:A:317:ASN:ND2	2.18	0.75
1:M:839:GLU:CB	5:M:2224:HOH:O	2.33	0.75
1:M:939:ARG:HD3	5:M:2291:HOH:O	1.86	0.75
2:C:1519:SER:O	2:X:1499:ARG:NE	2.19	0.75
2:K:1499:ARG:NE	2:O:1519:SER:O	2.19	0.75
2:S:1348:THR:HG21	5:S:2066:HOH:O	1.87	0.75
5:Q:2254:HOH:O	2:S:22:PHE:HE1	1.67	0.75
2:G:1281:THR:HB	5:G:2151:HOH:O	1.86	0.75
1:A:306:LEU:HG	5:A:2322:HOH:O	1.87	0.75
1:U:360:GLY:CA	5:U:2337:HOH:O	2.31	0.75
2:S:1739:THR:HG21	5:S:2196:HOH:O	1.85	0.75
2:X:1582:LYS:NZ	2:X:1596:MET:SD	2.59	0.75
1:M:377:ASN:OD1	1:M:405:ASN:ND2	2.19	0.75
1:M:1611:THR:HG23	5:M:2259:HOH:O	1.85	0.75
1:A:956:GLN:HB2	5:A:2231:HOH:O	1.87	0.75
2:C:798:MET:HE2	5:C:2170:HOH:O	1.86	0.75
1:U:371:GLU:HB3	5:U:2390:HOH:O	1.85	0.75
2:K:759:PRO:HD3	5:K:2260:HOH:O	1.87	0.75
2:K:356:SER:OG	2:S:356:SER:OG	1.92	0.74
2:X:759:PRO:CD	5:X:2234:HOH:O	2.32	0.74
1:U:723:ARG:NE	1:U:756:SER:O	2.20	0.74
2:O:339:GLN:O	2:O:343:VAL:HG23	1.87	0.74
1:E:1721:ILE:HD13	5:E:2390:HOH:O	1.87	0.74
1:I:466:LYS:NZ	1:I:470:GLU:OE1	2.19	0.74
2:X:1086:LYS:HE3	5:X:2149:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLY:HA3	5:A:2364:HOH:O	1.87	0.74
1:Q:306:LEU:HG	5:Q:2353:HOH:O	1.86	0.74
1:Q:1244:GLU:CB	5:Q:2224:HOH:O	2.34	0.74
2:G:29:ILE:CD1	5:G:2113:HOH:O	2.34	0.74
2:X:412:VAL:HG12	4:X:1901:PKZ:C16	2.17	0.74
2:X:1223:LEU:CD2	5:X:2279:HOH:O	2.34	0.74
1:A:903:GLU:CD	2:C:1690:ARG:HH12	1.96	0.74
1:E:775:LYS:CB	5:E:2260:HOH:O	2.34	0.74
1:I:1244:GLU:CB	5:I:2217:HOH:O	2.34	0.74
1:U:1533:PRO:HD2	5:U:2249:HOH:O	1.85	0.74
2:O:1086:LYS:HE3	5:O:2092:HOH:O	1.88	0.74
2:S:348:LEU:HD22	5:S:2226:HOH:O	1.85	0.74
2:C:759:PRO:HD3	5:C:2116:HOH:O	1.87	0.74
2:G:344:LEU:HD13	2:O:344:LEU:CD1	2.18	0.74
2:K:1348:THR:HG21	5:K:2062:HOH:O	1.86	0.74
2:O:771:ILE:HG23	5:O:2192:HOH:O	1.86	0.74
1:A:723:ARG:NE	1:A:756:SER:O	2.21	0.74
1:A:1031:VAL:HA	5:A:2262:HOH:O	1.88	0.74
1:U:545:ALA:HB2	5:U:2352:HOH:O	1.85	0.74
1:U:1175:LYS:HA	5:U:2221:HOH:O	1.86	0.74
2:O:29:ILE:CD1	5:O:2116:HOH:O	2.33	0.74
2:C:1279:ILE:HD12	2:X:1279:ILE:HD12	1.70	0.74
1:A:657:ARG:NH1	1:A:661:TYR:O	2.21	0.74
1:E:1161:ILE:HG23	1:E:1554:VAL:HG23	1.70	0.74
1:Q:591:THR:CG2	5:Q:2212:HOH:O	2.34	0.74
2:C:390:GLN:HB2	5:C:2257:HOH:O	1.88	0.74
2:G:771:ILE:HG23	5:G:2184:HOH:O	1.87	0.74
1:M:577:ALA:HB2	5:M:2310:HOH:O	1.87	0.74
1:Q:1228:PRO:HB2	5:Q:2251:HOH:O	1.88	0.74
2:S:369:VAL:HG23	5:S:2217:HOH:O	1.87	0.74
1:E:544:TRP:HB3	5:E:2277:HOH:O	1.87	0.73
1:I:792:VAL:O	1:I:795:SER:OG	2.06	0.73
1:I:902:GLN:HB3	2:K:1690:ARG:NH1	2.02	0.73
2:C:845:SER:OG	2:O:845:SER:OG	2.06	0.73
1:E:1721:ILE:CD1	5:E:2390:HOH:O	2.37	0.73
1:U:463:ARG:HE	1:U:467:LEU:CD1	2.02	0.73
2:K:412:VAL:HG12	4:K:1901:PKZ:C16	2.18	0.73
2:O:369:VAL:HG23	5:O:2260:HOH:O	1.88	0.73
1:E:57:GLU:CB	5:E:2396:HOH:O	2.35	0.73
1:M:1161:ILE:HG23	1:M:1554:VAL:HG23	1.69	0.73
2:C:412:VAL:HG12	4:C:1901:PKZ:C16	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:344:LEU:CD1	2:O:344:LEU:HD11	2.17	0.73
2:O:343:VAL:HG13	5:O:2267:HOH:O	1.87	0.73
2:X:1691:TYR:CE1	5:X:2279:HOH:O	2.41	0.73
1:I:879:ILE:HG21	1:I:898:VAL:HG23	1.70	0.73
1:M:57:GLU:CB	5:M:2395:HOH:O	2.36	0.73
1:M:723:ARG:NE	1:M:756:SER:O	2.21	0.73
2:C:1716:GLN:C	2:C:1717:PRO:CG	2.61	0.73
2:G:845:SER:OG	2:X:845:SER:OG	2.05	0.73
2:G:1527:ARG:NH2	2:G:1568:LEU:O	2.21	0.73
2:X:759:PRO:HD3	5:X:2234:HOH:O	1.88	0.73
1:A:360:GLY:CA	5:A:2348:HOH:O	2.34	0.73
1:A:1591:VAL:HG11	5:A:2413:HOH:O	1.88	0.73
1:I:630:PRO:CG	1:I:630:PRO:N	2.50	0.73
1:U:976:PRO:HG3	5:U:2307:HOH:O	1.88	0.73
2:G:1086:LYS:HE3	5:G:2085:HOH:O	1.88	0.73
2:S:412:VAL:HG12	4:S:1901:PKZ:C16	2.18	0.73
2:S:534:MET:SD	2:S:893:VAL:CG1	2.77	0.73
2:S:759:PRO:HD3	5:S:2260:HOH:O	1.87	0.73
1:E:306:LEU:HD21	1:E:310:MET:HE3	1.70	0.73
1:E:723:ARG:NE	1:E:756:SER:O	2.22	0.73
1:E:939:ARG:HD3	5:E:2289:HOH:O	1.86	0.73
1:E:1444:PHE:CB	5:E:2393:HOH:O	2.36	0.73
1:I:723:ARG:NE	1:I:756:SER:O	2.22	0.73
1:Q:723:ARG:NE	1:Q:756:SER:O	2.22	0.73
1:M:1721:ILE:HD13	5:M:2391:HOH:O	1.87	0.73
1:A:956:GLN:CB	5:A:2231:HOH:O	2.35	0.72
1:A:956:GLN:CG	5:A:2231:HOH:O	2.36	0.72
1:A:371:GLU:HB3	5:A:2398:HOH:O	1.88	0.72
1:A:569:LYS:NZ	1:A:748:SER:O	2.23	0.72
1:E:1090:TYR:CE2	1:E:1140:ALA:HB2	2.23	0.72
1:I:839:GLU:CB	5:I:2233:HOH:O	2.37	0.72
1:M:544:TRP:HB3	5:M:2277:HOH:O	1.87	0.72
1:M:1721:ILE:CD1	5:M:2391:HOH:O	2.37	0.72
1:M:1444:PHE:CB	5:M:2397:HOH:O	2.37	0.72
1:U:867:LEU:HD22	5:U:2348:HOH:O	1.90	0.72
1:U:1225:LYS:HE2	1:U:1225:LYS:HA	1.69	0.72
2:K:628:GLN:CA	2:K:628:GLN:O	2.37	0.72
1:I:591:THR:CG2	5:I:2206:HOH:O	2.37	0.72
1:I:630:PRO:CG	1:I:630:PRO:CB	2.66	0.72
1:U:657:ARG:NH1	1:U:661:TYR:O	2.22	0.72
2:K:534:MET:SD	2:K:893:VAL:CG1	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:656:LYS:HE2	5:O:2149:HOH:O	1.89	0.72
1:M:136:LEU:HA	5:M:2282:HOH:O	1.88	0.72
1:M:839:GLU:CA	5:M:2224:HOH:O	2.37	0.72
1:U:285:THR:HG21	5:U:2419:HOH:O	1.89	0.72
1:U:956:GLN:HB2	5:U:2218:HOH:O	1.86	0.72
1:U:1721:ILE:HG12	5:U:2223:HOH:O	1.90	0.72
2:K:337:ALA:HB2	2:X:348:LEU:HG	1.72	0.72
2:K:344:LEU:HD11	2:X:340:GLN:HB3	1.71	0.72
2:K:369:VAL:HG23	5:K:2207:HOH:O	1.88	0.72
1:A:834:ARG:CG	5:A:2391:HOH:O	2.35	0.72
1:Q:879:ILE:HG21	1:Q:898:VAL:HG23	1.70	0.72
1:Q:1794:GLY:O	1:Q:2001:ASN:ND2	2.22	0.72
2:C:1546:HIS:CD2	5:C:2015:HOH:O	2.10	0.72
1:A:850:MET:HA	1:A:850:MET:HE3	1.70	0.72
2:G:376:LEU:HD21	5:G:2188:HOH:O	1.88	0.72
1:E:839:GLU:CA	5:E:2223:HOH:O	2.37	0.72
2:C:1288:MET:HE1	2:X:1417:VAL:HG22	1.71	0.72
5:C:2003:HOH:O	2:S:348:LEU:HB2	1.90	0.72
2:X:35:PHE:O	2:X:41:THR:OG1	2.07	0.72
1:M:1090:TYR:CE2	1:M:1140:ALA:HB2	2.24	0.72
2:C:339:GLN:N	2:O:349:GLN:HE22	1.87	0.72
1:A:903:GLU:OE2	2:C:1690:ARG:CZ	2.38	0.72
1:E:867:LEU:HD22	5:E:2358:HOH:O	1.90	0.72
2:G:369:VAL:HG23	5:G:2266:HOH:O	1.90	0.72
2:G:1279:ILE:HD12	2:S:1279:ILE:HD12	1.72	0.72
1:E:657:ARG:NH1	1:E:661:TYR:O	2.23	0.71
1:I:1533:PRO:HD2	5:I:2232:HOH:O	1.89	0.71
1:Q:792:VAL:O	1:Q:795:SER:OG	2.06	0.71
2:G:337:ALA:HB2	2:O:348:LEU:HG	1.72	0.71
2:G:718:THR:CG2	5:G:2195:HOH:O	2.37	0.71
2:K:35:PHE:O	2:K:41:THR:OG1	2.08	0.71
2:K:779:GLU:HG2	5:K:2061:HOH:O	1.89	0.71
1:I:124:LYS:HA	1:I:124:LYS:CE	2.17	0.71
1:I:688:THR:HG23	5:I:2426:HOH:O	1.89	0.71
1:Q:688:THR:HG23	5:Q:2416:HOH:O	1.90	0.71
2:K:348:LEU:HG	2:X:337:ALA:HB2	1.71	0.71
2:O:1527:ARG:NH2	2:O:1568:LEU:O	2.22	0.71
2:X:778:PRO:O	2:X:790:LYS:NZ	2.23	0.71
1:E:136:LEU:HA	5:E:2282:HOH:O	1.90	0.71
1:Q:902:GLN:HB3	2:S:1690:ARG:NH1	2.06	0.71
1:U:463:ARG:HE	1:U:467:LEU:HD11	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:569:LYS:NZ	1:U:748:SER:O	2.23	0.71
2:K:1635:ILE:CD1	5:K:2289:HOH:O	2.33	0.71
2:S:1493:ARG:CG	5:S:2037:HOH:O	2.35	0.71
1:Q:657:ARG:NH1	1:Q:661:TYR:O	2.22	0.71
1:U:1031:VAL:HA	5:U:2278:HOH:O	1.89	0.71
1:A:1021:SER:HB3	5:A:2228:HOH:O	1.90	0.71
1:U:879:ILE:HG21	1:U:898:VAL:HG23	1.73	0.71
2:O:1281:THR:HB	5:O:2144:HOH:O	1.90	0.71
1:M:657:ARG:NH1	1:M:661:TYR:O	2.23	0.71
2:S:893:VAL:CG2	5:S:2080:HOH:O	2.38	0.71
1:M:569:LYS:NZ	1:M:748:SER:O	2.24	0.71
2:C:778:PRO:O	2:C:790:LYS:NZ	2.23	0.71
1:A:976:PRO:HG3	5:A:2317:HOH:O	1.90	0.71
1:E:888:LYS:HE2	5:E:2409:HOH:O	1.91	0.71
1:E:333:ILE:HG13	1:E:364:LEU:HD21	1.72	0.70
2:K:1211:THR:HG23	5:K:2046:HOH:O	1.91	0.70
2:O:1730:LYS:CB	5:O:2013:HOH:O	2.39	0.70
2:C:1499:ARG:NE	2:X:1519:SER:O	2.23	0.70
1:A:1469:THR:HB	5:A:2327:HOH:O	1.91	0.70
1:E:1591:VAL:HG11	5:E:2404:HOH:O	1.92	0.70
1:I:136:LEU:HA	5:I:2267:HOH:O	1.91	0.70
1:I:569:LYS:NZ	1:I:748:SER:O	2.24	0.70
1:Q:675:ILE:O	1:Q:679:THR:OG1	2.09	0.70
2:C:1701:MET:HA	2:C:1701:MET:HE3	1.71	0.70
2:K:893:VAL:CG2	5:K:2077:HOH:O	2.38	0.70
2:S:1211:THR:HG23	5:S:2051:HOH:O	1.91	0.70
1:A:956:GLN:HG2	5:A:2231:HOH:O	1.90	0.70
1:Q:447:THR:HG22	1:Q:467:LEU:HD23	1.72	0.70
1:U:1090:TYR:CE2	1:U:1140:ALA:HB2	2.26	0.70
2:C:1223:LEU:HB3	5:C:2177:HOH:O	1.90	0.70
2:S:35:PHE:O	2:S:41:THR:OG1	2.08	0.70
1:M:879:ILE:HG21	1:M:898:VAL:HG23	1.73	0.70
1:Q:569:LYS:NZ	1:Q:748:SER:O	2.25	0.70
1:Q:1533:PRO:HD2	5:Q:2236:HOH:O	1.89	0.70
2:O:718:THR:CG2	5:O:2200:HOH:O	2.37	0.70
2:S:1716:GLN:CA	2:S:1717:PRO:HG3	2.21	0.70
2:K:1716:GLN:OE1	2:O:1563:ASN:ND2	2.24	0.70
2:S:759:PRO:CD	5:S:2260:HOH:O	2.38	0.70
1:A:1592:ARG:CZ	5:A:2242:HOH:O	2.39	0.70
1:M:792:VAL:O	1:M:795:SER:OG	2.08	0.70
1:U:473:VAL:HG22	5:U:2232:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:675:ILE:O	1:U:679:THR:OG1	2.10	0.70
1:U:850:MET:HA	1:U:850:MET:HE3	1.72	0.70
2:C:337:ALA:HB2	2:S:348:LEU:HG	1.74	0.70
1:A:172:GLY:HA3	5:A:2273:HOH:O	1.92	0.70
1:E:614:PRO:HG3	1:E:648:TRP:HB2	1.73	0.70
1:M:867:LEU:HD22	5:M:2357:HOH:O	1.90	0.70
2:C:834:GLY:HA3	5:C:2086:HOH:O	1.91	0.70
5:G:2092:HOH:O	2:X:376:LEU:HD11	1.92	0.70
2:O:45:ILE:HD12	2:O:88:ILE:HD13	1.72	0.70
1:E:792:VAL:O	1:E:795:SER:OG	2.09	0.70
1:E:1708:PHE:O	1:E:1714:ARG:NH1	2.25	0.70
2:X:1223:LEU:HB3	5:X:2279:HOH:O	1.90	0.70
1:A:99:VAL:HG11	1:A:531:HIS:ND1	2.07	0.70
1:E:569:LYS:NZ	1:E:748:SER:O	2.25	0.70
1:U:1635:LEU:HD22	1:U:1636:PRO:CD	2.22	0.70
2:G:1129:ASP:OD1	2:K:347:TYR:OH	2.10	0.70
2:K:1279:ILE:HD12	2:O:1279:ILE:HD12	1.73	0.70
1:A:1845:VAL:CG1	5:A:2394:HOH:O	2.39	0.69
1:M:1708:PHE:O	1:M:1714:ARG:NH1	2.25	0.69
2:C:376:LEU:HD11	5:O:2117:HOH:O	1.91	0.69
1:U:1469:THR:HB	5:U:2297:HOH:O	1.92	0.69
2:K:759:PRO:CD	5:K:2260:HOH:O	2.38	0.69
2:S:1135:CYS:HB2	5:S:2263:HOH:O	1.92	0.69
1:E:379:ASN:HB2	5:E:2353:HOH:O	1.92	0.69
2:S:474:GLN:CD	5:S:2052:HOH:O	2.35	0.69
1:A:319:GLU:OE1	1:A:320:GLY:N	2.26	0.69
1:I:1228:PRO:HB2	5:I:2246:HOH:O	1.89	0.69
1:M:203:LEU:O	1:M:207:LYS:HG2	1.92	0.69
1:M:888:LYS:HE2	5:M:2406:HOH:O	1.91	0.69
2:C:1281:THR:CB	5:C:2114:HOH:O	2.40	0.69
2:G:344:LEU:HD11	2:O:340:GLN:HB3	1.74	0.69
2:G:1730:LYS:CB	5:G:2015:HOH:O	2.39	0.69
2:K:824:LEU:HG	5:K:2270:HOH:O	1.92	0.69
2:C:1275:GLN:HE21	2:X:1417:VAL:CG2	2.05	0.69
2:G:1004:ILE:HG13	5:G:2075:HOH:O	1.92	0.69
1:M:1714:ARG:NH2	2:C:918:GLN:OE1	2.26	0.69
1:U:463:ARG:HH21	1:U:467:LEU:HD11	1.57	0.69
1:U:985:GLU:HB3	5:X:2265:HOH:O	1.90	0.69
2:O:686:ALA:HB3	5:O:2137:HOH:O	1.93	0.69
1:A:879:ILE:HG21	1:A:898:VAL:HG23	1.73	0.69
1:A:1444:PHE:CB	5:A:2397:HOH:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1236:TYR:HA	5:G:2006:HOH:O	1.92	0.69
2:X:834:GLY:HA3	5:X:2079:HOH:O	1.92	0.69
1:A:285:THR:HG21	5:A:2427:HOH:O	1.92	0.69
1:E:879:ILE:HG21	1:E:898:VAL:HG23	1.74	0.69
1:I:99:VAL:HG11	1:I:531:HIS:ND1	2.08	0.69
1:I:675:ILE:O	1:I:679:THR:OG1	2.10	0.69
2:C:1352:ILE:CG2	5:C:2288:HOH:O	2.41	0.69
2:K:798:MET:CE	5:K:2142:HOH:O	2.24	0.69
2:K:1135:CYS:HB2	5:K:2256:HOH:O	1.92	0.69
2:K:1493:ARG:CG	5:K:2031:HOH:O	2.36	0.69
1:I:1779:ASP:OD2	2:K:89:TYR:OH	2.06	0.69
2:G:1716:GLN:CB	2:G:1717:PRO:HG3	2.20	0.69
2:O:1004:ILE:HG13	5:O:2078:HOH:O	1.91	0.69
2:X:1281:THR:HB	5:X:2126:HOH:O	1.90	0.69
5:A:2431:HOH:O	2:C:22:PHE:HZ	1.72	0.68
1:I:319:GLU:OE1	1:I:320:GLY:N	2.25	0.68
2:G:348:LEU:HG	2:O:337:ALA:HB2	1.75	0.68
2:G:686:ALA:HB3	5:G:2131:HOH:O	1.93	0.68
1:M:319:GLU:OE1	1:M:320:GLY:N	2.27	0.68
2:G:718:THR:HG22	5:G:2195:HOH:O	1.93	0.68
2:K:1422:LYS:CE	5:K:2275:HOH:O	2.41	0.68
1:E:480:ASN:HD22	1:E:480:ASN:C	2.00	0.68
1:E:1714:ARG:NH2	2:X:918:GLN:OE1	2.26	0.68
1:Q:21:PRO:O	1:Q:25:PHE:N	2.26	0.68
1:Q:136:LEU:HA	5:Q:2274:HOH:O	1.92	0.68
1:U:1093:GLY:HA3	5:U:2395:HOH:O	1.94	0.68
5:G:2092:HOH:O	2:X:376:LEU:HD21	1.92	0.68
2:S:814:PRO:HB2	5:S:2049:HOH:O	1.92	0.68
2:S:1717:PRO:CG	2:S:1717:PRO:CB	2.65	0.68
1:E:889:PRO:HB3	5:E:2316:HOH:O	1.91	0.68
1:A:21:PRO:O	1:A:25:PHE:N	2.26	0.68
1:A:481:HIS:HB3	5:A:2209:HOH:O	1.93	0.68
1:A:867:LEU:HD22	5:A:2350:HOH:O	1.93	0.68
1:I:1528:LEU:HD21	1:I:1612:MET:SD	2.34	0.68
1:Q:319:GLU:OE1	1:Q:320:GLY:N	2.25	0.68
2:K:474:GLN:CD	5:K:2052:HOH:O	2.35	0.68
2:K:1334:PHE:HA	5:K:2030:HOH:O	1.93	0.68
2:K:1498:TYR:HD2	5:K:2114:HOH:O	1.76	0.68
2:S:778:PRO:O	2:S:790:LYS:NZ	2.26	0.68
1:A:1090:TYR:CE2	1:A:1140:ALA:HB2	2.29	0.68
2:C:1223:LEU:HD22	5:C:2177:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:HD13	2:C:1690:ARG:HH21	1.56	0.68
1:A:1419:VAL:HG21	5:A:2304:HOH:O	1.92	0.68
1:E:798:SER:CB	5:E:2376:HOH:O	2.36	0.68
1:A:1456:LYS:O	1:A:1464:SER:N	2.27	0.68
1:E:21:PRO:O	1:E:25:PHE:N	2.26	0.68
1:Q:839:GLU:CB	5:Q:2235:HOH:O	2.40	0.68
1:U:1021:SER:HB3	5:U:2242:HOH:O	1.92	0.68
2:G:1129:ASP:OD1	2:G:1129:ASP:N	2.22	0.68
2:S:824:LEU:HG	5:S:2273:HOH:O	1.93	0.68
1:M:889:PRO:HB3	5:M:2318:HOH:O	1.92	0.68
1:M:956:GLN:HB2	5:M:2209:HOH:O	1.94	0.68
1:Q:99:VAL:HG11	1:Q:531:HIS:ND1	2.09	0.68
1:U:319:GLU:OE1	1:U:320:GLY:N	2.26	0.68
2:X:1631:PRO:HB2	5:X:2277:HOH:O	1.93	0.68
1:A:1093:GLY:HA3	5:A:2389:HOH:O	1.94	0.68
1:E:956:GLN:HB2	5:E:2209:HOH:O	1.94	0.68
1:U:360:GLY:C	5:U:2337:HOH:O	2.37	0.68
2:C:841:GLU:OE1	2:C:841:GLU:N	2.27	0.68
2:K:814:PRO:CB	5:K:2045:HOH:O	2.42	0.68
2:O:1582:LYS:NZ	2:O:1596:MET:SD	2.67	0.68
2:S:1498:TYR:HD2	5:S:2112:HOH:O	1.76	0.68
1:E:319:GLU:OE1	1:E:320:GLY:N	2.26	0.67
1:I:1456:LYS:O	1:I:1464:SER:N	2.27	0.67
1:M:122:TYR:O	1:M:126:VAL:HG23	1.94	0.67
2:C:53:LEU:HD23	2:C:56:MET:HE3	1.76	0.67
2:C:376:LEU:HD21	5:O:2117:HOH:O	1.93	0.67
2:S:1701:MET:HB2	5:S:2042:HOH:O	1.95	0.67
1:U:405:ASN:HB3	5:U:2241:HOH:O	1.94	0.67
2:K:778:PRO:O	2:K:790:LYS:NZ	2.26	0.67
2:K:814:PRO:HB2	5:K:2045:HOH:O	1.93	0.67
1:A:473:VAL:HG22	5:A:2235:HOH:O	1.95	0.67
1:I:589:VAL:O	1:I:611:TYR:OH	2.11	0.67
1:Q:1673:VAL:HG13	5:Q:2426:HOH:O	1.95	0.67
1:U:21:PRO:O	1:U:25:PHE:N	2.27	0.67
1:I:21:PRO:O	1:I:25:PHE:N	2.27	0.67
2:G:1197:TYR:HE1	5:G:2239:HOH:O	1.78	0.67
2:O:1197:TYR:HE1	5:O:2242:HOH:O	1.77	0.67
2:S:814:PRO:CB	5:S:2049:HOH:O	2.42	0.67
2:X:512:GLU:OE1	2:X:873:ARG:NH1	2.27	0.67
1:I:164:ARG:NH2	1:I:212:THR:OG1	2.28	0.67
1:M:21:PRO:O	1:M:25:PHE:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:955:LEU:HB3	5:M:2291:HOH:O	1.95	0.67
1:M:1175:LYS:HA	5:M:2245:HOH:O	1.94	0.67
1:U:306:LEU:HG	5:U:2339:HOH:O	1.94	0.67
2:O:1503:ARG:HD3	5:O:2050:HOH:O	1.93	0.67
1:I:1367:VAL:HG11	5:I:2247:HOH:O	1.94	0.67
1:M:99:VAL:HG11	1:M:531:HIS:ND1	2.10	0.67
1:Q:1159:HIS:CE1	5:Q:2365:HOH:O	2.47	0.67
1:Q:1456:LYS:O	1:Q:1464:SER:N	2.27	0.67
2:G:1582:LYS:NZ	2:G:1596:MET:SD	2.68	0.67
2:S:1334:PHE:HA	5:S:2031:HOH:O	1.93	0.67
1:A:982:LEU:HD13	2:C:1690:ARG:NE	2.09	0.67
1:Q:1367:VAL:HG11	5:Q:2247:HOH:O	1.94	0.67
2:X:1442:LEU:CD1	5:X:2274:HOH:O	2.36	0.67
2:G:377:TRP:CE3	2:X:377:TRP:CZ3	2.83	0.67
2:S:345:ALA:O	2:S:349:GLN:HG3	1.95	0.67
1:E:565:TYR:CE2	1:E:576:ARG:HA	2.29	0.67
1:M:1456:LYS:O	1:M:1464:SER:N	2.28	0.67
2:C:1352:ILE:HG21	5:C:2288:HOH:O	1.95	0.67
2:G:1120:MET:CE	2:S:1263:ARG:O	2.42	0.67
2:S:1211:THR:CG2	5:S:2051:HOH:O	2.42	0.67
1:E:956:GLN:CB	5:E:2209:HOH:O	2.43	0.67
2:C:512:GLU:OE1	2:C:873:ARG:NH1	2.28	0.67
2:G:1364:MET:HE1	5:G:2070:HOH:O	1.95	0.67
2:O:343:VAL:CG1	5:O:2267:HOH:O	2.43	0.67
1:A:675:ILE:O	1:A:679:THR:OG1	2.10	0.66
1:E:1175:LYS:HA	5:E:2244:HOH:O	1.94	0.66
1:U:99:VAL:HG11	1:U:531:HIS:ND1	2.09	0.66
2:K:875:THR:HA	5:K:2226:HOH:O	1.95	0.66
2:O:1369:THR:HG23	5:O:2238:HOH:O	1.95	0.66
2:S:1730:LYS:CB	5:S:2121:HOH:O	2.43	0.66
1:I:839:GLU:CA	5:I:2233:HOH:O	2.43	0.66
1:Q:423:THR:O	1:Q:427:LEU:HD22	1.95	0.66
2:C:1442:LEU:CD1	5:C:2236:HOH:O	2.32	0.66
2:S:467:LEU:HA	2:S:470:ARG:HE	1.60	0.66
2:C:875:THR:HA	5:C:2207:HOH:O	1.95	0.66
2:O:1020:VAL:CG2	2:O:1403:LEU:HD21	2.25	0.66
2:S:875:THR:HA	5:S:2230:HOH:O	1.95	0.66
1:E:1237:GLU:HG2	1:E:1239:MET:SD	2.34	0.66
1:Q:1779:ASP:OD2	2:S:89:TYR:OH	2.06	0.66
1:U:480:ASN:OD1	1:U:480:ASN:O	2.12	0.66
2:K:1211:THR:CG2	5:K:2046:HOH:O	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1364:MET:HE1	5:O:2074:HOH:O	1.94	0.66
2:S:526:TYR:CE1	5:S:2014:HOH:O	2.49	0.66
1:E:122:TYR:O	1:E:126:VAL:HG23	1.94	0.66
1:I:1237:GLU:HG2	1:I:1239:MET:SD	2.36	0.66
1:U:1237:GLU:HG2	1:U:1239:MET:SD	2.35	0.66
2:C:1621:LEU:H	2:C:1621:LEU:HD12	1.61	0.66
2:G:1020:VAL:CG2	2:G:1403:LEU:HD21	2.25	0.66
5:G:2034:HOH:O	2:K:347:TYR:CE1	2.48	0.66
2:K:1410:THR:OG1	2:O:1293:SER:O	2.13	0.66
1:A:1146:ARG:CD	5:A:2245:HOH:O	2.44	0.66
1:U:793:MET:HE1	3:U:2101:FMN:HM73	1.78	0.66
2:G:377:TRP:CZ3	2:X:377:TRP:HE3	2.14	0.66
2:G:1696:ILE:HG21	5:G:2013:HOH:O	1.94	0.66
1:Q:122:TYR:O	1:Q:126:VAL:HG23	1.96	0.66
1:Q:164:ARG:NH2	1:Q:212:THR:OG1	2.28	0.66
1:Q:164:ARG:NH1	1:Q:205:TRP:O	2.29	0.66
1:U:164:ARG:NH2	1:U:212:THR:OG1	2.28	0.66
2:O:894:ARG:NH2	2:O:900:GLU:OE1	2.29	0.66
2:S:1582:LYS:NZ	2:S:1596:MET:SD	2.69	0.66
1:E:1856:ASP:CB	5:E:2237:HOH:O	2.44	0.66
1:U:1456:LYS:O	1:U:1464:SER:N	2.29	0.66
2:K:1582:LYS:NZ	2:K:1596:MET:SD	2.69	0.66
1:A:1682:ASP:HB3	1:A:1683:ARG:HH11	1.61	0.65
1:E:955:LEU:HB3	5:E:2289:HOH:O	1.94	0.65
1:E:1456:LYS:O	1:E:1464:SER:N	2.28	0.65
1:E:1975:PRO:HB2	5:E:2254:HOH:O	1.96	0.65
1:I:867:LEU:HD22	5:I:2311:HOH:O	1.97	0.65
1:I:1673:VAL:HG13	5:I:2420:HOH:O	1.95	0.65
1:Q:360:GLY:HA2	5:Q:2362:HOH:O	1.95	0.65
2:G:35:PHE:O	2:G:41:THR:OG1	2.14	0.65
2:K:834:GLY:HA3	5:S:2118:HOH:O	1.96	0.65
2:S:412:VAL:CG1	4:S:1901:PKZ:C14	2.75	0.65
1:A:1721:ILE:HG12	5:A:2236:HOH:O	1.96	0.65
1:E:1367:VAL:HG11	5:E:2217:HOH:O	1.96	0.65
1:I:122:TYR:O	1:I:126:VAL:HG23	1.96	0.65
1:I:423:THR:O	1:I:427:LEU:HD22	1.95	0.65
1:I:1159:HIS:CE1	5:I:2367:HOH:O	2.49	0.65
1:Q:867:LEU:HD22	5:Q:2319:HOH:O	1.96	0.65
1:A:982:LEU:HD13	2:C:1690:ARG:CZ	2.27	0.65
2:G:940:THR:HG22	5:G:2132:HOH:O	1.97	0.65
1:A:164:ARG:NH2	1:A:212:THR:OG1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1541:ILE:HD11	5:E:2366:HOH:O	1.93	0.65
1:M:675:ILE:O	1:M:679:THR:OG1	2.13	0.65
2:G:1503:ARG:HD3	5:G:2047:HOH:O	1.96	0.65
2:O:1551:VAL:HG23	5:O:2235:HOH:O	1.97	0.65
1:M:1367:VAL:HG11	5:M:2232:HOH:O	1.96	0.65
2:G:778:PRO:O	2:G:790:LYS:NZ	2.29	0.65
2:K:1730:LYS:CB	5:K:2117:HOH:O	2.44	0.65
2:X:1004:ILE:HG13	5:X:2066:HOH:O	1.95	0.65
1:Q:839:GLU:CA	5:Q:2235:HOH:O	2.44	0.65
1:Q:2001:ASN:OD1	2:S:26:VAL:CG2	2.44	0.65
2:K:412:VAL:CG1	4:K:1901:PKZ:C14	2.75	0.65
2:O:29:ILE:HD11	5:O:2116:HOH:O	1.95	0.65
1:A:480:ASN:O	1:A:480:ASN:OD1	2.14	0.65
1:E:337:GLU:O	1:E:341:GLU:HG2	1.97	0.65
1:M:956:GLN:CB	5:M:2209:HOH:O	2.44	0.65
2:G:894:ARG:NH2	2:G:900:GLU:OE1	2.29	0.65
2:O:778:PRO:O	2:O:790:LYS:NZ	2.29	0.65
1:E:1688:ASN:HB2	5:E:2272:HOH:O	1.94	0.65
1:M:1541:ILE:HD11	5:M:2366:HOH:O	1.93	0.65
1:M:1856:ASP:CB	5:M:2236:HOH:O	2.44	0.65
2:G:1:MET:HE1	2:G:5:ILE:HG22	1.78	0.65
5:K:2109:HOH:O	2:S:834:GLY:HA3	1.97	0.65
2:O:1197:TYR:CE1	5:O:2242:HOH:O	2.50	0.65
1:A:1174:LYS:C	5:A:2202:HOH:O	2.38	0.65
1:M:774:GLU:CA	5:M:2290:HOH:O	2.45	0.65
2:K:1263:ARG:O	2:O:1120:MET:CE	2.44	0.65
2:S:651:GLY:CA	5:S:2056:HOH:O	2.45	0.65
1:Q:1504:SER:HB2	5:Q:2239:HOH:O	1.98	0.64
2:C:527:GLU:OE2	2:C:894:ARG:NH2	2.30	0.64
2:C:1503:ARG:HE	2:X:1519:SER:HB3	1.61	0.64
2:G:1132:PRO:HD3	2:G:1165:ARG:HD3	1.79	0.64
2:K:651:GLY:CA	5:K:2053:HOH:O	2.45	0.64
2:X:1621:LEU:H	2:X:1621:LEU:HD12	1.61	0.64
1:E:99:VAL:HG11	1:E:531:HIS:ND1	2.11	0.64
1:U:960:GLN:HG3	5:U:2288:HOH:O	1.96	0.64
2:C:1067:GLN:CB	5:C:2183:HOH:O	2.45	0.64
2:O:718:THR:HG22	5:O:2200:HOH:O	1.93	0.64
1:I:164:ARG:NH1	1:I:205:TRP:O	2.30	0.64
1:I:997:ARG:HD2	1:I:998:PRO:O	1.98	0.64
1:U:1444:PHE:CB	5:U:2401:HOH:O	2.45	0.64
1:U:1465:SER:HB3	5:U:2283:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:340:GLN:HB3	2:O:344:LEU:HD22	1.80	0.64
2:G:1369:THR:HG23	5:G:2234:HOH:O	1.96	0.64
2:X:407:TRP:O	2:X:411:ASP:OD1	2.15	0.64
1:A:172:GLY:CA	5:A:2273:HOH:O	2.44	0.64
1:E:1278:ILE:HG23	1:E:1283:ILE:HD11	1.80	0.64
2:C:788:ASP:HA	5:C:2275:HOH:O	1.96	0.64
2:G:1292:SER:O	2:G:1292:SER:OG	2.13	0.64
2:K:696:LEU:O	2:K:700:ILE:HG23	1.98	0.64
2:X:1352:ILE:CG2	5:X:2289:HOH:O	2.44	0.64
1:A:63:ILE:HD11	1:A:79:LEU:HG	1.78	0.64
1:E:589:VAL:O	1:E:611:TYR:OH	2.12	0.64
1:U:589:VAL:O	1:U:611:TYR:OH	2.15	0.64
2:S:696:LEU:O	2:S:700:ILE:HG23	1.98	0.64
2:S:1561:ILE:HD11	2:S:1646:THR:HG21	1.80	0.64
1:M:1278:ILE:HG23	1:M:1283:ILE:HD11	1.80	0.64
2:G:1551:VAL:HG23	5:G:2236:HOH:O	1.97	0.64
2:S:1212:LEU:CD2	5:S:2025:HOH:O	2.46	0.64
1:A:360:GLY:C	5:A:2348:HOH:O	2.40	0.64
1:M:337:GLU:O	1:M:341:GLU:HG2	1.97	0.64
1:M:1975:PRO:HB2	5:M:2247:HOH:O	1.96	0.64
2:O:1677:TYR:O	2:O:1681:VAL:HG23	1.98	0.64
1:M:1237:GLU:HG2	1:M:1239:MET:SD	2.38	0.64
2:K:1212:LEU:CD2	5:K:2020:HOH:O	2.46	0.64
2:O:940:THR:CG2	5:O:2139:HOH:O	2.46	0.64
1:A:405:ASN:HB3	5:A:2248:HOH:O	1.97	0.64
1:U:2018:TYR:CD1	1:U:2027:LYS:HD3	2.33	0.64
2:C:380:GLU:OE2	2:O:745:LYS:N	2.30	0.64
2:O:1281:THR:CB	5:O:2144:HOH:O	2.45	0.64
2:S:1560:THR:HG23	5:S:2210:HOH:O	1.98	0.64
2:X:1670:ASP:OD1	2:X:1673:THR:OG1	2.05	0.64
1:E:774:GLU:CA	5:E:2291:HOH:O	2.46	0.63
1:M:589:VAL:O	1:M:611:TYR:OH	2.13	0.63
1:Q:1810:MET:HE3	1:Q:1984:ILE:HD13	1.77	0.63
2:X:1352:ILE:HG21	5:X:2289:HOH:O	1.98	0.63
1:Q:997:ARG:HD2	1:Q:998:PRO:O	1.97	0.63
2:C:693:ALA:CB	5:C:2111:HOH:O	2.46	0.63
2:K:1677:TYR:O	2:K:1681:VAL:HG23	1.98	0.63
2:O:940:THR:HG22	5:O:2139:HOH:O	1.97	0.63
2:X:651:GLY:CA	5:X:2016:HOH:O	2.45	0.63
1:I:906:TYR:HD2	1:I:941:VAL:HG22	1.64	0.63
1:Q:1554:VAL:CG1	5:Q:2276:HOH:O	2.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:LYS:N	2:X:380:GLU:OE2	2.31	0.63
2:K:526:TYR:CE1	5:K:2012:HOH:O	2.50	0.63
2:K:834:GLY:CA	5:S:2118:HOH:O	2.46	0.63
2:O:1:MET:HE1	2:O:5:ILE:HG22	1.79	0.63
2:X:464:THR:CG2	5:X:2024:HOH:O	2.31	0.63
2:C:1129:ASP:OD1	2:G:347:TYR:OH	2.08	0.63
2:K:861:LYS:HA	5:K:2095:HOH:O	1.98	0.63
1:Q:1291:GLY:HA2	5:Q:2320:HOH:O	1.98	0.63
2:K:1560:THR:HG23	5:K:2205:HOH:O	1.97	0.63
2:S:1677:TYR:O	2:S:1681:VAL:HG23	1.98	0.63
1:A:847:ARG:NH2	1:A:1035:ASP:OD2	2.32	0.63
1:I:1124:GLN:HA	5:I:2412:HOH:O	1.98	0.63
1:M:1592:ARG:CZ	5:M:2225:HOH:O	2.46	0.63
1:Q:1124:GLN:HA	5:Q:2418:HOH:O	1.98	0.63
1:U:1721:ILE:CD1	5:U:2416:HOH:O	2.46	0.63
2:C:1004:ILE:HG13	5:C:2063:HOH:O	1.99	0.63
2:G:1677:TYR:O	2:G:1681:VAL:HG23	1.98	0.63
2:K:1561:ILE:HD11	2:K:1646:THR:HG21	1.80	0.63
1:E:447:THR:HG22	1:E:467:LEU:CD2	2.28	0.63
1:I:847:ARG:NH2	1:I:1035:ASP:OD2	2.32	0.63
2:C:1631:PRO:HB2	5:C:2260:HOH:O	1.97	0.63
2:G:499:LYS:HE3	2:G:513:THR:HG21	1.80	0.63
1:E:601:GLY:HA3	5:E:2250:HOH:O	1.99	0.63
1:E:615:VAL:HG23	5:E:2378:HOH:O	1.98	0.63
1:M:340:ILE:HD11	1:M:366:LEU:HD22	1.79	0.63
2:G:504:ALA:HB3	2:G:505:LYS:NZ	2.14	0.63
2:O:412:VAL:CG1	4:O:1901:PKZ:C14	2.77	0.63
2:X:1631:PRO:CB	5:X:2277:HOH:O	2.45	0.63
1:I:1291:GLY:HA2	5:I:2317:HOH:O	1.98	0.62
1:Q:1278:ILE:HG23	1:Q:1283:ILE:HD11	1.81	0.62
1:U:847:ARG:NH2	1:U:1035:ASP:OD2	2.32	0.62
2:C:759:PRO:HD2	5:C:2116:HOH:O	1.96	0.62
2:K:745:LYS:N	2:S:380:GLU:OE2	2.32	0.62
2:K:1293:SER:O	2:O:1410:THR:OG1	2.17	0.62
2:X:875:THR:HA	5:X:2207:HOH:O	1.98	0.62
1:A:960:GLN:HG3	5:A:2274:HOH:O	1.99	0.62
1:I:360:GLY:HA2	5:I:2365:HOH:O	1.99	0.62
1:I:850:MET:HA	1:I:850:MET:HE3	1.81	0.62
1:M:1528:LEU:HD21	1:M:1612:MET:SD	2.38	0.62
1:Q:481:HIS:CE1	1:Q:505:LYS:HD2	2.34	0.62
2:X:412:VAL:CG1	4:X:1901:PKZ:C14	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1281:THR:CB	5:X:2126:HOH:O	2.46	0.62
1:M:615:VAL:HG23	5:M:2376:HOH:O	1.98	0.62
1:M:1588:ALA:O	1:M:1591:VAL:HG22	1.99	0.62
1:U:164:ARG:NH1	1:U:205:TRP:O	2.33	0.62
2:G:412:VAL:CG1	4:G:1901:PKZ:C14	2.77	0.62
2:K:1701:MET:HB2	5:K:2040:HOH:O	2.00	0.62
2:O:388:GLY:O	2:O:741:ASN:ND2	2.31	0.62
2:O:968:VAL:CG1	5:O:2052:HOH:O	2.47	0.62
2:O:1426:THR:HA	2:O:1429:ARG:HE	1.64	0.62
2:O:1561:ILE:HD11	2:O:1646:THR:HG21	1.80	0.62
2:O:1716:GLN:CB	2:O:1717:PRO:HG3	2.28	0.62
1:A:903:GLU:CD	2:C:1690:ARG:NH2	2.54	0.62
1:E:340:ILE:HD11	1:E:366:LEU:HD22	1.81	0.62
1:I:1504:SER:HB2	5:I:2237:HOH:O	1.99	0.62
1:Q:847:ARG:NH2	1:Q:1035:ASP:OD2	2.32	0.62
1:U:139:HIS:CA	5:U:2205:HOH:O	2.47	0.62
2:C:1670:ASP:OD1	2:C:1673:THR:OG1	2.05	0.62
1:Q:1431:ARG:NH2	1:Q:1440:LYS:O	2.32	0.62
2:O:1355:PHE:CD1	5:O:2074:HOH:O	2.52	0.62
2:S:1716:GLN:HB2	2:S:1717:PRO:HG3	1.81	0.62
1:A:1721:ILE:CD1	5:A:2419:HOH:O	2.47	0.62
1:E:1528:LEU:HD21	1:E:1612:MET:SD	2.38	0.62
5:U:2300:HOH:O	2:X:26:VAL:HG11	1.98	0.62
2:O:875:THR:HA	5:O:2224:HOH:O	2.00	0.62
1:A:164:ARG:NH1	1:A:205:TRP:O	2.33	0.62
1:A:903:GLU:CD	2:C:1690:ARG:NH1	2.57	0.62
1:E:675:ILE:O	1:E:679:THR:OG1	2.17	0.62
1:I:325:MET:HG3	1:I:410:ILE:HG21	1.82	0.62
1:M:847:ARG:NH2	1:M:1035:ASP:OD2	2.32	0.62
1:M:1431:ARG:NH2	1:M:1440:LYS:O	2.33	0.62
1:Q:1787:PRO:HB3	5:Q:2347:HOH:O	1.98	0.62
2:C:835:PHE:CE1	5:C:2086:HOH:O	2.51	0.62
2:G:377:TRP:CZ3	2:X:377:TRP:CE3	2.87	0.62
2:G:940:THR:CG2	5:G:2132:HOH:O	2.47	0.62
2:S:861:LYS:HA	5:S:2096:HOH:O	1.98	0.62
1:A:1225:LYS:HD2	1:A:1238:ILE:HD11	1.81	0.62
2:G:407:TRP:O	2:G:411:ASP:OD1	2.18	0.62
1:E:847:ARG:NH2	1:E:1035:ASP:OD2	2.32	0.62
1:I:1278:ILE:HG23	1:I:1283:ILE:HD11	1.81	0.62
1:Q:857:ASP:O	1:Q:861:ASN:ND2	2.32	0.62
1:U:122:TYR:O	1:U:126:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:VAL:CG1	4:C:1901:PKZ:C14	2.78	0.62
2:C:1223:LEU:CD2	5:C:2177:HOH:O	2.45	0.62
2:G:1410:THR:OG1	2:S:1293:SER:O	2.17	0.62
2:O:407:TRP:O	2:O:411:ASP:OD1	2.18	0.62
1:A:793:MET:HE2	1:A:1043:HIS:HD2	1.64	0.62
1:E:423:THR:O	1:E:427:LEU:HD22	2.00	0.62
1:Q:906:TYR:HD2	1:Q:941:VAL:HG22	1.64	0.62
2:C:464:THR:CG2	5:C:2005:HOH:O	2.39	0.62
2:G:1197:TYR:CE1	5:G:2239:HOH:O	2.50	0.62
2:K:380:GLU:OE2	2:S:745:LYS:N	2.32	0.62
2:O:1364:MET:SD	5:O:2074:HOH:O	2.56	0.62
2:S:534:MET:SD	2:S:893:VAL:HG13	2.40	0.62
2:S:758:GLU:HB3	5:S:2260:HOH:O	2.00	0.62
1:A:1361:LYS:CD	5:A:2224:HOH:O	2.38	0.61
1:E:1592:ARG:CZ	5:E:2219:HOH:O	2.47	0.61
1:M:423:THR:O	1:M:427:LEU:HD22	2.00	0.61
1:M:1465:SER:HB3	5:M:2351:HOH:O	1.99	0.61
1:Q:1571:SER:O	1:Q:1575:ILE:HD12	2.00	0.61
1:Q:1575:ILE:HD13	1:Q:1638:LEU:HD22	1.82	0.61
2:C:467:LEU:HA	2:C:470:ARG:NE	2.15	0.61
2:G:1355:PHE:CD1	5:G:2070:HOH:O	2.52	0.61
2:G:1431:HIS:ND1	2:S:1721:ASP:OD1	2.31	0.61
2:G:1746:TYR:OH	2:S:1522:ARG:NH1	2.32	0.61
2:O:483:LEU:O	2:O:484:THR:OG1	2.17	0.61
2:O:504:ALA:HB3	2:O:505:LYS:NZ	2.14	0.61
2:O:1387:MET:HE1	2:O:1395:MET:SD	2.40	0.61
1:A:1679:ASP:O	1:A:1683:ARG:HD3	1.99	0.61
1:A:1725:PHE:CD2	1:A:1825:THR:HG23	2.35	0.61
1:E:1465:SER:HB3	5:E:2354:HOH:O	1.99	0.61
1:U:906:TYR:HD2	1:U:941:VAL:HG22	1.65	0.61
2:S:760:LYS:HE2	2:S:761:LYS:HZ2	1.65	0.61
1:A:688:THR:HG23	5:A:2324:HOH:O	2.00	0.61
1:A:1884:GLN:HB3	5:C:2096:HOH:O	1.98	0.61
1:I:371:GLU:HB3	5:I:2431:HOH:O	2.00	0.61
1:M:1395:GLN:CG	5:M:2229:HOH:O	2.47	0.61
2:C:341:LEU:CD2	5:S:2267:HOH:O	2.48	0.61
2:G:819:PRO:HG3	5:G:2008:HOH:O	2.00	0.61
2:K:1426:THR:HA	2:K:1429:ARG:HE	1.65	0.61
2:O:819:PRO:HG3	5:O:2007:HOH:O	1.99	0.61
2:S:534:MET:HE1	2:S:933:ILE:HG12	1.82	0.61
2:S:1527:ARG:NH2	2:S:1568:LEU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PRO:HD3	1:A:648:TRP:CE3	2.35	0.61
1:I:166:LEU:HD21	1:I:234:CYS:CB	2.30	0.61
1:Q:1127:LEU:HD13	5:Q:2365:HOH:O	1.99	0.61
2:K:758:GLU:HB3	5:K:2260:HOH:O	1.99	0.61
1:A:447:THR:HG22	5:A:2235:HOH:O	2.00	0.61
1:A:1845:VAL:HG22	5:A:2394:HOH:O	1.98	0.61
1:E:1395:GLN:CG	5:E:2231:HOH:O	2.48	0.61
1:I:1431:ARG:NH2	1:I:1440:LYS:O	2.33	0.61
1:M:613:SER:C	1:M:614:PRO:CG	2.72	0.61
1:M:850:MET:HA	1:M:850:MET:HE3	1.83	0.61
1:U:914:VAL:HG23	1:U:934:TYR:HE2	1.65	0.61
2:C:369:VAL:HG23	5:C:2187:HOH:O	2.00	0.61
2:G:1387:MET:HE1	2:G:1395:MET:SD	2.41	0.61
2:K:814:PRO:C	5:K:2045:HOH:O	2.42	0.61
2:X:757:ASP:O	2:X:765:GLY:N	2.32	0.61
1:I:397:SER:HB2	5:I:2261:HOH:O	2.00	0.61
2:C:528:MET:HE1	2:C:894:ARG:HD2	1.83	0.61
5:K:2109:HOH:O	2:S:834:GLY:CA	2.47	0.61
2:X:693:ALA:CB	5:X:2112:HOH:O	2.49	0.61
1:A:1431:ARG:NH2	1:A:1440:LYS:O	2.34	0.61
1:I:799:HIS:HA	5:I:2376:HOH:O	2.01	0.61
1:M:601:GLY:HA3	5:M:2249:HOH:O	1.99	0.61
1:M:939:ARG:CD	5:M:2291:HOH:O	2.46	0.61
1:U:857:ASP:O	1:U:861:ASN:ND2	2.34	0.61
2:G:1281:THR:CB	5:G:2151:HOH:O	2.44	0.61
2:K:483:LEU:O	2:K:484:THR:OG1	2.17	0.61
2:K:534:MET:SD	2:K:893:VAL:HG13	2.40	0.61
2:O:441:ARG:NH1	2:O:726:ALA:O	2.33	0.61
2:O:757:ASP:O	2:O:765:GLY:N	2.33	0.61
2:X:1085:GLU:HA	2:X:1088:ILE:HD13	1.82	0.61
1:I:1554:VAL:CG1	5:I:2286:HOH:O	2.41	0.61
1:M:906:TYR:HD2	1:M:941:VAL:HG22	1.66	0.61
1:Q:371:GLU:HB3	5:Q:2433:HOH:O	1.99	0.61
2:K:964:GLU:CG	5:K:2148:HOH:O	2.42	0.61
1:E:956:GLN:CG	5:E:2209:HOH:O	2.49	0.61
1:Q:1237:GLU:HG2	1:Q:1239:MET:SD	2.41	0.61
5:G:2086:HOH:O	2:S:1500:GLU:HG2	2.01	0.61
2:S:964:GLU:CG	5:S:2160:HOH:O	2.43	0.61
2:X:759:PRO:HD2	5:X:2234:HOH:O	1.95	0.61
2:X:1503:ARG:HD3	5:X:2011:HOH:O	2.01	0.61
1:A:906:TYR:HD2	1:A:941:VAL:HG22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:956:GLN:HG2	5:M:2209:HOH:O	2.01	0.61
1:Q:807:LEU:HD22	1:Q:1041:ILE:HD13	1.83	0.61
1:Q:850:MET:HA	1:Q:850:MET:HE3	1.81	0.61
1:U:466:LYS:NZ	1:U:470:GLU:OE1	2.26	0.61
1:U:872:ASN:O	1:U:875:ARG:HG2	2.00	0.61
2:C:483:LEU:O	2:C:484:THR:OG1	2.19	0.61
2:O:834:GLY:HA3	5:O:2103:HOH:O	2.01	0.61
2:O:1004:ILE:HD11	5:O:2291:HOH:O	2.00	0.61
2:O:1020:VAL:HG23	2:O:1403:LEU:HD21	1.82	0.61
1:I:1575:ILE:HD13	1:I:1638:LEU:HD22	1.83	0.60
2:C:651:GLY:CA	5:C:2029:HOH:O	2.49	0.60
2:G:875:THR:HA	5:G:2223:HOH:O	2.00	0.60
2:G:1014:LEU:HD21	2:G:1668:VAL:CG2	2.31	0.60
2:G:1020:VAL:HG23	2:G:1403:LEU:HD21	1.82	0.60
2:K:338:LYS:HD2	2:S:349:GLN:HG2	1.83	0.60
2:K:1721:ASP:OD1	2:O:1431:HIS:ND1	2.32	0.60
2:O:515:LYS:CE	5:O:2034:HOH:O	2.49	0.60
1:A:1465:SER:HB3	5:A:2306:HOH:O	2.01	0.60
1:I:1588:ALA:O	1:I:1591:VAL:HG22	2.01	0.60
1:U:1431:ARG:NH2	1:U:1440:LYS:O	2.33	0.60
2:G:1021:THR:HG21	2:G:1397:VAL:HG21	1.83	0.60
2:K:534:MET:HE1	2:K:933:ILE:HG12	1.82	0.60
2:S:1332:ASP:OD2	2:S:1590:GLY:N	2.34	0.60
1:E:1431:ARG:NH2	1:E:1440:LYS:O	2.33	0.60
1:I:1127:LEU:HD13	5:I:2367:HOH:O	2.00	0.60
1:Q:996:ALA:CB	5:Q:2440:HOH:O	2.49	0.60
2:G:441:ARG:NH1	2:G:726:ALA:O	2.33	0.60
2:S:1132:PRO:HD3	2:S:1165:ARG:HE	1.66	0.60
2:X:758:GLU:HB3	5:X:2234:HOH:O	2.00	0.60
1:I:857:ASP:O	1:I:861:ASN:ND2	2.35	0.60
1:Q:1588:ALA:O	1:Q:1591:VAL:HG22	2.01	0.60
2:C:341:LEU:HD23	5:S:2267:HOH:O	1.99	0.60
2:K:1132:PRO:HD3	2:K:1165:ARG:HE	1.65	0.60
2:O:432:ILE:HD13	4:O:1901:PKZ:CEP	2.32	0.60
2:O:522:GLU:N	2:O:522:GLU:OE2	2.35	0.60
2:O:651:GLY:CA	5:O:2104:HOH:O	2.50	0.60
2:S:483:LEU:O	2:S:484:THR:OG1	2.17	0.60
1:A:857:ASP:O	1:A:861:ASN:ND2	2.34	0.60
1:E:956:GLN:HG2	5:E:2209:HOH:O	2.01	0.60
1:I:820:GLU:HB2	5:I:2425:HOH:O	2.02	0.60
1:M:306:LEU:HD11	1:M:310:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:693:ALA:HA	5:C:2111:HOH:O	1.99	0.60
2:G:1720:LEU:HD22	2:S:1567:HIS:CG	2.37	0.60
2:O:968:VAL:HG12	5:O:2052:HOH:O	2.02	0.60
2:O:1278:PHE:O	2:O:1281:THR:HG22	2.02	0.60
2:S:774:PHE:CE1	2:S:825:PRO:HB3	2.37	0.60
2:X:1691:TYR:HE1	5:X:2279:HOH:O	1.80	0.60
2:G:432:ILE:HD13	4:G:1901:PKZ:CEP	2.32	0.60
2:K:432:ILE:HD13	4:K:1901:PKZ:CEP	2.31	0.60
1:E:906:TYR:HD2	1:E:941:VAL:HG22	1.67	0.60
1:M:478:ALA:CB	5:M:2401:HOH:O	2.40	0.60
2:C:1288:MET:HE1	2:X:1417:VAL:CG2	2.31	0.60
1:A:1304:ALA:C	5:A:2205:HOH:O	2.45	0.60
1:I:807:LEU:HD22	1:I:1041:ILE:HD13	1.84	0.60
1:U:423:THR:O	1:U:427:LEU:HD22	2.02	0.60
1:U:1174:LYS:C	5:U:2221:HOH:O	2.44	0.60
2:C:1503:ARG:HD3	5:C:2020:HOH:O	2.00	0.60
5:I:2253:HOH:O	2:K:968:VAL:CG2	2.35	0.60
1:Q:601:GLY:HA3	5:Q:2273:HOH:O	2.01	0.60
1:U:1826:MET:SD	2:X:22:PHE:CE2	2.94	0.60
2:C:757:ASP:O	2:C:765:GLY:N	2.33	0.60
1:E:1214:ASP:O	1:E:1215:THR:HG22	2.02	0.60
1:M:571:SER:OG	1:M:576:ARG:O	2.18	0.60
2:G:515:LYS:CE	5:G:2032:HOH:O	2.49	0.60
2:G:834:GLY:HA3	5:G:2098:HOH:O	2.00	0.60
1:A:985:GLU:HB3	5:A:2374:HOH:O	2.02	0.59
1:I:480:ASN:O	1:I:480:ASN:OD1	2.18	0.59
1:M:814:VAL:HG21	1:M:827:THR:HB	1.83	0.59
1:U:333:ILE:HG13	1:U:364:LEU:HD21	1.84	0.59
2:G:1364:MET:SD	5:G:2070:HOH:O	2.56	0.59
2:K:760:LYS:HE2	2:K:761:LYS:HZ3	1.67	0.59
2:O:528:MET:HE3	2:O:641:PHE:HB2	1.84	0.59
2:X:369:VAL:HG23	5:X:2188:HOH:O	2.01	0.59
2:X:651:GLY:HA3	5:X:2016:HOH:O	2.02	0.59
1:I:1810:MET:HE3	1:I:1984:ILE:HD13	1.83	0.59
1:M:956:GLN:CG	5:M:2209:HOH:O	2.49	0.59
1:Q:447:THR:HG22	1:Q:467:LEU:CD2	2.32	0.59
2:G:632:SER:HA	5:G:2210:HOH:O	2.02	0.59
2:G:1355:PHE:CE1	5:G:2070:HOH:O	2.51	0.59
2:K:404:TYR:CE1	5:K:2228:HOH:O	2.52	0.59
2:K:1527:ARG:NH2	2:K:1568:LEU:O	2.33	0.59
2:X:788:ASP:OD1	2:X:791:SER:OG	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:THR:O	1:A:427:LEU:HD22	2.02	0.59
2:S:432:ILE:HD13	4:S:1901:PKZ:CEP	2.31	0.59
2:X:693:ALA:HA	5:X:2112:HOH:O	2.01	0.59
1:E:570:PHE:CZ	1:E:574:LEU:HD11	2.37	0.59
1:I:996:ALA:CB	5:I:2436:HOH:O	2.50	0.59
1:U:139:HIS:CB	5:U:2205:HOH:O	2.50	0.59
2:C:344:LEU:CD1	2:S:344:LEU:HD13	2.32	0.59
2:C:730:ALA:O	2:C:733:SER:OG	2.19	0.59
2:G:651:GLY:CA	5:G:2099:HOH:O	2.49	0.59
2:S:1059:ILE:HD13	2:S:1088:ILE:HD12	1.85	0.59
1:A:982:LEU:CD1	2:C:1690:ARG:NH2	2.63	0.59
1:E:814:VAL:HG21	1:E:827:THR:HB	1.84	0.59
1:I:774:GLU:CA	5:I:2307:HOH:O	2.50	0.59
1:Q:2001:ASN:OD1	2:S:26:VAL:HG23	2.02	0.59
1:U:340:ILE:HG22	1:U:376:PHE:CE2	2.38	0.59
1:U:340:ILE:HG22	1:U:376:PHE:CZ	2.38	0.59
2:C:1677:TYR:O	2:C:1681:VAL:HG23	2.02	0.59
2:K:1332:ASP:OD2	2:K:1590:GLY:N	2.35	0.59
2:O:788:ASP:HA	5:O:2237:HOH:O	2.03	0.59
2:X:483:LEU:O	2:X:484:THR:OG1	2.18	0.59
1:Q:872:ASN:O	1:Q:875:ARG:HG2	2.02	0.59
1:U:985:GLU:CB	5:X:2265:HOH:O	2.48	0.59
1:U:1591:VAL:HG11	5:U:2405:HOH:O	2.03	0.59
2:C:1631:PRO:CB	5:C:2260:HOH:O	2.49	0.59
1:U:1651:TYR:OH	1:U:1785:LEU:O	2.20	0.59
2:C:478:ASN:ND2	4:C:1901:PKZ:C1	2.66	0.59
2:O:913:ILE:HD13	5:O:2148:HOH:O	2.02	0.59
2:X:1067:GLN:CB	5:X:2206:HOH:O	2.51	0.59
1:Q:397:SER:HB2	5:Q:2356:HOH:O	2.01	0.59
1:Q:1504:SER:CB	5:Q:2239:HOH:O	2.50	0.59
2:G:29:ILE:HD11	5:G:2113:HOH:O	1.95	0.59
2:G:344:LEU:HD11	2:O:340:GLN:CB	2.33	0.59
2:G:913:ILE:HD13	5:G:2142:HOH:O	2.02	0.59
2:K:1035:ARG:NH2	2:K:1602:GLN:OE1	2.36	0.59
1:Q:578:PRO:HD2	5:Q:2403:HOH:O	2.03	0.59
2:C:990:PHE:CZ	2:C:1223:LEU:HD11	2.38	0.59
2:O:1021:THR:HG21	2:O:1397:VAL:HG21	1.84	0.59
1:E:939:ARG:CD	5:E:2289:HOH:O	2.46	0.59
1:Q:360:GLY:CA	5:Q:2362:HOH:O	2.50	0.59
2:K:1236:TYR:HA	5:K:2054:HOH:O	2.03	0.59
2:K:1588:PRO:HB2	5:K:2124:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:814:PRO:C	5:S:2049:HOH:O	2.44	0.59
1:E:305:SER:N	1:I:1293:LYS:O	2.24	0.58
1:E:613:SER:C	1:E:614:PRO:CG	2.73	0.58
2:K:774:PHE:CE1	2:K:825:PRO:HB3	2.38	0.58
1:E:1444:PHE:CA	5:E:2393:HOH:O	2.32	0.58
1:I:601:GLY:HA3	5:I:2264:HOH:O	2.02	0.58
1:U:1588:ALA:O	1:U:1591:VAL:HG22	2.02	0.58
1:I:578:PRO:HD2	5:I:2406:HOH:O	2.03	0.58
1:Q:1415:THR:CB	5:Q:2332:HOH:O	2.51	0.58
1:U:306:LEU:HD21	1:U:310:MET:CE	2.33	0.58
1:U:1236:LEU:HB3	5:U:2422:HOH:O	2.04	0.58
1:U:1504:SER:HB2	5:U:2270:HOH:O	2.04	0.58
2:C:990:PHE:HE1	2:C:1692:MET:SD	2.26	0.58
2:G:377:TRP:HE3	2:X:377:TRP:CZ3	2.21	0.58
2:G:1278:PHE:O	2:G:1281:THR:HG22	2.02	0.58
1:A:437:PHE:HD2	1:A:461:ILE:HG13	1.67	0.58
1:A:615:VAL:CG2	5:A:2352:HOH:O	2.49	0.58
1:A:639:ILE:H	1:A:645:MET:HE3	1.67	0.58
1:A:1237:GLU:HG2	1:A:1239:MET:SD	2.44	0.58
1:I:1571:SER:O	1:I:1575:ILE:HD12	2.03	0.58
1:Q:139:HIS:CA	5:Q:2203:HOH:O	2.52	0.58
1:Q:774:GLU:CA	5:Q:2315:HOH:O	2.51	0.58
1:Q:875:ARG:HD2	5:Q:2255:HOH:O	2.03	0.58
1:Q:1288:HIS:CD2	5:Q:2233:HOH:O	2.56	0.58
1:Q:1673:VAL:CG1	5:Q:2426:HOH:O	2.49	0.58
1:U:544:TRP:HB3	5:U:2274:HOH:O	2.03	0.58
2:G:757:ASP:O	2:G:765:GLY:N	2.33	0.58
2:O:1014:LEU:HD21	2:O:1668:VAL:CG2	2.34	0.58
2:O:1144:LYS:HB2	2:O:1153:ILE:HD13	1.86	0.58
2:S:1014:LEU:HD21	2:S:1668:VAL:CG2	2.34	0.58
1:E:1159:HIS:O	1:E:1163:THR:OG1	2.22	0.58
1:Q:611:TYR:HA	5:Q:2412:HOH:O	2.03	0.58
1:Q:1161:ILE:HG23	1:Q:1554:VAL:HG23	1.84	0.58
2:G:522:GLU:OE1	2:G:522:GLU:N	2.34	0.58
2:G:1004:ILE:HD11	5:G:2292:HOH:O	2.01	0.58
1:I:360:GLY:C	5:I:2365:HOH:O	2.47	0.58
1:M:306:LEU:HG	5:M:2377:HOH:O	2.02	0.58
1:Q:360:GLY:C	5:Q:2362:HOH:O	2.46	0.58
2:G:338:LYS:HD3	2:X:348:LEU:HD12	1.84	0.58
2:G:483:LEU:O	2:G:484:THR:OG1	2.17	0.58
2:G:528:MET:HE3	2:G:641:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1720:LEU:HD22	2:O:1567:HIS:CD2	2.38	0.58
2:O:1035:ARG:NH2	2:O:1602:GLN:OE1	2.36	0.58
2:O:1129:ASP:OD1	2:O:1129:ASP:N	2.33	0.58
2:X:478:ASN:ND2	4:X:1901:PKZ:C1	2.66	0.58
2:X:528:MET:HE1	2:X:894:ARG:HD3	1.85	0.58
1:I:139:HIS:CA	5:I:2203:HOH:O	2.52	0.58
1:I:774:GLU:CB	5:I:2307:HOH:O	2.52	0.58
1:I:902:GLN:HB3	2:K:1690:ARG:HH11	1.69	0.58
1:Q:799:HIS:HA	5:Q:2375:HOH:O	2.03	0.58
1:U:2018:TYR:CG	1:U:2027:LYS:HD3	2.38	0.58
2:S:1236:TYR:HA	5:S:2057:HOH:O	2.03	0.58
1:E:1597:ASP:HB3	5:E:2327:HOH:O	2.04	0.58
1:Q:1651:TYR:OH	1:Q:1785:LEU:O	2.21	0.58
2:G:1014:LEU:HD21	2:G:1668:VAL:HG21	1.86	0.58
2:G:1086:LYS:HB2	5:G:2085:HOH:O	2.03	0.58
2:O:1086:LYS:HB2	5:O:2092:HOH:O	2.03	0.58
2:S:388:GLY:O	2:S:741:ASN:ND2	2.33	0.58
2:S:1014:LEU:HD21	2:S:1668:VAL:HG21	1.86	0.58
2:X:1035:ARG:NH2	2:X:1602:GLN:OE1	2.36	0.58
1:A:1588:ALA:O	1:A:1591:VAL:HG22	2.03	0.58
5:A:2431:HOH:O	2:C:22:PHE:CE2	2.55	0.58
2:X:965:GLN:HB3	5:X:2003:HOH:O	2.02	0.58
1:E:571:SER:OG	1:E:576:ARG:O	2.16	0.58
2:G:1021:THR:HG21	2:G:1397:VAL:CG2	2.34	0.58
2:K:1500:GLU:CG	5:O:2094:HOH:O	2.52	0.58
2:S:841:GLU:OE1	2:S:841:GLU:N	2.37	0.58
2:S:1035:ARG:NH2	2:S:1602:GLN:OE1	2.36	0.58
2:X:1014:LEU:HD21	2:X:1668:VAL:HG21	1.86	0.58
1:A:903:GLU:CA	2:C:1690:ARG:NH2	2.60	0.57
1:E:306:LEU:HG	5:E:2375:HOH:O	2.03	0.57
1:E:1469:THR:HB	5:E:2345:HOH:O	2.03	0.57
1:I:875:ARG:HD2	5:I:2256:HOH:O	2.02	0.57
1:M:1597:ASP:HB3	5:M:2331:HOH:O	2.04	0.57
1:Q:1469:THR:HB	5:Q:2331:HOH:O	2.04	0.57
1:U:146:LEU:O	1:U:255:LYS:N	2.36	0.57
2:C:1561:ILE:HD11	2:C:1646:THR:HG21	1.85	0.57
2:G:1561:ILE:HD11	2:G:1646:THR:HG21	1.85	0.57
2:K:700:ILE:HD11	2:K:728:TYR:HB2	1.86	0.57
1:A:960:GLN:HB2	5:A:2274:HOH:O	2.04	0.57
1:M:306:LEU:HD11	1:M:310:MET:CE	2.33	0.57
1:Q:1824:MET:HA	1:Q:1824:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:641:VAL:HG13	5:U:2216:HOH:O	2.04	0.57
2:C:388:GLY:O	2:C:741:ASN:ND2	2.35	0.57
2:C:996:LYS:HD2	5:C:2164:HOH:O	2.04	0.57
2:S:1588:PRO:HB2	5:S:2130:HOH:O	2.03	0.57
1:A:305:SER:N	1:E:1293:LYS:O	2.24	0.57
1:A:1682:ASP:O	1:A:1686:VAL:HG23	2.04	0.57
1:E:578:PRO:HD2	5:E:2395:HOH:O	2.05	0.57
1:I:1161:ILE:HG23	1:I:1554:VAL:HG23	1.85	0.57
1:M:527:TYR:HA	5:M:2201:HOH:O	2.04	0.57
1:Q:820:GLU:HB2	5:Q:2429:HOH:O	2.04	0.57
1:Q:1127:LEU:CD1	5:Q:2365:HOH:O	2.52	0.57
1:U:960:GLN:CG	5:U:2288:HOH:O	2.50	0.57
2:C:850:PHE:CE2	2:C:923:MET:HE2	2.39	0.57
5:G:2086:HOH:O	2:S:1500:GLU:CG	2.51	0.57
2:S:1212:LEU:HD21	5:S:2025:HOH:O	2.03	0.57
1:I:1504:SER:CB	5:I:2237:HOH:O	2.51	0.57
1:M:577:ALA:CB	5:M:2310:HOH:O	2.47	0.57
1:U:793:MET:HE1	3:U:2101:FMN:C7M	2.34	0.57
1:U:914:VAL:HG23	1:U:934:TYR:CE2	2.39	0.57
2:K:1014:LEU:HD21	2:K:1668:VAL:HG21	1.86	0.57
2:K:1014:LEU:HD21	2:K:1668:VAL:CG2	2.35	0.57
2:K:1567:HIS:CG	2:O:1720:LEU:HD22	2.39	0.57
2:O:632:SER:HA	5:O:2211:HOH:O	2.02	0.57
1:A:1948:LEU:HA	5:A:2261:HOH:O	2.05	0.57
1:M:807:LEU:HD22	1:M:1041:ILE:HD13	1.86	0.57
1:U:578:PRO:HD2	5:U:2393:HOH:O	2.05	0.57
2:K:478:ASN:ND2	4:K:1901:PKZ:C1	2.67	0.57
1:E:1611:THR:CG2	5:E:2256:HOH:O	2.50	0.57
2:K:1500:GLU:HG2	5:O:2094:HOH:O	2.03	0.57
1:A:437:PHE:CD2	1:A:461:ILE:HG13	2.40	0.57
1:A:960:GLN:CG	5:A:2274:HOH:O	2.53	0.57
1:E:478:ALA:CB	5:E:2411:HOH:O	2.41	0.57
1:I:447:THR:HG22	1:I:467:LEU:CD2	2.32	0.57
1:I:1673:VAL:CG1	5:I:2420:HOH:O	2.50	0.57
1:M:305:SER:N	1:Q:1293:LYS:O	2.26	0.57
5:M:2202:HOH:O	2:O:968:VAL:HG21	2.05	0.57
2:G:1332:ASP:OD2	2:G:1590:GLY:N	2.37	0.57
2:K:45:ILE:HD12	2:K:88:ILE:HD13	1.86	0.57
2:S:404:TYR:CE1	5:S:2231:HOH:O	2.52	0.57
2:X:1450:GLN:HA	2:X:1453:LYS:HZ3	1.70	0.57
2:X:1561:ILE:HD11	2:X:1646:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1682:ASP:O	1:U:1686:VAL:HG23	2.05	0.57
1:U:1948:LEU:HA	5:U:2248:HOH:O	2.04	0.57
2:G:380:GLU:OE2	2:X:745:LYS:N	2.38	0.57
2:G:788:ASP:HA	5:G:2235:HOH:O	2.04	0.57
2:X:1014:LEU:HD21	2:X:1668:VAL:CG2	2.35	0.57
1:A:319:GLU:OE2	1:A:377:ASN:ND2	2.37	0.57
1:M:857:ASP:O	1:M:861:ASN:ND2	2.38	0.57
1:E:333:ILE:HD12	1:E:333:ILE:H	1.69	0.57
1:E:857:ASP:O	1:E:861:ASN:ND2	2.38	0.57
1:I:872:ASN:O	1:I:875:ARG:HG2	2.05	0.57
1:M:1159:HIS:O	1:M:1163:THR:OG1	2.22	0.57
1:Q:902:GLN:OE1	1:Q:902:GLN:N	2.37	0.57
1:U:447:THR:HG22	5:U:2232:HOH:O	2.05	0.57
1:U:1884:GLN:HB3	5:X:2095:HOH:O	2.04	0.57
2:G:1035:ARG:NH2	2:G:1602:GLN:OE1	2.37	0.57
2:G:1083:ILE:HD13	5:G:2109:HOH:O	2.05	0.57
2:G:1093:GLU:HB3	5:G:2021:HOH:O	2.05	0.57
2:S:700:ILE:HD11	2:S:728:TYR:HB2	1.86	0.57
1:I:1721:ILE:CD1	5:I:2383:HOH:O	2.53	0.56
1:I:1787:PRO:HB3	5:I:2350:HOH:O	2.04	0.56
1:M:613:SER:HA	1:M:614:PRO:HG2	1.87	0.56
2:K:352:LEU:HD22	2:K:355:GLY:N	2.20	0.56
2:K:989:LYS:HB3	5:K:2153:HOH:O	2.05	0.56
2:K:1208:ASP:OD2	2:K:1210:ILE:HG22	2.05	0.56
2:K:1563:ASN:ND2	2:O:1716:GLN:OE1	2.38	0.56
2:X:53:LEU:HA	2:X:56:MET:HE3	1.87	0.56
2:X:1211:THR:HG22	5:X:2159:HOH:O	1.95	0.56
1:I:1415:THR:CB	5:I:2336:HOH:O	2.52	0.56
1:I:1533:PRO:CG	5:I:2422:HOH:O	2.47	0.56
2:C:1035:ARG:NH2	2:C:1602:GLN:OE1	2.37	0.56
2:O:835:PHE:CE1	5:O:2103:HOH:O	2.55	0.56
2:O:1355:PHE:CE1	5:O:2074:HOH:O	2.52	0.56
2:S:1208:ASP:OD2	2:S:1210:ILE:HG22	2.05	0.56
1:A:1146:ARG:CG	5:A:2245:HOH:O	2.37	0.56
1:I:571:SER:OG	1:I:576:ARG:O	2.18	0.56
1:I:1682:ASP:O	1:I:1686:VAL:HG23	2.06	0.56
1:M:282:ASN:O	1:M:285:THR:OG1	2.21	0.56
1:Q:248:GLY:HA2	1:Q:251:ARG:HH12	1.70	0.56
1:Q:1213:ALA:CB	5:Q:2249:HOH:O	2.54	0.56
1:U:1721:ILE:HD12	5:U:2416:HOH:O	2.03	0.56
2:C:377:TRP:CE3	2:O:377:TRP:CE3	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:745:LYS:N	2:O:380:GLU:OE2	2.38	0.56
2:C:1014:LEU:HD21	2:C:1668:VAL:CG2	2.35	0.56
2:K:1422:LYS:HE2	5:K:2275:HOH:O	2.04	0.56
2:K:1461:TRP:NE1	2:O:1450:GLN:OE1	2.37	0.56
2:S:441:ARG:NH1	2:S:726:ALA:O	2.39	0.56
2:S:478:ASN:ND2	4:S:1901:PKZ:C1	2.67	0.56
1:A:578:PRO:HD2	5:A:2381:HOH:O	2.05	0.56
1:Q:340:ILE:HG22	1:Q:376:PHE:CE2	2.40	0.56
2:C:651:GLY:HA3	5:C:2029:HOH:O	2.05	0.56
2:C:1143:TYR:OH	2:X:1124:ILE:HD11	2.05	0.56
2:C:1417:VAL:HG22	2:X:1288:MET:HE1	1.87	0.56
2:C:1720:LEU:HD23	2:X:1429:ARG:HH21	1.69	0.56
1:M:611:TYR:HA	5:M:2362:HOH:O	2.05	0.56
1:U:136:LEU:HA	5:U:2244:HOH:O	2.05	0.56
2:C:834:GLY:CA	5:C:2086:HOH:O	2.51	0.56
2:C:1431:HIS:ND1	2:X:1721:ASP:OD1	2.38	0.56
2:K:388:GLY:O	2:K:741:ASN:ND2	2.34	0.56
2:O:1083:ILE:HD13	5:O:2113:HOH:O	2.04	0.56
1:U:325:MET:HE1	1:U:414:PHE:HB2	1.88	0.56
2:G:388:GLY:O	2:G:741:ASN:ND2	2.33	0.56
1:E:527:TYR:HA	5:E:2201:HOH:O	2.03	0.56
2:C:1284:ALA:O	2:C:1288:MET:HG3	2.06	0.56
1:I:1469:THR:HB	5:I:2323:HOH:O	2.05	0.56
2:O:1021:THR:HG21	2:O:1397:VAL:CG2	2.36	0.56
2:O:1093:GLU:HB3	5:O:2022:HOH:O	2.05	0.56
2:X:835:PHE:CE1	5:X:2079:HOH:O	2.53	0.56
1:A:571:SER:OG	1:A:576:ARG:O	2.20	0.56
1:M:1469:THR:HB	5:M:2338:HOH:O	2.06	0.56
2:K:757:ASP:O	2:K:765:GLY:N	2.36	0.56
2:X:478:ASN:HD22	4:X:1901:PKZ:C1	2.16	0.56
1:E:1588:ALA:O	1:E:1591:VAL:HG22	2.06	0.56
1:I:584:MET:HE1	1:I:789:GLY:O	2.06	0.56
1:Q:1479:LYS:CB	5:Q:2261:HOH:O	2.52	0.56
2:G:1083:ILE:HD12	2:G:1091:LYS:CE	2.37	0.56
2:G:1315:ILE:HD11	2:G:1403:LEU:HD12	1.88	0.56
2:K:441:ARG:NH1	2:K:726:ALA:O	2.39	0.56
2:K:1212:LEU:HD21	5:K:2020:HOH:O	2.04	0.56
2:O:1014:LEU:HD21	2:O:1668:VAL:HG21	1.88	0.56
1:M:1444:PHE:CA	5:M:2397:HOH:O	2.32	0.55
1:Q:774:GLU:CB	5:Q:2315:HOH:O	2.53	0.55
2:O:693:ALA:HB1	5:O:2176:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1692:MET:HA	2:S:1701:MET:HE1	1.89	0.55
5:E:2202:HOH:O	2:G:968:VAL:HG21	2.05	0.55
1:I:1127:LEU:CD1	5:I:2367:HOH:O	2.54	0.55
1:I:1288:HIS:CD2	5:I:2234:HOH:O	2.58	0.55
1:M:1591:VAL:HG11	5:M:2415:HOH:O	2.06	0.55
2:C:913:ILE:HD13	5:C:2139:HOH:O	2.06	0.55
2:G:1425:LEU:O	2:G:1429:ARG:NH2	2.39	0.55
2:G:1721:ASP:OD1	2:S:1431:HIS:ND1	2.38	0.55
2:O:1234:TYR:OH	2:O:1291:LEU:O	2.21	0.55
1:A:122:TYR:O	1:A:126:VAL:HG23	2.05	0.55
1:A:146:LEU:O	1:A:255:LYS:N	2.35	0.55
1:A:1504:SER:HB2	5:A:2285:HOH:O	2.06	0.55
1:E:611:TYR:HA	5:E:2360:HOH:O	2.05	0.55
1:Q:167:TYR:CD1	1:Q:178:LEU:HD12	2.42	0.55
2:C:344:LEU:HD12	2:S:344:LEU:HD13	1.88	0.55
2:K:348:LEU:HD13	2:S:338:LYS:HZ2	1.71	0.55
2:O:1332:ASP:OD2	2:O:1590:GLY:N	2.38	0.55
2:X:388:GLY:O	2:X:741:ASN:ND2	2.35	0.55
2:X:1677:TYR:O	2:X:1681:VAL:HG23	2.05	0.55
1:E:807:LEU:HD22	1:E:1041:ILE:HD13	1.86	0.55
1:E:988:CYS:CB	5:E:2416:HOH:O	2.49	0.55
1:Q:902:GLN:HB3	2:S:1690:ARG:HH11	1.70	0.55
2:G:1429:ARG:HH21	2:S:1720:LEU:HD23	1.71	0.55
2:X:833:PHE:HB2	5:X:2242:HOH:O	2.06	0.55
2:X:893:VAL:CG2	5:X:2021:HOH:O	2.49	0.55
1:A:544:TRP:HB3	5:A:2298:HOH:O	2.05	0.55
1:Q:166:LEU:HD21	1:Q:234:CYS:CB	2.37	0.55
1:U:883:ASN:O	1:U:1038:ARG:NH2	2.40	0.55
2:C:1211:THR:HG22	5:C:2150:HOH:O	1.97	0.55
2:C:1275:GLN:HB2	2:X:1345:MET:HE1	1.89	0.55
2:G:504:ALA:HB3	2:G:505:LYS:HZ1	1.72	0.55
2:G:835:PHE:CE1	5:G:2098:HOH:O	2.55	0.55
1:E:167:TYR:CD1	1:E:178:LEU:HD12	2.41	0.55
1:I:319:GLU:OE2	1:I:377:ASN:ND2	2.39	0.55
1:Q:305:SER:N	1:U:1293:LYS:O	2.27	0.55
2:C:1006:PRO:HD3	5:C:2182:HOH:O	2.06	0.55
2:K:1567:HIS:CD2	2:O:1720:LEU:HD22	2.42	0.55
2:X:432:ILE:HD13	4:X:1901:PKZ:CEP	2.37	0.55
1:M:902:GLN:N	1:M:902:GLN:OE1	2.39	0.55
2:O:478:ASN:ND2	4:O:1901:PKZ:C1	2.70	0.55
2:O:1619:ASP:OD1	2:O:1621:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1716:GLN:HB3	2:O:1717:PRO:HG3	1.88	0.55
1:A:793:MET:HE2	1:A:1043:HIS:CD2	2.42	0.55
1:A:807:LEU:HD22	1:A:1041:ILE:HD13	1.88	0.55
1:M:126:VAL:HG11	5:M:2313:HOH:O	2.07	0.55
1:M:578:PRO:HD2	5:M:2398:HOH:O	2.05	0.55
2:K:1130:LEU:HD22	2:O:1130:LEU:HD22	1.88	0.55
2:K:1720:LEU:HD22	2:O:1567:HIS:CG	2.42	0.55
1:E:319:GLU:OE2	1:E:377:ASN:ND2	2.40	0.55
1:E:546:PRO:HD2	5:E:2221:HOH:O	2.07	0.55
1:I:360:GLY:CA	5:I:2365:HOH:O	2.53	0.55
1:Q:584:MET:HE1	1:Q:789:GLY:O	2.06	0.55
1:U:960:GLN:HB2	5:U:2288:HOH:O	2.06	0.55
2:G:1422:LYS:CE	5:S:2242:HOH:O	2.55	0.55
2:K:841:GLU:OE1	2:K:841:GLU:N	2.37	0.55
1:A:1175:LYS:CA	5:A:2202:HOH:O	2.50	0.55
1:A:1175:LYS:N	5:A:2202:HOH:O	2.40	0.55
1:U:1141:PHE:CE2	1:U:1158:LEU:HD21	2.42	0.55
2:X:1248:SER:HB3	2:X:1279:ILE:HG23	1.89	0.55
1:E:577:ALA:CB	5:E:2317:HOH:O	2.48	0.54
1:E:1650:THR:CG2	2:G:41:THR:HG21	2.37	0.54
1:I:466:LYS:NZ	1:I:470:GLU:CD	2.65	0.54
1:I:614:PRO:HD3	1:I:648:TRP:CE3	2.41	0.54
1:I:1541:ILE:HD11	5:I:2346:HOH:O	2.02	0.54
1:U:339:PHE:HB3	1:U:376:PHE:HE1	1.72	0.54
1:U:571:SER:OG	1:U:576:ARG:O	2.21	0.54
2:C:1014:LEU:HD21	2:C:1668:VAL:HG21	1.89	0.54
5:C:2037:HOH:O	2:X:1500:GLU:HG2	2.07	0.54
2:S:1197:TYR:HA	5:S:2042:HOH:O	2.07	0.54
2:X:1537:ILE:HD11	2:X:1565:MET:HE1	1.89	0.54
2:X:1619:ASP:OD1	2:X:1621:LEU:CD1	2.55	0.54
1:A:1651:TYR:OH	1:A:1785:LEU:O	2.25	0.54
1:I:1651:TYR:OH	1:I:1785:LEU:O	2.26	0.54
1:Q:319:GLU:OE2	1:Q:377:ASN:ND2	2.41	0.54
1:Q:1721:ILE:CD1	5:Q:2389:HOH:O	2.55	0.54
2:C:441:ARG:NH1	2:C:726:ALA:O	2.40	0.54
2:G:693:ALA:HB1	5:G:2164:HOH:O	2.06	0.54
2:G:1716:GLN:NE2	5:G:2003:HOH:O	2.40	0.54
2:O:1315:ILE:HD11	2:O:1403:LEU:HD12	1.88	0.54
1:U:463:ARG:NH2	1:U:467:LEU:HD11	2.22	0.54
2:C:432:ILE:HD13	4:C:1901:PKZ:CEP	2.37	0.54
2:C:1619:ASP:OD1	2:C:1621:LEU:CD1	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1692:MET:HA	2:G:1701:MET:HE1	1.89	0.54
1:A:282:ASN:O	1:A:285:THR:OG1	2.23	0.54
1:Q:589:VAL:O	1:Q:611:TYR:OH	2.22	0.54
1:Q:1682:ASP:O	1:Q:1686:VAL:HG23	2.06	0.54
2:C:377:TRP:CE3	2:O:377:TRP:CZ3	2.95	0.54
2:C:1334:PHE:HA	5:C:2027:HOH:O	2.07	0.54
2:C:1684:ARG:O	2:C:1688:THR:OG1	2.20	0.54
2:G:478:ASN:ND2	4:G:1901:PKZ:C1	2.70	0.54
2:G:1570:ARG:NE	2:G:1574:ASN:O	2.38	0.54
1:U:1541:ILE:CD1	5:U:2279:HOH:O	2.55	0.54
5:K:2251:HOH:O	2:X:341:LEU:CD2	2.56	0.54
2:O:1083:ILE:HD12	2:O:1091:LYS:CE	2.36	0.54
2:X:1179:ARG:CG	5:X:2107:HOH:O	2.37	0.54
1:E:902:GLN:N	1:E:902:GLN:OE1	2.40	0.54
1:I:1377:GLU:OE2	1:I:1395:GLN:NE2	2.36	0.54
1:M:167:TYR:CD1	1:M:178:LEU:HD12	2.43	0.54
1:M:306:LEU:HD21	1:M:310:MET:HE3	1.89	0.54
1:Q:588:THR:O	1:Q:588:THR:HG22	2.08	0.54
2:K:344:LEU:HD11	2:X:340:GLN:CB	2.37	0.54
2:X:834:GLY:CA	5:X:2079:HOH:O	2.51	0.54
1:A:883:ASN:O	1:A:1038:ARG:NH2	2.40	0.54
1:A:1278:ILE:HG23	1:A:1283:ILE:HD11	1.88	0.54
1:A:1451:CYS:HB2	5:A:2210:HOH:O	2.07	0.54
1:I:340:ILE:HG22	1:I:376:PHE:CE2	2.42	0.54
1:I:834:ARG:CG	5:I:2396:HOH:O	2.55	0.54
1:U:166:LEU:HD21	1:U:234:CYS:CB	2.38	0.54
1:U:319:GLU:OE2	1:U:377:ASN:ND2	2.40	0.54
2:K:1248:SER:HB3	2:K:1279:ILE:HG23	1.90	0.54
2:O:505:LYS:HE2	2:O:505:LYS:N	2.23	0.54
1:E:588:THR:O	1:E:588:THR:HG22	2.08	0.54
1:M:319:GLU:OE2	1:M:377:ASN:ND2	2.40	0.54
5:Q:2253:HOH:O	2:S:968:VAL:CG2	2.37	0.54
2:O:1692:MET:HA	2:O:1701:MET:HE1	1.89	0.54
1:E:164:ARG:NH1	1:E:205:TRP:O	2.41	0.54
1:E:761:ASP:N	1:E:761:ASP:OD1	2.41	0.54
1:I:588:THR:O	1:I:588:THR:HG22	2.08	0.54
1:Q:872:ASN:HA	1:Q:875:ARG:HG2	1.90	0.54
1:U:588:THR:HG22	1:U:588:THR:O	2.08	0.54
5:U:2300:HOH:O	2:X:26:VAL:CG2	2.33	0.54
2:G:1735:PHE:HZ	5:G:2212:HOH:O	1.91	0.54
2:O:693:ALA:CB	5:O:2176:HOH:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:989:LYS:HB3	5:S:2156:HOH:O	2.07	0.54
2:S:1696:ILE:HG21	5:S:2084:HOH:O	2.07	0.54
1:E:944:ARG:NH1	2:G:986:ALA:O	2.39	0.54
1:E:985:GLU:HA	5:E:2416:HOH:O	2.08	0.54
1:M:166:LEU:HD21	1:M:234:CYS:CB	2.38	0.54
1:U:139:HIS:N	5:U:2205:HOH:O	2.42	0.54
2:G:1033:ARG:NH2	2:G:1051:GLU:OE1	2.41	0.54
2:S:757:ASP:O	2:S:765:GLY:N	2.37	0.54
2:X:1006:PRO:HD3	5:X:2170:HOH:O	2.08	0.54
1:A:588:THR:O	1:A:588:THR:HG22	2.08	0.53
1:A:1141:PHE:CE2	1:A:1158:LEU:HD21	2.43	0.53
1:M:146:LEU:O	1:M:255:LYS:N	2.37	0.53
1:M:178:LEU:HD21	1:M:234:CYS:SG	2.48	0.53
1:M:761:ASP:OD1	1:M:761:ASP:N	2.41	0.53
1:M:1788:SER:O	1:M:1997:LYS:NZ	2.41	0.53
1:Q:2001:ASN:OD1	2:S:26:VAL:HG21	2.07	0.53
2:G:505:LYS:HE2	2:G:505:LYS:N	2.22	0.53
2:O:1735:PHE:HZ	5:O:2216:HOH:O	1.91	0.53
2:X:1278:PHE:O	2:X:1281:THR:HG22	2.08	0.53
1:E:166:LEU:HD21	1:E:234:CYS:CB	2.38	0.53
1:M:588:THR:O	1:M:588:THR:HG22	2.08	0.53
2:G:693:ALA:CB	5:G:2164:HOH:O	2.56	0.53
2:X:996:LYS:HD2	5:X:2169:HOH:O	2.07	0.53
1:A:1779:ASP:OD2	2:C:89:TYR:OH	2.13	0.53
1:E:306:LEU:HD12	1:E:311:LEU:HD23	1.89	0.53
1:E:1788:SER:O	1:E:1997:LYS:NZ	2.41	0.53
1:M:944:ARG:NH1	2:O:986:ALA:O	2.39	0.53
1:Q:146:LEU:O	1:Q:255:LYS:N	2.38	0.53
2:C:340:GLN:NE2	5:C:2003:HOH:O	2.41	0.53
2:C:346:ARG:HG3	2:O:342:GLU:OE1	2.08	0.53
2:C:851:ASN:ND2	2:O:830:HIS:O	2.39	0.53
2:O:1248:SER:HB3	2:O:1279:ILE:HG23	1.90	0.53
2:O:1472:GLU:C	5:O:2115:HOH:O	2.52	0.53
1:A:1031:VAL:CA	5:A:2262:HOH:O	2.53	0.53
1:I:426:ILE:O	1:I:430:VAL:HG23	2.08	0.53
1:M:626:SER:HA	5:M:2417:HOH:O	2.09	0.53
1:U:325:MET:SD	1:U:410:ILE:HD13	2.49	0.53
2:S:1212:LEU:HG	5:S:2025:HOH:O	2.08	0.53
1:A:325:MET:SD	1:A:410:ILE:HD13	2.49	0.53
1:A:614:PRO:HD3	1:A:648:TRP:CD2	2.43	0.53
1:A:1163:THR:HB	5:A:2201:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:902:GLN:OE1	1:I:902:GLN:N	2.41	0.53
1:U:601:GLY:HA3	5:U:2247:HOH:O	2.09	0.53
2:C:1275:GLN:HE21	2:X:1417:VAL:CB	2.22	0.53
2:G:833:PHE:HB2	5:G:2246:HOH:O	2.08	0.53
2:S:1248:SER:HB3	2:S:1279:ILE:HG23	1.90	0.53
2:S:1278:PHE:O	2:S:1281:THR:HG22	2.08	0.53
2:X:913:ILE:HD13	5:X:2140:HOH:O	2.07	0.53
2:X:1050:ILE:HG13	2:X:1088:ILE:HG21	1.89	0.53
1:A:1683:ARG:HD3	1:A:1683:ARG:N	2.23	0.53
1:Q:251:ARG:HB3	1:Q:251:ARG:NH1	2.23	0.53
2:C:1248:SER:HB3	2:C:1279:ILE:HG23	1.91	0.53
2:S:1680:LYS:HD2	5:S:2002:HOH:O	2.07	0.53
2:X:841:GLU:OE1	2:X:841:GLU:N	2.40	0.53
1:A:1553:ARG:NH1	5:A:2201:HOH:O	2.40	0.53
1:I:1824:MET:HA	1:I:1824:MET:HE3	1.89	0.53
2:X:441:ARG:NH1	2:X:726:ALA:O	2.42	0.53
1:A:80:LYS:HD3	1:A:80:LYS:N	2.23	0.53
1:I:139:HIS:N	5:I:2203:HOH:O	2.42	0.53
2:C:36:LEU:O	2:C:76:ARG:NH2	2.41	0.53
2:C:693:ALA:HB1	5:C:2111:HOH:O	2.09	0.53
2:C:1288:MET:CE	2:X:1417:VAL:HG22	2.38	0.53
2:G:1021:THR:CG2	2:G:1397:VAL:CG2	2.87	0.53
2:K:1212:LEU:HG	5:K:2020:HOH:O	2.09	0.53
2:K:1560:THR:CG2	5:K:2205:HOH:O	2.56	0.53
2:O:1570:ARG:NE	2:O:1574:ASN:O	2.38	0.53
2:X:1137:LYS:HG2	5:X:2210:HOH:O	2.08	0.53
1:A:555:THR:CG2	5:A:2212:HOH:O	2.56	0.53
1:U:1361:LYS:CD	5:U:2224:HOH:O	2.44	0.53
2:G:830:HIS:O	2:X:851:ASN:ND2	2.39	0.53
2:G:1213:TYR:CD2	5:G:2244:HOH:O	2.35	0.53
2:K:1197:TYR:HA	5:K:2040:HOH:O	2.09	0.53
2:X:1332:ASP:OD2	2:X:1590:GLY:N	2.42	0.53
2:X:1334:PHE:HA	5:X:2031:HOH:O	2.09	0.53
1:E:146:LEU:O	1:E:255:LYS:N	2.37	0.53
1:E:555:THR:CG2	5:E:2264:HOH:O	2.57	0.53
1:U:264:LEU:HD11	1:U:453:PHE:CE2	2.44	0.53
2:G:36:LEU:O	2:G:76:ARG:NH2	2.41	0.53
2:G:1719:TYR:HB3	2:S:1429:ARG:CZ	2.39	0.53
2:K:1422:LYS:HE3	5:K:2275:HOH:O	2.05	0.53
1:A:1595:LYS:HE2	1:A:1597:ASP:OD2	2.08	0.52
1:E:850:MET:HA	1:E:850:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1998:TYR:O	1:E:2007:PHE:N	2.40	0.52
1:I:614:PRO:HD3	1:I:648:TRP:CD2	2.44	0.52
1:M:546:PRO:HD2	5:M:2215:HOH:O	2.08	0.52
1:Q:571:SER:OG	1:Q:576:ARG:O	2.25	0.52
1:Q:614:PRO:HD3	1:Q:648:TRP:CE3	2.45	0.52
1:U:807:LEU:HD22	1:U:1041:ILE:HD13	1.89	0.52
1:U:906:TYR:CD2	1:U:941:VAL:HG22	2.44	0.52
2:K:377:TRP:CE3	2:S:377:TRP:CE3	2.97	0.52
2:K:1472:GLU:C	5:K:2134:HOH:O	2.53	0.52
2:O:1498:TYR:HD2	5:O:2029:HOH:O	1.91	0.52
2:S:474:GLN:CG	5:S:2052:HOH:O	2.57	0.52
1:A:256:TRP:CH2	5:A:2209:HOH:O	2.56	0.52
1:Q:1788:SER:O	1:Q:1997:LYS:NZ	2.42	0.52
1:U:615:VAL:CG2	5:U:2345:HOH:O	2.50	0.52
2:G:834:GLY:CA	5:G:2098:HOH:O	2.55	0.52
2:G:1248:SER:HB3	2:G:1279:ILE:HG23	1.91	0.52
2:K:1444:ILE:HG13	5:K:2152:HOH:O	2.09	0.52
2:O:833:PHE:HB2	5:O:2244:HOH:O	2.08	0.52
1:A:641:VAL:HG13	5:A:2226:HOH:O	2.09	0.52
1:A:1305:THR:N	5:A:2205:HOH:O	2.41	0.52
1:I:463:ARG:HE	1:I:467:LEU:HD11	1.75	0.52
2:C:1132:PRO:HD3	2:C:1165:ARG:HG2	1.92	0.52
2:C:1557:GLU:HB2	5:C:2105:HOH:O	2.09	0.52
2:G:1619:ASP:OD1	2:G:1621:LEU:HD12	2.10	0.52
2:S:530:GLN:OE1	2:S:530:GLN:HA	2.10	0.52
1:A:264:LEU:HD11	1:A:453:PHE:CE2	2.44	0.52
1:E:883:ASN:O	1:E:1038:ARG:NH2	2.43	0.52
1:E:1651:TYR:OH	1:E:1785:LEU:O	2.27	0.52
1:I:282:ASN:O	1:I:285:THR:OG1	2.26	0.52
1:Q:139:HIS:N	5:Q:2203:HOH:O	2.42	0.52
1:Q:1249:PHE:HZ	1:Q:1548:PRO:HG2	1.74	0.52
1:U:282:ASN:O	1:U:285:THR:OG1	2.24	0.52
1:U:944:ARG:NH1	2:X:986:ALA:O	2.41	0.52
2:G:851:ASN:ND2	2:X:830:HIS:O	2.40	0.52
2:K:1210:ILE:O	2:K:1214:VAL:HG23	2.10	0.52
2:O:36:LEU:O	2:O:76:ARG:NH2	2.42	0.52
2:O:504:ALA:HB3	2:O:505:LYS:HZ1	1.72	0.52
2:O:834:GLY:CA	5:O:2103:HOH:O	2.55	0.52
1:A:306:LEU:HD11	1:A:310:MET:CE	2.39	0.52
1:A:1788:SER:O	1:A:1997:LYS:NZ	2.42	0.52
1:E:932:ASN:ND2	5:E:2203:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:LEU:O	1:I:255:LYS:N	2.38	0.52
1:I:466:LYS:NZ	1:I:470:GLU:OE2	2.41	0.52
2:C:446:LEU:O	2:C:450:MET:HG3	2.10	0.52
2:C:1570:ARG:NE	2:C:1574:ASN:O	2.38	0.52
2:K:29:ILE:HD11	5:K:2235:HOH:O	2.08	0.52
2:K:1522:ARG:NH1	2:O:1746:TYR:OH	2.42	0.52
1:A:325:MET:HE1	1:A:414:PHE:HB2	1.91	0.52
1:Q:139:HIS:CB	5:Q:2203:HOH:O	2.58	0.52
1:Q:340:ILE:HG22	1:Q:376:PHE:CZ	2.44	0.52
1:Q:906:TYR:CD2	1:Q:941:VAL:HG22	2.44	0.52
2:G:1144:LYS:HB2	2:G:1153:ILE:HD13	1.91	0.52
2:G:1210:ILE:HG13	5:G:2244:HOH:O	2.09	0.52
2:G:1291:LEU:HG	5:G:2238:HOH:O	2.10	0.52
2:G:1498:TYR:HD2	5:G:2027:HOH:O	1.91	0.52
2:K:530:GLN:OE1	2:K:530:GLN:HA	2.10	0.52
5:K:2230:HOH:O	2:O:1422:LYS:CE	2.57	0.52
2:S:1006:PRO:HD3	5:S:2115:HOH:O	2.09	0.52
2:S:1210:ILE:O	2:S:1214:VAL:HG23	2.09	0.52
2:X:708:VAL:HG23	5:X:2002:HOH:O	2.09	0.52
1:I:139:HIS:CB	5:I:2203:HOH:O	2.57	0.52
1:U:586:PRO:HD2	3:U:2101:FMN:H6	1.92	0.52
1:U:1504:SER:CB	5:U:2270:HOH:O	2.56	0.52
2:C:758:GLU:HB3	5:C:2116:HOH:O	2.09	0.52
2:G:656:LYS:HE2	5:G:2133:HOH:O	2.09	0.52
2:G:1472:GLU:C	5:G:2112:HOH:O	2.52	0.52
2:O:1021:THR:CG2	2:O:1397:VAL:CG2	2.87	0.52
1:A:437:PHE:CE2	1:A:461:ILE:HD11	2.44	0.52
1:A:603:HIS:HA	5:A:2341:HOH:O	2.09	0.52
1:A:814:VAL:HG21	1:A:827:THR:HB	1.91	0.52
1:M:733:PHE:HZ	5:M:2410:HOH:O	1.92	0.52
1:Q:1870:THR:HG22	5:Q:2439:HOH:O	2.10	0.52
2:K:522:GLU:OE2	2:K:522:GLU:N	2.42	0.52
2:K:855:SER:O	2:S:937:LYS:NZ	2.39	0.52
2:K:1006:PRO:HD3	5:K:2106:HOH:O	2.09	0.52
1:I:906:TYR:CD2	1:I:941:VAL:HG22	2.44	0.52
1:M:164:ARG:NH1	1:M:205:TRP:O	2.43	0.52
1:M:1651:TYR:OH	1:M:1785:LEU:O	2.27	0.52
1:Q:396:PHE:N	1:Q:820:GLU:OE1	2.42	0.52
1:Q:614:PRO:HD3	1:Q:648:TRP:CD2	2.45	0.52
2:K:36:LEU:O	2:K:76:ARG:NH2	2.43	0.52
2:O:1033:ARG:NH2	2:O:1051:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1716:GLN:NE2	5:O:2010:HOH:O	2.43	0.52
2:X:983:GLU:HB2	5:X:2004:HOH:O	1.79	0.52
1:A:166:LEU:HD21	1:A:234:CYS:CB	2.40	0.52
1:A:761:ASP:OD1	1:A:761:ASP:N	2.42	0.52
1:A:1650:THR:CG2	2:C:44:ILE:HD13	2.40	0.52
1:I:1870:THR:HG22	5:I:2434:HOH:O	2.10	0.52
1:M:1141:PHE:CE2	1:M:1158:LEU:HD21	2.45	0.52
1:Q:883:ASN:O	1:Q:1038:ARG:NH2	2.43	0.52
1:U:725:GLY:HA3	5:U:2363:HOH:O	2.09	0.52
1:U:1788:SER:O	1:U:1997:LYS:NZ	2.43	0.52
5:C:2169:HOH:O	2:O:376:LEU:CD1	2.47	0.52
2:K:651:GLY:HA3	5:K:2053:HOH:O	2.09	0.52
2:K:1144:LYS:HB2	2:K:1153:ILE:HD13	1.92	0.52
2:K:1429:ARG:HD2	2:O:1720:LEU:HA	1.91	0.52
2:S:1564:MET:HG3	2:S:1565:MET:HE2	1.92	0.52
2:X:841:GLU:O	2:X:845:SER:OG	2.21	0.52
1:M:1799:GLU:OE2	1:M:1998:TYR:OH	2.28	0.51
1:Q:956:GLN:HG3	2:S:979:LYS:CE	2.39	0.51
2:C:830:HIS:O	2:O:851:ASN:ND2	2.40	0.51
2:K:29:ILE:CD1	5:K:2235:HOH:O	2.58	0.51
1:E:340:ILE:HD11	1:E:366:LEU:CD2	2.39	0.51
1:E:586:PRO:HD2	3:E:2101:FMN:H6	1.92	0.51
1:M:1611:THR:CG2	5:M:2259:HOH:O	2.50	0.51
1:M:1998:TYR:O	1:M:2007:PHE:N	2.40	0.51
2:C:1278:PHE:O	2:C:1281:THR:HG22	2.10	0.51
5:C:2169:HOH:O	2:O:376:LEU:CD2	2.52	0.51
2:G:771:ILE:CG2	5:G:2184:HOH:O	2.53	0.51
2:K:1692:MET:HA	2:K:1701:MET:HE1	1.92	0.51
2:O:1129:ASP:OD1	2:S:347:TYR:OH	2.25	0.51
2:S:522:GLU:N	2:S:522:GLU:OE2	2.42	0.51
2:X:1570:ARG:NE	2:X:1574:ASN:O	2.39	0.51
1:I:1788:SER:O	1:I:1997:LYS:NZ	2.43	0.51
1:M:340:ILE:HD11	1:M:366:LEU:CD2	2.40	0.51
1:M:555:THR:CG2	5:M:2257:HOH:O	2.57	0.51
1:M:1214:ASP:O	1:M:1215:THR:HG22	2.10	0.51
1:U:494:VAL:O	1:U:499:VAL:HG21	2.10	0.51
2:C:983:GLU:CG	5:C:2014:HOH:O	2.09	0.51
2:K:1431:HIS:ND1	2:O:1721:ASP:OD1	2.37	0.51
2:X:662:TYR:OH	2:X:904:ASN:O	2.27	0.51
1:A:59:TYR:O	1:A:63:ILE:HG22	2.11	0.51
1:E:906:TYR:CD2	1:E:941:VAL:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1417:VAL:HG21	1:E:1503:LEU:HB3	1.92	0.51
1:I:964:PRO:HD2	5:I:2338:HOH:O	2.09	0.51
1:I:1141:PHE:CE2	1:I:1158:LEU:HD21	2.46	0.51
1:Q:703:VAL:HG11	1:Q:717:LEU:CD1	2.41	0.51
1:Q:996:ALA:HB3	5:Q:2440:HOH:O	2.09	0.51
1:Q:1144:THR:O	1:Q:1156:ASN:ND2	2.42	0.51
1:U:925:TRP:HH2	1:U:934:TYR:CD2	2.28	0.51
2:C:1332:ASP:OD2	2:C:1590:GLY:N	2.43	0.51
2:G:1450:GLN:OE1	2:S:1461:TRP:NE1	2.37	0.51
2:K:474:GLN:CG	5:K:2052:HOH:O	2.57	0.51
2:K:1223:LEU:HD22	2:K:1691:TYR:HE2	1.76	0.51
2:S:29:ILE:HD11	5:S:2240:HOH:O	2.10	0.51
2:X:1236:TYR:HA	5:X:2036:HOH:O	2.10	0.51
1:A:123:TYR:OH	1:A:242:VAL:HG22	2.11	0.51
1:A:1293:LYS:O	1:I:305:SER:N	2.27	0.51
1:E:1727:THR:OG1	1:E:1728:ILE:N	2.42	0.51
1:M:1504:SER:HB2	5:M:2255:HOH:O	2.10	0.51
1:Q:481:HIS:CE1	1:Q:505:LYS:CD	2.93	0.51
1:Q:814:VAL:HG21	1:Q:827:THR:HB	1.93	0.51
1:Q:964:PRO:HD2	5:Q:2342:HOH:O	2.11	0.51
2:C:407:TRP:O	2:C:411:ASP:OD1	2.28	0.51
2:K:687:GLY:O	2:K:690:SER:OG	2.28	0.51
2:K:1278:PHE:O	2:K:1281:THR:HG22	2.10	0.51
2:S:36:LEU:O	2:S:76:ARG:NH2	2.43	0.51
2:S:759:PRO:HD2	5:S:2260:HOH:O	2.06	0.51
2:S:1144:LYS:HB2	2:S:1153:ILE:HD13	1.92	0.51
2:X:36:LEU:O	2:X:76:ARG:NH2	2.42	0.51
2:X:1147:HIS:HB2	2:X:1151:CYS:SG	2.50	0.51
1:A:906:TYR:CD2	1:A:941:VAL:HG22	2.45	0.51
1:I:703:VAL:HG11	1:I:717:LEU:CD1	2.40	0.51
1:I:996:ALA:HB3	5:I:2436:HOH:O	2.11	0.51
1:I:1090:TYR:CE1	1:I:1140:ALA:HB2	2.46	0.51
1:M:1417:VAL:HG21	1:M:1503:LEU:HB3	1.92	0.51
1:U:463:ARG:NE	1:U:467:LEU:HD11	2.24	0.51
2:C:437:GLN:HG3	5:C:2002:HOH:O	2.11	0.51
2:C:1147:HIS:HB2	2:C:1151:CYS:SG	2.50	0.51
2:G:1333:ASP:OD1	2:G:1379:GLN:NE2	2.44	0.51
2:X:983:GLU:N	5:X:2004:HOH:O	2.41	0.51
1:A:1144:THR:O	1:A:1156:ASN:ND2	2.44	0.51
1:E:282:ASN:O	1:E:285:THR:OG1	2.25	0.51
1:E:1504:SER:HB2	5:E:2253:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:LEU:HD21	1:I:234:CYS:HB3	1.92	0.51
1:Q:466:LYS:NZ	1:Q:470:GLU:OE1	2.34	0.51
1:U:839:GLU:CB	5:U:2421:HOH:O	2.59	0.51
2:G:1716:GLN:N	2:G:1717:PRO:HG3	2.13	0.51
2:K:1426:THR:HA	2:K:1429:ARG:NE	2.25	0.51
2:S:746:GLN:NE2	5:S:2013:HOH:O	2.44	0.51
1:A:223:VAL:O	1:A:227:VAL:HG23	2.11	0.51
1:M:264:LEU:HD11	1:M:453:PHE:CE2	2.45	0.51
1:M:1727:THR:OG1	1:M:1728:ILE:N	2.42	0.51
2:C:467:LEU:HA	2:C:470:ARG:HE	1.74	0.51
2:G:1067:GLN:CB	5:G:2257:HOH:O	2.58	0.51
2:G:1720:LEU:HA	2:S:1429:ARG:HD3	1.91	0.51
2:K:939:PHE:CE1	2:K:943:LEU:HD22	2.46	0.51
2:K:1720:LEU:HA	2:O:1429:ARG:HD2	1.91	0.51
2:O:651:GLY:C	5:O:2104:HOH:O	2.54	0.51
2:O:712:ARG:HH11	2:O:712:ARG:HG3	1.75	0.51
2:O:1333:ASP:OD1	2:O:1379:GLN:NE2	2.44	0.51
1:A:601:GLY:HA3	5:A:2243:HOH:O	2.11	0.51
1:A:902:GLN:OE1	1:A:902:GLN:N	2.44	0.51
1:M:223:VAL:O	1:M:227:VAL:HG23	2.11	0.51
1:M:1523:SER:O	1:M:1528:LEU:HD22	2.11	0.51
1:Q:306:LEU:HD23	5:Q:2446:HOH:O	2.11	0.51
1:Q:1278:ILE:CG2	1:Q:1283:ILE:HD11	2.41	0.51
2:C:478:ASN:HD22	4:C:1901:PKZ:C1	2.16	0.51
2:C:1281:THR:CA	5:C:2114:HOH:O	2.59	0.51
2:C:1551:VAL:HG23	5:C:2245:HOH:O	2.11	0.51
5:C:2037:HOH:O	2:X:1500:GLU:CG	2.59	0.51
2:O:1426:THR:HA	2:O:1429:ARG:NE	2.24	0.51
2:S:1426:THR:HA	2:S:1429:ARG:NE	2.26	0.51
1:E:626:SER:HA	5:E:2420:HOH:O	2.09	0.51
1:I:883:ASN:O	1:I:1038:ARG:NH2	2.44	0.51
1:M:883:ASN:O	1:M:1038:ARG:NH2	2.43	0.51
1:Q:304:THR:HG23	1:U:1300:ARG:NH2	2.26	0.51
1:Q:1141:PHE:CZ	1:Q:1158:LEU:HD11	2.46	0.51
1:U:1779:ASP:OD2	2:X:89:TYR:OH	2.19	0.51
2:G:1684:ARG:O	2:G:1688:THR:OG1	2.27	0.51
2:S:1560:THR:CG2	5:S:2210:HOH:O	2.57	0.51
1:A:1141:PHE:CE2	1:A:1195:ILE:HG21	2.46	0.50
1:A:1430:LEU:HD21	1:A:1502:TYR:OH	2.11	0.50
1:A:1541:ILE:CD1	5:A:2253:HOH:O	2.59	0.50
1:I:339:PHE:HB3	1:I:376:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1144:THR:O	1:I:1156:ASN:ND2	2.44	0.50
1:Q:265:VAL:O	1:Q:269:THR:OG1	2.29	0.50
2:C:1322:LYS:NZ	2:X:1312:ASP:OD1	2.44	0.50
2:K:657:LYS:H	2:K:657:LYS:CE	2.24	0.50
2:O:1696:ILE:HG21	5:O:2037:HOH:O	2.10	0.50
2:S:45:ILE:HD12	2:S:88:ILE:HD13	1.91	0.50
2:X:1017:VAL:HG11	2:X:1665:LEU:CD1	2.41	0.50
1:A:589:VAL:O	1:A:611:TYR:OH	2.23	0.50
1:E:1141:PHE:CE2	1:E:1158:LEU:HD21	2.46	0.50
1:M:1174:LYS:C	5:M:2245:HOH:O	2.55	0.50
1:Q:1523:SER:O	1:Q:1528:LEU:HD22	2.11	0.50
2:C:339:GLN:CA	2:O:349:GLN:HE22	2.24	0.50
2:C:502:VAL:O	2:C:954:ARG:NH2	2.44	0.50
2:C:686:ALA:HB3	5:C:2006:HOH:O	2.10	0.50
2:C:1716:GLN:N	2:C:1717:PRO:HG3	2.26	0.50
2:G:376:LEU:CD1	5:G:2188:HOH:O	2.47	0.50
2:G:651:GLY:C	5:G:2099:HOH:O	2.54	0.50
2:G:824:LEU:HG	5:G:2194:HOH:O	2.11	0.50
2:G:1006:PRO:HD3	5:G:2122:HOH:O	2.11	0.50
2:O:1684:ARG:O	2:O:1688:THR:OG1	2.26	0.50
1:A:982:LEU:HD13	2:C:1690:ARG:HE	1.74	0.50
1:E:1174:LYS:C	5:E:2244:HOH:O	2.54	0.50
1:I:544:TRP:HB3	5:I:2275:HOH:O	2.12	0.50
1:M:586:PRO:HD2	3:M:2101:FMN:H6	1.92	0.50
1:M:990:TYR:HD1	5:O:2279:HOH:O	1.95	0.50
1:Q:544:TRP:HB3	5:Q:2283:HOH:O	2.11	0.50
1:Q:1090:TYR:CE1	1:Q:1140:ALA:HB2	2.46	0.50
1:U:603:HIS:HA	5:U:2331:HOH:O	2.10	0.50
2:C:708:VAL:HG23	5:C:2006:HOH:O	2.10	0.50
2:S:352:LEU:HD22	2:S:355:GLY:N	2.27	0.50
2:S:691:ILE:HG22	2:S:695:ILE:HD12	1.94	0.50
2:X:996:LYS:HE3	2:X:1000:GLU:OE2	2.11	0.50
1:A:265:VAL:O	1:A:269:THR:OG1	2.27	0.50
1:E:1504:SER:CB	5:E:2253:HOH:O	2.60	0.50
1:M:1130:LEU:CD2	1:M:1162:LEU:HD12	2.41	0.50
1:Q:264:LEU:HD11	1:Q:453:PHE:CE2	2.46	0.50
1:Q:370:PRO:HG2	5:Q:2446:HOH:O	2.12	0.50
1:U:1163:THR:HB	5:U:2213:HOH:O	2.10	0.50
2:C:475:LEU:HD22	4:C:1901:PKZ:C7	2.41	0.50
2:K:953:ILE:CG2	5:K:2250:HOH:O	2.40	0.50
2:S:1472:GLU:C	5:S:2138:HOH:O	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PHE:N	1:A:820:GLU:OE2	2.44	0.50
1:A:1504:SER:CB	5:A:2285:HOH:O	2.59	0.50
1:I:306:LEU:HD23	5:I:2442:HOH:O	2.12	0.50
1:I:814:VAL:HG21	1:I:827:THR:HB	1.92	0.50
1:I:1845:VAL:HG12	1:I:1954:VAL:HG12	1.93	0.50
1:Q:546:PRO:HD2	5:Q:2207:HOH:O	2.11	0.50
1:U:902:GLN:N	1:U:902:GLN:OE1	2.44	0.50
2:C:342:GLU:OE2	2:O:351:ARG:CZ	2.58	0.50
2:C:1144:LYS:HB2	2:C:1153:ILE:HD13	1.93	0.50
2:C:1210:ILE:O	2:C:1214:VAL:HG23	2.11	0.50
2:C:1499:ARG:NH1	5:C:2013:HOH:O	2.44	0.50
2:G:1239:VAL:HG13	5:G:2212:HOH:O	2.11	0.50
2:X:1089:LYS:CB	5:X:2077:HOH:O	2.41	0.50
1:A:722:GLY:CA	5:A:2305:HOH:O	2.40	0.50
1:I:1141:PHE:CZ	1:I:1158:LEU:HD11	2.46	0.50
1:M:1504:SER:CB	5:M:2255:HOH:O	2.60	0.50
1:U:1759:LEU:O	1:U:1765:THR:OG1	2.29	0.50
2:C:1197:TYR:HE1	5:C:2147:HOH:O	1.94	0.50
2:C:1461:TRP:NE1	2:X:1450:GLN:OE1	2.38	0.50
2:G:662:TYR:HA	2:G:913:ILE:HD11	1.94	0.50
2:G:1369:THR:CG2	5:G:2234:HOH:O	2.57	0.50
2:K:952:ASP:OD1	2:K:953:ILE:N	2.45	0.50
2:O:1006:PRO:HD3	5:O:2127:HOH:O	2.11	0.50
2:X:475:LEU:HD22	4:X:1901:PKZ:C7	2.41	0.50
2:X:1684:ARG:O	2:X:1688:THR:OG1	2.23	0.50
1:I:333:ILE:HG13	1:I:364:LEU:HD21	1.94	0.50
1:Q:282:ASN:O	1:Q:285:THR:OG1	2.25	0.50
1:Q:333:ILE:HG13	1:Q:364:LEU:HD21	1.94	0.50
1:Q:339:PHE:HB3	1:Q:376:PHE:HE1	1.77	0.50
1:U:822:THR:OG1	1:U:830:ILE:O	2.30	0.50
2:K:478:ASN:HD22	4:K:1901:PKZ:C1	2.17	0.50
1:A:903:GLU:CD	2:C:1690:ARG:CZ	2.85	0.50
1:A:1845:VAL:HG13	5:A:2394:HOH:O	2.07	0.50
1:M:1201:ASN:CB	5:M:2268:HOH:O	2.58	0.50
1:Q:1141:PHE:CE2	1:Q:1158:LEU:HD21	2.46	0.50
1:Q:1541:ILE:HD12	5:Q:2360:HOH:O	2.04	0.50
1:Q:1727:THR:OG1	1:Q:1728:ILE:N	2.45	0.50
2:C:1017:VAL:HG11	2:C:1665:LEU:CD1	2.41	0.50
2:C:1695:ALA:HB3	2:C:1701:MET:SD	2.51	0.50
2:K:888:ILE:HD12	2:K:939:PHE:CE1	2.47	0.50
2:O:798:MET:CE	5:O:2001:HOH:O	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:534:MET:SD	2:S:932:PHE:HB2	2.52	0.50
1:A:822:THR:OG1	1:A:830:ILE:O	2.30	0.50
1:E:733:PHE:HZ	5:E:2410:HOH:O	1.93	0.50
1:E:1523:SER:O	1:E:1528:LEU:HD22	2.11	0.50
1:I:80:LYS:HD3	1:I:80:LYS:N	2.26	0.50
1:I:774:GLU:HA	5:I:2307:HOH:O	2.11	0.50
1:I:1141:PHE:CE2	1:I:1195:ILE:HG21	2.47	0.50
1:I:1278:ILE:CG2	1:I:1283:ILE:HD11	2.41	0.50
1:U:1430:LEU:HD21	1:U:1502:TYR:OH	2.12	0.50
2:G:1364:MET:CE	5:G:2070:HOH:O	2.57	0.50
2:K:1017:VAL:HG11	2:K:1665:LEU:CD1	2.42	0.50
2:S:336:LEU:CD2	5:S:2178:HOH:O	2.51	0.50
2:X:686:ALA:HB3	5:X:2002:HOH:O	2.11	0.50
1:A:340:ILE:HG22	1:A:376:PHE:CE2	2.46	0.49
1:E:1130:LEU:CD2	1:E:1162:LEU:HD12	2.42	0.49
1:I:264:LEU:HD11	1:I:453:PHE:CE2	2.46	0.49
1:I:1244:GLU:C	5:I:2217:HOH:O	2.54	0.49
1:M:1565:ILE:HD12	1:M:1565:ILE:O	2.12	0.49
1:U:688:THR:HG23	5:U:2351:HOH:O	2.11	0.49
2:C:1275:GLN:HE21	2:X:1417:VAL:HB	1.76	0.49
2:C:1619:ASP:OD1	2:C:1621:LEU:HD13	2.12	0.49
2:G:1686:LYS:O	2:G:1690:ARG:HG3	2.12	0.49
2:O:662:TYR:HA	2:O:913:ILE:HD11	1.94	0.49
2:O:1624:GLN:HG2	5:O:2245:HOH:O	2.11	0.49
2:X:502:VAL:O	2:X:954:ARG:NH2	2.45	0.49
1:A:494:VAL:O	1:A:499:VAL:HG21	2.12	0.49
1:E:264:LEU:HD11	1:E:453:PHE:CE2	2.47	0.49
1:I:1650:THR:HG21	2:K:35:PHE:HB2	1.93	0.49
1:M:1144:THR:O	1:M:1156:ASN:ND2	2.46	0.49
1:Q:1211:ARG:NH1	1:Q:1537:GLU:OE2	2.46	0.49
1:Q:1581:GLU:OE2	1:Q:1586:ASN:ND2	2.43	0.49
2:G:1293:SER:HB3	5:G:2238:HOH:O	2.13	0.49
2:K:534:MET:SD	2:K:932:PHE:HB2	2.52	0.49
2:K:691:ILE:HG22	2:K:695:ILE:HD12	1.94	0.49
2:K:1429:ARG:CZ	2:O:1719:TYR:HB3	2.42	0.49
2:O:1369:THR:CG2	5:O:2238:HOH:O	2.57	0.49
2:X:687:GLY:O	2:X:690:SER:OG	2.30	0.49
1:A:63:ILE:HD11	1:A:125:ALA:HB1	1.94	0.49
1:E:178:LEU:HD21	1:E:234:CYS:SG	2.51	0.49
1:E:1565:ILE:HD12	1:E:1565:ILE:O	2.12	0.49
1:M:2017:VAL:HG21	2:O:13:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:153:GLN:HG2	1:Q:410:ILE:HD12	1.93	0.49
1:Q:591:THR:N	5:Q:2212:HOH:O	2.45	0.49
1:Q:761:ASP:OD1	1:Q:761:ASP:N	2.45	0.49
1:U:774:GLU:CA	5:U:2318:HOH:O	2.60	0.49
2:O:824:LEU:HG	5:O:2196:HOH:O	2.11	0.49
2:O:1239:VAL:HG13	5:O:2216:HOH:O	2.12	0.49
2:S:1129:ASP:N	2:S:1129:ASP:OD1	2.44	0.49
2:X:1468:TYR:CB	5:X:2247:HOH:O	2.60	0.49
1:E:1759:LEU:O	1:E:1765:THR:OG1	2.25	0.49
1:I:265:VAL:O	1:I:269:THR:OG1	2.29	0.49
1:I:1211:ARG:NH1	1:I:1537:GLU:OE2	2.45	0.49
1:I:1523:SER:O	1:I:1528:LEU:HD22	2.12	0.49
1:I:1727:THR:OG1	1:I:1728:ILE:N	2.45	0.49
1:M:1141:PHE:CE2	1:M:1195:ILE:HG21	2.48	0.49
1:U:1451:CYS:HB2	5:U:2209:HOH:O	2.11	0.49
2:C:1450:GLN:OE1	2:X:1461:TRP:NE1	2.39	0.49
2:G:1720:LEU:HD22	2:S:1567:HIS:CD2	2.46	0.49
2:O:1067:GLN:CB	5:O:2256:HOH:O	2.58	0.49
2:S:1444:ILE:HG13	5:S:2149:HOH:O	2.12	0.49
2:X:1551:VAL:HG23	5:X:2255:HOH:O	2.11	0.49
1:A:703:VAL:HG11	1:A:717:LEU:CD1	2.43	0.49
1:I:591:THR:N	5:I:2206:HOH:O	2.44	0.49
1:Q:760:SER:OG	1:Q:763:ASP:OD1	2.18	0.49
1:Q:1650:THR:HG21	2:S:35:PHE:HB2	1.93	0.49
1:U:703:VAL:HG11	1:U:717:LEU:CD1	2.43	0.49
2:C:1468:TYR:CB	5:C:2244:HOH:O	2.60	0.49
2:K:528:MET:HE3	2:K:641:PHE:HB2	1.94	0.49
2:K:824:LEU:CG	5:K:2270:HOH:O	2.56	0.49
2:O:475:LEU:HD22	4:O:1901:PKZ:C7	2.43	0.49
2:S:687:GLY:O	2:S:690:SER:OG	2.30	0.49
2:S:1017:VAL:HG11	2:S:1665:LEU:CD1	2.42	0.49
2:X:831:GLY:N	2:X:840:SER:OG	2.46	0.49
1:A:875:ARG:CG	5:A:2251:HOH:O	2.48	0.49
1:E:223:VAL:O	1:E:227:VAL:HG23	2.12	0.49
1:E:570:PHE:CE1	1:E:574:LEU:HD11	2.48	0.49
1:U:446:ASP:N	1:U:451:SER:O	2.44	0.49
2:C:1721:ASP:OD1	2:X:1431:HIS:ND1	2.42	0.49
2:O:818:ARG:NH2	5:O:2019:HOH:O	2.45	0.49
2:O:1444:ILE:HG13	5:O:2163:HOH:O	2.11	0.49
2:S:528:MET:HE1	2:S:894:ARG:HD3	1.95	0.49
2:X:1370:THR:HG23	5:X:2050:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG12	1:A:125:ALA:HB2	1.94	0.49
1:I:340:ILE:HG22	1:I:376:PHE:CZ	2.47	0.49
1:U:223:VAL:O	1:U:227:VAL:HG23	2.12	0.49
1:U:814:VAL:HG21	1:U:827:THR:HB	1.93	0.49
1:U:940:ARG:NH2	5:U:2201:HOH:O	2.41	0.49
2:C:891:LEU:CD1	2:C:933:ILE:HD11	2.42	0.49
2:G:1291:LEU:CG	5:G:2238:HOH:O	2.57	0.49
2:K:1719:TYR:HB3	2:O:1429:ARG:CZ	2.43	0.49
2:O:1004:ILE:HG13	5:O:2291:HOH:O	2.13	0.49
2:X:1141:GLU:HB2	5:X:2158:HOH:O	2.11	0.49
1:I:166:LEU:HD21	1:I:234:CYS:HB2	1.94	0.49
1:U:1137:TRP:CD1	1:U:1197:LEU:HD22	2.48	0.49
1:U:1725:PHE:CD2	1:U:1825:THR:HG23	2.47	0.49
2:C:841:GLU:O	2:C:845:SER:OG	2.23	0.49
2:G:1265:ALA:HB1	2:G:1267:LYS:HE2	1.93	0.49
2:O:80:CYS:HB2	5:O:2097:HOH:O	2.13	0.49
2:O:1017:VAL:HG11	2:O:1665:LEU:CD1	2.43	0.49
1:E:703:VAL:HG11	1:E:717:LEU:CD1	2.43	0.49
1:E:1144:THR:O	1:E:1156:ASN:ND2	2.45	0.49
1:M:906:TYR:CD2	1:M:941:VAL:HG22	2.46	0.49
1:M:1172:ILE:HD12	1:M:1172:ILE:N	2.28	0.49
1:U:1523:SER:OG	1:U:1528:LEU:HD13	2.13	0.49
1:U:1708:PHE:O	1:U:1714:ARG:NH1	2.46	0.49
2:C:348:LEU:HD12	2:O:338:LYS:HD3	1.94	0.49
2:C:1236:TYR:HA	5:C:2043:HOH:O	2.12	0.49
2:K:1450:GLN:OE1	2:O:1461:TRP:NE1	2.39	0.49
2:S:29:ILE:CD1	5:S:2240:HOH:O	2.60	0.49
1:E:126:VAL:HG11	5:E:2307:HOH:O	2.10	0.49
1:E:822:THR:OG1	1:E:830:ILE:O	2.31	0.49
1:I:822:THR:OG1	1:I:830:ILE:O	2.31	0.49
1:I:1998:TYR:O	1:I:2007:PHE:N	2.44	0.49
1:M:703:VAL:HG11	1:M:717:LEU:CD1	2.43	0.49
1:M:822:THR:OG1	1:M:830:ILE:O	2.31	0.49
1:Q:1141:PHE:CE2	1:Q:1195:ILE:HG21	2.48	0.49
1:U:1144:THR:O	1:U:1156:ASN:ND2	2.46	0.49
2:C:952:ASP:OD1	2:C:953:ILE:N	2.46	0.49
2:G:787:ILE:HD12	2:G:838:LEU:HD12	1.95	0.49
2:G:1004:ILE:HG13	5:G:2292:HOH:O	2.13	0.49
2:G:1141:GLU:HB2	5:G:2214:HOH:O	2.12	0.49
2:K:475:LEU:HD22	4:K:1901:PKZ:C7	2.43	0.49
2:K:759:PRO:HD2	5:K:2260:HOH:O	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1265:ALA:HB1	2:O:1267:LYS:HE2	1.93	0.49
2:S:528:MET:HE3	2:S:641:PHE:HB2	1.94	0.49
2:S:944:ARG:HD3	5:S:2225:HOH:O	2.13	0.49
2:S:1503:ARG:CD	5:S:2009:HOH:O	2.43	0.49
2:X:53:LEU:HD23	2:X:56:MET:HE3	1.95	0.49
1:A:1415:THR:CB	5:A:2260:HOH:O	2.61	0.48
1:I:325:MET:HE3	1:I:367:SER:OG	2.13	0.48
1:M:2001:ASN:OD1	2:O:26:VAL:HG13	2.12	0.48
1:U:1795:HIS:CE1	5:U:2300:HOH:O	2.65	0.48
2:C:708:VAL:CG2	5:C:2006:HOH:O	2.60	0.48
2:C:1370:THR:HG23	5:C:2047:HOH:O	2.13	0.48
2:C:1503:ARG:HE	2:X:1519:SER:CB	2.23	0.48
2:G:1017:VAL:HG11	2:G:1665:LEU:CD1	2.42	0.48
2:K:534:MET:HE3	2:K:891:LEU:CD1	2.43	0.48
2:K:851:ASN:ND2	2:S:830:HIS:O	2.46	0.48
2:S:1557:GLU:HB2	5:S:2203:HOH:O	2.13	0.48
2:X:952:ASP:OD1	2:X:953:ILE:N	2.46	0.48
2:X:963:ILE:HG23	5:X:2173:HOH:O	2.14	0.48
1:E:73:GLN:N	5:E:2211:HOH:O	2.45	0.48
1:E:2001:ASN:OD1	2:G:26:VAL:HG13	2.12	0.48
1:I:1595:LYS:HE2	1:I:1597:ASP:OD2	2.13	0.48
1:Q:178:LEU:HD21	1:Q:234:CYS:SG	2.53	0.48
1:Q:1618:ILE:HG22	1:Q:1623:ILE:HG12	1.96	0.48
2:C:1234:TYR:OH	2:C:1291:LEU:O	2.27	0.48
2:G:1641:LYS:CE	5:G:2134:HOH:O	2.45	0.48
2:K:746:GLN:NE2	5:K:2013:HOH:O	2.44	0.48
2:O:478:ASN:HD22	4:O:1901:PKZ:C1	2.20	0.48
2:O:1641:LYS:CE	5:O:2140:HOH:O	2.45	0.48
2:S:534:MET:HE3	2:S:891:LEU:CD1	2.43	0.48
2:S:1570:ARG:NE	2:S:1574:ASN:O	2.40	0.48
2:X:708:VAL:CG2	5:X:2002:HOH:O	2.60	0.48
1:I:546:PRO:HD2	5:I:2202:HOH:O	2.12	0.48
1:Q:822:THR:OG1	1:Q:830:ILE:O	2.31	0.48
1:U:761:ASP:OD1	1:U:761:ASP:N	2.42	0.48
2:C:787:ILE:HD12	2:C:838:LEU:HD12	1.94	0.48
2:G:475:LEU:HD22	4:G:1901:PKZ:C7	2.43	0.48
2:K:830:HIS:O	2:S:851:ASN:ND2	2.47	0.48
2:K:1315:ILE:HB	5:O:2096:HOH:O	2.14	0.48
2:O:952:ASP:OD1	2:O:953:ILE:N	2.46	0.48
2:O:1471:GLU:OE1	2:O:1471:GLU:N	2.46	0.48
2:X:468:ALA:CB	5:X:2261:HOH:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1565:ILE:HD12	1:A:1565:ILE:O	2.13	0.48
1:A:1974:LYS:HB3	1:A:1974:LYS:NZ	2.27	0.48
1:E:1172:ILE:HD12	1:E:1172:ILE:N	2.28	0.48
1:I:466:LYS:HZ3	1:I:470:GLU:CD	2.21	0.48
1:M:1779:ASP:OD2	2:O:89:TYR:OH	2.28	0.48
1:Q:1595:LYS:HE2	1:Q:1597:ASP:OD2	2.13	0.48
2:C:1695:ALA:HB1	2:C:1701:MET:HA	1.94	0.48
2:G:1444:ILE:HG13	5:G:2149:HOH:O	2.12	0.48
2:K:351:ARG:NH1	2:S:346:ARG:HH22	2.11	0.48
2:K:512:GLU:OE1	2:K:873:ARG:NH1	2.46	0.48
2:O:1084:ASP:HB3	2:O:1087:ASP:OD2	2.12	0.48
1:A:136:LEU:HA	5:A:2257:HOH:O	2.13	0.48
1:A:1225:LYS:HE2	1:A:1225:LYS:HA	1.94	0.48
1:A:1998:TYR:O	1:A:2007:PHE:N	2.43	0.48
1:I:668:ILE:HD13	1:I:673:PRO:HG2	1.95	0.48
1:Q:1244:GLU:C	5:Q:2224:HOH:O	2.55	0.48
1:U:639:ILE:HG12	1:U:645:MET:HE2	1.95	0.48
1:U:668:ILE:HD13	1:U:673:PRO:HG2	1.95	0.48
1:U:1141:PHE:CE2	1:U:1195:ILE:HG21	2.49	0.48
1:U:1435:TRP:CE3	1:U:1487:VAL:HG13	2.48	0.48
1:U:1553:ARG:NH1	5:U:2213:HOH:O	2.46	0.48
2:C:1537:ILE:HD11	2:C:1565:MET:HE1	1.94	0.48
2:C:1719:TYR:OH	2:X:1411:ASP:O	2.32	0.48
2:G:891:LEU:CD1	2:G:933:ILE:HD11	2.43	0.48
2:G:1471:GLU:OE1	2:G:1471:GLU:N	2.47	0.48
2:G:1716:GLN:HB2	2:G:1717:PRO:HG3	1.93	0.48
2:S:475:LEU:HD22	4:S:1901:PKZ:C7	2.43	0.48
2:S:1135:CYS:CB	5:S:2263:HOH:O	2.54	0.48
1:A:447:THR:HG23	1:A:473:VAL:HG13	1.95	0.48
1:I:834:ARG:HG2	5:I:2396:HOH:O	2.13	0.48
1:M:73:GLN:N	5:M:2217:HOH:O	2.47	0.48
1:Q:1479:LYS:CA	5:Q:2261:HOH:O	2.51	0.48
1:Q:1810:MET:HE3	1:Q:1984:ILE:CD1	2.44	0.48
1:U:1201:ASN:O	1:U:1225:LYS:HE2	2.13	0.48
2:G:1693:HIS:HA	2:G:1696:ILE:HG22	1.95	0.48
2:K:433:ASN:OD1	2:K:437:GLN:NE2	2.44	0.48
2:K:1373:ASN:ND2	5:K:2005:HOH:O	2.46	0.48
2:X:693:ALA:CA	5:X:2112:HOH:O	2.61	0.48
2:X:1210:ILE:O	2:X:1214:VAL:HG23	2.14	0.48
1:I:1565:ILE:HD12	1:I:1565:ILE:O	2.14	0.48
1:Q:1010:ASP:OD2	1:Q:1012:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:522:GLU:OE2	2:C:522:GLU:N	2.47	0.48
2:G:795:HIS:ND1	2:G:842:SER:OG	2.43	0.48
2:G:1084:ASP:HB3	2:G:1087:ASP:OD2	2.13	0.48
2:K:1693:HIS:HA	2:K:1696:ILE:HG22	1.94	0.48
2:K:1696:ILE:HG21	5:K:2074:HOH:O	2.12	0.48
2:O:1427:THR:OG1	2:O:1656:GLN:OE1	2.16	0.48
2:S:1373:ASN:ND2	5:S:2007:HOH:O	2.46	0.48
2:X:891:LEU:CD1	2:X:933:ILE:HD11	2.44	0.48
2:X:1619:ASP:OD1	2:X:1621:LEU:HD13	2.13	0.48
1:A:937:PHE:O	1:A:941:VAL:HG23	2.14	0.48
1:E:265:VAL:O	1:E:269:THR:OG1	2.28	0.48
1:E:2017:VAL:HG21	2:G:13:LEU:HD11	1.96	0.48
1:I:889:PRO:HB3	5:I:2331:HOH:O	2.14	0.48
1:Q:1159:HIS:O	1:Q:1163:THR:OG1	2.31	0.48
1:U:1635:LEU:HD22	1:U:1636:PRO:HD2	1.93	0.48
2:G:818:ARG:NH2	5:G:2026:HOH:O	2.47	0.48
2:K:1135:CYS:CB	5:K:2256:HOH:O	2.54	0.48
2:S:534:MET:HE1	2:S:933:ILE:CG1	2.44	0.48
2:S:1693:HIS:HA	2:S:1696:ILE:HG22	1.95	0.48
1:A:944:ARG:NH1	2:C:986:ALA:O	2.41	0.48
1:E:570:PHE:CE2	1:E:578:PRO:HA	2.48	0.48
1:E:679:THR:HG22	1:E:683:GLU:OE1	2.14	0.48
1:E:914:VAL:HG23	1:E:934:TYR:CE2	2.49	0.48
1:I:370:PRO:HG2	5:I:2442:HOH:O	2.12	0.48
1:M:1298:VAL:HG21	1:U:304:THR:HG22	1.96	0.48
1:M:1419:VAL:HG21	5:M:2204:HOH:O	2.14	0.48
1:Q:1526:GLU:O	1:Q:1529:THR:OG1	2.23	0.48
1:Q:1565:ILE:HD12	1:Q:1565:ILE:O	2.14	0.48
1:U:166:LEU:HD21	1:U:234:CYS:HB3	1.95	0.48
1:U:255:LYS:HE3	1:U:256:TRP:CD1	2.49	0.48
1:U:306:LEU:HD12	1:U:311:LEU:HD23	1.96	0.48
1:U:722:GLY:CA	5:U:2309:HOH:O	2.40	0.48
1:U:1565:ILE:HD12	1:U:1565:ILE:O	2.13	0.48
2:C:1450:GLN:HA	2:C:1453:LYS:HZ3	1.78	0.48
2:G:1537:ILE:HD11	2:G:1565:MET:HE1	1.96	0.48
2:O:771:ILE:CG2	5:O:2192:HOH:O	2.53	0.48
2:X:499:LYS:HE3	2:X:513:THR:HG21	1.95	0.48
2:X:651:GLY:N	5:X:2016:HOH:O	2.46	0.48
2:X:1093:GLU:O	2:X:1097:LEU:HD22	2.14	0.48
1:A:914:VAL:HG23	1:A:934:TYR:CE2	2.49	0.48
1:A:1300:ARG:NH2	1:I:304:THR:HG23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:616:MET:HB3	5:I:2230:HOH:O	2.14	0.48
1:I:871:LEU:O	1:I:875:ARG:HB3	2.14	0.48
1:Q:889:PRO:HB3	5:Q:2333:HOH:O	2.13	0.48
1:U:1826:MET:SD	2:X:22:PHE:CZ	3.06	0.48
2:K:341:LEU:HD23	2:X:344:LEU:HD22	1.96	0.48
2:K:528:MET:HE1	2:K:894:ARG:HD3	1.95	0.48
2:K:987:ASN:HB3	5:K:2068:HOH:O	2.12	0.48
2:X:522:GLU:OE1	2:X:522:GLU:N	2.46	0.48
1:A:256:TRP:HZ2	5:A:2209:HOH:O	1.81	0.47
1:E:1592:ARG:NH2	5:E:2219:HOH:O	2.47	0.47
1:I:487:LEU:CD2	1:I:533:ILE:HD12	2.44	0.47
1:I:660:GLY:O	1:I:1153:HIS:N	2.47	0.47
1:I:1147:ILE:HG22	1:I:1154:VAL:HG23	1.96	0.47
1:Q:1435:TRP:CE3	1:Q:1487:VAL:HG13	2.49	0.47
2:C:1137:LYS:HG2	5:C:2201:HOH:O	2.12	0.47
2:K:760:LYS:HE2	2:K:761:LYS:NZ	2.29	0.47
2:K:1471:GLU:N	2:K:1471:GLU:OE1	2.47	0.47
2:O:1739:THR:HG21	5:O:2181:HOH:O	2.14	0.47
2:S:774:PHE:CD1	2:S:825:PRO:HB3	2.49	0.47
2:X:1018:VAL:HG11	2:X:1315:ILE:CD1	2.45	0.47
2:X:1402:VAL:HG11	2:X:1533:PHE:CZ	2.49	0.47
2:X:1557:GLU:HB2	5:X:2100:HOH:O	2.12	0.47
1:E:565:TYR:HE2	1:E:577:ALA:N	2.12	0.47
1:M:872:ASN:ND2	5:M:2212:HOH:O	2.45	0.47
1:Q:668:ILE:HD13	1:Q:673:PRO:HG2	1.96	0.47
1:Q:1721:ILE:HD13	5:Q:2389:HOH:O	2.14	0.47
1:U:444:VAL:N	1:U:452:ASP:OD1	2.43	0.47
1:U:871:LEU:O	1:U:875:ARG:HB3	2.14	0.47
2:C:514:GLN:HB3	5:C:2042:HOH:O	2.12	0.47
2:C:1471:GLU:N	2:C:1471:GLU:OE1	2.47	0.47
2:G:784:LEU:HD21	2:X:806:LEU:HB3	1.97	0.47
2:G:952:ASP:OD1	2:G:953:ILE:N	2.46	0.47
2:O:891:LEU:CD1	2:O:933:ILE:HD11	2.43	0.47
2:S:987:ASN:HB3	5:S:2072:HOH:O	2.14	0.47
2:X:787:ILE:HD12	2:X:838:LEU:HD12	1.95	0.47
1:I:620:ALA:O	1:I:624:ILE:HG13	2.14	0.47
1:I:761:ASP:OD1	1:I:761:ASP:N	2.45	0.47
1:Q:166:LEU:HD21	1:Q:234:CYS:HB3	1.95	0.47
1:Q:616:MET:HB3	5:Q:2232:HOH:O	2.14	0.47
1:U:306:LEU:HD21	1:U:310:MET:HE1	1.96	0.47
1:U:1635:LEU:HD22	1:U:1636:PRO:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1210:ILE:O	2:G:1214:VAL:HG23	2.14	0.47
2:K:1653:LYS:HE3	2:O:1297:ILE:O	2.15	0.47
1:A:1435:TRP:CE3	1:A:1487:VAL:HG13	2.50	0.47
1:E:304:THR:HG22	1:I:1298:VAL:HG21	1.96	0.47
1:E:306:LEU:HD21	1:E:310:MET:CE	2.41	0.47
1:E:1141:PHE:CE2	1:E:1195:ILE:HG21	2.49	0.47
1:M:265:VAL:O	1:M:269:THR:OG1	2.29	0.47
1:M:839:GLU:N	5:M:2224:HOH:O	2.48	0.47
1:M:1435:TRP:CE3	1:M:1487:VAL:HG13	2.49	0.47
1:Q:760:SER:O	1:Q:764:THR:OG1	2.26	0.47
1:U:1665:MET:O	1:U:1669:ASN:OD1	2.32	0.47
1:U:1826:MET:SD	2:X:22:PHE:HE2	2.37	0.47
2:C:662:TYR:HA	2:C:913:ILE:HD11	1.96	0.47
2:C:1141:GLU:HB2	5:C:2142:HOH:O	2.15	0.47
2:G:1461:TRP:NE1	2:S:1450:GLN:OE1	2.39	0.47
2:G:1739:THR:HG21	5:G:2171:HOH:O	2.14	0.47
5:G:2090:HOH:O	2:S:1315:ILE:HB	2.14	0.47
2:K:944:ARG:HD3	5:K:2224:HOH:O	2.14	0.47
2:K:1570:ARG:NE	2:K:1574:ASN:O	2.40	0.47
2:S:349:GLN:HB2	2:S:351:ARG:HG3	1.97	0.47
2:S:1207:VAL:C	5:S:2025:HOH:O	2.58	0.47
1:A:1141:PHE:CZ	1:A:1158:LEU:HD11	2.50	0.47
1:M:668:ILE:HD13	1:M:673:PRO:HG2	1.95	0.47
1:Q:223:VAL:O	1:Q:227:VAL:HG23	2.14	0.47
1:Q:914:VAL:HG23	1:Q:934:TYR:CE2	2.50	0.47
1:U:447:THR:HG23	1:U:473:VAL:HG13	1.96	0.47
2:C:693:ALA:CA	5:C:2111:HOH:O	2.58	0.47
2:G:377:TRP:HH2	2:X:381:HIS:HB2	1.78	0.47
2:G:1522:ARG:NH2	2:S:1496:GLU:OE2	2.48	0.47
2:K:657:LYS:H	2:K:657:LYS:HE2	1.79	0.47
2:S:433:ASN:OD1	2:S:437:GLN:NE2	2.44	0.47
1:E:872:ASN:ND2	5:E:2216:HOH:O	2.46	0.47
1:I:1010:ASP:OD2	1:I:1012:ARG:NH1	2.48	0.47
1:M:937:PHE:O	1:M:941:VAL:HG23	2.14	0.47
1:U:555:THR:CG2	5:U:2246:HOH:O	2.63	0.47
1:U:1175:LYS:CA	5:U:2221:HOH:O	2.55	0.47
2:C:1410:THR:OG1	2:X:1293:SER:O	2.17	0.47
2:G:80:CYS:HB2	5:G:2093:HOH:O	2.13	0.47
2:S:659:SER:O	2:S:663:LEU:HD22	2.14	0.47
2:X:1132:PRO:HD3	2:X:1165:ARG:HE	1.79	0.47
1:A:251:ARG:HD2	1:A:442:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:974:LYS:HG3	1:E:975:PHE:CE2	2.50	0.47
1:E:1435:TRP:CE3	1:E:1487:VAL:HG13	2.49	0.47
1:I:914:VAL:HG23	1:I:934:TYR:CE2	2.49	0.47
1:M:379:ASN:HB2	5:M:2356:HOH:O	2.15	0.47
1:M:446:ASP:N	1:M:451:SER:O	2.43	0.47
1:M:914:VAL:HG23	1:M:934:TYR:CE2	2.49	0.47
1:M:974:LYS:HG3	1:M:975:PHE:CE2	2.50	0.47
1:M:1514:VAL:O	1:M:1617:MET:N	2.48	0.47
1:U:265:VAL:O	1:U:269:THR:OG1	2.29	0.47
1:U:1191:PRO:O	1:U:1210:HIS:NE2	2.45	0.47
2:C:709:THR:HG23	2:C:740:PHE:HB3	1.97	0.47
2:C:806:LEU:HB3	2:O:784:LEU:HD21	1.97	0.47
2:G:1035:ARG:NH1	2:G:1039:GLU:OE1	2.46	0.47
2:G:1624:GLN:HG2	5:G:2261:HOH:O	2.15	0.47
2:K:338:LYS:HD3	2:S:348:LEU:HD12	1.96	0.47
2:K:442:ALA:HA	2:K:446:LEU:HD23	1.96	0.47
2:K:937:LYS:NZ	2:S:855:SER:O	2.40	0.47
2:O:59:ARG:NE	5:O:2030:HOH:O	2.48	0.47
2:O:348:LEU:C	2:O:348:LEU:HD13	2.40	0.47
1:A:463:ARG:HE	1:A:467:LEU:HD11	1.80	0.47
1:A:1721:ILE:HD12	5:A:2419:HOH:O	2.11	0.47
1:E:668:ILE:HD13	1:E:673:PRO:HG2	1.95	0.47
1:E:1799:GLU:OE2	1:E:1998:TYR:OH	2.30	0.47
1:M:304:THR:HG22	1:Q:1298:VAL:HG21	1.96	0.47
1:M:974:LYS:HD2	1:M:974:LYS:O	2.15	0.47
1:M:1780:ILE:HG22	1:M:1786:ILE:HD11	1.97	0.47
1:U:1998:TYR:O	1:U:2007:PHE:N	2.44	0.47
2:C:784:LEU:HD21	2:O:806:LEU:HB3	1.97	0.47
2:K:795:HIS:CE1	2:K:842:SER:HG	2.32	0.47
2:O:787:ILE:HD12	2:O:838:LEU:HD12	1.96	0.47
2:O:1021:THR:CG2	2:O:1397:VAL:HB	2.45	0.47
2:O:1141:GLU:HB2	5:O:2221:HOH:O	2.14	0.47
2:S:760:LYS:HE2	2:S:761:LYS:NZ	2.29	0.47
2:S:798:MET:CE	5:S:2059:HOH:O	2.06	0.47
2:X:1471:GLU:OE1	2:X:1471:GLU:N	2.48	0.47
1:A:265:VAL:HG12	1:A:464:VAL:HG11	1.97	0.47
1:A:1444:PHE:CA	5:A:2397:HOH:O	2.62	0.47
1:A:1505:ARG:NH2	2:C:963:ILE:HG21	2.29	0.47
1:A:1683:ARG:N	1:A:1683:ARG:CD	2.77	0.47
1:I:1721:ILE:HD13	5:I:2383:HOH:O	2.15	0.47
1:Q:304:THR:HG22	1:U:1298:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1471:GLU:N	2:S:1471:GLU:OE1	2.47	0.47
1:A:1419:VAL:CB	5:A:2304:HOH:O	2.60	0.47
1:Q:1845:VAL:HG12	1:Q:1954:VAL:HG12	1.95	0.47
1:U:898:VAL:CG2	5:U:2427:HOH:O	2.37	0.47
1:U:1175:LYS:N	5:U:2221:HOH:O	2.48	0.47
1:U:1762:THR:HG21	1:U:1826:MET:HE2	1.97	0.47
2:C:691:ILE:HG22	2:C:695:ILE:HD12	1.97	0.47
2:C:1312:ASP:OD1	2:X:1322:LYS:NZ	2.48	0.47
2:G:1086:LYS:CE	5:G:2085:HOH:O	2.56	0.47
2:K:36:LEU:HD22	2:K:61:ILE:CG2	2.45	0.47
2:S:1670:ASP:OD1	2:S:1673:THR:OG1	2.25	0.47
1:A:466:LYS:NZ	1:A:470:GLU:OE1	2.35	0.46
1:A:1583:ALA:HB1	1:A:1644:ILE:HD13	1.97	0.46
1:A:1892:LEU:HD23	1:A:1946:ILE:H	1.79	0.46
1:I:479:THR:O	1:I:481:HIS:N	2.47	0.46
1:I:1526:GLU:O	1:I:1529:THR:OG1	2.25	0.46
1:Q:1612:MET:HE3	1:Q:1626:VAL:HG23	1.96	0.46
1:Q:1998:TYR:O	1:Q:2007:PHE:N	2.44	0.46
1:U:1278:ILE:HG23	1:U:1283:ILE:HD11	1.96	0.46
1:U:1583:ALA:HB1	1:U:1644:ILE:HD13	1.97	0.46
2:G:433:ASN:OD1	2:G:437:GLN:NE2	2.45	0.46
2:G:1129:ASP:CG	2:K:347:TYR:OH	2.57	0.46
2:K:1557:GLU:HB2	5:K:2191:HOH:O	2.14	0.46
2:O:528:MET:HE1	2:O:894:ARG:HD3	1.97	0.46
2:X:1094:GLU:OE2	2:X:1095:GLU:HG3	2.15	0.46
1:A:304:THR:HG21	1:E:1295:ASP:HA	1.97	0.46
1:A:1607:THR:HG23	1:A:1631:VAL:HB	1.96	0.46
1:E:265:VAL:HG12	1:E:464:VAL:HG11	1.96	0.46
1:I:1248:GLU:HA	1:I:1261:TYR:CE1	2.51	0.46
1:I:1607:THR:HG23	1:I:1631:VAL:HB	1.97	0.46
1:Q:265:VAL:HG12	1:Q:464:VAL:HG11	1.97	0.46
2:C:1018:VAL:HG11	2:C:1315:ILE:CD1	2.45	0.46
2:K:774:PHE:CD1	2:K:825:PRO:HB3	2.51	0.46
5:K:2127:HOH:O	2:O:1135:CYS:HB3	2.14	0.46
2:S:348:LEU:O	2:S:348:LEU:HD13	2.16	0.46
2:S:442:ALA:HA	2:S:446:LEU:HD23	1.95	0.46
1:I:937:PHE:O	1:I:941:VAL:HG23	2.15	0.46
1:Q:1248:GLU:HA	1:Q:1261:TYR:CE1	2.50	0.46
1:Q:1533:PRO:CG	5:Q:2434:HOH:O	2.52	0.46
1:U:1031:VAL:CA	5:U:2278:HOH:O	2.56	0.46
1:U:1159:HIS:O	1:U:1163:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1892:LEU:HD23	1:U:1946:ILE:H	1.78	0.46
2:K:910:THR:OG1	2:K:913:ILE:HD13	2.15	0.46
2:S:779:GLU:CG	5:S:2071:HOH:O	2.50	0.46
2:S:802:LEU:O	2:S:806:LEU:HD13	2.14	0.46
1:A:960:GLN:CB	5:A:2274:HOH:O	2.63	0.46
1:A:1295:ASP:HA	1:I:304:THR:HG21	1.97	0.46
1:E:903:GLU:HG3	5:E:2415:HOH:O	2.15	0.46
1:I:1514:VAL:O	1:I:1617:MET:N	2.49	0.46
1:Q:1607:THR:HG23	1:Q:1631:VAL:HB	1.97	0.46
1:U:265:VAL:HG12	1:U:464:VAL:HG11	1.97	0.46
1:U:463:ARG:O	1:U:467:LEU:HD13	2.15	0.46
1:U:1607:THR:HG23	1:U:1631:VAL:HB	1.98	0.46
2:G:1250:MET:HE1	2:S:1274:LEU:HD11	1.96	0.46
2:K:1496:GLU:OE2	2:O:1522:ARG:NH2	2.48	0.46
2:K:1695:ALA:HB1	2:K:1701:MET:HA	1.97	0.46
2:O:1004:ILE:CG1	5:O:2291:HOH:O	2.64	0.46
2:O:1265:ALA:CB	2:O:1267:LYS:HE2	2.45	0.46
2:S:478:ASN:HD22	4:S:1901:PKZ:C1	2.17	0.46
1:A:1298:VAL:HG21	1:I:304:THR:HG22	1.97	0.46
1:E:304:THR:HG23	1:I:1300:ARG:NH2	2.30	0.46
1:I:265:VAL:HG12	1:I:464:VAL:HG11	1.96	0.46
1:I:1435:TRP:CE3	1:I:1487:VAL:HG13	2.50	0.46
1:Q:774:GLU:HA	5:Q:2315:HOH:O	2.12	0.46
1:U:619:ARG:HA	5:U:2409:HOH:O	2.16	0.46
1:U:1565:ILE:HG21	1:U:1601:MET:HG2	1.98	0.46
1:U:1892:LEU:HD21	1:U:1946:ILE:O	2.15	0.46
2:C:338:LYS:HZ3	2:O:348:LEU:HD11	1.81	0.46
2:C:1120:MET:CE	2:C:1176:LYS:HE3	2.46	0.46
2:G:474:GLN:CD	5:G:2071:HOH:O	2.59	0.46
2:G:528:MET:HE1	2:G:894:ARG:HD3	1.98	0.46
2:G:741:ASN:HB3	2:G:747:ASP:OD2	2.16	0.46
2:K:908:LEU:HD11	2:K:924:ALA:HB2	1.97	0.46
2:O:1210:ILE:O	2:O:1214:VAL:HG23	2.15	0.46
1:A:304:THR:HG22	1:E:1298:VAL:HG21	1.98	0.46
1:A:814:VAL:HG12	1:A:815:PRO:O	2.16	0.46
1:E:937:PHE:O	1:E:941:VAL:HG23	2.15	0.46
1:M:65:PHE:C	1:M:65:PHE:CD1	2.94	0.46
1:Q:698:ASP:O	1:Q:702:GLN:HG3	2.16	0.46
1:Q:871:LEU:O	1:Q:875:ARG:HB3	2.14	0.46
2:G:35:PHE:CD1	2:G:44:ILE:HD11	2.50	0.46
2:G:1265:ALA:CB	2:G:1267:LYS:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:30:GLU:CB	5:O:2116:HOH:O	2.35	0.46
2:O:741:ASN:HB3	2:O:747:ASP:OD2	2.16	0.46
2:S:1333:ASP:OD1	2:S:1379:GLN:NE2	2.48	0.46
2:X:989:LYS:HB3	5:X:2178:HOH:O	2.15	0.46
1:A:1523:SER:OG	1:A:1528:LEU:HD13	2.15	0.46
1:E:1072:ARG:HH11	1:E:1072:ARG:HG3	1.81	0.46
1:M:1211:ARG:NH1	1:M:1537:GLU:OE2	2.49	0.46
2:C:989:LYS:HB3	5:C:2202:HOH:O	2.14	0.46
2:G:376:LEU:CD2	5:G:2188:HOH:O	2.54	0.46
2:K:514:GLN:HB3	5:K:2098:HOH:O	2.15	0.46
2:O:369:VAL:O	2:O:372:LYS:HG2	2.15	0.46
2:O:1403:LEU:N	2:O:1403:LEU:HD23	2.30	0.46
2:S:357:LEU:O	2:S:357:LEU:HD13	2.16	0.46
2:S:435:CYS:O	2:S:439:MET:HG3	2.15	0.46
2:X:446:LEU:O	2:X:450:MET:HG3	2.16	0.46
1:A:475:TRP:O	1:A:479:THR:HG22	2.16	0.46
1:A:1078:TYR:O	1:A:1084:LYS:HD3	2.16	0.46
1:A:1581:GLU:HG3	1:A:1582:TRP:CD1	2.50	0.46
1:E:166:LEU:HD21	1:E:234:CYS:HB3	1.97	0.46
1:E:1569:MET:HA	1:E:1569:MET:HE3	1.98	0.46
1:E:1845:VAL:HG12	1:E:1954:VAL:HG12	1.98	0.46
1:I:1523:SER:HB3	1:I:1582:TRP:CE3	2.51	0.46
1:M:265:VAL:HG12	1:M:464:VAL:HG11	1.97	0.46
1:Q:1877:VAL:HG11	1:Q:1889:ALA:HB3	1.98	0.46
1:U:1727:THR:OG1	1:U:1728:ILE:N	2.48	0.46
2:C:347:TYR:OH	2:K:1129:ASP:CG	2.56	0.46
2:C:1496:GLU:HG3	2:X:1522:ARG:NH2	2.31	0.46
1:A:982:LEU:HD21	5:C:2045:HOH:O	2.15	0.46
1:A:1191:PRO:O	1:A:1210:HIS:NE2	2.45	0.46
1:E:839:GLU:N	5:E:2223:HOH:O	2.48	0.46
1:E:1514:VAL:O	1:E:1617:MET:N	2.48	0.46
1:E:1621:ARG:NH1	1:E:1643:GLU:OE1	2.49	0.46
1:U:1093:GLY:CA	5:U:2395:HOH:O	2.57	0.46
1:U:1710:GLY:O	1:U:1714:ARG:HG2	2.16	0.46
2:C:967:VAL:HG23	5:C:2144:HOH:O	2.15	0.46
2:K:1401:ALA:HB1	2:K:1659:VAL:HG12	1.98	0.46
2:X:1144:LYS:HB2	2:X:1153:ILE:HD13	1.97	0.46
2:X:1717:PRO:HB2	2:X:1740:ILE:HG21	1.97	0.46
1:E:126:VAL:CG1	5:E:2307:HOH:O	2.64	0.46
1:E:851:PHE:CE1	1:E:855:LEU:HD11	2.51	0.46
1:E:1779:ASP:OD2	2:G:89:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:LEU:HD21	1:M:234:CYS:HB3	1.98	0.46
1:M:1072:ARG:HH11	1:M:1072:ARG:HG3	1.81	0.46
1:M:1191:PRO:O	1:M:1210:HIS:NE2	2.46	0.46
1:M:1618:ILE:HG22	1:M:1623:ILE:HG12	1.98	0.46
2:G:937:LYS:NZ	2:X:855:SER:O	2.42	0.46
2:K:435:CYS:O	2:K:439:MET:HG3	2.15	0.46
2:K:534:MET:HE1	2:K:933:ILE:CG1	2.44	0.46
2:K:1207:VAL:C	5:K:2020:HOH:O	2.57	0.46
2:O:1035:ARG:NH1	2:O:1039:GLU:OE2	2.46	0.46
2:X:36:LEU:HD22	2:X:61:ILE:CG2	2.46	0.46
2:X:528:MET:HE1	2:X:894:ARG:CD	2.46	0.46
1:A:334:LYS:NZ	1:A:335:GLN:HG2	2.31	0.45
1:M:304:THR:HG21	1:Q:1295:ASP:HA	1.99	0.45
1:Q:122:TYR:CE1	1:Q:126:VAL:HG21	2.52	0.45
1:Q:304:THR:HG21	1:U:1295:ASP:HA	1.97	0.45
1:Q:937:PHE:O	1:Q:941:VAL:HG23	2.16	0.45
1:Q:1595:LYS:HD2	1:Q:1641:GLU:OE1	2.17	0.45
1:U:1845:VAL:HG12	1:U:1954:VAL:HG12	1.98	0.45
2:O:35:PHE:CD1	2:O:44:ILE:HD11	2.50	0.45
1:E:1842:MET:HG2	1:E:1889:ALA:HB2	1.99	0.45
1:M:126:VAL:CG1	5:M:2313:HOH:O	2.63	0.45
1:M:1010:ASP:OD2	1:M:1012:ARG:NH1	2.50	0.45
1:M:1621:ARG:NH1	1:M:1643:GLU:OE1	2.49	0.45
1:Q:123:TYR:OH	1:Q:242:VAL:HG22	2.16	0.45
1:Q:1541:ILE:HD11	5:Q:2360:HOH:O	2.05	0.45
2:C:855:SER:O	2:O:937:LYS:NZ	2.44	0.45
2:C:1093:GLU:O	2:C:1097:LEU:HD22	2.16	0.45
2:C:1696:ILE:HG21	5:C:2090:HOH:O	2.16	0.45
2:G:891:LEU:HD13	2:G:933:ILE:HD11	1.99	0.45
2:G:1401:ALA:HB3	2:G:1601:ILE:CD1	2.47	0.45
2:G:1403:LEU:N	2:G:1403:LEU:HD23	2.30	0.45
2:K:450:MET:HG2	4:K:1901:PKZ:C14	2.47	0.45
2:K:1303:ALA:CA	5:K:2051:HOH:O	2.64	0.45
2:O:474:GLN:CD	5:O:2075:HOH:O	2.58	0.45
2:O:908:LEU:HD11	2:O:924:ALA:HB2	1.98	0.45
2:S:526:TYR:CD1	5:S:2014:HOH:O	2.68	0.45
2:S:908:LEU:HD11	2:S:924:ALA:HB2	1.97	0.45
1:A:1239:MET:O	1:A:1242:ARG:HB2	2.16	0.45
1:E:931:ARG:NH1	1:E:962:ASN:OD1	2.50	0.45
1:I:122:TYR:CE1	1:I:126:VAL:HG21	2.51	0.45
1:Q:1421:PHE:HZ	1:Q:1447:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1650:THR:HG21	2:X:35:PHE:HB2	1.98	0.45
2:G:1:MET:CE	2:G:6:GLU:HA	2.47	0.45
2:G:1312:ASP:OD1	2:S:1322:LYS:NZ	2.50	0.45
2:K:526:TYR:CD1	5:K:2012:HOH:O	2.69	0.45
2:O:891:LEU:HD13	2:O:933:ILE:HD11	1.99	0.45
2:O:1537:ILE:HD13	2:O:1568:LEU:HD13	1.98	0.45
2:O:1672:SER:O	2:O:1676:GLU:HG3	2.16	0.45
2:S:1116:LYS:HB2	5:S:2270:HOH:O	2.17	0.45
1:A:732:ASP:OD2	1:A:735:GLN:NE2	2.49	0.45
1:A:875:ARG:HD3	5:A:2251:HOH:O	2.17	0.45
1:I:519:ASP:OD1	1:I:520:SER:N	2.50	0.45
1:I:655:ASP:O	1:I:658:GLU:HG3	2.16	0.45
1:I:814:VAL:HG12	1:I:815:PRO:O	2.17	0.45
1:M:304:THR:HG23	1:Q:1300:ARG:NH2	2.32	0.45
1:M:814:VAL:HG12	1:M:815:PRO:O	2.16	0.45
1:M:1141:PHE:HE2	1:M:1195:ILE:HG21	1.82	0.45
1:M:1300:ARG:NH2	1:U:304:THR:HG23	2.31	0.45
1:M:1592:ARG:NH2	5:M:2225:HOH:O	2.48	0.45
1:U:239:THR:HG23	1:U:533:ILE:HD11	1.97	0.45
1:U:937:PHE:O	1:U:941:VAL:HG23	2.16	0.45
1:U:1211:ARG:NH1	1:U:1537:GLU:OE2	2.49	0.45
2:C:1315:ILE:HB	5:C:2007:HOH:O	2.17	0.45
2:C:1401:ALA:HB3	2:C:1601:ILE:CD1	2.46	0.45
2:G:348:LEU:CD1	2:X:338:LYS:HZ3	2.29	0.45
2:G:1021:THR:CG2	2:G:1397:VAL:HB	2.45	0.45
2:K:338:LYS:NZ	2:S:348:LEU:HD13	2.32	0.45
2:K:348:LEU:HD13	2:S:338:LYS:NZ	2.31	0.45
2:K:1132:PRO:HD3	2:K:1165:ARG:NE	2.32	0.45
2:O:1561:ILE:HD13	2:O:1564:MET:SD	2.57	0.45
2:S:938:ASP:OD1	2:S:938:ASP:N	2.49	0.45
2:X:1197:TYR:HE1	5:X:2143:HOH:O	2.00	0.45
1:A:353:ILE:HD11	1:A:372:SER:CB	2.46	0.45
1:A:586:PRO:HD2	3:A:2101:FMN:H6	1.98	0.45
1:A:774:GLU:CA	5:A:2340:HOH:O	2.64	0.45
1:A:982:LEU:CD1	2:C:1690:ARG:CZ	2.94	0.45
1:A:1565:ILE:HG21	1:A:1601:MET:HG2	1.97	0.45
1:E:1607:THR:HG23	1:E:1631:VAL:HB	1.99	0.45
1:I:1421:PHE:HZ	1:I:1447:LEU:HD12	1.81	0.45
1:I:1621:ARG:NH1	1:I:1643:GLU:OE1	2.49	0.45
1:M:679:THR:HG22	1:M:683:GLU:OE2	2.17	0.45
1:M:1650:THR:HG21	2:O:35:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:944:ARG:NH2	1:U:987:ASP:OD1	2.49	0.45
2:G:1:MET:HE3	2:G:6:GLU:CA	2.47	0.45
2:G:806:LEU:HB3	2:X:784:LEU:HD21	1.98	0.45
2:K:1333:ASP:OD1	2:K:1379:GLN:NE2	2.48	0.45
2:O:36:LEU:HD22	2:O:61:ILE:CG2	2.46	0.45
2:O:1086:LYS:CE	5:O:2092:HOH:O	2.56	0.45
2:O:1278:PHE:O	2:O:1282:MET:HE1	2.17	0.45
2:X:1197:TYR:O	2:X:1701:MET:N	2.49	0.45
1:A:166:LEU:HD21	1:A:234:CYS:HB3	1.99	0.45
1:A:1618:ILE:HG22	1:A:1623:ILE:HG12	1.97	0.45
1:E:1780:ILE:HG22	1:E:1786:ILE:HD11	1.98	0.45
1:E:1824:MET:HA	1:E:1824:MET:HE3	1.98	0.45
1:I:698:ASP:O	1:I:702:GLN:HG3	2.16	0.45
1:I:875:ARG:HG3	1:I:876:ASP:N	2.32	0.45
1:I:1566:THR:HB	5:I:2232:HOH:O	2.17	0.45
1:I:1977:GLN:NE2	2:K:16:GLU:OE2	2.48	0.45
1:M:447:THR:HG23	1:M:473:VAL:HG13	1.98	0.45
1:M:1824:MET:HA	1:M:1824:MET:HE3	1.98	0.45
2:G:1054:TRP:NE1	2:G:1696:ILE:O	2.50	0.45
2:G:1426:THR:HA	2:G:1429:ARG:CZ	2.47	0.45
2:K:806:LEU:HB3	2:S:784:LEU:HD21	1.99	0.45
2:K:1279:ILE:HA	2:K:1282:MET:HE1	1.99	0.45
2:K:1588:PRO:O	2:K:1592:ALA:HB2	2.16	0.45
2:O:708:VAL:HG23	5:O:2137:HOH:O	2.16	0.45
2:S:467:LEU:HA	2:S:470:ARG:NE	2.28	0.45
2:S:1540:ILE:O	2:S:1570:ARG:NH2	2.46	0.45
2:X:709:THR:HG23	2:X:740:PHE:HB3	1.97	0.45
2:X:1265:ALA:HB1	2:X:1267:LYS:HE2	1.98	0.45
1:A:1845:VAL:HG21	5:A:2394:HOH:O	2.07	0.45
1:E:1618:ILE:HG22	1:E:1623:ILE:HG12	1.98	0.45
1:Q:1191:PRO:O	1:Q:1210:HIS:NE2	2.44	0.45
2:K:338:LYS:HZ2	2:S:348:LEU:HD13	1.81	0.45
2:K:500:THR:HG21	2:K:947:LEU:HD21	1.97	0.45
2:O:346:ARG:CZ	2:O:353:LYS:HA	2.47	0.45
2:O:696:LEU:HD11	2:O:735:LEU:HD13	1.98	0.45
2:O:1018:VAL:HG11	2:O:1315:ILE:CD1	2.47	0.45
2:S:448:LYS:NZ	5:S:2021:HOH:O	2.47	0.45
2:S:450:MET:HG2	4:S:1901:PKZ:C14	2.47	0.45
2:S:1083:ILE:HD12	2:S:1091:LYS:HD3	1.98	0.45
1:A:97:PHE:CE1	1:A:101:LEU:HD11	2.52	0.45
1:E:1239:MET:O	1:E:1242:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:487:LEU:HD21	1:I:533:ILE:HD12	1.98	0.45
1:M:251:ARG:HE	1:M:441:LYS:HB2	1.81	0.45
1:M:1682:ASP:O	1:M:1686:VAL:HG23	2.17	0.45
1:M:1845:VAL:HG12	1:M:1954:VAL:HG12	1.98	0.45
1:Q:586:PRO:HD2	3:Q:2101:FMN:H6	1.99	0.45
1:Q:1514:VAL:O	1:Q:1617:MET:N	2.49	0.45
1:U:1248:GLU:HA	1:U:1261:TYR:CE1	2.52	0.45
1:U:1505:ARG:NH2	2:X:963:ILE:HG21	2.31	0.45
2:C:442:ALA:HA	2:C:446:LEU:HD23	1.98	0.45
2:K:913:ILE:HD13	5:K:2026:HOH:O	2.16	0.45
2:O:1:MET:HE3	2:O:6:GLU:CA	2.47	0.45
2:S:795:HIS:ND1	2:S:842:SER:OG	2.44	0.45
2:S:1391:LEU:O	2:S:1395:MET:HG3	2.17	0.45
1:E:304:THR:HG21	1:I:1295:ASP:HA	1.99	0.45
1:E:616:MET:CB	5:E:2360:HOH:O	2.65	0.45
1:E:1139:GLN:HB2	5:E:2204:HOH:O	2.16	0.45
1:I:1595:LYS:HD2	1:I:1641:GLU:OE1	2.17	0.45
1:M:931:ARG:NH1	1:M:962:ASN:OD1	2.50	0.45
1:M:1523:SER:HB3	1:M:1582:TRP:CE3	2.52	0.45
1:U:960:GLN:CB	5:U:2288:HOH:O	2.64	0.45
2:C:338:LYS:CD	2:O:348:LEU:HD12	2.47	0.45
2:C:1402:VAL:HG11	2:C:1533:PHE:CZ	2.52	0.45
2:K:891:LEU:HD11	2:K:893:VAL:HG22	1.99	0.45
2:K:938:ASP:OD1	2:K:938:ASP:N	2.50	0.45
2:K:1322:LYS:NZ	2:O:1312:ASP:OD1	2.50	0.45
2:S:651:GLY:HA3	5:S:2056:HOH:O	2.10	0.45
1:A:887:GLN:NE2	5:A:2228:HOH:O	2.50	0.45
1:E:1140:ALA:O	1:E:1144:THR:OG1	2.18	0.45
1:I:586:PRO:HD2	3:I:2101:FMN:H6	1.98	0.45
1:I:760:SER:O	1:I:764:THR:OG1	2.25	0.45
1:I:1877:VAL:HG11	1:I:1889:ALA:HB3	1.99	0.45
1:M:851:PHE:CE1	1:M:855:LEU:HD11	2.51	0.45
1:M:1139:GLN:HB2	5:M:2203:HOH:O	2.17	0.45
1:M:1565:ILE:HG21	1:M:1601:MET:HG2	1.99	0.45
1:M:1569:MET:HA	1:M:1569:MET:HE3	1.97	0.45
1:U:1591:VAL:HG23	1:U:1591:VAL:O	2.17	0.45
1:U:1595:LYS:HD3	1:U:1641:GLU:H	1.82	0.45
2:G:1132:PRO:HD3	2:G:1165:ARG:HG2	1.99	0.45
2:G:1250:MET:CE	2:S:1274:LEU:HD11	2.47	0.45
2:K:657:LYS:HE2	2:K:657:LYS:HB2	1.84	0.45
2:O:1401:ALA:HB3	2:O:1601:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:415:MET:HE1	2:S:424:LEU:HD13	1.99	0.45
2:S:1272:ASP:OD1	2:S:1272:ASP:N	2.50	0.45
2:S:1588:PRO:O	2:S:1592:ALA:HB2	2.16	0.45
1:A:145:LYS:N	5:A:2223:HOH:O	2.49	0.44
1:A:1725:PHE:CE1	1:A:1727:THR:OG1	2.70	0.44
1:I:97:PHE:CE1	1:I:101:LEU:HD11	2.51	0.44
2:C:526:TYR:O	2:C:530:GLN:HG2	2.17	0.44
2:C:662:TYR:OH	2:C:904:ASN:O	2.35	0.44
2:G:36:LEU:HD22	2:G:61:ILE:CG2	2.46	0.44
2:G:1018:VAL:HG11	2:G:1315:ILE:CD1	2.47	0.44
2:K:1116:LYS:HB2	5:K:2268:HOH:O	2.17	0.44
2:O:1:MET:CE	2:O:6:GLU:HA	2.46	0.44
2:O:348:LEU:HD13	2:O:348:LEU:O	2.17	0.44
2:O:411:ASP:OD2	2:O:1633:ARG:NH2	2.50	0.44
2:S:369:VAL:CG2	5:S:2217:HOH:O	2.55	0.44
2:S:534:MET:CE	2:S:891:LEU:CD1	2.95	0.44
2:S:913:ILE:HD13	5:S:2041:HOH:O	2.16	0.44
1:E:974:LYS:HD2	1:E:974:LYS:O	2.16	0.44
1:I:668:ILE:HD13	1:I:673:PRO:CG	2.47	0.44
1:M:1679:ASP:O	1:M:1683:ARG:HD3	2.17	0.44
1:Q:668:ILE:HD13	1:Q:673:PRO:CG	2.48	0.44
1:Q:875:ARG:HG3	1:Q:876:ASP:N	2.32	0.44
2:C:339:GLN:O	2:C:343:VAL:HG23	2.17	0.44
2:C:908:LEU:HD11	2:C:924:ALA:HB2	1.99	0.44
2:G:1004:ILE:CD1	5:G:2292:HOH:O	2.61	0.44
2:G:1132:PRO:HD3	2:G:1165:ARG:CD	2.46	0.44
2:S:1425:LEU:HB3	2:S:1429:ARG:NH2	2.32	0.44
2:X:657:LYS:HE3	5:X:2091:HOH:O	2.17	0.44
2:X:662:TYR:HA	2:X:913:ILE:HD11	1.98	0.44
1:A:1710:GLY:O	1:A:1714:ARG:HG2	2.18	0.44
1:A:1845:VAL:HG12	1:A:1954:VAL:HG12	1.98	0.44
1:E:1565:ILE:HG21	1:E:1601:MET:HG2	1.99	0.44
1:I:725:GLY:HA3	5:I:2403:HOH:O	2.15	0.44
1:I:1679:ASP:O	1:I:1683:ARG:HD3	2.18	0.44
1:M:1591:VAL:HG23	1:M:1591:VAL:O	2.16	0.44
1:Q:353:ILE:HD11	1:Q:372:SER:CB	2.47	0.44
1:Q:814:VAL:HG12	1:Q:815:PRO:O	2.17	0.44
1:U:406:ARG:HD3	5:U:2287:HOH:O	2.17	0.44
1:U:1421:PHE:CZ	1:U:1447:LEU:HG	2.51	0.44
1:U:1447:LEU:HD23	1:U:1474:LEU:HD13	2.00	0.44
2:C:792:GLU:OE1	2:O:804:ARG:NH2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1391:LEU:O	2:C:1395:MET:HG3	2.17	0.44
2:K:1087:ASP:O	2:K:1091:LYS:HG2	2.17	0.44
2:O:1391:LEU:O	2:O:1395:MET:HG3	2.18	0.44
2:S:1401:ALA:HB1	2:S:1659:VAL:HG12	1.99	0.44
2:X:693:ALA:HB1	5:X:2112:HOH:O	2.11	0.44
2:X:1366:ARG:NH2	2:X:1371:THR:O	2.50	0.44
1:A:985:GLU:OE1	2:C:1694:ASN:OD1	2.35	0.44
1:A:1172:ILE:N	1:A:1172:ILE:HD12	2.31	0.44
1:E:251:ARG:HE	1:E:441:LYS:HB2	1.81	0.44
1:E:814:VAL:HG12	1:E:815:PRO:O	2.16	0.44
1:E:1682:ASP:O	1:E:1686:VAL:HG23	2.17	0.44
1:I:1591:VAL:HG23	1:I:1591:VAL:O	2.17	0.44
1:M:614:PRO:N	1:M:614:PRO:HG2	2.08	0.44
1:Q:527:TYR:HA	5:Q:2227:HOH:O	2.17	0.44
1:Q:1140:ALA:O	1:Q:1144:THR:OG1	2.20	0.44
1:U:685:LEU:HD12	1:U:687:LEU:HD11	1.98	0.44
2:C:742:GLN:O	2:C:801:ASN:ND2	2.51	0.44
2:C:1716:GLN:CA	2:C:1717:PRO:HG3	2.47	0.44
2:G:348:LEU:HD12	2:X:338:LYS:HD3	1.99	0.44
2:K:534:MET:CE	2:K:891:LEU:CD1	2.96	0.44
2:K:802:LEU:O	2:K:806:LEU:HD13	2.18	0.44
2:K:1391:LEU:O	2:K:1395:MET:HG3	2.17	0.44
1:A:479:THR:O	1:A:481:HIS:N	2.51	0.44
1:E:1211:ARG:NH1	1:E:1537:GLU:OE1	2.50	0.44
1:I:353:ILE:HD11	1:I:372:SER:CB	2.47	0.44
1:I:1621:ARG:NH1	1:I:1621:ARG:HB2	2.32	0.44
1:M:353:ILE:HD11	1:M:372:SER:CB	2.48	0.44
1:Q:1523:SER:HB3	1:Q:1582:TRP:CE3	2.53	0.44
1:U:250:PHE:CD1	1:U:250:PHE:C	2.93	0.44
1:U:353:ILE:HD11	1:U:372:SER:CB	2.47	0.44
2:C:718:THR:HG21	5:C:2205:HOH:O	2.10	0.44
2:C:891:LEU:HD13	2:C:933:ILE:HD11	1.99	0.44
2:G:411:ASP:OD2	2:G:1633:ARG:NH2	2.50	0.44
2:G:499:LYS:HG2	2:G:511:GLU:OE1	2.18	0.44
2:O:410:GLN:NE2	2:O:1633:ARG:NH2	2.66	0.44
2:S:1410:THR:HG22	2:S:1652:GLN:O	2.17	0.44
2:X:871:TRP:CD1	2:X:895:THR:HG23	2.52	0.44
2:X:1391:LEU:O	2:X:1395:MET:HG3	2.18	0.44
1:A:406:ARG:HD3	5:A:2264:HOH:O	2.16	0.44
1:A:741:TYR:HB3	1:A:781:MET:HE2	2.00	0.44
1:A:1725:PHE:CD2	1:A:1828:VAL:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ILE:CG1	1:E:364:LEU:HD21	2.46	0.44
1:E:1010:ASP:OD2	1:E:1012:ARG:NH1	2.50	0.44
1:Q:1147:ILE:HD11	1:Q:1235:ILE:HG22	1.99	0.44
1:Q:1591:VAL:HG23	1:Q:1591:VAL:O	2.18	0.44
1:U:732:ASP:OD2	1:U:735:GLN:NE2	2.50	0.44
1:U:774:GLU:CB	5:U:2318:HOH:O	2.65	0.44
2:C:1197:TYR:O	2:C:1701:MET:N	2.51	0.44
2:C:1281:THR:HA	5:C:2114:HOH:O	2.18	0.44
2:C:1711:SER:O	2:C:1715:GLU:N	2.51	0.44
2:G:965:GLN:O	2:G:969:ASN:ND2	2.35	0.44
2:G:1004:ILE:CG1	5:G:2292:HOH:O	2.64	0.44
2:G:1422:LYS:HE3	5:S:2242:HOH:O	2.18	0.44
2:O:651:GLY:HA3	5:O:2104:HOH:O	2.17	0.44
2:O:718:THR:HG21	5:O:2200:HOH:O	2.13	0.44
2:O:1693:HIS:HA	2:O:1696:ILE:HG22	1.99	0.44
2:S:514:GLN:HB3	5:S:2102:HOH:O	2.16	0.44
2:X:514:GLN:HB3	5:X:2028:HOH:O	2.18	0.44
2:X:1281:THR:CA	5:X:2126:HOH:O	2.66	0.44
1:A:305:SER:O	1:E:1586:ASN:ND2	2.51	0.44
1:A:845:ALA:CA	5:A:2377:HOH:O	2.42	0.44
1:E:166:LEU:HD21	1:E:234:CYS:HB2	2.00	0.44
1:E:353:ILE:HD11	1:E:372:SER:CB	2.48	0.44
1:E:512:ILE:O	1:E:528:GLY:N	2.43	0.44
1:M:191:SER:N	5:M:2228:HOH:O	2.50	0.44
1:M:685:LEU:HD12	1:M:687:LEU:HD11	1.99	0.44
1:Q:123:TYR:CZ	1:Q:242:VAL:HG22	2.53	0.44
1:Q:1566:THR:HB	5:Q:2236:HOH:O	2.17	0.44
1:Q:1665:MET:O	1:Q:1668:TYR:N	2.51	0.44
1:U:639:ILE:H	1:U:645:MET:HE3	1.82	0.44
1:U:668:ILE:HD11	1:U:681:TYR:CD2	2.53	0.44
1:U:847:ARG:NH1	1:U:884:ASN:O	2.51	0.44
2:C:530:GLN:OE1	2:C:530:GLN:HA	2.18	0.44
2:C:1444:ILE:HG13	5:C:2078:HOH:O	2.16	0.44
2:G:59:ARG:NE	5:G:2037:HOH:O	2.49	0.44
2:G:478:ASN:HD22	4:G:1901:PKZ:C1	2.20	0.44
2:G:1094:GLU:OE1	2:G:1095:GLU:HG3	2.18	0.44
2:S:500:THR:HG21	2:S:947:LEU:HD21	1.99	0.44
1:A:305:SER:C	1:E:1586:ASN:HD21	2.26	0.44
1:A:931:ARG:NH1	1:A:962:ASN:OD1	2.51	0.44
1:A:1093:GLY:CA	5:A:2389:HOH:O	2.58	0.44
1:A:1361:LYS:HE2	5:A:2224:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:685:LEU:HD12	1:E:687:LEU:HD11	1.99	0.44
1:E:1033:ASP:OD1	1:E:1033:ASP:N	2.51	0.44
1:E:1130:LEU:HD21	1:E:1162:LEU:HD12	2.00	0.44
1:E:1141:PHE:HE2	1:E:1195:ILE:HG21	1.83	0.44
1:E:1719:ASN:O	1:E:1723:MET:HG3	2.18	0.44
1:I:524:ASP:OD1	1:I:524:ASP:N	2.45	0.44
1:I:685:LEU:HD12	1:I:687:LEU:HD11	1.99	0.44
1:I:1618:ILE:HG22	1:I:1623:ILE:HG12	1.99	0.44
1:I:1665:MET:O	1:I:1668:TYR:N	2.51	0.44
1:M:668:ILE:HD13	1:M:673:PRO:CG	2.48	0.44
1:M:1295:ASP:HA	1:U:304:THR:HG21	2.00	0.44
1:U:668:ILE:HD13	1:U:673:PRO:CG	2.47	0.44
2:C:338:LYS:HB3	2:O:349:GLN:NE2	2.33	0.44
2:K:1059:ILE:HD13	2:K:1088:ILE:HD12	1.99	0.44
2:K:1095:GLU:OE1	2:K:1099:HIS:NE2	2.47	0.44
2:O:1303:ALA:N	5:O:2040:HOH:O	2.51	0.44
2:S:1303:ALA:CA	5:S:2038:HOH:O	2.65	0.44
2:S:1425:LEU:CD1	2:S:1564:MET:HB3	2.47	0.44
2:X:1693:HIS:HA	2:X:1696:ILE:HG22	1.99	0.44
1:E:1796:SER:H	1:E:2001:ASN:HD21	1.66	0.44
1:I:115:LYS:O	1:I:118:ILE:HG22	2.18	0.44
1:Q:519:ASP:OD1	1:Q:520:SER:N	2.51	0.44
1:Q:725:GLY:HA3	5:Q:2401:HOH:O	2.17	0.44
1:Q:1213:ALA:HB2	5:Q:2249:HOH:O	2.17	0.44
1:U:1033:ASP:OD1	1:U:1033:ASP:N	2.51	0.44
1:U:1452:GLU:C	1:U:1452:GLU:OE1	2.60	0.44
1:U:1618:ILE:HG22	1:U:1623:ILE:HG12	2.00	0.44
2:G:696:LEU:HD11	2:G:735:LEU:HD13	1.98	0.44
5:K:2251:HOH:O	2:X:341:LEU:HD23	2.17	0.44
2:O:1425:LEU:O	2:O:1429:ARG:NE	2.50	0.44
2:O:1721:ASP:HB3	2:O:1724:ALA:HB2	2.00	0.44
2:S:51:PRO:HD3	2:S:80:CYS:SG	2.57	0.44
2:S:340:GLN:HA	2:S:343:VAL:HG22	1.99	0.44
1:A:1523:SER:HB3	1:A:1582:TRP:CE3	2.53	0.43
1:E:1137:TRP:CD1	1:E:1197:LEU:HD22	2.53	0.43
1:E:1654:THR:HG23	2:G:52:THR:HG22	2.00	0.43
1:I:1021:SER:HB3	5:I:2358:HOH:O	2.18	0.43
1:M:879:ILE:HG21	1:M:898:VAL:CG2	2.46	0.43
1:M:1665:MET:O	1:M:1669:ASN:OD1	2.35	0.43
1:U:178:LEU:HD21	1:U:234:CYS:SG	2.57	0.43
1:U:931:ARG:NH1	1:U:962:ASN:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:651:GLY:N	5:C:2029:HOH:O	2.51	0.43
2:C:1653:LYS:HD2	5:X:2138:HOH:O	2.18	0.43
2:G:1391:LEU:O	2:G:1395:MET:HG3	2.18	0.43
2:K:784:LEU:HD21	2:S:806:LEU:HB3	2.00	0.43
2:O:1004:ILE:CD1	5:O:2291:HOH:O	2.59	0.43
2:O:1364:MET:CE	5:O:2074:HOH:O	2.57	0.43
2:O:1588:PRO:O	2:O:1592:ALA:HB2	2.18	0.43
2:X:891:LEU:HD13	2:X:933:ILE:HD11	2.00	0.43
2:X:1400:HIS:O	2:X:1605:GLU:OE2	2.37	0.43
1:A:446:ASP:N	1:A:451:SER:O	2.44	0.43
1:A:982:LEU:HD11	2:C:1686:LYS:HB3	1.98	0.43
1:A:1265:ILE:HG22	5:A:2345:HOH:O	2.17	0.43
1:A:1419:VAL:HG13	1:A:1421:PHE:CE1	2.53	0.43
1:E:1679:ASP:O	1:E:1683:ARG:HD3	2.17	0.43
1:I:668:ILE:HD11	1:I:681:TYR:CD2	2.53	0.43
1:Q:325:MET:HE3	1:Q:367:SER:OG	2.18	0.43
1:U:1592:ARG:NH2	5:U:2231:HOH:O	2.50	0.43
2:G:708:VAL:HG23	5:G:2131:HOH:O	2.16	0.43
2:G:908:LEU:HD11	2:G:924:ALA:HB2	1.98	0.43
2:G:1223:LEU:CD2	2:G:1701:MET:HE2	2.48	0.43
5:G:2226:HOH:O	2:S:1288:MET:SD	2.62	0.43
2:K:448:LYS:NZ	5:K:2016:HOH:O	2.47	0.43
2:K:1312:ASP:OD1	2:O:1322:LYS:NZ	2.51	0.43
2:S:1279:ILE:HA	2:S:1282:MET:HE1	1.99	0.43
2:X:339:GLN:O	2:X:343:VAL:HG22	2.18	0.43
2:X:534:MET:HE3	5:X:2017:HOH:O	2.18	0.43
1:A:1708:PHE:O	1:A:1714:ARG:NH1	2.52	0.43
1:E:668:ILE:HD13	1:E:673:PRO:CG	2.48	0.43
1:I:1159:HIS:O	1:I:1163:THR:OG1	2.35	0.43
1:M:166:LEU:HD21	1:M:234:CYS:HB2	2.00	0.43
1:M:336:VAL:O	1:M:340:ILE:HD13	2.17	0.43
1:Q:598:LEU:HD23	1:Q:598:LEU:C	2.43	0.43
1:Q:668:ILE:HD11	1:Q:681:TYR:CD2	2.53	0.43
2:C:36:LEU:HD22	2:C:61:ILE:CG2	2.48	0.43
2:C:1179:ARG:CG	5:C:2133:HOH:O	2.40	0.43
2:G:410:GLN:NE2	2:G:1633:ARG:NH2	2.66	0.43
2:G:442:ALA:HA	2:G:446:LEU:HD23	2.00	0.43
2:K:348:LEU:HD12	2:S:338:LYS:HD3	2.00	0.43
2:S:1083:ILE:HD13	5:S:2154:HOH:O	2.18	0.43
2:X:803:LEU:HD21	5:X:2099:HOH:O	2.18	0.43
1:A:166:LEU:HD21	1:A:234:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:ARG:HA	5:A:2424:HOH:O	2.19	0.43
1:A:760:SER:OG	1:A:763:ASP:OD1	2.17	0.43
1:A:1223:LEU:HB3	1:A:1238:ILE:HD12	1.99	0.43
1:A:1284:SER:HA	5:A:2321:HOH:O	2.18	0.43
1:A:1974:LYS:HB3	1:A:1974:LYS:HZ1	1.84	0.43
5:A:2323:HOH:O	2:C:986:ALA:HB3	2.17	0.43
1:E:1304:ALA:CA	5:E:2384:HOH:O	2.67	0.43
1:E:1304:ALA:HA	5:E:2384:HOH:O	2.18	0.43
1:I:689:HIS:CE1	5:I:2266:HOH:O	2.71	0.43
1:Q:685:LEU:HD12	1:Q:687:LEU:HD11	1.99	0.43
1:Q:1016:PHE:HZ	5:Q:2323:HOH:O	2.00	0.43
1:U:306:LEU:HD12	1:U:311:LEU:HB3	2.00	0.43
1:U:334:LYS:NZ	1:U:335:GLN:HG2	2.34	0.43
2:G:1322:LYS:NZ	2:S:1312:ASP:OD1	2.51	0.43
2:G:1540:ILE:O	2:G:1570:ARG:NH2	2.47	0.43
2:G:1588:PRO:O	2:G:1592:ALA:HB2	2.18	0.43
2:G:1695:ALA:HB1	2:G:1700:THR:C	2.43	0.43
2:K:415:MET:HE1	2:K:424:LEU:HD13	1.99	0.43
2:O:1181:ASP:HB3	2:O:1350:ASN:OD1	2.18	0.43
2:O:1376:MET:O	2:O:1587:HIS:N	2.48	0.43
2:S:891:LEU:HD11	2:S:893:VAL:HG22	1.99	0.43
1:A:871:LEU:O	1:A:875:ARG:HB3	2.18	0.43
1:E:613:SER:CA	1:E:614:PRO:HG2	2.48	0.43
1:M:340:ILE:CD1	1:M:376:PHE:CZ	2.96	0.43
1:M:1759:LEU:O	1:M:1765:THR:OG1	2.30	0.43
2:C:795:HIS:CE1	2:C:842:SER:HG	2.35	0.43
2:G:792:GLU:OE1	2:X:804:ARG:NH2	2.45	0.43
2:K:534:MET:HE1	2:K:933:ILE:CD1	2.49	0.43
2:O:802:LEU:O	2:O:806:LEU:HD13	2.19	0.43
1:A:847:ARG:NH1	1:A:884:ASN:O	2.51	0.43
1:A:1595:LYS:HD3	1:A:1641:GLU:H	1.84	0.43
1:E:1523:SER:HB3	1:E:1582:TRP:CE3	2.53	0.43
1:E:1671:SER:OG	1:E:1674:ALA:CB	2.66	0.43
1:I:703:VAL:HG11	1:I:717:LEU:HD12	2.01	0.43
1:M:1719:ASN:O	1:M:1723:MET:HG3	2.18	0.43
1:M:1877:VAL:HG11	1:M:1889:ALA:HB3	2.01	0.43
1:Q:166:LEU:HD21	1:Q:234:CYS:HB2	2.00	0.43
1:Q:703:VAL:HG11	1:Q:717:LEU:HD12	2.01	0.43
1:Q:931:ARG:NH1	1:Q:962:ASN:OD1	2.52	0.43
1:U:1654:THR:HG23	2:X:52:THR:CG2	2.48	0.43
2:C:534:MET:HE3	5:C:2018:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:937:LYS:NZ	2:O:855:SER:O	2.44	0.43
2:C:1621:LEU:HD12	2:C:1621:LEU:N	2.31	0.43
2:G:1281:THR:CA	5:G:2151:HOH:O	2.65	0.43
2:G:1429:ARG:HH12	2:S:1719:TYR:HB3	1.84	0.43
2:K:349:GLN:HB3	2:K:351:ARG:HG3	2.00	0.43
2:K:439:MET:HE3	2:K:478:ASN:HB3	2.01	0.43
1:A:123:TYR:CZ	1:A:242:VAL:HG22	2.54	0.43
1:A:856:ASP:HB2	5:A:2400:HOH:O	2.19	0.43
1:A:1591:VAL:HG23	1:A:1591:VAL:O	2.19	0.43
1:E:191:SER:N	5:E:2230:HOH:O	2.50	0.43
1:E:587:THR:HG23	5:E:2376:HOH:O	2.07	0.43
1:M:1607:THR:HG23	1:M:1631:VAL:HB	2.00	0.43
1:Q:1617:MET:HE3	1:Q:1785:LEU:HD23	2.00	0.43
1:U:1444:PHE:CA	5:U:2401:HOH:O	2.67	0.43
2:G:687:GLY:O	2:G:690:SER:OG	2.34	0.43
2:G:802:LEU:O	2:G:806:LEU:HD13	2.19	0.43
2:K:1692:MET:O	2:K:1696:ILE:HG22	2.19	0.43
2:X:986:ALA:HB3	5:X:2165:HOH:O	2.17	0.43
1:E:333:ILE:HG13	1:E:364:LEU:HD11	2.01	0.43
1:E:446:ASP:N	1:E:451:SER:O	2.47	0.43
1:I:668:ILE:HD11	1:I:681:TYR:HD2	1.84	0.43
1:I:1284:SER:HA	5:I:2364:HOH:O	2.19	0.43
1:I:1565:ILE:HG21	1:I:1601:MET:HG2	2.00	0.43
1:M:616:MET:CB	5:M:2362:HOH:O	2.66	0.43
1:U:1671:SER:OG	1:U:1674:ALA:HB3	2.19	0.43
1:U:1780:ILE:HG22	1:U:1786:ILE:HD11	1.99	0.43
2:C:990:PHE:CE1	2:C:1223:LEU:HD11	2.54	0.43
2:C:1716:GLN:H	2:C:1717:PRO:HG3	1.84	0.43
2:G:694:GLU:HB2	2:G:902:ALA:HB2	2.01	0.43
2:G:1692:MET:HE1	5:G:2296:HOH:O	2.18	0.43
2:K:787:ILE:HD12	2:K:838:LEU:HD12	2.00	0.43
2:O:1094:GLU:OE1	2:O:1095:GLU:HG3	2.18	0.43
2:S:36:LEU:HD22	2:S:61:ILE:CG2	2.48	0.43
2:X:1031:ASN:ND2	2:X:1031:ASN:H	2.16	0.43
1:A:668:ILE:HD13	1:A:673:PRO:HG2	2.00	0.43
1:A:1419:VAL:CG2	5:A:2304:HOH:O	2.61	0.43
1:E:1031:VAL:O	1:E:1033:ASP:N	2.52	0.43
1:I:221:VAL:HG21	1:I:412:ALA:HB3	2.01	0.43
1:I:931:ARG:NH1	1:I:962:ASN:OD1	2.52	0.43
1:M:1842:MET:HG2	1:M:1889:ALA:HB2	2.01	0.43
1:Q:181:ILE:HD12	1:Q:287:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:668:ILE:HD11	1:Q:681:TYR:HD2	1.84	0.43
1:U:660:GLY:O	1:U:1153:HIS:N	2.52	0.43
1:U:1141:PHE:HE2	1:U:1195:ILE:HG21	1.84	0.43
1:U:1617:MET:HE3	1:U:1785:LEU:HD23	2.01	0.43
2:O:439:MET:CE	2:O:482:VAL:HG21	2.49	0.43
2:O:1208:ASP:OD1	2:O:1208:ASP:N	2.46	0.43
2:O:1281:THR:CA	5:O:2144:HOH:O	2.66	0.43
2:S:439:MET:HE3	2:S:478:ASN:HB3	2.01	0.43
2:S:953:ILE:CG2	5:S:2257:HOH:O	2.40	0.43
2:X:442:ALA:HA	2:X:446:LEU:HD23	1.99	0.43
2:X:1265:ALA:CB	2:X:1267:LYS:HE2	2.48	0.43
1:A:982:LEU:CD1	2:C:1686:LYS:HB3	2.49	0.43
1:A:1033:ASP:N	1:A:1033:ASP:OD1	2.52	0.43
1:A:1463:TYR:CD2	1:A:1466:ILE:HD11	2.54	0.43
1:A:1595:LYS:HD2	1:A:1641:GLU:OE1	2.19	0.43
1:E:623:ASP:OD1	1:E:627:ARG:NH2	2.52	0.43
1:E:660:GLY:O	1:E:1153:HIS:N	2.52	0.43
1:I:720:THR:HG21	3:I:2101:FMN:O3'	2.19	0.43
1:I:1031:VAL:O	1:I:1033:ASP:N	2.52	0.43
1:I:1595:LYS:HD3	1:I:1641:GLU:H	1.83	0.43
1:M:1581:GLU:HG3	1:M:1582:TRP:CD1	2.54	0.43
1:Q:944:ARG:NH1	2:S:986:ALA:O	2.45	0.43
1:Q:1595:LYS:HD3	1:Q:1641:GLU:H	1.83	0.43
1:U:221:VAL:HG21	1:U:412:ALA:HB3	2.01	0.43
1:U:668:ILE:HD11	1:U:681:TYR:HD2	1.84	0.43
2:C:433:ASN:OD1	2:C:437:GLN:NE2	2.43	0.43
2:C:687:GLY:O	2:C:690:SER:OG	2.30	0.43
2:C:1693:HIS:HA	2:C:1696:ILE:HG22	2.00	0.43
2:K:1056:MET:HE1	2:K:1099:HIS:HB2	2.01	0.43
2:O:357:LEU:O	2:O:357:LEU:HD13	2.19	0.43
2:S:657:LYS:H	2:S:657:LYS:HE2	1.83	0.43
2:S:1303:ALA:N	5:S:2038:HOH:O	2.51	0.43
2:X:691:ILE:HG22	2:X:695:ILE:HD12	2.00	0.43
2:X:840:SER:HA	5:X:2069:HOH:O	2.18	0.43
2:X:983:GLU:CG	5:X:2020:HOH:O	2.11	0.43
1:A:660:GLY:O	1:A:1153:HIS:N	2.51	0.42
1:E:176:ASP:OD1	1:E:176:ASP:C	2.62	0.42
1:E:668:ILE:HD11	1:E:681:TYR:HD2	1.84	0.42
1:E:999:GLY:HA3	5:E:2239:HOH:O	2.18	0.42
1:E:1031:VAL:O	1:E:1031:VAL:HG23	2.19	0.42
1:E:1591:VAL:HG23	1:E:1591:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1191:PRO:O	1:I:1210:HIS:NE2	2.45	0.42
1:I:1842:MET:HG2	1:I:1889:ALA:HB2	2.00	0.42
1:M:999:GLY:HA3	5:M:2237:HOH:O	2.18	0.42
1:Q:1505:ARG:NH2	2:S:963:ILE:HG21	2.34	0.42
1:Q:1621:ARG:NH1	1:Q:1621:ARG:HB2	2.33	0.42
1:U:814:VAL:HG12	1:U:815:PRO:O	2.19	0.42
1:U:850:MET:HE1	1:U:853:LYS:HD2	2.01	0.42
1:U:2017:VAL:HG21	2:X:13:LEU:HD11	2.01	0.42
1:U:2018:TYR:CE1	1:U:2027:LYS:HD3	2.53	0.42
2:C:1540:ILE:O	2:C:1570:ARG:NH2	2.48	0.42
2:G:855:SER:O	2:X:937:LYS:NZ	2.45	0.42
2:G:1049:ALA:CB	5:G:2073:HOH:O	2.52	0.42
2:G:1129:ASP:OD1	2:K:347:TYR:CZ	2.72	0.42
2:O:499:LYS:HG3	2:O:511:GLU:OE2	2.17	0.42
2:O:1091:LYS:HE3	2:O:1092:TYR:CZ	2.54	0.42
2:S:723:ASN:ND2	5:S:2039:HOH:O	2.51	0.42
2:X:64:LYS:HE2	2:X:64:LYS:HB2	1.81	0.42
1:A:159:TYR:CD1	1:A:159:TYR:C	2.97	0.42
1:A:265:VAL:HG11	1:A:289:LEU:HD22	2.01	0.42
1:A:685:LEU:HD12	1:A:687:LEU:HD11	2.01	0.42
1:E:1304:ALA:HB1	5:E:2384:HOH:O	2.19	0.42
1:E:1505:ARG:NH2	2:G:963:ILE:HG21	2.34	0.42
1:I:527:TYR:HA	5:I:2225:HOH:O	2.17	0.42
1:M:871:LEU:O	1:M:875:ARG:HB3	2.19	0.42
1:M:1033:ASP:OD1	1:M:1033:ASP:N	2.51	0.42
1:Q:689:HIS:CE1	5:Q:2267:HOH:O	2.71	0.42
1:Q:1583:ALA:HB1	1:Q:1644:ILE:HD13	2.01	0.42
1:Q:1679:ASP:O	1:Q:1683:ARG:HD3	2.18	0.42
2:C:1019:VAL:HB	2:C:1399:ILE:HG23	2.01	0.42
2:O:687:GLY:O	2:O:690:SER:OG	2.33	0.42
2:X:447:ILE:O	2:X:451:GLN:HG3	2.19	0.42
2:X:908:LEU:HD11	2:X:924:ALA:HB2	2.00	0.42
2:X:910:THR:OG1	2:X:913:ILE:HD13	2.19	0.42
2:X:910:THR:O	2:X:914:VAL:HG23	2.19	0.42
1:A:304:THR:HG23	1:E:1300:ARG:NH2	2.34	0.42
1:A:774:GLU:CB	5:A:2340:HOH:O	2.66	0.42
1:A:850:MET:HE1	1:A:853:LYS:HD2	2.00	0.42
1:E:336:VAL:O	1:E:340:ILE:HD13	2.19	0.42
1:E:668:ILE:HD11	1:E:681:TYR:CD2	2.53	0.42
1:E:879:ILE:HG21	1:E:898:VAL:CG2	2.46	0.42
1:I:872:ASN:HA	1:I:875:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1617:MET:HE3	1:I:1785:LEU:HD23	2.00	0.42
1:M:623:ASP:OD1	1:M:627:ARG:NH2	2.52	0.42
1:M:668:ILE:HD11	1:M:681:TYR:CD2	2.53	0.42
1:Q:623:ASP:OD1	1:Q:627:ARG:NH2	2.53	0.42
1:Q:720:THR:HG21	3:Q:2101:FMN:O3'	2.19	0.42
1:Q:1565:ILE:HG21	1:Q:1601:MET:HG2	2.01	0.42
2:C:963:ILE:HG23	5:C:2144:HOH:O	2.19	0.42
2:C:1286:VAL:HG12	2:C:1291:LEU:HD23	2.00	0.42
2:C:1450:GLN:CD	2:C:1453:LYS:HZ3	2.26	0.42
2:G:965:GLN:HB3	5:G:2033:HOH:O	2.20	0.42
2:O:871:TRP:CD1	2:O:895:THR:HG23	2.54	0.42
2:S:824:LEU:CG	5:S:2273:HOH:O	2.56	0.42
2:S:1056:MET:HE1	2:S:1099:HIS:HB2	2.01	0.42
2:X:1401:ALA:HB3	2:X:1601:ILE:CD1	2.48	0.42
1:A:1141:PHE:HE2	1:A:1195:ILE:HG21	1.82	0.42
1:A:1447:LEU:HD23	1:A:1474:LEU:HD13	2.01	0.42
1:A:2028:SER:O	1:A:2032:ASN:OD1	2.38	0.42
1:E:1877:VAL:HG11	1:E:1889:ALA:HB3	2.00	0.42
1:I:623:ASP:OD1	1:I:627:ARG:NH2	2.53	0.42
1:M:613:SER:CA	1:M:614:PRO:CG	2.98	0.42
1:M:1031:VAL:HG23	1:M:1031:VAL:O	2.19	0.42
1:M:1304:ALA:HA	5:M:2381:HOH:O	2.19	0.42
1:Q:1333:LEU:N	5:Q:2206:HOH:O	2.43	0.42
1:U:1862:VAL:HA	1:U:1928:LEU:HD21	2.02	0.42
2:C:910:THR:OG1	2:C:913:ILE:HD13	2.20	0.42
2:C:996:LYS:HE3	2:C:1000:GLU:OE1	2.19	0.42
2:G:662:TYR:OH	2:G:904:ASN:O	2.37	0.42
2:O:662:TYR:OH	2:O:904:ASN:O	2.37	0.42
2:O:1603:ILE:CG2	2:O:1640:ILE:HD13	2.50	0.42
2:S:787:ILE:HD12	2:S:838:LEU:HD12	2.00	0.42
1:E:1522:LEU:HD21	1:E:1583:ALA:HA	2.01	0.42
1:I:1031:VAL:O	1:I:1031:VAL:HG23	2.19	0.42
1:M:660:GLY:O	1:M:1153:HIS:N	2.52	0.42
1:Q:111:ILE:HG22	1:Q:112:ALA:H	1.84	0.42
1:Q:907:LYS:HE3	5:Q:2231:HOH:O	2.18	0.42
1:Q:1031:VAL:O	1:Q:1033:ASP:N	2.52	0.42
2:C:1716:GLN:HB2	5:C:2140:HOH:O	2.19	0.42
2:K:1332:ASP:OD2	2:K:1590:GLY:CA	2.67	0.42
2:S:910:THR:OG1	2:S:913:ILE:HD13	2.19	0.42
2:S:1212:LEU:CG	5:S:2025:HOH:O	2.65	0.42
2:X:854:TYR:OH	2:X:920:GLU:OE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1019:VAL:HB	2:X:1399:ILE:HG23	2.01	0.42
2:X:1054:TRP:NE1	2:X:1696:ILE:O	2.52	0.42
2:X:1315:ILE:HB	5:X:2006:HOH:O	2.18	0.42
1:A:306:LEU:HD11	1:A:310:MET:HE3	2.00	0.42
1:E:974:LYS:C	1:E:974:LYS:CD	2.93	0.42
1:M:974:LYS:CD	1:M:974:LYS:C	2.93	0.42
1:M:1796:SER:H	1:M:2001:ASN:HD21	1.67	0.42
1:Q:1031:VAL:O	1:Q:1031:VAL:HG23	2.19	0.42
1:U:147:VAL:O	1:U:487:LEU:HD12	2.20	0.42
1:U:1415:THR:CB	5:U:2239:HOH:O	2.66	0.42
1:U:1877:VAL:HG11	1:U:1889:ALA:HB3	2.00	0.42
2:C:35:PHE:CD1	2:C:44:ILE:HD11	2.54	0.42
2:C:1410:THR:HG22	2:C:1652:GLN:O	2.20	0.42
2:G:1603:ILE:CG2	2:G:1640:ILE:HD13	2.50	0.42
2:G:1695:ALA:HB1	2:G:1701:MET:HA	2.01	0.42
2:K:1059:ILE:HG22	2:K:1083:ILE:HD13	2.01	0.42
2:O:694:GLU:HB2	2:O:902:ALA:HB2	2.01	0.42
2:O:996:LYS:CD	5:O:2168:HOH:O	2.67	0.42
2:O:1200:PRO:HD3	5:O:2232:HOH:O	2.19	0.42
2:X:412:VAL:HG13	4:X:1901:PKZ:C14	2.49	0.42
2:X:1250:MET:HE2	2:X:1589:LYS:HE3	2.02	0.42
2:X:1444:ILE:HG13	5:X:2072:HOH:O	2.19	0.42
1:A:720:THR:HG21	3:A:2101:FMN:O3'	2.19	0.42
1:A:1608:LEU:CD2	1:A:1637:VAL:HG21	2.49	0.42
1:E:616:MET:CG	5:E:2360:HOH:O	2.44	0.42
1:M:512:ILE:O	1:M:528:GLY:N	2.43	0.42
1:M:1522:LEU:HD21	1:M:1583:ALA:HA	2.00	0.42
1:Q:1874:LEU:HD21	1:Q:1895:LEU:HD12	2.02	0.42
1:U:320:GLY:HA3	5:U:2407:HOH:O	2.20	0.42
1:U:639:ILE:HG12	1:U:645:MET:CE	2.49	0.42
2:C:1049:ALA:CB	5:C:2056:HOH:O	2.47	0.42
2:C:1691:TYR:CD1	2:C:1691:TYR:C	2.98	0.42
2:K:1239:VAL:HG13	5:K:2156:HOH:O	2.18	0.42
2:K:1540:ILE:O	2:K:1540:ILE:HG22	2.20	0.42
2:O:433:ASN:OD1	2:O:437:GLN:NE2	2.45	0.42
2:S:1603:ILE:CG2	2:S:1640:ILE:HD13	2.50	0.42
2:X:1200:PRO:HD3	5:X:2156:HOH:O	2.19	0.42
2:X:1588:PRO:O	2:X:1592:ALA:HB2	2.19	0.42
1:A:221:VAL:HG21	1:A:412:ALA:HB3	2.00	0.42
1:A:265:VAL:HG13	1:A:468:ILE:HD11	2.02	0.42
1:A:1081:ASP:CB	1:A:1084:LYS:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:HIS:NE2	2:K:67:SER:OG	2.53	0.42
1:I:315:LEU:HD21	1:I:321:ARG:CZ	2.50	0.42
1:I:1228:PRO:CB	5:I:2246:HOH:O	2.60	0.42
1:I:1874:LEU:HD21	1:I:1895:LEU:HD12	2.02	0.42
1:M:176:ASP:C	1:M:176:ASP:OD1	2.63	0.42
1:M:1031:VAL:O	1:M:1033:ASP:N	2.52	0.42
1:M:1505:ARG:NH2	2:O:963:ILE:HG21	2.34	0.42
1:Q:1620:GLY:N	1:Q:1784:GLY:O	2.50	0.42
1:Q:1621:ARG:NH1	1:Q:1643:GLU:OE1	2.52	0.42
1:U:879:ILE:HG21	1:U:898:VAL:CG2	2.47	0.42
2:C:499:LYS:HE3	2:C:513:THR:HG21	2.01	0.42
2:G:428:ASP:CB	2:G:430:GLU:OE1	2.68	0.42
2:G:989:LYS:HB3	5:G:2247:HOH:O	2.20	0.42
2:G:1059:ILE:HD13	2:G:1088:ILE:HD12	2.02	0.42
2:G:1200:PRO:HD3	5:G:2232:HOH:O	2.18	0.42
2:K:1197:TYR:HE1	5:K:2165:HOH:O	2.03	0.42
2:K:1368:THR:OG1	2:K:1622:LEU:HD13	2.20	0.42
2:O:965:GLN:HB3	5:O:2035:HOH:O	2.20	0.42
2:S:534:MET:HE1	2:S:933:ILE:CD1	2.49	0.42
2:S:1692:MET:O	2:S:1696:ILE:HG22	2.20	0.42
2:X:1417:VAL:HG13	2:X:1651:GLY:HA2	2.01	0.42
1:A:56:ALA:HB3	1:A:97:PHE:HZ	1.85	0.42
1:A:880:LYS:NZ	5:A:2238:HOH:O	2.53	0.42
1:E:116:GLU:HB3	1:E:169:LEU:HD13	2.01	0.42
1:E:306:LEU:HD12	1:E:311:LEU:HB3	2.02	0.42
1:E:985:GLU:CD	2:G:1694:ASN:HA	2.45	0.42
1:I:179:VAL:HG13	1:I:183:GLU:OE1	2.20	0.42
1:I:203:LEU:O	1:I:207:LYS:HG2	2.19	0.42
1:I:1279:SER:O	1:I:1283:ILE:HG12	2.20	0.42
1:I:1505:ARG:NH2	2:K:963:ILE:HG21	2.34	0.42
1:M:346:HIS:NE2	2:S:67:SER:OG	2.53	0.42
1:Q:97:PHE:CE1	1:Q:101:LEU:HD11	2.55	0.42
1:Q:221:VAL:HG21	1:Q:412:ALA:HB3	2.01	0.42
2:C:348:LEU:HD13	2:O:338:LYS:NZ	2.34	0.42
2:G:1402:VAL:HG11	2:G:1533:PHE:CZ	2.55	0.42
2:K:723:ASN:ND2	5:K:2035:HOH:O	2.52	0.42
2:K:990:PHE:CZ	2:K:1223:LEU:HD11	2.55	0.42
2:K:1425:LEU:O	2:K:1429:ARG:NE	2.51	0.42
5:K:2109:HOH:O	2:S:835:PHE:CE1	2.72	0.42
2:O:656:LYS:CE	5:O:2149:HOH:O	2.59	0.42
2:S:1332:ASP:OD2	2:S:1590:GLY:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1540:ILE:O	2:S:1540:ILE:HG22	2.20	0.42
1:A:306:LEU:HD21	1:A:310:MET:CE	2.50	0.42
1:A:623:ASP:OD1	1:A:627:ARG:NH2	2.52	0.42
1:A:1421:PHE:CZ	1:A:1447:LEU:HG	2.55	0.42
1:E:603:HIS:HA	5:E:2346:HOH:O	2.20	0.42
1:E:1323:ALA:HB1	1:E:1364:ILE:HG12	2.02	0.42
1:E:1874:LEU:HD21	1:E:1895:LEU:HD12	2.02	0.42
1:M:603:HIS:HA	5:M:2346:HOH:O	2.19	0.42
1:M:668:ILE:HD11	1:M:681:TYR:HD2	1.84	0.42
1:M:764:THR:OG1	1:M:1069:HIS:NE2	2.48	0.42
1:M:1395:GLN:HG2	5:M:2229:HOH:O	2.16	0.42
1:M:1845:VAL:HG21	1:M:1859:LEU:HD11	2.02	0.42
1:U:760:SER:OG	1:U:763:ASP:OD1	2.20	0.42
2:C:344:LEU:HD11	2:S:340:GLN:C	2.44	0.42
2:C:435:CYS:SG	2:C:475:LEU:HD13	2.60	0.42
2:C:1054:TRP:NE1	2:C:1696:ILE:O	2.53	0.42
2:K:528:MET:CE	2:K:642:LEU:HG	2.50	0.42
2:X:338:LYS:HA	2:X:341:LEU:HD12	2.02	0.42
2:X:1449:ARG:O	2:X:1453:LYS:HD3	2.20	0.42
1:A:982:LEU:CD1	2:C:1690:ARG:HH21	2.25	0.41
1:A:1031:VAL:O	1:A:1033:ASP:N	2.53	0.41
1:A:1877:VAL:HG11	1:A:1889:ALA:HB3	2.01	0.41
1:E:239:THR:HG23	1:E:533:ILE:HD11	2.01	0.41
1:E:449:ASP:OD2	1:E:451:SER:OG	2.28	0.41
1:E:475:TRP:O	1:E:479:THR:HG22	2.20	0.41
1:E:871:LEU:O	1:E:875:ARG:HB3	2.19	0.41
1:M:1874:LEU:HD21	1:M:1895:LEU:HD12	2.02	0.41
1:U:524:ASP:OD1	1:U:524:ASP:N	2.46	0.41
1:U:1031:VAL:HG23	1:U:1031:VAL:O	2.20	0.41
1:U:1528:LEU:HD21	1:U:1612:MET:HE3	2.02	0.41
2:C:1303:ALA:CA	5:C:2065:HOH:O	2.68	0.41
2:C:1366:ARG:NH2	2:C:1371:THR:O	2.49	0.41
2:C:1502:LYS:HD3	2:C:1503:ARG:HH12	1.84	0.41
2:C:1537:ILE:HD13	2:C:1568:LEU:HD13	2.01	0.41
2:G:1332:ASP:OD2	2:G:1590:GLY:CA	2.68	0.41
2:G:1695:ALA:HB1	2:G:1701:MET:N	2.35	0.41
2:O:1059:ILE:HD13	2:O:1088:ILE:HD12	2.02	0.41
2:O:1286:VAL:HG12	2:O:1291:LEU:CD2	2.50	0.41
2:S:1086:LYS:HB2	5:S:2132:HOH:O	2.20	0.41
2:X:433:ASN:OD1	2:X:437:GLN:NE2	2.42	0.41
2:X:1137:LYS:O	2:X:1141:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1695:ALA:HB1	2:X:1701:MET:HA	2.01	0.41
1:A:1683:ARG:HD3	1:A:1683:ARG:H	1.85	0.41
1:A:1874:LEU:HD21	1:A:1895:LEU:HD12	2.03	0.41
1:E:1151:SER:O	1:E:1151:SER:OG	2.34	0.41
1:E:1523:SER:CB	1:E:1582:TRP:CE3	3.03	0.41
1:I:762:GLU:HA	1:I:1072:ARG:HH22	1.85	0.41
1:M:1687:ASN:ND2	5:M:2226:HOH:O	2.48	0.41
1:Q:115:LYS:O	1:Q:118:ILE:HG22	2.20	0.41
1:Q:839:GLU:N	5:Q:2235:HOH:O	2.53	0.41
1:U:512:ILE:O	1:U:528:GLY:N	2.45	0.41
1:U:1874:LEU:HD21	1:U:1895:LEU:HD12	2.02	0.41
1:U:1977:GLN:NE2	2:X:16:GLU:OE2	2.48	0.41
2:C:910:THR:O	2:C:914:VAL:HG23	2.20	0.41
2:C:986:ALA:HB2	2:C:1050:ILE:CD1	2.50	0.41
2:G:1091:LYS:HE3	2:G:1092:TYR:CZ	2.54	0.41
2:K:1223:LEU:CD2	2:K:1701:MET:HE2	2.50	0.41
2:O:428:ASP:CB	2:O:430:GLU:OE2	2.68	0.41
2:O:442:ALA:HA	2:O:446:LEU:HD23	2.02	0.41
2:O:1692:MET:HE1	5:O:2295:HOH:O	2.21	0.41
2:S:451:GLN:O	2:S:455:ASP:OD1	2.39	0.41
1:A:1323:ALA:HB1	1:A:1364:ILE:HG12	2.03	0.41
1:A:2032:ASN:OD1	1:A:2032:ASN:N	2.53	0.41
1:E:1136:ASN:ND2	5:E:2204:HOH:O	2.52	0.41
1:E:1209:GLU:OE1	1:E:1552:SER:OG	2.26	0.41
1:I:944:ARG:NH1	2:K:986:ALA:O	2.45	0.41
1:I:1333:LEU:N	5:I:2204:HOH:O	2.42	0.41
1:I:1714:ARG:NH2	2:S:918:GLN:OE1	2.53	0.41
1:M:1523:SER:CB	1:M:1582:TRP:CE3	3.04	0.41
1:U:166:LEU:HD21	1:U:234:CYS:HB2	2.01	0.41
1:U:479:THR:O	1:U:481:HIS:N	2.53	0.41
2:C:1588:PRO:O	2:C:1592:ALA:HB2	2.20	0.41
2:C:1603:ILE:CG2	2:C:1640:ILE:HD13	2.50	0.41
2:C:1695:ALA:HB1	2:C:1701:MET:N	2.35	0.41
2:G:697:GLN:NE2	2:G:724:MET:SD	2.93	0.41
2:K:986:ALA:HB2	2:K:1050:ILE:HD13	2.02	0.41
2:K:1342:PHE:HB3	2:K:1348:THR:HG23	2.02	0.41
2:K:1695:ALA:HB1	2:K:1701:MET:N	2.35	0.41
2:O:1023:PHE:CE1	2:O:1601:ILE:HG21	2.56	0.41
2:O:1179:ARG:CG	5:O:2189:HOH:O	2.49	0.41
2:S:964:GLU:CD	5:S:2160:HOH:O	2.63	0.41
2:X:340:GLN:HA	2:X:343:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1441:LEU:HD21	2:X:1516:PHE:O	2.21	0.41
1:A:1618:ILE:O	1:A:1618:ILE:HG23	2.21	0.41
1:E:340:ILE:CD1	1:E:376:PHE:CZ	2.96	0.41
1:E:613:SER:CA	1:E:614:PRO:CG	2.98	0.41
1:I:2017:VAL:HG21	2:K:13:LEU:HD11	2.02	0.41
1:M:116:GLU:HB3	1:M:169:LEU:HD13	2.03	0.41
1:M:449:ASP:OD2	1:M:451:SER:OG	2.30	0.41
1:M:1304:ALA:CA	5:M:2381:HOH:O	2.68	0.41
1:Q:524:ASP:OD1	1:Q:524:ASP:N	2.46	0.41
1:Q:1284:SER:HA	5:Q:2368:HOH:O	2.20	0.41
1:U:265:VAL:HG13	1:U:468:ILE:HD11	2.02	0.41
1:U:623:ASP:OD1	1:U:627:ARG:NH2	2.54	0.41
1:U:1225:LYS:HA	1:U:1225:LYS:CE	2.46	0.41
1:U:1671:SER:OG	1:U:1674:ALA:CB	2.68	0.41
2:C:1701:MET:HE3	2:C:1701:MET:CA	2.45	0.41
2:K:1011:MET:HE2	2:K:1011:MET:HB3	1.95	0.41
2:K:1309:GLU:OE1	2:K:1653:LYS:HE2	2.20	0.41
2:K:1315:ILE:HD11	2:K:1403:LEU:CD1	2.51	0.41
2:K:1603:ILE:CG2	2:K:1640:ILE:HD13	2.50	0.41
2:S:528:MET:CE	2:S:642:LEU:HG	2.50	0.41
1:A:60:GLY:HA2	1:A:63:ILE:HG22	2.02	0.41
1:A:430:VAL:HG11	1:A:461:ILE:HG21	2.01	0.41
1:E:1862:VAL:HA	1:E:1928:LEU:HD21	2.03	0.41
1:I:1522:LEU:O	1:I:1522:LEU:HD23	2.20	0.41
1:I:1845:VAL:HG21	1:I:1859:LEU:HD11	2.02	0.41
1:M:265:VAL:HG13	1:M:468:ILE:HD11	2.03	0.41
1:M:957:ASN:HA	5:M:2302:HOH:O	2.21	0.41
1:M:1136:ASN:ND2	5:M:2203:HOH:O	2.53	0.41
1:Q:1522:LEU:HD21	1:Q:1583:ALA:HA	2.03	0.41
1:Q:1862:VAL:HA	1:Q:1928:LEU:HD21	2.02	0.41
1:Q:2036:TYR:HD1	2:S:5:ILE:HG23	1.85	0.41
1:U:159:TYR:CD1	1:U:159:TYR:C	2.98	0.41
1:U:1421:PHE:HD2	1:U:1442:VAL:O	2.04	0.41
1:U:1514:VAL:O	1:U:1617:MET:N	2.53	0.41
2:C:871:TRP:CD1	2:C:895:THR:HG23	2.55	0.41
2:G:871:TRP:CD1	2:G:895:THR:HG23	2.55	0.41
2:G:1696:ILE:CG2	5:G:2013:HOH:O	2.62	0.41
2:K:428:ASP:CB	2:K:430:GLU:OE2	2.68	0.41
2:K:451:GLN:O	2:K:455:ASP:OD1	2.38	0.41
2:K:1376:MET:O	2:K:1587:HIS:N	2.47	0.41
2:O:1670:ASP:OD1	2:O:1673:THR:OG1	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:345:ALA:O	2:X:349:GLN:HG3	2.21	0.41
1:A:336:VAL:O	1:A:340:ILE:HG23	2.19	0.41
1:A:1147:ILE:HG22	1:A:1154:VAL:HG23	2.02	0.41
1:A:1892:LEU:HD21	1:A:1946:ILE:O	2.20	0.41
1:E:479:THR:O	1:E:479:THR:HG23	2.21	0.41
1:I:512:ILE:O	1:I:528:GLY:N	2.46	0.41
1:I:1151:SER:O	1:I:1151:SER:OG	2.31	0.41
1:Q:306:LEU:HD11	1:Q:310:MET:CE	2.51	0.41
2:C:381:HIS:HB2	2:O:377:TRP:HH2	1.86	0.41
2:G:412:VAL:HG13	4:G:1901:PKZ:C14	2.50	0.41
2:G:1366:ARG:NH2	2:G:1371:THR:O	2.54	0.41
2:K:659:SER:O	2:K:663:LEU:HD22	2.21	0.41
2:K:1143:TYR:OH	2:O:1124:ILE:HD11	2.20	0.41
2:O:697:GLN:NE2	2:O:724:MET:SD	2.92	0.41
2:O:1332:ASP:OD2	2:O:1590:GLY:CA	2.69	0.41
2:S:888:ILE:HD12	2:S:939:PHE:CE2	2.56	0.41
2:X:357:LEU:O	2:X:357:LEU:HD13	2.21	0.41
1:A:1759:LEU:O	1:A:1765:THR:OG1	2.29	0.41
1:E:65:PHE:C	1:E:65:PHE:CD1	2.99	0.41
1:E:1278:ILE:CG2	1:E:1283:ILE:HD11	2.50	0.41
1:I:1862:VAL:HA	1:I:1928:LEU:HD21	2.02	0.41
1:M:353:ILE:HD11	1:M:372:SER:HB2	2.03	0.41
1:M:1130:LEU:HD21	1:M:1162:LEU:HD12	2.01	0.41
1:M:1323:ALA:HB1	1:M:1364:ILE:HG12	2.02	0.41
1:M:1650:THR:CG2	2:O:41:THR:HG21	2.51	0.41
1:Q:116:GLU:OE1	1:Q:169:LEU:HD13	2.21	0.41
1:Q:839:GLU:CB	5:Q:2381:HOH:O	2.68	0.41
1:Q:1845:VAL:HG21	1:Q:1859:LEU:HD11	2.03	0.41
1:U:1031:VAL:O	1:U:1033:ASP:N	2.53	0.41
2:C:795:HIS:ND1	2:C:842:SER:OG	2.52	0.41
2:C:1368:THR:OG1	2:C:1622:LEU:HD13	2.21	0.41
2:G:708:VAL:CG1	2:G:737:VAL:HG22	2.51	0.41
2:G:996:LYS:CD	5:G:2158:HOH:O	2.69	0.41
2:G:1018:VAL:HG11	2:G:1315:ILE:HD13	2.02	0.41
2:G:1242:VAL:HG11	5:G:2238:HOH:O	2.21	0.41
2:K:1002:LYS:NZ	2:K:1007:GLU:OE1	2.52	0.41
2:X:1426:THR:HA	2:X:1429:ARG:CZ	2.50	0.41
1:A:679:THR:HG22	1:A:683:GLU:OE2	2.21	0.41
1:A:1031:VAL:O	1:A:1031:VAL:HG23	2.20	0.41
1:E:265:VAL:HG13	1:E:468:ILE:HD11	2.02	0.41
1:I:97:PHE:CZ	1:I:101:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:PHE:CD1	1:I:97:PHE:C	2.97	0.41
1:I:265:VAL:HG13	1:I:468:ILE:HD11	2.03	0.41
1:I:306:LEU:HD11	1:I:310:MET:CE	2.50	0.41
1:I:1016:PHE:HZ	5:I:2322:HOH:O	2.01	0.41
1:I:1725:PHE:CD2	1:I:1825:THR:HG23	2.55	0.41
1:I:1759:LEU:O	1:I:1765:THR:OG1	2.26	0.41
1:M:209:PRO:O	1:M:212:THR:HG22	2.20	0.41
1:Q:76:GLU:O	1:Q:80:LYS:HD3	2.20	0.41
1:Q:265:VAL:HG13	1:Q:468:ILE:HD11	2.03	0.41
1:Q:660:GLY:O	1:Q:1153:HIS:N	2.53	0.41
1:U:336:VAL:O	1:U:340:ILE:HG23	2.21	0.41
1:U:1323:ALA:HB1	1:U:1364:ILE:HG12	2.02	0.41
2:C:680:TYR:O	2:C:769:ASP:N	2.51	0.41
2:C:1013:ASP:OD1	2:C:1015:GLU:OE2	2.39	0.41
2:C:1137:LYS:O	2:C:1141:GLU:HG3	2.20	0.41
2:G:342:GLU:OE2	2:X:346:ARG:HG2	2.21	0.41
2:G:1292:SER:HB2	2:S:1413:ILE:HG12	2.03	0.41
2:G:1641:LYS:CD	5:G:2134:HOH:O	2.68	0.41
2:K:964:GLU:CD	5:K:2148:HOH:O	2.62	0.41
2:O:439:MET:HE3	2:O:482:VAL:HG21	2.03	0.41
2:S:1002:LYS:NZ	2:S:1007:GLU:OE1	2.52	0.41
2:X:967:VAL:HG23	5:X:2173:HOH:O	2.21	0.41
2:X:1181:ASP:HB3	2:X:1350:ASN:OD1	2.21	0.41
2:X:1303:ALA:CA	5:X:2062:HOH:O	2.69	0.41
1:A:97:PHE:CD1	1:A:97:PHE:C	2.99	0.41
1:A:668:ILE:HD11	1:A:681:TYR:CD2	2.56	0.41
1:A:879:ILE:HG21	1:A:898:VAL:CG2	2.48	0.41
1:A:1629:ARG:HG2	5:A:2386:HOH:O	2.20	0.41
1:A:1845:VAL:HG21	1:A:1859:LEU:HD11	2.03	0.41
1:A:1862:VAL:HA	1:A:1928:LEU:HD21	2.02	0.41
1:E:353:ILE:HD11	1:E:372:SER:HB2	2.03	0.41
1:E:613:SER:HA	1:E:614:PRO:HG2	2.03	0.41
1:E:957:ASN:HA	5:E:2300:HOH:O	2.20	0.41
1:I:1046:VAL:O	1:I:1049:GLN:NE2	2.46	0.41
1:I:1367:VAL:N	1:I:1409:PHE:O	2.50	0.41
1:I:1583:ALA:HB1	1:I:1644:ILE:HD13	2.03	0.41
1:M:239:THR:HG23	1:M:533:ILE:HD11	2.02	0.41
1:M:720:THR:HG21	3:M:2101:FMN:O3'	2.21	0.41
1:M:969:ALA:O	1:M:973:GLU:OE2	2.39	0.41
1:Q:153:GLN:NE2	1:Q:225:CYS:SG	2.94	0.41
1:Q:875:ARG:CD	5:Q:2255:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1021:SER:HB3	5:Q:2337:HOH:O	2.21	0.41
1:Q:1279:SER:O	1:Q:1283:ILE:HG12	2.20	0.41
1:Q:1810:MET:CE	1:Q:1984:ILE:HD13	2.47	0.41
1:U:255:LYS:CE	1:U:256:TRP:CD1	3.03	0.41
1:U:774:GLU:HA	5:U:2318:HOH:O	2.20	0.41
1:U:1172:ILE:HD12	1:U:1172:ILE:N	2.35	0.41
1:U:1452:GLU:OE1	1:U:1452:GLU:O	2.39	0.41
1:U:1523:SER:HB3	1:U:1582:TRP:CE3	2.56	0.41
1:U:1523:SER:CB	1:U:1582:TRP:CE3	3.04	0.41
1:U:1650:THR:CG2	2:X:41:THR:HG21	2.51	0.41
1:U:1863:VAL:HG13	1:U:1874:LEU:HD13	2.03	0.41
2:C:1035:ARG:NH1	2:C:1039:GLU:OE1	2.54	0.41
2:G:1:MET:HE2	2:G:9:LEU:HD12	2.02	0.41
2:G:651:GLY:HA3	5:G:2099:HOH:O	2.17	0.41
2:G:1023:PHE:CE1	2:G:1601:ILE:HG21	2.56	0.41
2:G:1637:THR:HG22	2:G:1638:ASP:N	2.36	0.41
2:K:815:THR:N	5:K:2045:HOH:O	2.54	0.41
5:K:2251:HOH:O	2:X:341:LEU:HD21	2.19	0.41
2:O:708:VAL:CG1	2:O:737:VAL:HG22	2.51	0.41
2:O:969:ASN:ND2	5:O:2052:HOH:O	2.54	0.41
2:O:1129:ASP:OD1	2:S:347:TYR:CZ	2.74	0.41
2:O:1129:ASP:CG	2:S:347:TYR:HH	2.26	0.41
2:O:1402:VAL:HG11	2:O:1533:PHE:CZ	2.56	0.41
2:O:1637:THR:HG22	2:O:1638:ASP:N	2.36	0.41
2:S:512:GLU:OE2	2:S:873:ARG:NH1	2.54	0.41
2:S:1008:LEU:HD23	2:S:1668:VAL:HG12	2.03	0.41
2:S:1368:THR:OG1	2:S:1622:LEU:HD13	2.20	0.41
2:S:1411:ASP:OD2	2:S:1652:GLN:HG2	2.21	0.41
2:X:931:GLN:NE2	5:X:2035:HOH:O	2.53	0.41
2:X:1129:ASP:OD1	2:X:1129:ASP:N	2.53	0.41
1:A:33:ASP:HA	1:A:36:ILE:HG22	2.03	0.41
1:A:900:ASP:OD2	1:A:902:GLN:OE1	2.39	0.41
1:A:1324:ILE:HD12	1:A:1333:LEU:HD21	2.03	0.41
1:E:123:TYR:OH	1:E:242:VAL:HG22	2.21	0.41
1:E:598:LEU:HD11	1:E:633:GLY:O	2.21	0.41
1:I:1702:ASN:ND2	1:I:1754:SER:O	2.53	0.41
1:M:703:VAL:HG11	1:M:717:LEU:HD12	2.03	0.41
1:M:1175:LYS:CA	5:M:2245:HOH:O	2.64	0.41
1:M:1324:ILE:HD12	1:M:1333:LEU:HD21	2.03	0.41
1:Q:374:TYR:CE2	1:Q:378:LEU:HD11	2.56	0.41
1:Q:898:VAL:CG1	5:Q:2260:HOH:O	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1016:PHE:CE2	5:Q:2323:HOH:O	2.74	0.41
1:Q:1725:PHE:CD2	1:Q:1825:THR:HG23	2.56	0.41
1:U:1395:GLN:CG	5:U:2320:HOH:O	2.68	0.41
2:C:1502:LYS:HD3	2:C:1503:ARG:NH1	2.35	0.41
2:K:499:LYS:HG2	2:K:511:GLU:OE1	2.20	0.41
2:O:937:LYS:NZ	5:O:2003:HOH:O	2.41	0.41
2:O:1013:ASP:OD1	2:O:1015:GLU:OE1	2.38	0.41
2:O:1054:TRP:NE1	2:O:1696:ILE:O	2.53	0.41
2:O:1366:ARG:NH2	2:O:1371:THR:O	2.54	0.41
2:S:455:ASP:OD1	2:S:455:ASP:N	2.54	0.41
2:S:1019:VAL:HB	2:S:1399:ILE:HG23	2.03	0.41
2:X:398:SER:HB2	2:X:738:VAL:HG12	2.03	0.41
2:X:435:CYS:SG	2:X:475:LEU:HD13	2.61	0.41
2:X:1603:ILE:CG2	2:X:1640:ILE:HD13	2.50	0.41
1:A:123:TYR:OH	1:A:242:VAL:HG13	2.21	0.40
1:A:764:THR:OG1	1:A:1069:HIS:NE2	2.48	0.40
1:E:29:SER:O	1:E:33:ASP:OD1	2.39	0.40
1:E:221:VAL:HG21	1:E:412:ALA:HB3	2.02	0.40
1:E:1249:PHE:HA	5:E:2227:HOH:O	2.20	0.40
1:E:1845:VAL:HG21	1:E:1859:LEU:HD11	2.02	0.40
1:M:221:VAL:HG21	1:M:412:ALA:HB3	2.02	0.40
1:M:1161:ILE:HG22	1:M:1162:LEU:HD22	2.03	0.40
1:M:1395:GLN:HG3	5:M:2229:HOH:O	2.17	0.40
1:Q:1367:VAL:O	1:Q:1409:PHE:N	2.52	0.40
1:Q:2017:VAL:HG21	2:S:13:LEU:HD11	2.02	0.40
1:U:586:PRO:CD	3:U:2101:FMN:H6	2.51	0.40
1:U:1317:TRP:O	1:U:1321:ILE:HG22	2.21	0.40
2:G:1195:ARG:HH21	2:G:1199:ILE:C	2.29	0.40
2:K:534:MET:HE3	2:K:891:LEU:HD13	2.03	0.40
2:K:1019:VAL:HB	2:K:1399:ILE:HG23	2.03	0.40
2:K:1197:TYR:O	2:K:1701:MET:N	2.54	0.40
2:S:1315:ILE:HD11	2:S:1403:LEU:CD1	2.51	0.40
1:A:1395:GLN:CG	5:A:2338:HOH:O	2.69	0.40
1:A:2017:VAL:HG21	2:C:13:LEU:HD11	2.02	0.40
1:E:613:SER:HA	1:E:614:PRO:CG	2.51	0.40
1:E:703:VAL:HG11	1:E:717:LEU:HD12	2.03	0.40
1:E:1324:ILE:HD12	1:E:1333:LEU:HD21	2.03	0.40
1:E:1528:LEU:HD23	1:E:1610:THR:O	2.22	0.40
1:I:374:TYR:CE2	1:I:378:LEU:HD11	2.57	0.40
1:I:907:LYS:HE3	5:I:2229:HOH:O	2.20	0.40
1:I:1068:GLY:O	1:I:1072:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1074:ILE:HD12	1:M:1078:TYR:HB2	2.03	0.40
1:Q:956:GLN:CD	2:S:979:LYS:HE2	2.46	0.40
1:U:265:VAL:HG11	1:U:289:LEU:HD22	2.03	0.40
1:U:909:VAL:HG21	1:U:983:ILE:HD11	2.03	0.40
2:C:1089:LYS:CB	5:C:2093:HOH:O	2.45	0.40
2:C:1708:ALA:HB1	2:C:1709:PRO:HD2	2.04	0.40
2:K:377:TRP:CE3	2:S:377:TRP:CZ3	3.09	0.40
2:K:1302:GLY:HA2	2:K:1653:LYS:HD3	2.03	0.40
2:O:1019:VAL:HB	2:O:1399:ILE:HG23	2.03	0.40
2:S:428:ASP:CB	2:S:430:GLU:OE2	2.69	0.40
2:X:1018:VAL:HG11	2:X:1315:ILE:HD13	2.03	0.40
1:A:1317:TRP:O	1:A:1321:ILE:HG22	2.21	0.40
1:A:1332:ASP:HB2	5:A:2426:HOH:O	2.19	0.40
1:E:598:LEU:HD21	1:E:632:TYR:HB3	2.03	0.40
1:E:1796:SER:H	1:E:2001:ASN:ND2	2.18	0.40
1:I:430:VAL:HG11	1:I:461:ILE:HG21	2.03	0.40
1:I:839:GLU:N	5:I:2233:HOH:O	2.54	0.40
1:I:1016:PHE:CE2	5:I:2322:HOH:O	2.74	0.40
1:I:1522:LEU:HD21	1:I:1583:ALA:HA	2.03	0.40
1:M:586:PRO:CD	3:M:2101:FMN:H6	2.51	0.40
1:Q:179:VAL:HG13	1:Q:183:GLU:OE1	2.21	0.40
1:Q:487:LEU:CD2	1:Q:533:ILE:HD12	2.51	0.40
1:U:1024:GLN:OE1	1:U:1024:GLN:N	2.52	0.40
1:U:1324:ILE:HD12	1:U:1333:LEU:HD21	2.02	0.40
1:U:1899:THR:OG1	1:U:1954:VAL:HG21	2.22	0.40
2:C:339:GLN:N	2:O:349:GLN:NE2	2.63	0.40
2:G:1013:ASP:OD1	2:G:1015:GLU:OE1	2.39	0.40
2:G:1129:ASP:HB3	2:G:1167:LEU:HA	2.03	0.40
2:K:835:PHE:CE1	5:S:2118:HOH:O	2.73	0.40
2:O:1276:GLU:HA	2:O:1281:THR:HG21	2.03	0.40
2:S:1197:TYR:O	2:S:1701:MET:N	2.54	0.40
2:X:348:LEU:HD13	2:X:348:LEU:O	2.22	0.40
2:X:1303:ALA:HB1	2:X:1650:PHE:HD2	1.86	0.40
1:E:969:ALA:O	1:E:973:GLU:OE2	2.39	0.40
1:E:1149:GLN:HG2	1:E:1239:MET:SD	2.61	0.40
1:M:613:SER:HA	1:M:614:PRO:CG	2.52	0.40
1:M:1522:LEU:HD23	1:M:1522:LEU:O	2.22	0.40
1:M:1862:VAL:HA	1:M:1928:LEU:HD21	2.03	0.40
1:Q:1323:ALA:HB1	1:Q:1364:ILE:HG12	2.03	0.40
1:U:845:ALA:CA	5:U:2391:HOH:O	2.48	0.40
2:C:1426:THR:HB	2:C:1429:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:MET:CE	2:G:9:LEU:HD12	2.51	0.40
2:G:1091:LYS:HG2	2:G:1092:TYR:CE1	2.57	0.40
2:K:1564:MET:CG	2:K:1565:MET:HE2	2.50	0.40
2:K:1637:THR:HG22	2:K:1638:ASP:N	2.36	0.40
2:S:1095:GLU:OE1	2:S:1099:HIS:NE2	2.49	0.40
2:X:1035:ARG:NH1	2:X:1039:GLU:OE1	2.53	0.40
1:A:1046:VAL:O	1:A:1049:GLN:NE2	2.47	0.40
1:E:1284:SER:HA	5:E:2325:HOH:O	2.21	0.40
1:I:1774:LYS:NZ	1:I:1778:GLU:OE2	2.53	0.40
1:M:760:SER:OG	1:M:763:ASP:OD1	2.20	0.40
1:M:1833:ASP:N	1:M:1837:ARG:O	2.51	0.40
1:Q:251:ARG:HB3	1:Q:251:ARG:CZ	2.52	0.40
1:Q:265:VAL:HG11	1:Q:289:LEU:HD22	2.04	0.40
1:U:250:PHE:O	1:U:250:PHE:HD1	2.05	0.40
1:U:405:ASN:N	5:U:2241:HOH:O	2.54	0.40
1:U:1284:SER:HA	5:U:2311:HOH:O	2.21	0.40
2:C:342:GLU:HG3	2:O:342:GLU:OE2	2.21	0.40
2:C:433:ASN:CG	2:C:437:GLN:HE22	2.28	0.40
2:K:990:PHE:HE1	2:K:1692:MET:SD	2.44	0.40
2:K:1695:ALA:HB1	2:K:1700:THR:C	2.46	0.40
2:S:1342:PHE:HB3	2:S:1348:THR:HG23	2.03	0.40
2:S:1366:ARG:NH2	2:S:1371:THR:O	2.54	0.40
2:X:1200:PRO:CD	5:X:2156:HOH:O	2.70	0.40
2:X:1368:THR:OG1	2:X:1622:LEU:HD13	2.21	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	1985/2037 (97%)	1884 (95%)	97 (5%)	4 (0%)	44 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1985/2037 (97%)	1884 (95%)	98 (5%)	3 (0%)	44	65
1	I	1985/2037 (97%)	1884 (95%)	97 (5%)	4 (0%)	44	65
1	M	1985/2037 (97%)	1884 (95%)	98 (5%)	3 (0%)	44	65
1	Q	1985/2037 (97%)	1883 (95%)	99 (5%)	3 (0%)	44	65
1	U	1985/2037 (97%)	1885 (95%)	96 (5%)	4 (0%)	44	65
2	C	1369/1885 (73%)	1325 (97%)	43 (3%)	1 (0%)	48	70
2	G	1369/1885 (73%)	1326 (97%)	42 (3%)	1 (0%)	48	70
2	K	1369/1885 (73%)	1322 (97%)	45 (3%)	2 (0%)	48	70
2	O	1369/1885 (73%)	1330 (97%)	38 (3%)	1 (0%)	48	70
2	S	1369/1885 (73%)	1322 (97%)	46 (3%)	1 (0%)	48	70
2	X	1369/1885 (73%)	1325 (97%)	43 (3%)	1 (0%)	48	70
All	All	20124/23532 (86%)	19254 (96%)	842 (4%)	28 (0%)	50	70

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1166	LYS
1	E	1166	LYS
1	I	1166	LYS
1	M	1166	LYS
1	Q	1166	LYS
1	U	1166	LYS
2	C	650	ASP
2	G	650	ASP
2	K	650	ASP
2	O	650	ASP
2	S	650	ASP
2	X	650	ASP
1	A	896	ASN
1	A	1032	VAL
1	E	896	ASN
1	E	1032	VAL
1	I	896	ASN
1	I	1032	VAL
1	M	896	ASN
1	M	1032	VAL
1	Q	896	ASN
1	Q	1032	VAL

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Mol	Chain	Res	Type
1	U	896	ASN
1	U	1032	VAL
1	I	480	ASN
1	U	480	ASN
1	A	480	ASN
2	K	629	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1613/1784 (90%)	1583 (98%)	30 (2%)	52	75
1	E	1613/1784 (90%)	1589 (98%)	24 (2%)	60	80
1	I	1613/1784 (90%)	1584 (98%)	29 (2%)	54	76
1	M	1613/1784 (90%)	1588 (98%)	25 (2%)	60	80
1	Q	1613/1784 (90%)	1588 (98%)	25 (2%)	60	80
1	U	1613/1784 (90%)	1582 (98%)	31 (2%)	52	75
2	C	1141/1580 (72%)	1126 (99%)	15 (1%)	65	83
2	G	1141/1580 (72%)	1116 (98%)	25 (2%)	47	70
2	K	1141/1580 (72%)	1120 (98%)	21 (2%)	54	76
2	O	1141/1580 (72%)	1115 (98%)	26 (2%)	45	69
2	S	1141/1580 (72%)	1119 (98%)	22 (2%)	52	75
2	X	1141/1580 (72%)	1123 (98%)	18 (2%)	58	78
All	All	16524/20184 (82%)	16233 (98%)	291 (2%)	54	76

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	111	ILE
1	A	221	VAL
1	A	240	CYS

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Mol	Chain	Res	Type
1	A	305	SER
1	A	306	LEU
1	A	340	ILE
1	A	425	LEU
1	A	435	LEU
1	A	517	THR
1	A	685	LEU
1	A	875	ARG
1	A	929	SER
1	A	954	LEU
1	A	985	GLU
1	A	1138	LEU
1	A	1160	ASP
1	A	1185	ILE
1	A	1215	THR
1	A	1242	ARG
1	A	1280	SER
1	A	1328	SER
1	A	1363	GLU
1	A	1375	LEU
1	A	1464	SER
1	A	1509	THR
1	A	1552	SER
1	A	1636	PRO
1	A	1760	SER
1	A	1845	VAL
1	E	96	SER
1	E	111	ILE
1	E	221	VAL
1	E	305	SER
1	E	435	LEU
1	E	480	ASN
1	E	685	LEU
1	E	811	CYS
1	E	875	ARG
1	E	898	VAL
1	E	929	SER
1	E	1128	ASP
1	E	1242	ARG
1	E	1280	SER
1	E	1328	SER
1	E	1464	SER

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Mol	Chain	Res	Type
1	E	1509	THR
1	E	1597	ASP
1	E	1608	LEU
1	E	1623	ILE
1	E	1727	THR
1	E	1760	SER
1	E	1790	ILE
1	E	1845	VAL
1	I	96	SER
1	I	111	ILE
1	I	183	GLU
1	I	221	VAL
1	I	305	SER
1	I	340	ILE
1	I	517	THR
1	I	533	ILE
1	I	685	LEU
1	I	764	THR
1	I	811	CYS
1	I	898	VAL
1	I	929	SER
1	I	957	ASN
1	I	1215	THR
1	I	1280	SER
1	I	1328	SER
1	I	1375	LEU
1	I	1417	VAL
1	I	1464	SER
1	I	1509	THR
1	I	1552	SER
1	I	1608	LEU
1	I	1623	ILE
1	I	1727	THR
1	I	1760	SER
1	I	1790	ILE
1	I	1845	VAL
1	I	2001	ASN
1	M	96	SER
1	M	111	ILE
1	M	221	VAL
1	M	305	SER
1	M	376	PHE

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Mol	Chain	Res	Type
1	M	435	LEU
1	M	685	LEU
1	M	811	CYS
1	M	875	ARG
1	M	898	VAL
1	M	929	SER
1	M	1128	ASP
1	M	1215	THR
1	M	1280	SER
1	M	1328	SER
1	M	1464	SER
1	M	1509	THR
1	M	1597	ASP
1	M	1608	LEU
1	M	1623	ILE
1	M	1688	ASN
1	M	1727	THR
1	M	1760	SER
1	M	1790	ILE
1	M	1845	VAL
1	Q	96	SER
1	Q	221	VAL
1	Q	305	SER
1	Q	435	LEU
1	Q	517	THR
1	Q	647	GLN
1	Q	685	LEU
1	Q	764	THR
1	Q	811	CYS
1	Q	898	VAL
1	Q	929	SER
1	Q	1215	THR
1	Q	1280	SER
1	Q	1328	SER
1	Q	1375	LEU
1	Q	1417	VAL
1	Q	1464	SER
1	Q	1509	THR
1	Q	1552	SER
1	Q	1608	LEU
1	Q	1612	MET
1	Q	1727	THR

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Mol	Chain	Res	Type
1	Q	1760	SER
1	Q	1790	ILE
1	Q	1845	VAL
1	U	68	ASN
1	U	96	SER
1	U	111	ILE
1	U	221	VAL
1	U	340	ILE
1	U	435	LEU
1	U	495	SER
1	U	517	THR
1	U	634	LEU
1	U	685	LEU
1	U	893	LYS
1	U	898	VAL
1	U	929	SER
1	U	954	LEU
1	U	1185	ILE
1	U	1215	THR
1	U	1236	LEU
1	U	1280	SER
1	U	1328	SER
1	U	1363	GLU
1	U	1375	LEU
1	U	1417	VAL
1	U	1464	SER
1	U	1509	THR
1	U	1623	ILE
1	U	1635	LEU
1	U	1636	PRO
1	U	1727	THR
1	U	1760	SER
1	U	1790	ILE
1	U	1845	VAL
2	C	30	GLU
2	C	88	ILE
2	C	338	LYS
2	C	344	LEU
2	C	349	GLN
2	C	437	GLN
2	C	663	LEU
2	C	744	SER

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Mol	Chain	Res	Type
2	C	861	LYS
2	C	862	LEU
2	C	997	SER
2	C	1223	LEU
2	C	1237	VAL
2	C	1659	VAL
2	C	1679	THR
2	G	30	GLU
2	G	338	LYS
2	G	349	GLN
2	G	419	ILE
2	G	663	LEU
2	G	709	THR
2	G	757	ASP
2	G	861	LYS
2	G	862	LEU
2	G	997	SER
2	G	1081	THR
2	G	1090	SER
2	G	1097	LEU
2	G	1129	ASP
2	G	1130	LEU
2	G	1151	CYS
2	G	1223	LEU
2	G	1237	VAL
2	G	1292	SER
2	G	1406	THR
2	G	1444	ILE
2	G	1501	SER
2	G	1647	SER
2	G	1659	VAL
2	G	1742	SER
2	K	30	GLU
2	K	338	LYS
2	K	349	GLN
2	K	444	PRO
2	K	527	GLU
2	K	663	LEU
2	K	709	THR
2	K	744	SER
2	K	827	SER
2	K	862	LEU

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Mol	Chain	Res	Type
2	K	990	PHE
2	K	997	SER
2	K	1081	THR
2	K	1097	LEU
2	K	1122	GLN
2	K	1237	VAL
2	K	1369	THR
2	K	1444	ILE
2	K	1526	LEU
2	K	1564	MET
2	K	1659	VAL
2	O	30	GLU
2	O	56	MET
2	O	338	LYS
2	O	362	LYS
2	O	419	ILE
2	O	663	LEU
2	O	709	THR
2	O	757	ASP
2	O	792	GLU
2	O	861	LYS
2	O	862	LEU
2	O	997	SER
2	O	1081	THR
2	O	1090	SER
2	O	1097	LEU
2	O	1130	LEU
2	O	1223	LEU
2	O	1237	VAL
2	O	1406	THR
2	O	1420	PRO
2	O	1444	ILE
2	O	1501	SER
2	O	1564	MET
2	O	1647	SER
2	O	1659	VAL
2	O	1742	SER
2	S	30	GLU
2	S	66	GLU
2	S	338	LYS
2	S	339	GLN
2	S	344	LEU

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Mol	Chain	Res	Type
2	S	444	PRO
2	S	527	GLU
2	S	663	LEU
2	S	709	THR
2	S	744	SER
2	S	827	SER
2	S	862	LEU
2	S	997	SER
2	S	1081	THR
2	S	1097	LEU
2	S	1122	GLN
2	S	1130	LEU
2	S	1237	VAL
2	S	1369	THR
2	S	1387	MET
2	S	1526	LEU
2	S	1659	VAL
2	X	30	GLU
2	X	88	ILE
2	X	349	GLN
2	X	437	GLN
2	X	663	LEU
2	X	827	SER
2	X	861	LYS
2	X	862	LEU
2	X	997	SER
2	X	1083	ILE
2	X	1223	LEU
2	X	1237	VAL
2	X	1429	ARG
2	X	1453	LYS
2	X	1506	SER
2	X	1526	LEU
2	X	1653	LYS
2	X	1659	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	117	ASN
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	346	HIS
1	A	433	HIS
1	A	480	ASN
1	A	689	HIS
1	A	884	ASN
1	A	932	ASN
1	A	1288	HIS
1	A	1586	ASN
1	A	1808	ASN
1	A	1900	ASN
1	E	121	ASN
1	E	739	GLN
1	E	872	ASN
1	E	932	ASN
1	E	960	GLN
1	E	1227	ASN
1	E	1281	GLN
1	E	1609	GLN
1	E	1688	ASN
1	E	1885	GLN
1	E	1900	ASN
1	I	117	ASN
1	I	312	GLN
1	I	335	GLN
1	I	572	GLN
1	I	884	ASN
1	I	960	GLN
1	I	1159	HIS
1	I	1288	HIS
1	I	1609	GLN
1	I	1656	GLN
1	I	1808	ASN
1	I	1900	ASN
1	M	121	ASN
1	M	739	GLN
1	M	872	ASN
1	M	884	ASN
1	M	960	GLN
1	M	1227	ASN
1	M	1609	GLN
1	M	1688	ASN
1	M	1885	GLN

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Mol	Chain	Res	Type
1	M	1900	ASN
1	Q	117	ASN
1	Q	312	GLN
1	Q	335	GLN
1	Q	572	GLN
1	Q	884	ASN
1	Q	960	GLN
1	Q	1159	HIS
1	Q	1227	ASN
1	Q	1288	HIS
1	Q	1609	GLN
1	Q	1656	GLN
1	Q	1900	ASN
1	U	121	ASN
1	U	335	GLN
1	U	433	HIS
1	U	480	ASN
1	U	932	ASN
1	U	960	GLN
1	U	1227	ASN
1	U	1586	ASN
1	U	1808	ASN
1	U	1885	GLN
1	U	1900	ASN
2	C	340	GLN
2	C	507	ASN
2	C	915	GLN
2	C	935	ASN
2	C	1003	GLN
2	C	1206	GLN
2	C	1270	GLN
2	C	1275	GLN
2	C	1350	ASN
2	C	1546	HIS
2	C	1553	ASN
2	C	1563	ASN
2	G	40	ASN
2	G	371	GLN
2	G	637	GLN
2	G	915	GLN
2	G	1003	GLN
2	G	1270	GLN

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Mol	Chain	Res	Type
2	G	1350	ASN
2	G	1563	ASN
2	G	1685	ASN
2	G	1716	GLN
2	K	39	HIS
2	K	40	ASN
2	K	697	GLN
2	K	851	ASN
2	K	915	GLN
2	K	1003	GLN
2	K	1016	ASN
2	K	1119	GLN
2	K	1206	GLN
2	K	1270	GLN
2	K	1346	ASN
2	K	1384	GLN
2	K	1504	GLN
2	K	1553	ASN
2	K	1563	ASN
2	K	1624	GLN
2	O	40	ASN
2	O	349	GLN
2	O	637	GLN
2	O	969	ASN
2	O	1003	GLN
2	O	1270	GLN
2	O	1563	ASN
2	O	1624	GLN
2	O	1685	ASN
2	O	1694	ASN
2	O	1716	GLN
2	S	39	HIS
2	S	40	ASN
2	S	58	ASN
2	S	371	GLN
2	S	697	GLN
2	S	851	ASN
2	S	904	ASN
2	S	915	GLN
2	S	1003	GLN
2	S	1119	GLN
2	S	1206	GLN

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Mol	Chain	Res	Type
2	S	1270	GLN
2	S	1346	ASN
2	S	1373	ASN
2	S	1504	GLN
2	S	1553	ASN
2	X	915	GLN
2	X	935	ASN
2	X	1003	GLN
2	X	1031	ASN
2	X	1099	HIS
2	X	1206	GLN
2	X	1270	GLN
2	X	1546	HIS
2	X	1553	ASN
2	X	1563	ASN
2	X	1716	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FMN	U	2101	-	33,33,33	1.17	2 (6%)	48,50,50	1.46	10 (20%)
4	PKZ	K	1901	-	36,38,67	2.10	10 (27%)	43,47,93	1.61	9 (20%)
3	FMN	Q	2101	-	33,33,33	1.05	2 (6%)	48,50,50	1.36	9 (18%)
4	PKZ	G	1901	-	36,38,67	2.10	10 (27%)	43,47,93	1.60	9 (20%)
3	FMN	I	2101	-	33,33,33	1.05	2 (6%)	48,50,50	1.37	8 (16%)
4	PKZ	S	1901	-	36,38,67	2.10	10 (27%)	43,47,93	1.61	9 (20%)
3	FMN	E	2101	-	33,33,33	1.04	2 (6%)	48,50,50	1.34	8 (16%)
3	FMN	A	2101	-	33,33,33	1.05	2 (6%)	48,50,50	1.38	8 (16%)
3	FMN	M	2101	-	33,33,33	1.04	2 (6%)	48,50,50	1.34	8 (16%)
4	PKZ	O	1901	-	36,38,67	2.09	10 (27%)	43,47,93	1.61	9 (20%)
4	PKZ	X	1901	-	36,38,67	2.10	10 (27%)	43,47,93	1.61	9 (20%)
4	PKZ	C	1901	-	36,38,67	2.10	10 (27%)	43,47,93	1.61	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	U	2101	-	-	0/18/18/18	0/3/3/3
4	PKZ	K	1901	-	-	23/45/45/82	-
3	FMN	Q	2101	-	-	0/18/18/18	0/3/3/3
4	PKZ	G	1901	-	-	23/45/45/82	-
3	FMN	I	2101	-	-	0/18/18/18	0/3/3/3
4	PKZ	S	1901	-	-	23/45/45/82	-
3	FMN	E	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	A	2101	-	-	0/18/18/18	0/3/3/3
3	FMN	M	2101	-	-	0/18/18/18	0/3/3/3
4	PKZ	O	1901	-	-	23/45/45/82	-
4	PKZ	X	1901	-	-	23/45/45/82	-
4	PKZ	C	1901	-	-	23/45/45/82	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1901	PKZ	P2A-O6A	6.91	1.82	1.60
4	S	1901	PKZ	P2A-O6A	6.90	1.82	1.60
4	X	1901	PKZ	P2A-O6A	6.89	1.82	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1901	PKZ	P2A-O6A	6.89	1.82	1.60
4	C	1901	PKZ	P2A-O6A	6.88	1.82	1.60
4	O	1901	PKZ	P2A-O6A	6.86	1.82	1.60
4	O	1901	PKZ	C1-S1P	4.67	1.87	1.76
4	K	1901	PKZ	C1-S1P	4.65	1.87	1.76
4	S	1901	PKZ	C1-S1P	4.65	1.87	1.76
4	G	1901	PKZ	C1-S1P	4.64	1.87	1.76
4	C	1901	PKZ	C1-S1P	4.63	1.87	1.76
4	X	1901	PKZ	C1-S1P	4.63	1.87	1.76
4	C	1901	PKZ	C5P-N4P	4.15	1.43	1.33
4	G	1901	PKZ	C5P-N4P	4.15	1.43	1.33
4	K	1901	PKZ	C5P-N4P	4.14	1.43	1.33
4	S	1901	PKZ	C5P-N4P	4.14	1.43	1.33
4	O	1901	PKZ	C5P-N4P	4.11	1.43	1.33
4	X	1901	PKZ	C5P-N4P	4.09	1.43	1.33
4	K	1901	PKZ	O6A-CCP	-3.56	1.32	1.43
4	S	1901	PKZ	O6A-CCP	-3.56	1.32	1.43
4	G	1901	PKZ	O6A-CCP	-3.56	1.32	1.43
4	O	1901	PKZ	O6A-CCP	-3.56	1.32	1.43
4	X	1901	PKZ	O6A-CCP	-3.56	1.32	1.43
4	C	1901	PKZ	O6A-CCP	-3.55	1.32	1.43
4	C	1901	PKZ	CCP-CBP	3.44	1.58	1.52
4	X	1901	PKZ	CCP-CBP	3.44	1.58	1.52
4	O	1901	PKZ	CCP-CBP	3.44	1.58	1.52
4	K	1901	PKZ	CCP-CBP	3.41	1.58	1.52
4	S	1901	PKZ	CCP-CBP	3.41	1.58	1.52
4	G	1901	PKZ	CCP-CBP	3.40	1.58	1.52
4	C	1901	PKZ	C2-C1	3.39	1.54	1.50
4	G	1901	PKZ	C2-C1	3.37	1.54	1.50
4	K	1901	PKZ	C2-C1	3.33	1.54	1.50
4	S	1901	PKZ	C2-C1	3.33	1.54	1.50
4	X	1901	PKZ	C2-C1	3.33	1.54	1.50
4	O	1901	PKZ	C2-C1	3.26	1.54	1.50
3	U	2101	FMN	C4A-N5	3.25	1.37	1.30
3	E	2101	FMN	C4A-N5	3.25	1.37	1.30
3	M	2101	FMN	C4A-N5	3.23	1.37	1.30
3	I	2101	FMN	C4A-N5	3.19	1.37	1.30
3	Q	2101	FMN	C4A-N5	3.18	1.37	1.30
3	A	2101	FMN	C4A-N5	3.15	1.37	1.30
4	G	1901	PKZ	C9P-N8P	2.71	1.40	1.33
4	C	1901	PKZ	C9P-N8P	2.71	1.40	1.33
4	S	1901	PKZ	C9P-N8P	2.71	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1901	PKZ	C9P-N8P	2.70	1.40	1.33
4	X	1901	PKZ	C9P-N8P	2.69	1.40	1.33
4	O	1901	PKZ	C9P-N8P	2.68	1.39	1.33
3	E	2101	FMN	C10-N1	2.63	1.38	1.33
4	X	1901	PKZ	OAP-CAP	-2.63	1.37	1.42
4	S	1901	PKZ	OAP-CAP	-2.62	1.37	1.42
3	M	2101	FMN	C10-N1	2.61	1.38	1.33
4	C	1901	PKZ	OAP-CAP	-2.60	1.37	1.42
3	U	2101	FMN	C10-N1	2.59	1.38	1.33
4	K	1901	PKZ	OAP-CAP	-2.58	1.37	1.42
4	G	1901	PKZ	OAP-CAP	-2.56	1.37	1.42
4	O	1901	PKZ	OAP-CAP	-2.56	1.37	1.42
3	A	2101	FMN	C10-N1	2.55	1.38	1.33
3	I	2101	FMN	C10-N1	2.51	1.38	1.33
3	Q	2101	FMN	C10-N1	2.49	1.38	1.33
4	C	1901	PKZ	P2A-O4A	-2.12	1.46	1.54
4	X	1901	PKZ	P2A-O3A	-2.12	1.46	1.54
4	G	1901	PKZ	P2A-O4A	-2.11	1.46	1.54
4	O	1901	PKZ	P2A-O3A	-2.11	1.46	1.54
4	K	1901	PKZ	P2A-O4A	-2.11	1.47	1.54
4	S	1901	PKZ	P2A-O3A	-2.11	1.47	1.54
4	C	1901	PKZ	P2A-O3A	2.10	1.62	1.54
4	K	1901	PKZ	P2A-O3A	2.10	1.62	1.54
4	O	1901	PKZ	P2A-O4A	2.09	1.62	1.54
4	X	1901	PKZ	P2A-O4A	2.09	1.62	1.54
4	G	1901	PKZ	P2A-O3A	2.09	1.62	1.54
4	S	1901	PKZ	P2A-O4A	2.09	1.62	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	1901	PKZ	C2-C1-S1P	4.89	119.23	113.40
4	O	1901	PKZ	C2-C1-S1P	4.87	119.21	113.40
4	K	1901	PKZ	C2-C1-S1P	4.87	119.21	113.40
4	S	1901	PKZ	C2-C1-S1P	4.87	119.21	113.40
4	C	1901	PKZ	C2-C1-S1P	4.87	119.20	113.40
4	G	1901	PKZ	C2-C1-S1P	4.85	119.18	113.40
3	I	2101	FMN	C4-N3-C2	-3.86	118.80	125.64
3	A	2101	FMN	C4-N3-C2	-3.82	118.86	125.64
3	Q	2101	FMN	C4-N3-C2	-3.81	118.87	125.64
3	M	2101	FMN	C4-N3-C2	-3.72	119.03	125.64
3	E	2101	FMN	C4-N3-C2	-3.71	119.05	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2101	FMN	C4-N3-C2	-3.71	119.05	125.64
4	C	1901	PKZ	O4A-P2A-O5A	3.67	125.12	110.83
4	G	1901	PKZ	O4A-P2A-O5A	3.66	125.11	110.83
4	X	1901	PKZ	O3A-P2A-O5A	3.66	125.11	110.83
4	K	1901	PKZ	O4A-P2A-O5A	3.66	125.11	110.83
4	S	1901	PKZ	O3A-P2A-O5A	3.66	125.09	110.83
4	O	1901	PKZ	O3A-P2A-O5A	3.65	125.08	110.83
4	S	1901	PKZ	O9P-C9P-N8P	-3.45	115.68	122.98
4	X	1901	PKZ	O9P-C9P-N8P	-3.44	115.70	122.98
4	K	1901	PKZ	O9P-C9P-N8P	-3.44	115.71	122.98
4	C	1901	PKZ	O9P-C9P-N8P	-3.44	115.71	122.98
4	G	1901	PKZ	O9P-C9P-N8P	-3.43	115.72	122.98
4	O	1901	PKZ	O9P-C9P-N8P	-3.43	115.72	122.98
4	O	1901	PKZ	C2P-S1P-C1	3.13	111.08	101.84
4	C	1901	PKZ	C2P-S1P-C1	3.12	111.07	101.84
4	X	1901	PKZ	C2P-S1P-C1	3.12	111.07	101.84
4	K	1901	PKZ	C2P-S1P-C1	3.12	111.06	101.84
4	S	1901	PKZ	C2P-S1P-C1	3.12	111.06	101.84
4	G	1901	PKZ	C2P-S1P-C1	3.11	111.03	101.84
4	S	1901	PKZ	O6A-P2A-O5A	-2.98	98.40	106.44
4	G	1901	PKZ	O6A-P2A-O5A	-2.97	98.41	106.44
4	X	1901	PKZ	O6A-P2A-O5A	-2.97	98.42	106.44
4	O	1901	PKZ	O6A-P2A-O5A	-2.97	98.42	106.44
4	K	1901	PKZ	O6A-P2A-O5A	-2.97	98.43	106.44
4	C	1901	PKZ	O6A-P2A-O5A	-2.96	98.45	106.44
3	A	2101	FMN	C4A-C4-N3	2.89	120.60	113.25
3	I	2101	FMN	C4A-C4-N3	2.88	120.59	113.25
3	M	2101	FMN	C4A-C4-N3	2.87	120.56	113.25
3	U	2101	FMN	C4A-C4-N3	2.86	120.54	113.25
3	E	2101	FMN	C4A-C4-N3	2.86	120.54	113.25
3	Q	2101	FMN	C4A-C4-N3	2.86	120.53	113.25
3	I	2101	FMN	C4A-C10-N10	2.77	120.44	116.48
3	A	2101	FMN	C4A-C10-N10	2.76	120.44	116.48
3	Q	2101	FMN	C4A-C10-N10	2.72	120.37	116.48
3	E	2101	FMN	C4A-C10-N10	2.68	120.32	116.48
3	Q	2101	FMN	O4-C4-C4A	-2.66	119.51	126.53
3	U	2101	FMN	C4A-C10-N10	2.64	120.27	116.48
3	I	2101	FMN	O4-C4-C4A	-2.64	119.57	126.53
3	M	2101	FMN	C4A-C10-N10	2.62	120.24	116.48
3	A	2101	FMN	O4-C4-C4A	-2.61	119.63	126.53
3	M	2101	FMN	O4-C4-C4A	-2.61	119.64	126.53
3	Q	2101	FMN	C4A-C10-N1	-2.61	118.19	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2101	FMN	O4-C4-C4A	-2.59	119.68	126.53
3	A	2101	FMN	C4A-C10-N1	-2.58	118.27	124.59
3	I	2101	FMN	C4A-C10-N1	-2.58	118.27	124.59
3	E	2101	FMN	C4A-C10-N1	-2.56	118.31	124.59
3	U	2101	FMN	C4A-C10-N1	-2.56	118.31	124.59
4	O	1901	PKZ	O1-C1-S1P	-2.56	119.43	122.68
3	U	2101	FMN	O4-C4-C4A	-2.56	119.78	126.53
3	M	2101	FMN	C4A-C10-N1	-2.56	118.32	124.59
3	U	2101	FMN	C8M-C8-C9	-2.54	115.10	119.57
4	X	1901	PKZ	O1-C1-S1P	-2.52	119.48	122.68
4	K	1901	PKZ	O1-C1-S1P	-2.52	119.48	122.68
4	S	1901	PKZ	O1-C1-S1P	-2.52	119.48	122.68
4	G	1901	PKZ	O1-C1-S1P	-2.48	119.52	122.68
4	C	1901	PKZ	O1-C1-S1P	-2.48	119.53	122.68
4	C	1901	PKZ	O1-C1-C2	-2.35	121.27	123.98
4	X	1901	PKZ	O1-C1-C2	-2.33	121.29	123.98
4	G	1901	PKZ	O1-C1-C2	-2.32	121.30	123.98
4	K	1901	PKZ	O1-C1-C2	-2.31	121.31	123.98
4	S	1901	PKZ	O1-C1-C2	-2.31	121.31	123.98
3	E	2101	FMN	C10-C4A-N5	-2.30	120.11	124.81
3	U	2101	FMN	C10-C4A-N5	-2.29	120.13	124.81
3	M	2101	FMN	C10-C4A-N5	-2.28	120.15	124.81
4	O	1901	PKZ	O1-C1-C2	-2.26	121.37	123.98
3	U	2101	FMN	C7M-C7-C6	-2.25	115.61	119.57
3	A	2101	FMN	C10-C4A-N5	-2.22	120.27	124.81
3	A	2101	FMN	C5A-C9A-N10	2.21	119.97	117.97
3	Q	2101	FMN	C10-C4A-N5	-2.20	120.32	124.81
3	I	2101	FMN	C10-C4A-N5	-2.20	120.32	124.81
4	S	1901	PKZ	O3A-P2A-O6A	-2.18	100.98	106.67
4	C	1901	PKZ	O4A-P2A-O6A	-2.18	100.98	106.67
4	K	1901	PKZ	O4A-P2A-O6A	-2.17	101.01	106.67
4	G	1901	PKZ	O4A-P2A-O6A	-2.17	101.01	106.67
4	C	1901	PKZ	O6A-CCP-CBP	2.17	114.03	110.55
4	K	1901	PKZ	O6A-CCP-CBP	2.17	114.03	110.55
4	S	1901	PKZ	O6A-CCP-CBP	2.17	114.03	110.55
4	X	1901	PKZ	O3A-P2A-O6A	-2.17	101.02	106.67
4	O	1901	PKZ	O3A-P2A-O6A	-2.16	101.03	106.67
3	I	2101	FMN	C5A-C9A-N10	2.16	119.92	117.97
4	X	1901	PKZ	O6A-CCP-CBP	2.16	114.02	110.55
4	O	1901	PKZ	O6A-CCP-CBP	2.16	114.01	110.55
4	G	1901	PKZ	O6A-CCP-CBP	2.14	113.99	110.55
3	U	2101	FMN	C8M-C8-C7	2.14	125.12	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2101	FMN	C4-C4A-C10	2.10	120.53	116.93
3	Q	2101	FMN	C5A-C9A-N10	2.08	119.85	117.97
3	I	2101	FMN	C4-C4A-C10	2.07	120.47	116.93
3	U	2101	FMN	C10-N1-C2	2.06	121.31	116.85
3	A	2101	FMN	C4-C4A-C10	2.05	120.45	116.93
3	E	2101	FMN	C4-C4A-C10	2.03	120.41	116.93
3	E	2101	FMN	C10-N1-C2	2.02	121.23	116.85
3	Q	2101	FMN	C10-N1-C2	2.02	121.23	116.85
3	M	2101	FMN	C10-N1-C2	2.02	121.21	116.85
3	M	2101	FMN	C4-C4A-C10	2.00	120.37	116.93

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1901	PKZ	C1-C2-C3-C4
4	C	1901	PKZ	CCP-O6A-P2A-O3A
4	C	1901	PKZ	CCP-O6A-P2A-O4A
4	C	1901	PKZ	CCP-O6A-P2A-O5A
4	C	1901	PKZ	OAP-CAP-CBP-CCP
4	C	1901	PKZ	C9P-CAP-CBP-CCP
4	C	1901	PKZ	OAP-CAP-CBP-CDP
4	C	1901	PKZ	C9P-CAP-CBP-CDP
4	C	1901	PKZ	OAP-CAP-CBP-CEP
4	C	1901	PKZ	C9P-CAP-CBP-CEP
4	C	1901	PKZ	CAP-C9P-N8P-C7P
4	C	1901	PKZ	C5P-C6P-C7P-N8P
4	G	1901	PKZ	C1-C2-C3-C4
4	G	1901	PKZ	CCP-O6A-P2A-O3A
4	G	1901	PKZ	CCP-O6A-P2A-O4A
4	G	1901	PKZ	CCP-O6A-P2A-O5A
4	G	1901	PKZ	OAP-CAP-CBP-CCP
4	G	1901	PKZ	C9P-CAP-CBP-CCP
4	G	1901	PKZ	OAP-CAP-CBP-CDP
4	G	1901	PKZ	C9P-CAP-CBP-CDP
4	G	1901	PKZ	OAP-CAP-CBP-CEP
4	G	1901	PKZ	C9P-CAP-CBP-CEP
4	G	1901	PKZ	CAP-C9P-N8P-C7P
4	G	1901	PKZ	C5P-C6P-C7P-N8P
4	K	1901	PKZ	C1-C2-C3-C4
4	K	1901	PKZ	CCP-O6A-P2A-O3A
4	K	1901	PKZ	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
4	K	1901	PKZ	CCP-O6A-P2A-O5A
4	K	1901	PKZ	OAP-CAP-CBP-CCP
4	K	1901	PKZ	C9P-CAP-CBP-CCP
4	K	1901	PKZ	OAP-CAP-CBP-CDP
4	K	1901	PKZ	C9P-CAP-CBP-CDP
4	K	1901	PKZ	OAP-CAP-CBP-CEP
4	K	1901	PKZ	C9P-CAP-CBP-CEP
4	K	1901	PKZ	CAP-C9P-N8P-C7P
4	K	1901	PKZ	C5P-C6P-C7P-N8P
4	O	1901	PKZ	C1-C2-C3-C4
4	O	1901	PKZ	CCP-O6A-P2A-O3A
4	O	1901	PKZ	CCP-O6A-P2A-O4A
4	O	1901	PKZ	CCP-O6A-P2A-O5A
4	O	1901	PKZ	OAP-CAP-CBP-CCP
4	O	1901	PKZ	C9P-CAP-CBP-CCP
4	O	1901	PKZ	OAP-CAP-CBP-CDP
4	O	1901	PKZ	C9P-CAP-CBP-CDP
4	O	1901	PKZ	OAP-CAP-CBP-CEP
4	O	1901	PKZ	C9P-CAP-CBP-CEP
4	O	1901	PKZ	CAP-C9P-N8P-C7P
4	O	1901	PKZ	C5P-C6P-C7P-N8P
4	S	1901	PKZ	C1-C2-C3-C4
4	S	1901	PKZ	CCP-O6A-P2A-O3A
4	S	1901	PKZ	CCP-O6A-P2A-O4A
4	S	1901	PKZ	CCP-O6A-P2A-O5A
4	S	1901	PKZ	OAP-CAP-CBP-CCP
4	S	1901	PKZ	C9P-CAP-CBP-CCP
4	S	1901	PKZ	OAP-CAP-CBP-CDP
4	S	1901	PKZ	C9P-CAP-CBP-CDP
4	S	1901	PKZ	OAP-CAP-CBP-CEP
4	S	1901	PKZ	C9P-CAP-CBP-CEP
4	S	1901	PKZ	CAP-C9P-N8P-C7P
4	S	1901	PKZ	C5P-C6P-C7P-N8P
4	X	1901	PKZ	C1-C2-C3-C4
4	X	1901	PKZ	CCP-O6A-P2A-O3A
4	X	1901	PKZ	CCP-O6A-P2A-O4A
4	X	1901	PKZ	CCP-O6A-P2A-O5A
4	X	1901	PKZ	OAP-CAP-CBP-CCP
4	X	1901	PKZ	C9P-CAP-CBP-CCP
4	X	1901	PKZ	OAP-CAP-CBP-CDP
4	X	1901	PKZ	C9P-CAP-CBP-CDP
4	X	1901	PKZ	OAP-CAP-CBP-CEP

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Mol	Chain	Res	Type	Atoms
4	X	1901	PKZ	C9P-CAP-CBP-CEP
4	X	1901	PKZ	CAP-C9P-N8P-C7P
4	X	1901	PKZ	C5P-C6P-C7P-N8P
4	C	1901	PKZ	O9P-C9P-N8P-C7P
4	G	1901	PKZ	O9P-C9P-N8P-C7P
4	K	1901	PKZ	O9P-C9P-N8P-C7P
4	O	1901	PKZ	O9P-C9P-N8P-C7P
4	S	1901	PKZ	O9P-C9P-N8P-C7P
4	X	1901	PKZ	O9P-C9P-N8P-C7P
4	C	1901	PKZ	C12-C13-C14-C15
4	G	1901	PKZ	C12-C13-C14-C15
4	K	1901	PKZ	C12-C13-C14-C15
4	O	1901	PKZ	C12-C13-C14-C15
4	S	1901	PKZ	C12-C13-C14-C15
4	X	1901	PKZ	C12-C13-C14-C15
4	C	1901	PKZ	C2-C3-C4-C5
4	G	1901	PKZ	C2-C3-C4-C5
4	K	1901	PKZ	C2-C3-C4-C5
4	O	1901	PKZ	C2-C3-C4-C5
4	S	1901	PKZ	C2-C3-C4-C5
4	X	1901	PKZ	C2-C3-C4-C5
4	C	1901	PKZ	C11-C12-C13-C14
4	G	1901	PKZ	C11-C12-C13-C14
4	K	1901	PKZ	C11-C12-C13-C14
4	O	1901	PKZ	C11-C12-C13-C14
4	S	1901	PKZ	C11-C12-C13-C14
4	X	1901	PKZ	C11-C12-C13-C14
4	O	1901	PKZ	C3-C4-C5-C6
4	G	1901	PKZ	C3-C4-C5-C6
4	C	1901	PKZ	C3-C4-C5-C6
4	K	1901	PKZ	C3-C4-C5-C6
4	S	1901	PKZ	C3-C4-C5-C6
4	X	1901	PKZ	C3-C4-C5-C6
4	G	1901	PKZ	C6-C7-C8-C9
4	K	1901	PKZ	C6-C7-C8-C9
4	O	1901	PKZ	C6-C7-C8-C9
4	S	1901	PKZ	C6-C7-C8-C9
4	X	1901	PKZ	C6-C7-C8-C9
4	C	1901	PKZ	C6-C7-C8-C9
4	C	1901	PKZ	C11-C10-C9-C8
4	G	1901	PKZ	C11-C10-C9-C8
4	K	1901	PKZ	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	O	1901	PKZ	C11-C10-C9-C8
4	S	1901	PKZ	C11-C10-C9-C8
4	X	1901	PKZ	C11-C10-C9-C8
4	C	1901	PKZ	C5-C6-C7-C8
4	G	1901	PKZ	C5-C6-C7-C8
4	K	1901	PKZ	C5-C6-C7-C8
4	O	1901	PKZ	C5-C6-C7-C8
4	S	1901	PKZ	C5-C6-C7-C8
4	X	1901	PKZ	C5-C6-C7-C8
4	G	1901	PKZ	C4-C5-C6-C7
4	O	1901	PKZ	C4-C5-C6-C7
4	K	1901	PKZ	C4-C5-C6-C7
4	S	1901	PKZ	C4-C5-C6-C7
4	X	1901	PKZ	C4-C5-C6-C7
4	C	1901	PKZ	C4-C5-C6-C7
4	S	1901	PKZ	C7-C8-C9-C10
4	O	1901	PKZ	C7-C8-C9-C10
4	X	1901	PKZ	C7-C8-C9-C10
4	C	1901	PKZ	C7-C8-C9-C10
4	G	1901	PKZ	C7-C8-C9-C10
4	K	1901	PKZ	C7-C8-C9-C10
4	C	1901	PKZ	N8P-C9P-CAP-OAP
4	G	1901	PKZ	N8P-C9P-CAP-OAP
4	K	1901	PKZ	N8P-C9P-CAP-OAP
4	O	1901	PKZ	N8P-C9P-CAP-OAP
4	S	1901	PKZ	N8P-C9P-CAP-OAP
4	X	1901	PKZ	N8P-C9P-CAP-OAP

There are no ring outliers.

12 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	2101	FMN	4	0
4	K	1901	PKZ	10	0
3	Q	2101	FMN	2	0
4	G	1901	PKZ	9	0
3	I	2101	FMN	2	0
4	S	1901	PKZ	10	0
3	E	2101	FMN	1	0
3	A	2101	FMN	2	0
3	M	2101	FMN	3	0
4	O	1901	PKZ	8	0

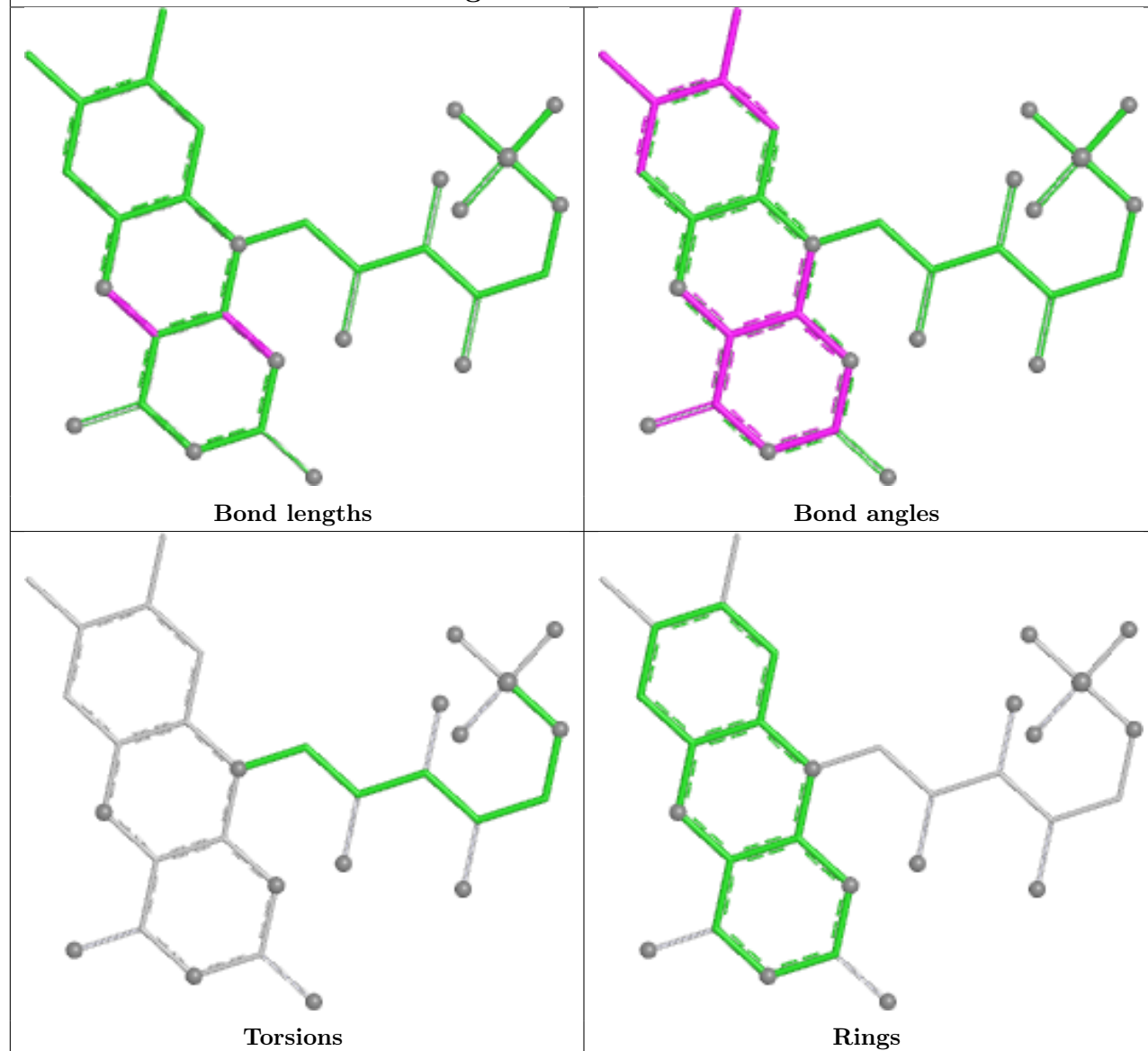
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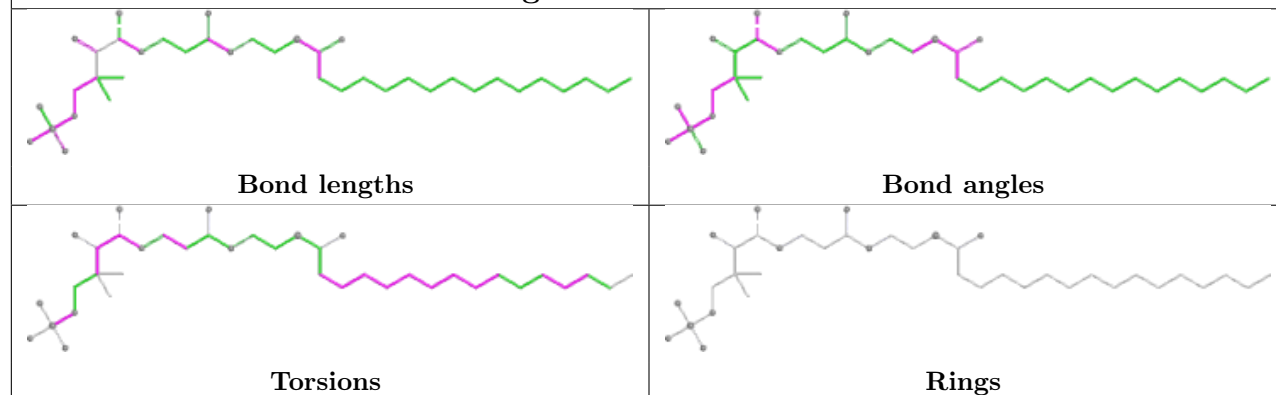
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	1901	PKZ	9	0
4	C	1901	PKZ	8	0

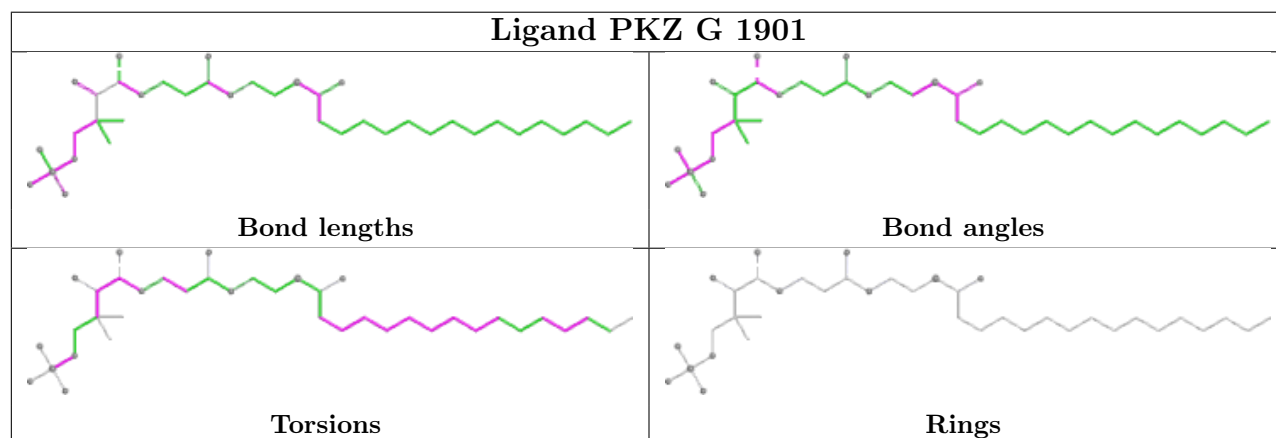
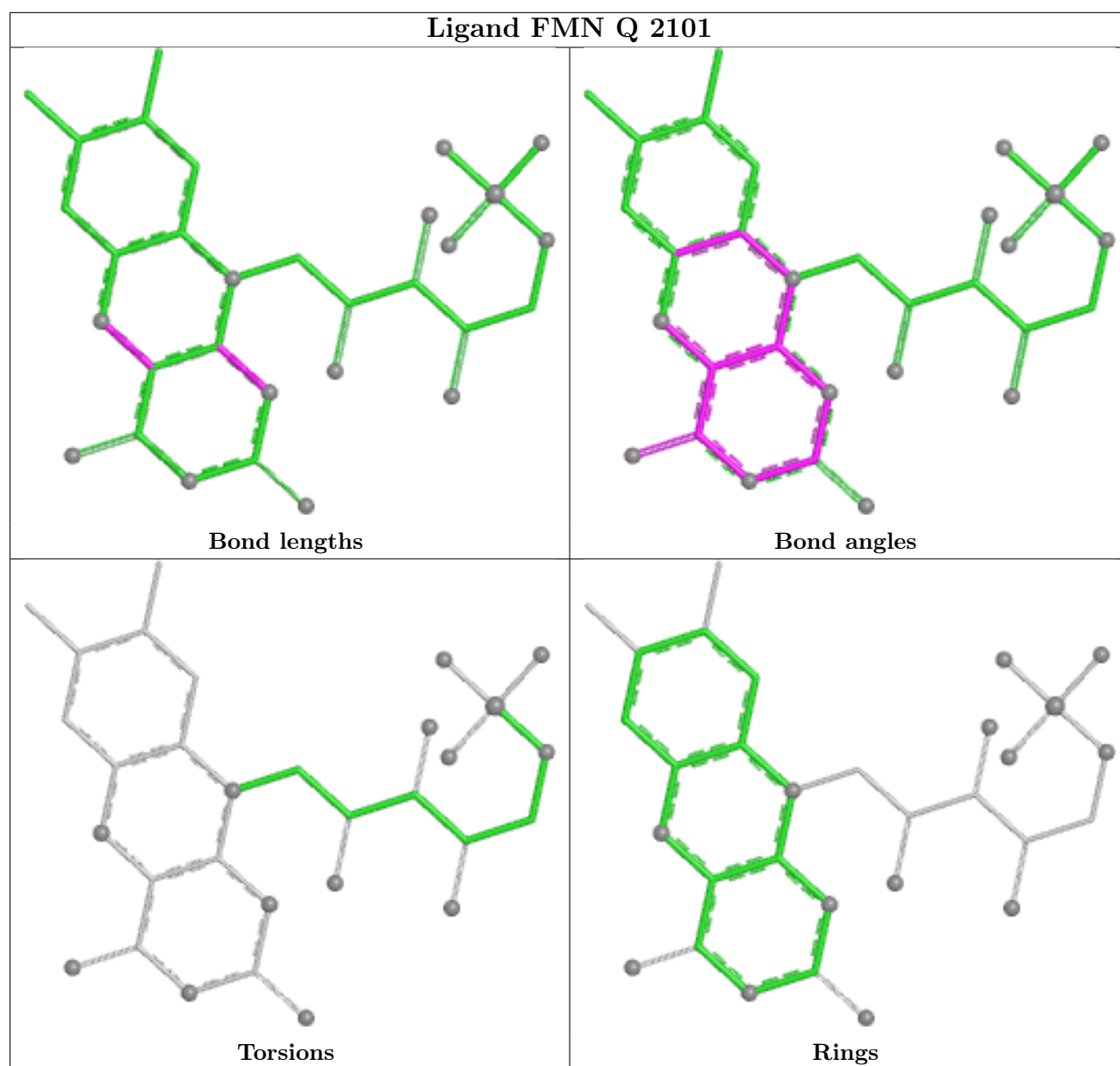
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

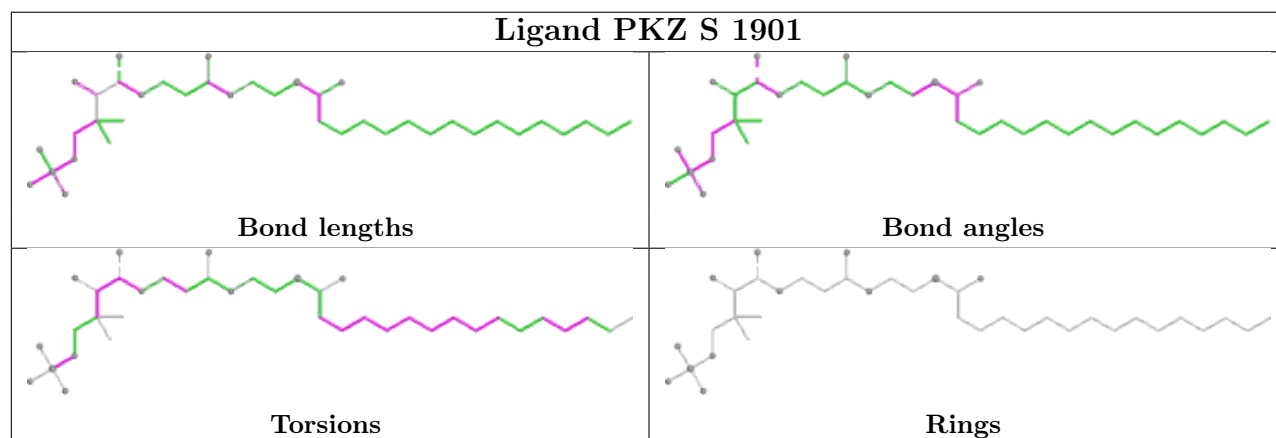
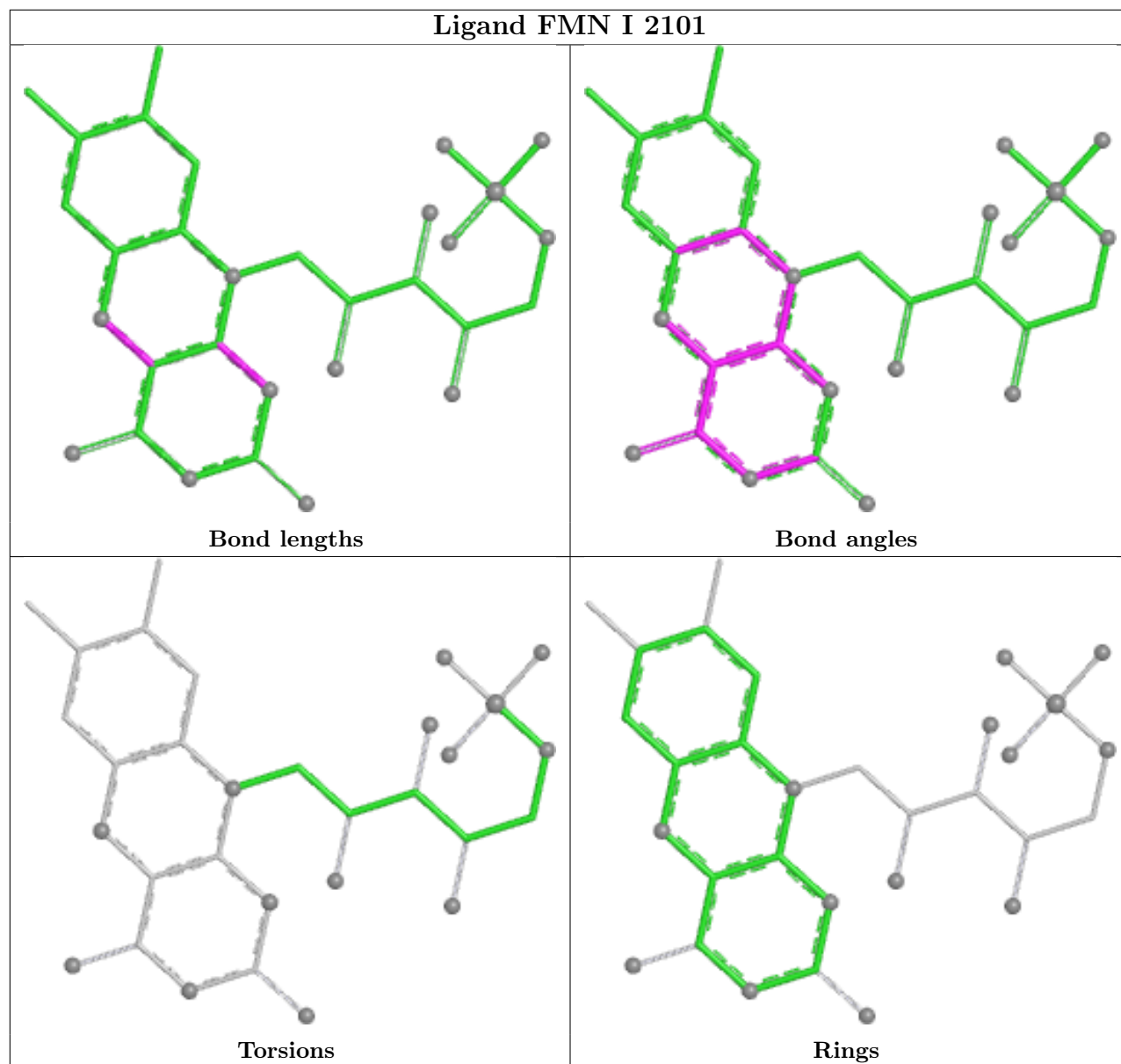
## Ligand FMN U 2101

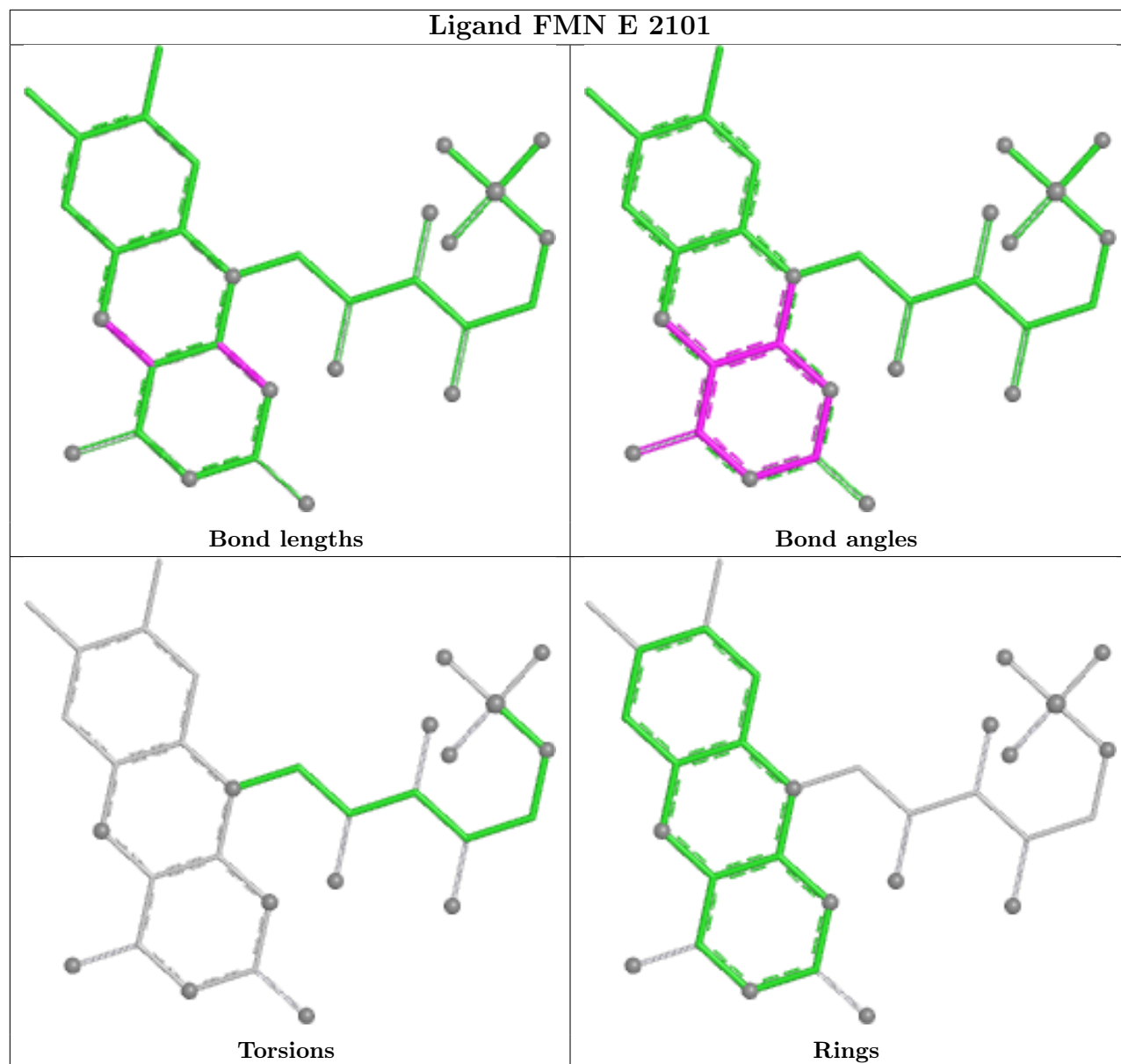


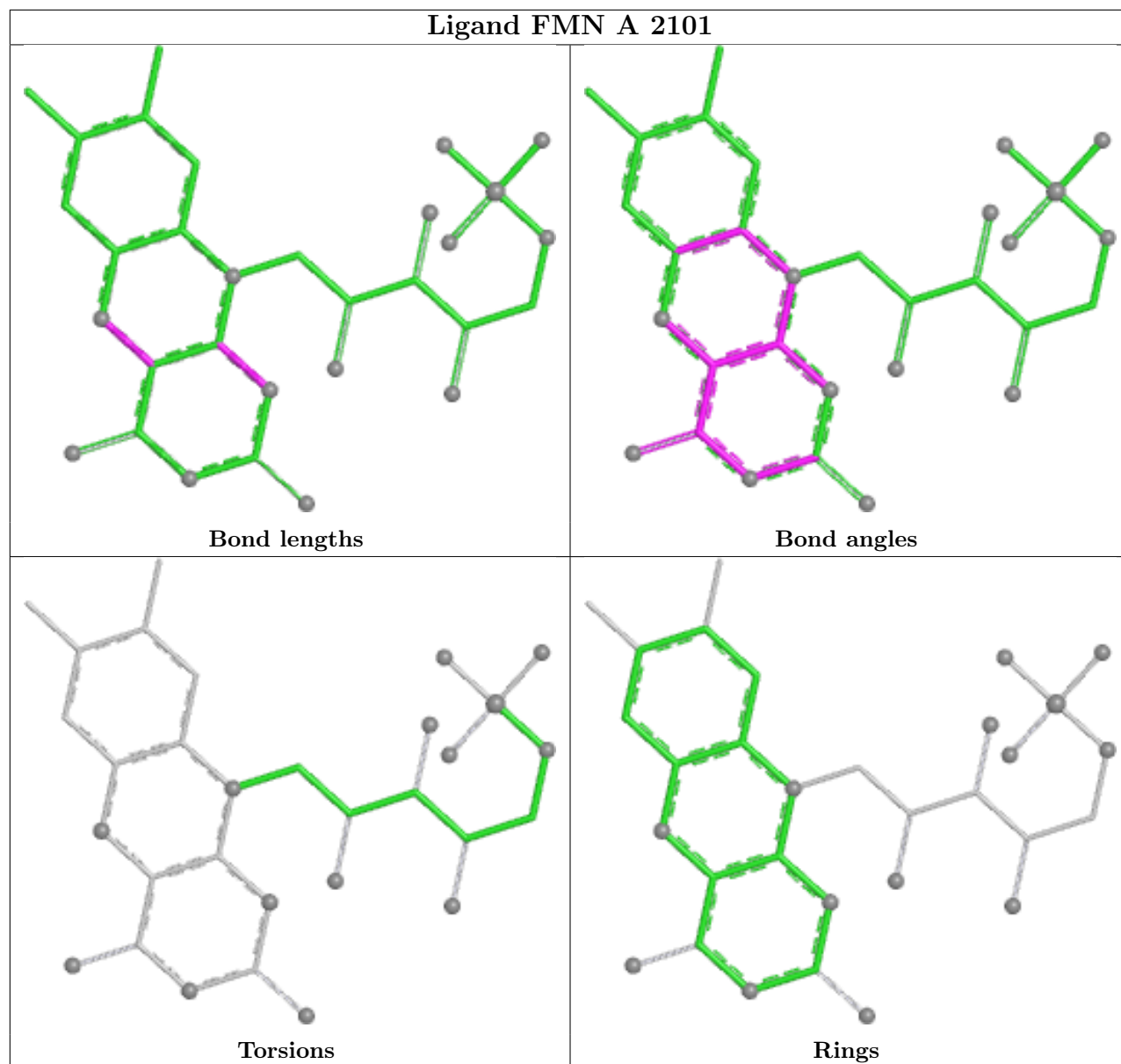
## Ligand PKZ K 1901



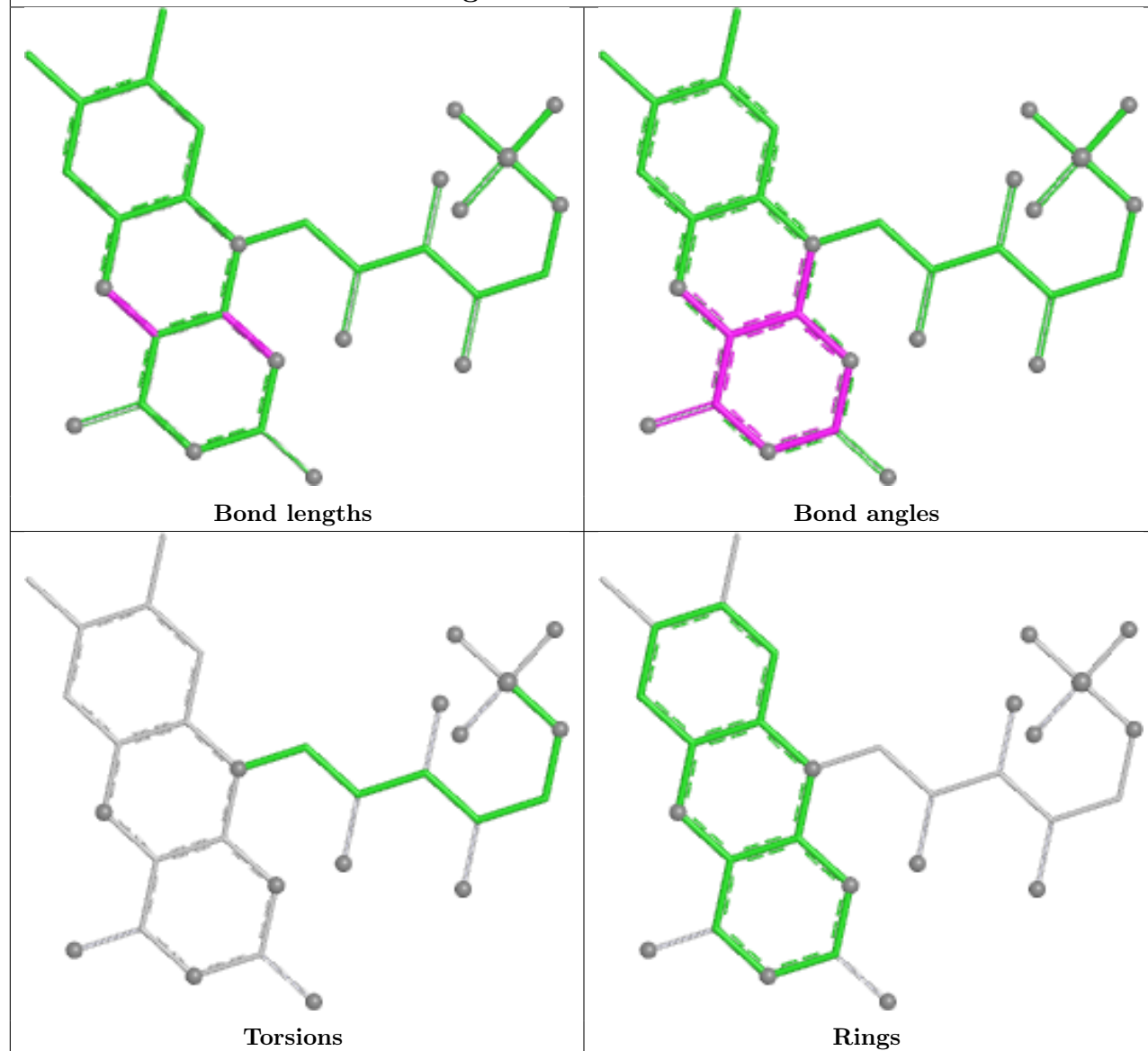




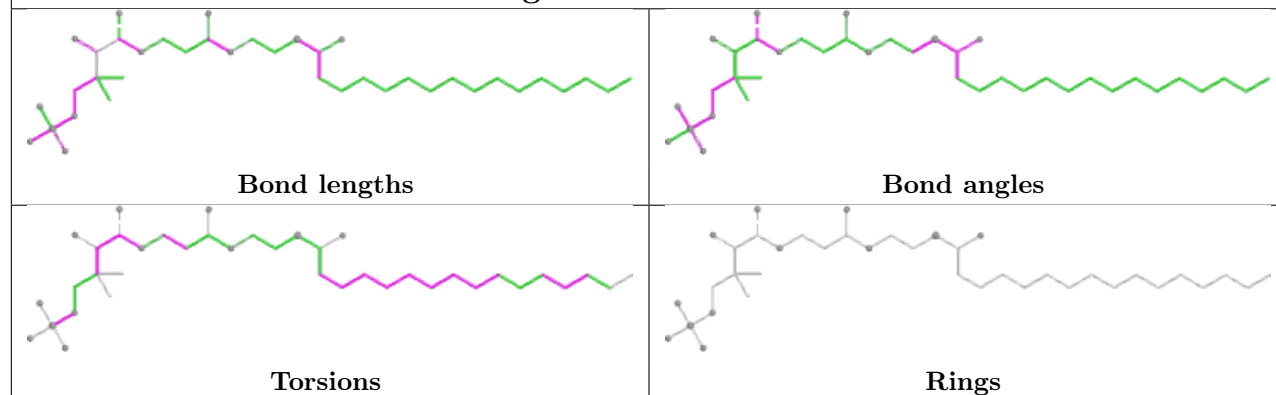




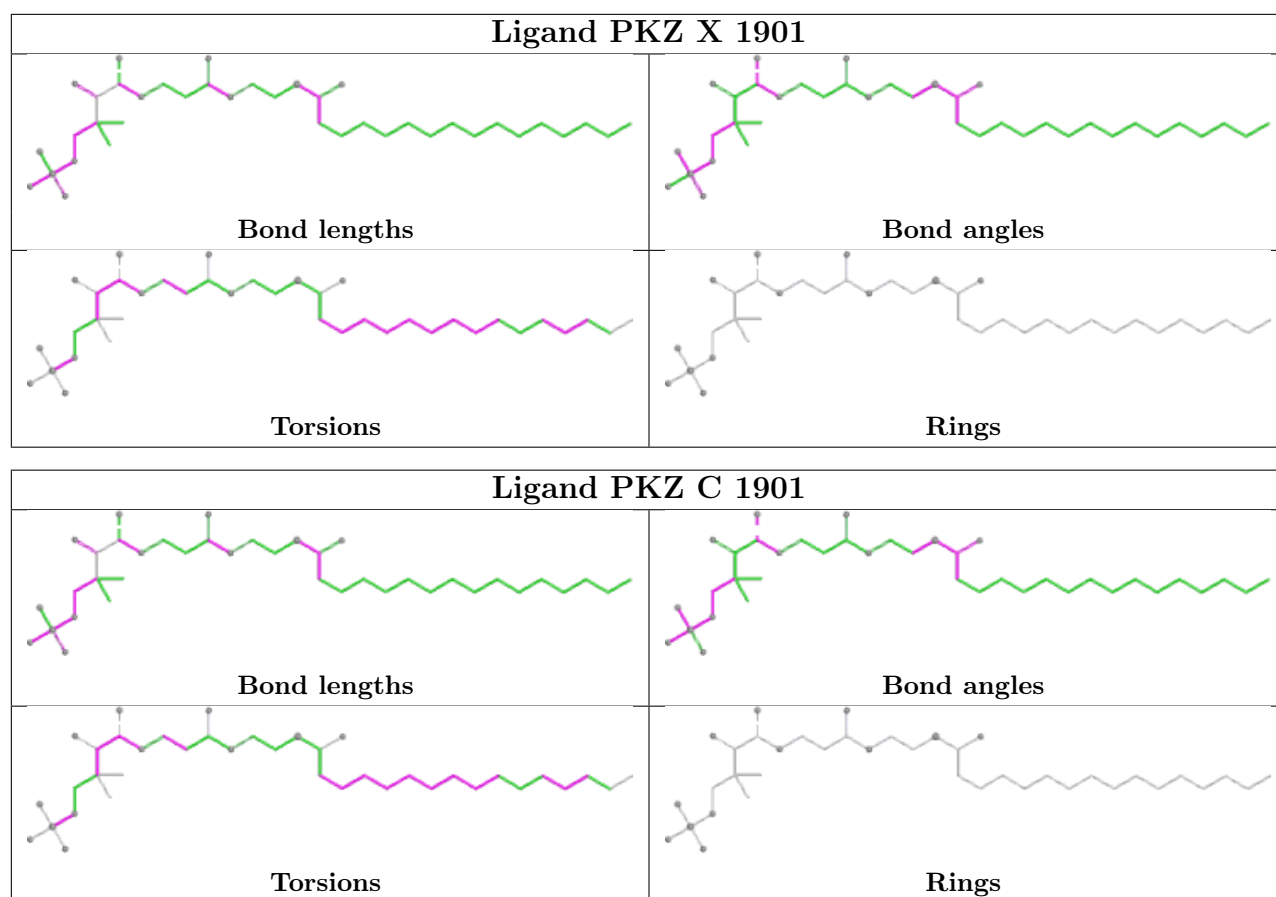
## Ligand FMN M 2101



## Ligand PKZ O 1901







## 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.

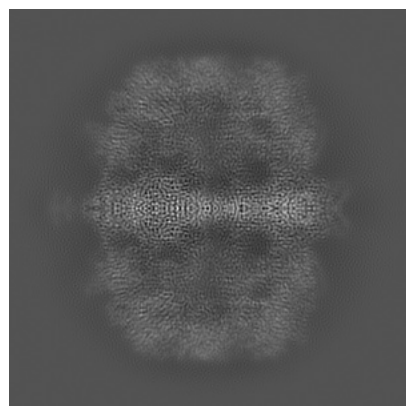
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46552. These allow visual inspection of the internal detail of the map and identification of artifacts.

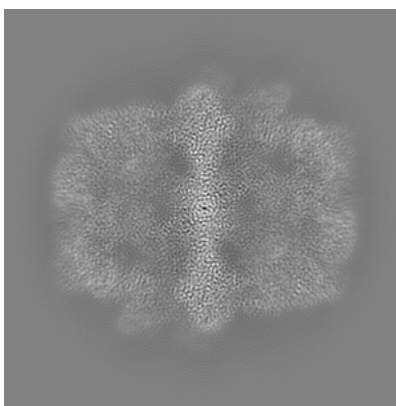
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

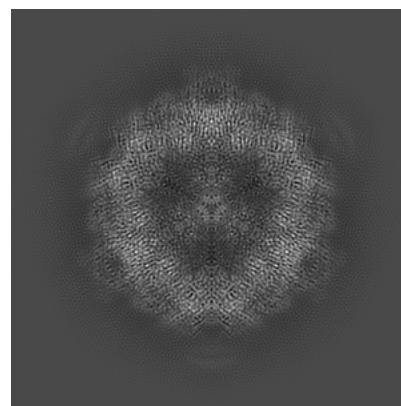
#### 6.1.1 Primary map



X

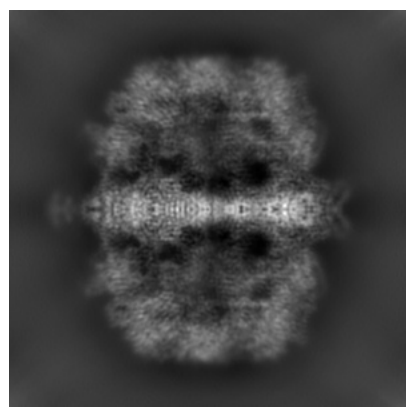


Y

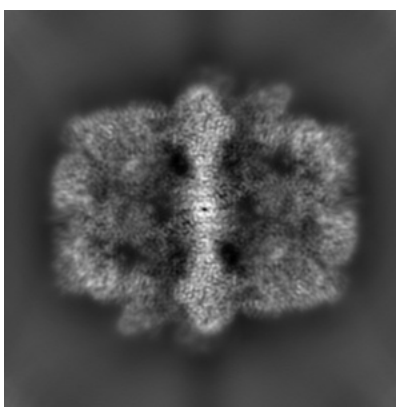


Z

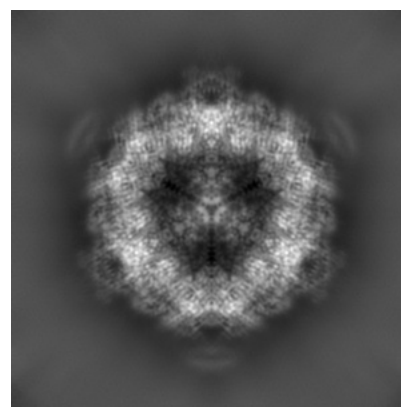
#### 6.1.2 Raw map



X



Y

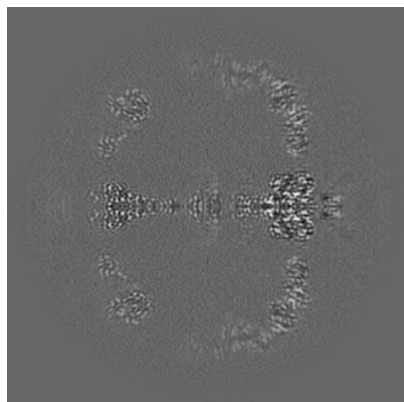


Z

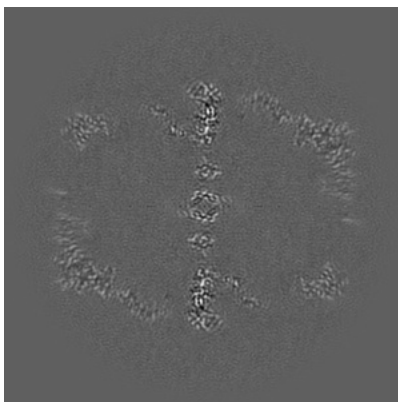
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

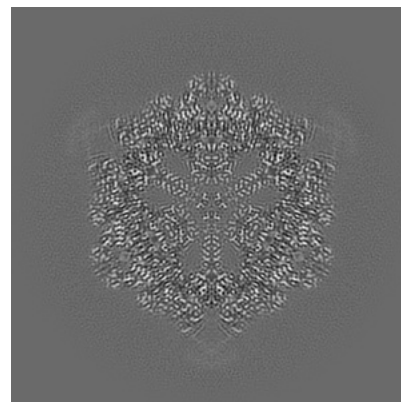
### 6.2.1 Primary map



X Index: 168

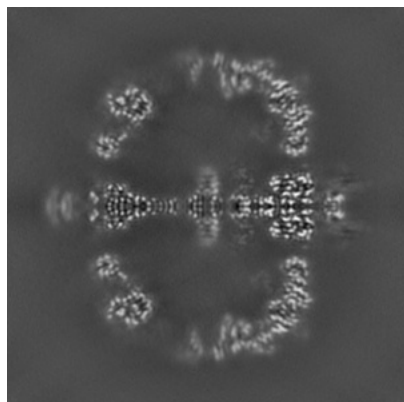


Y Index: 168

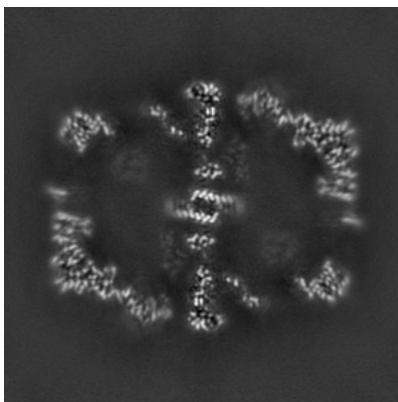


Z Index: 168

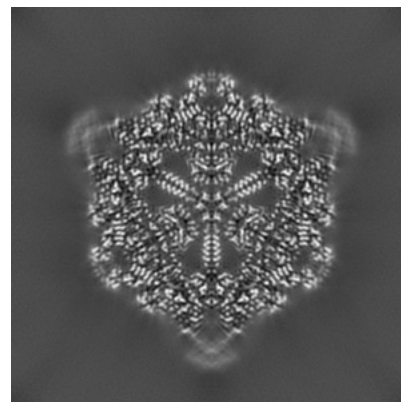
### 6.2.2 Raw map



X Index: 168



Y Index: 168

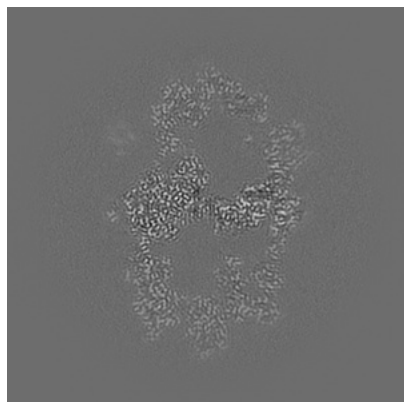


Z Index: 168

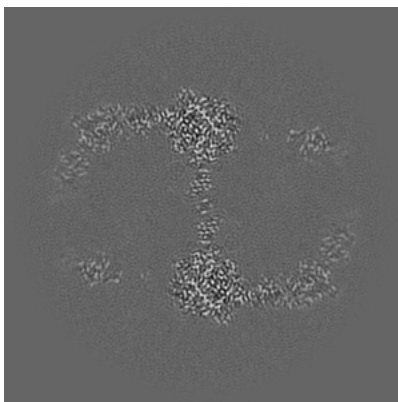
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

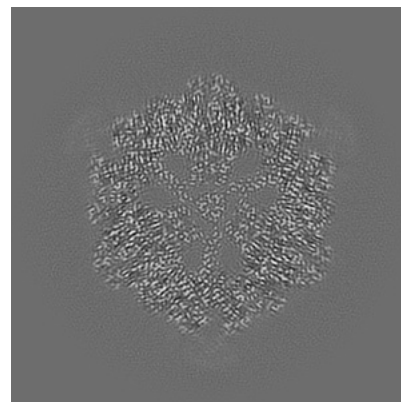
### 6.3.1 Primary map



X Index: 105

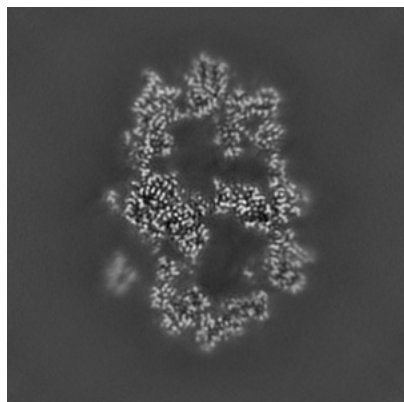


Y Index: 141

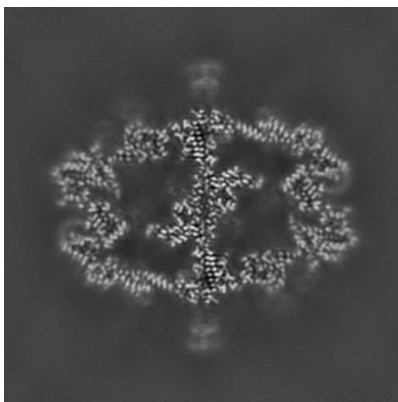


Z Index: 171

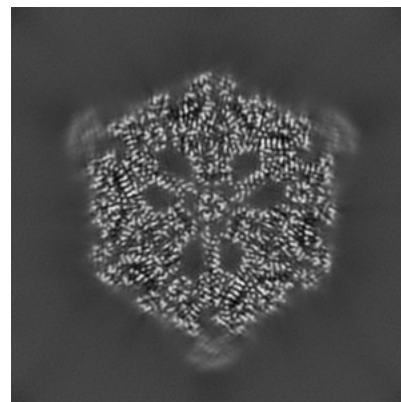
### 6.3.2 Raw map



X Index: 231



Y Index: 224

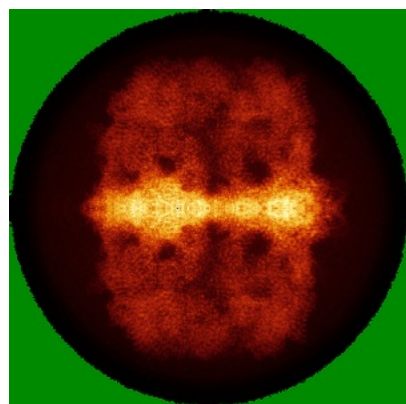


Z Index: 165

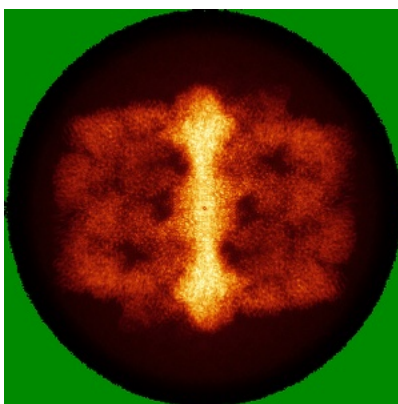
The images above show the largest variance slices of the map in three orthogonal directions.

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

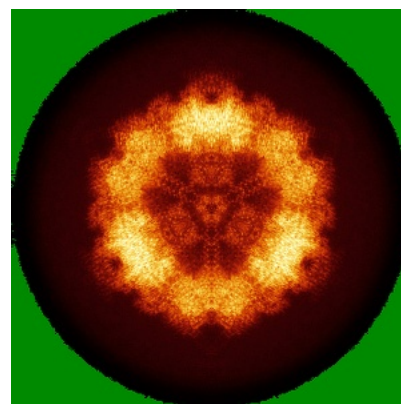
### 6.4.1 Primary map



X

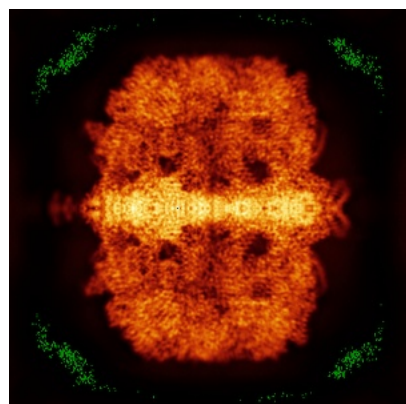


Y

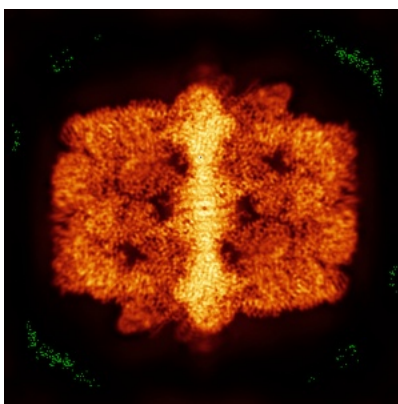


Z

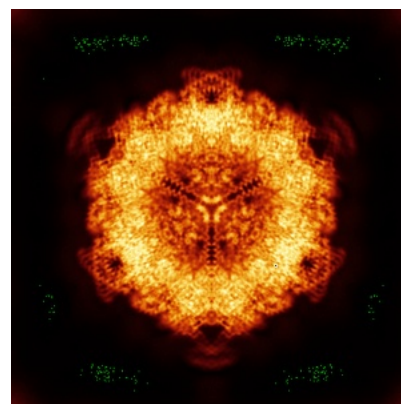
### 6.4.2 Raw map



X



Y



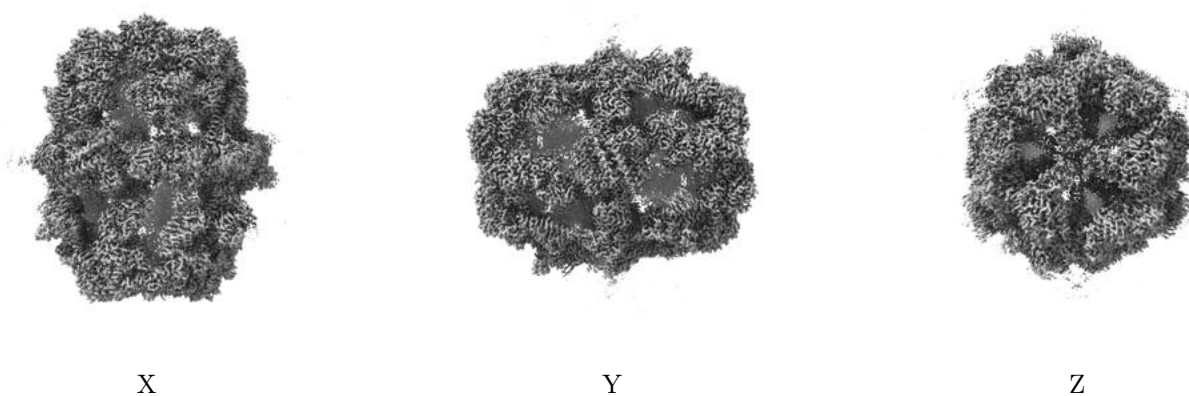
Z

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



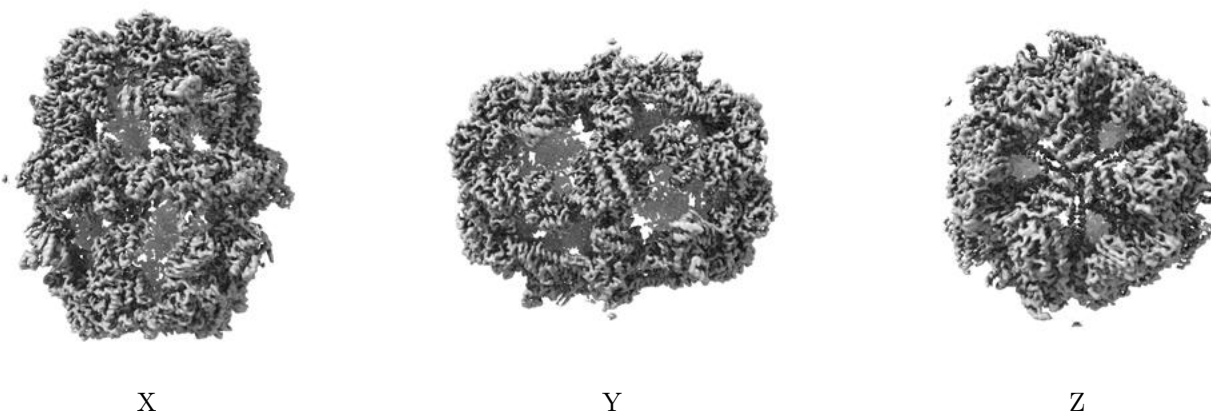
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

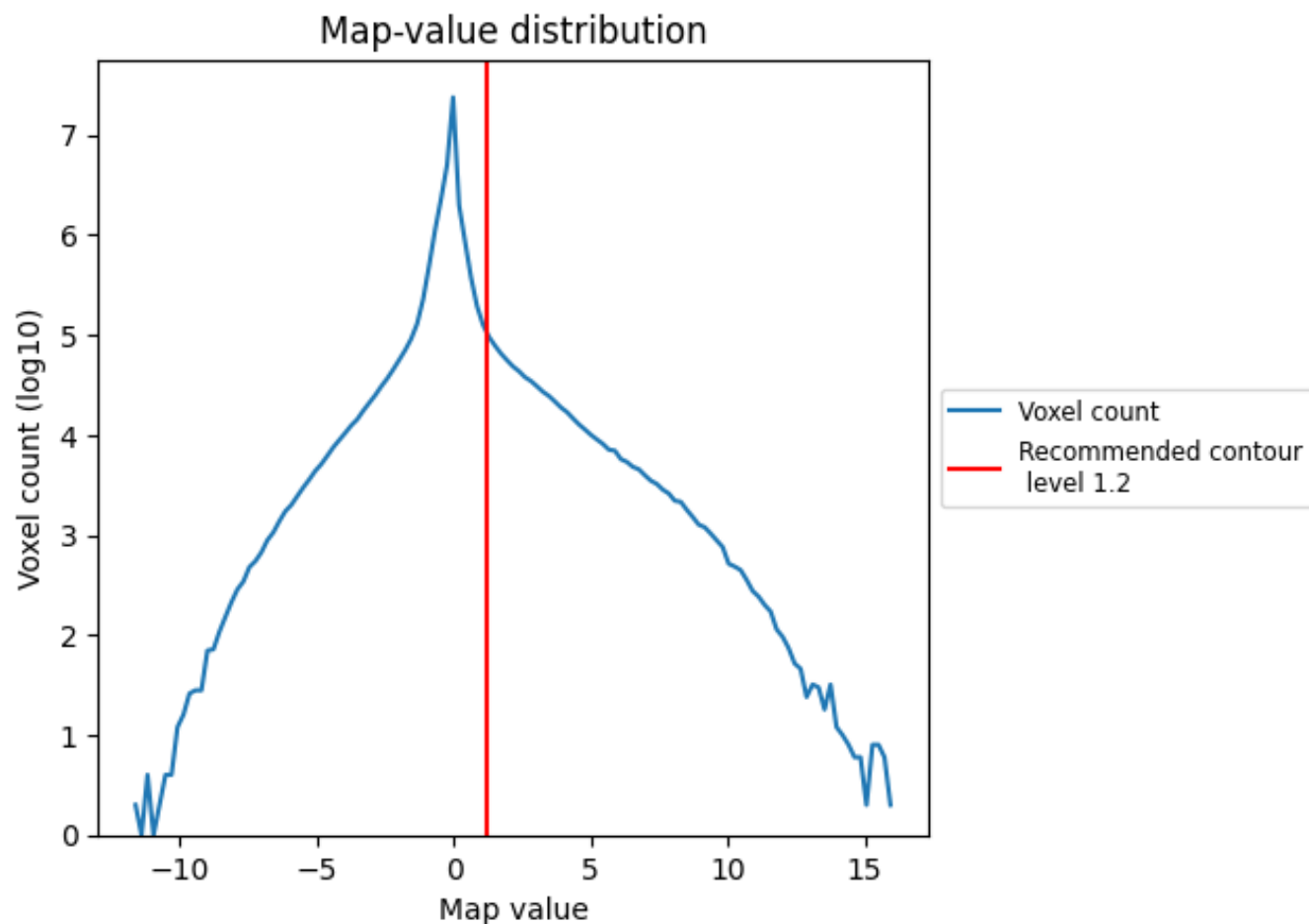
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

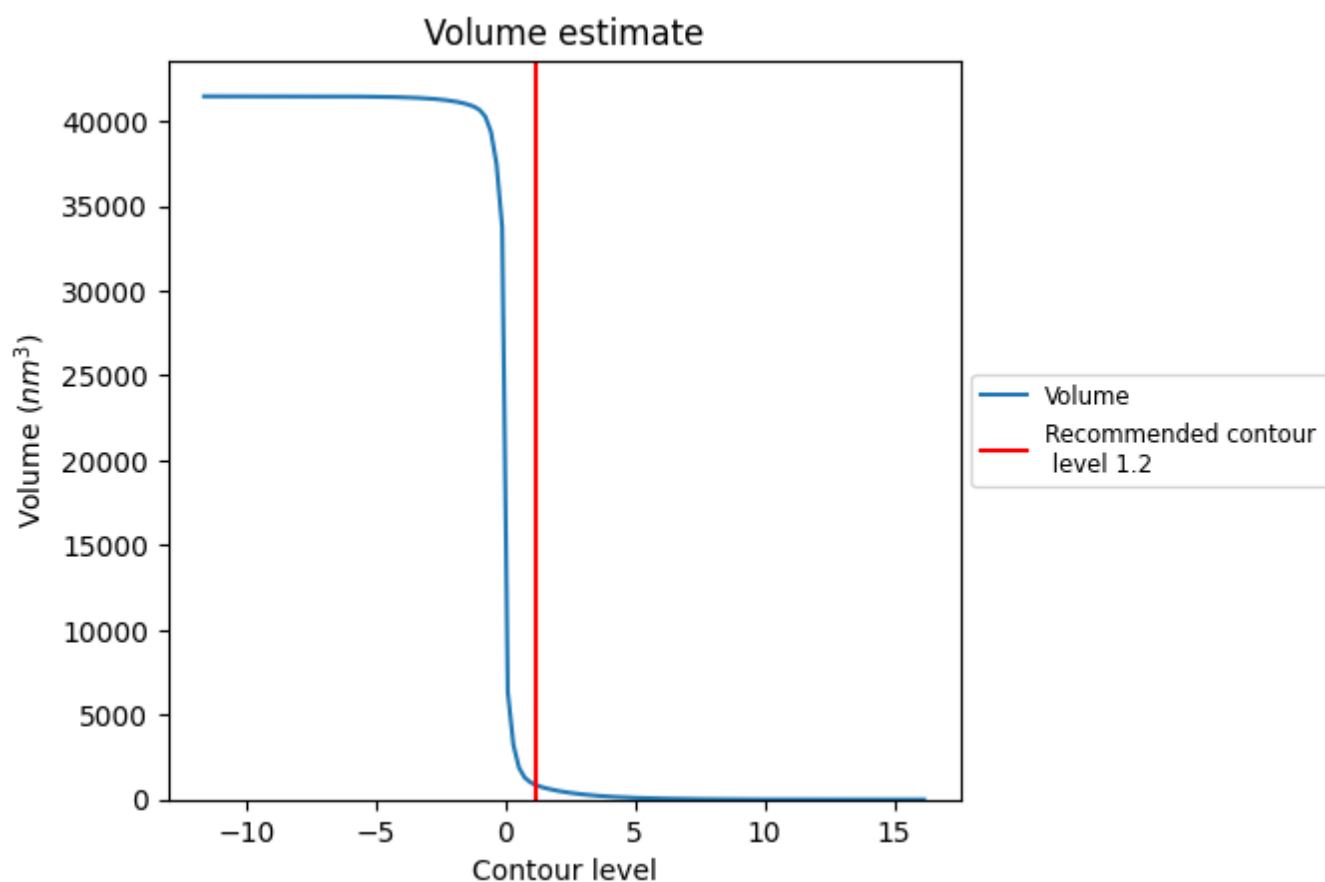
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

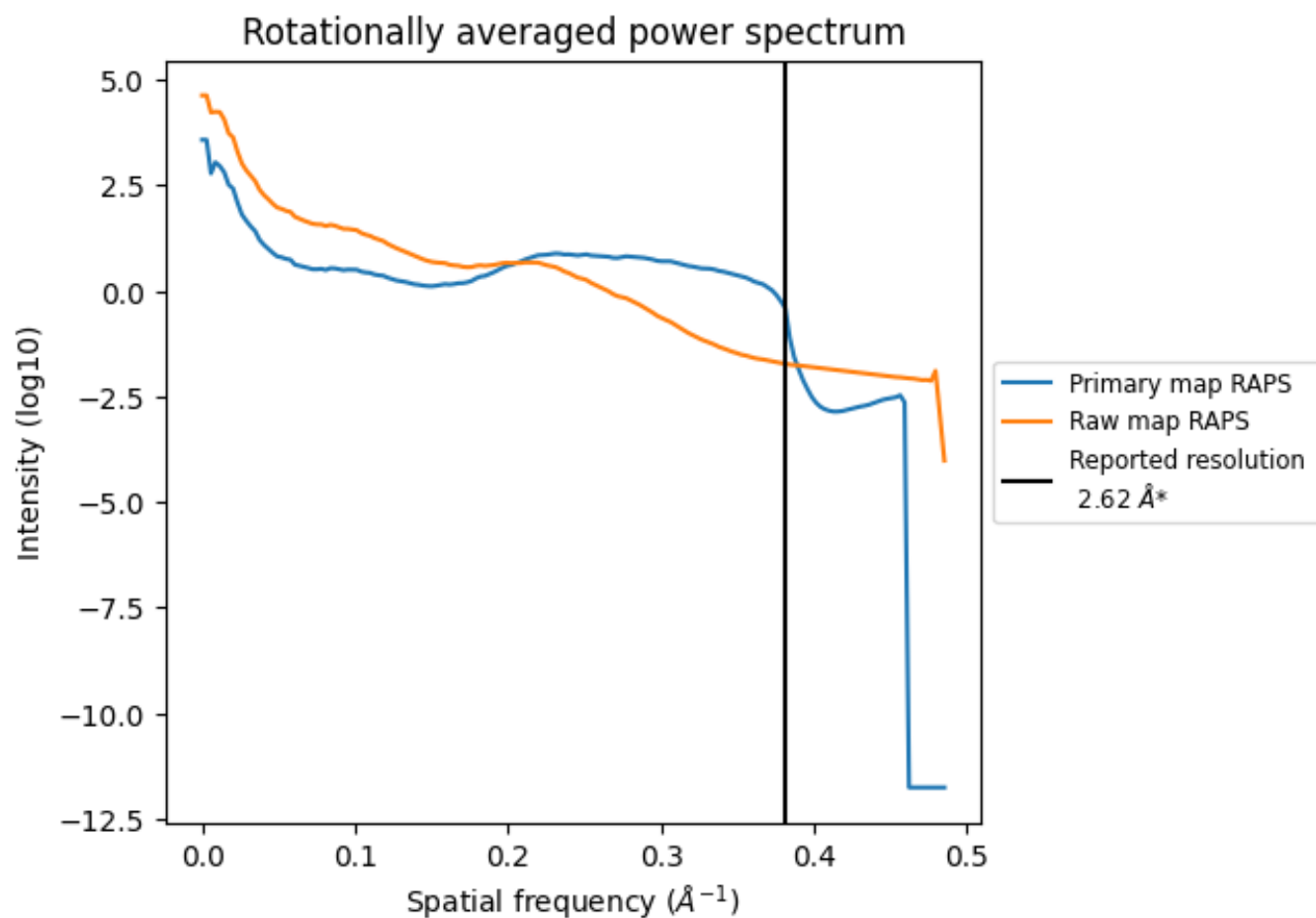


The volume at the recommended contour level is 853 nm<sup>3</sup>; this corresponds to an approximate mass of 771 kDa.

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 ⓘ

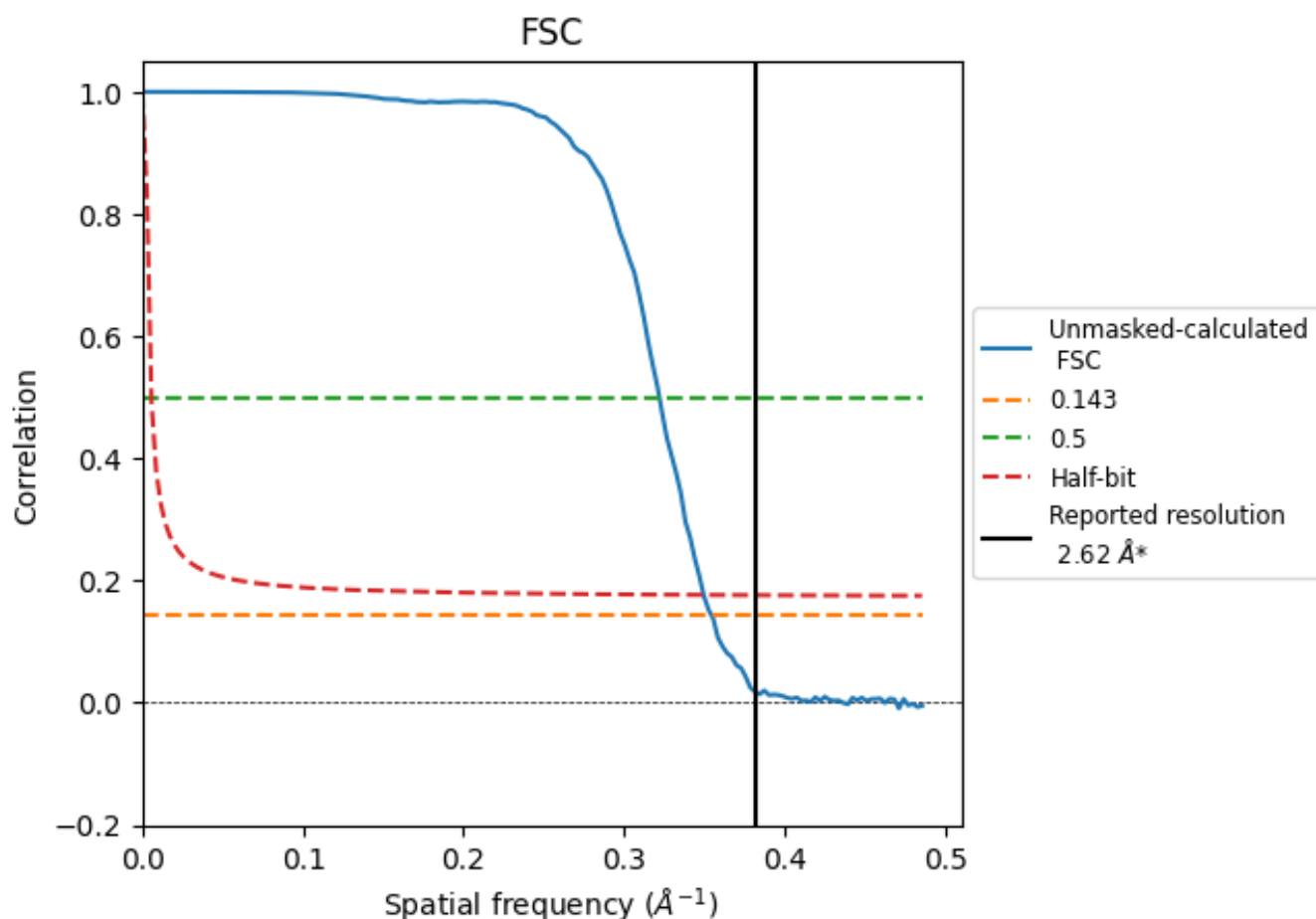


\*Reported resolution corresponds to spatial frequency of 0.382 Å<sup>-1</sup>

## 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 0.382  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

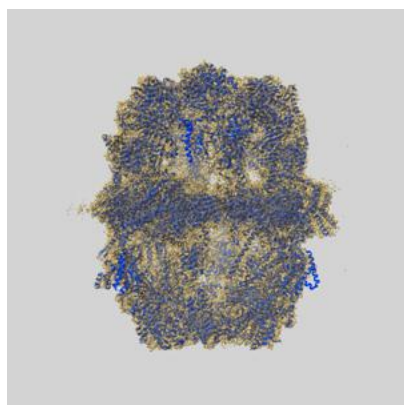
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.11	2.86

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

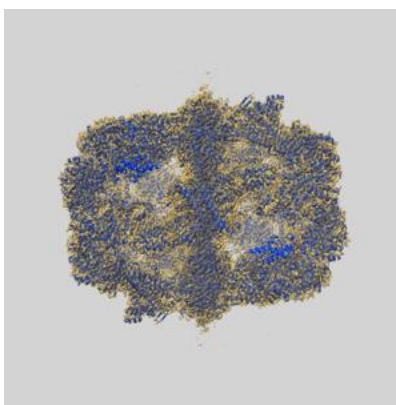
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46552 and PDB model 9D47. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

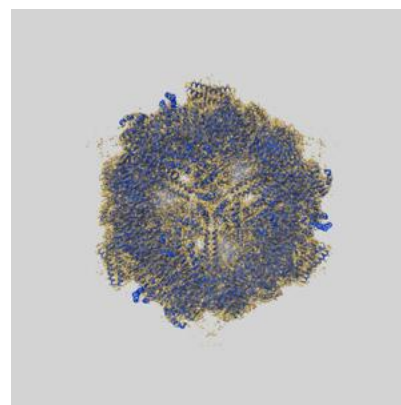
### 9.1 Map-model overlay [i](#)



X



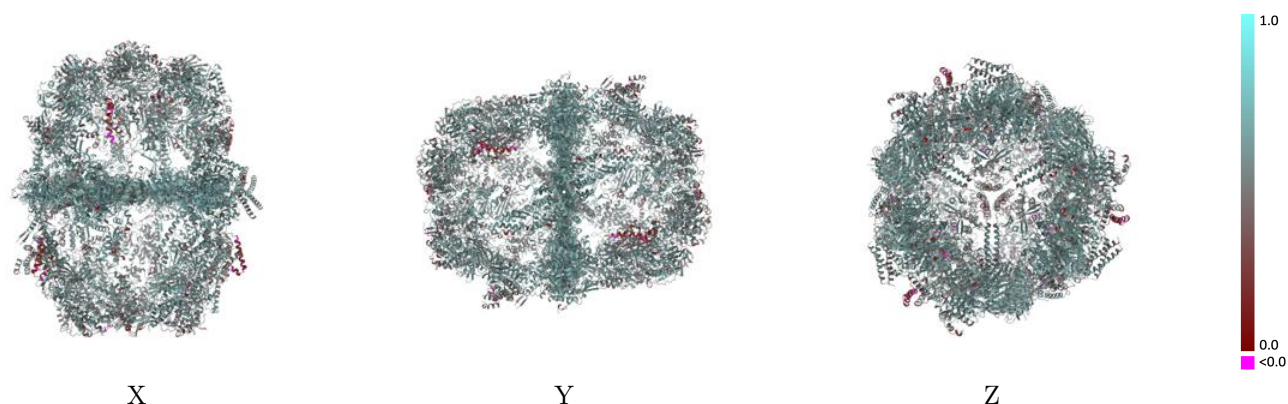
Y



Z

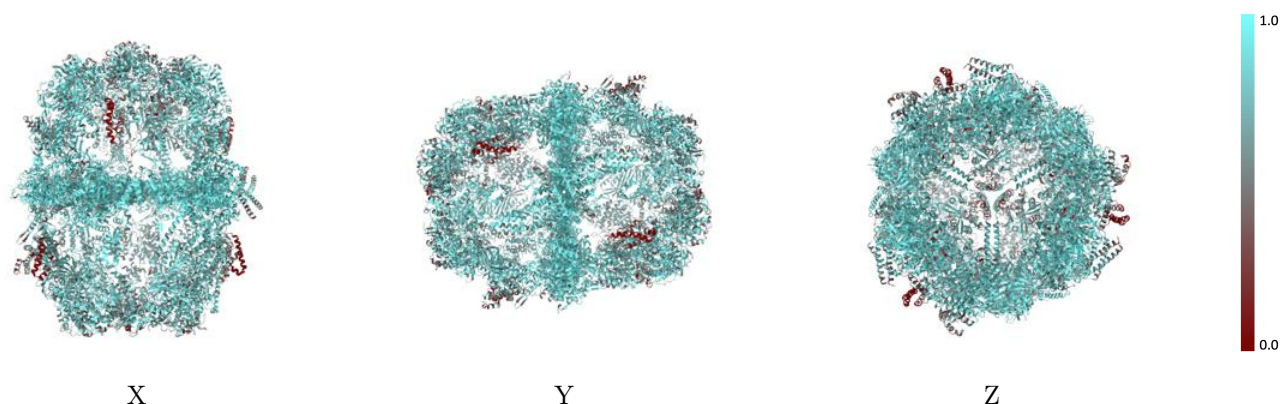
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



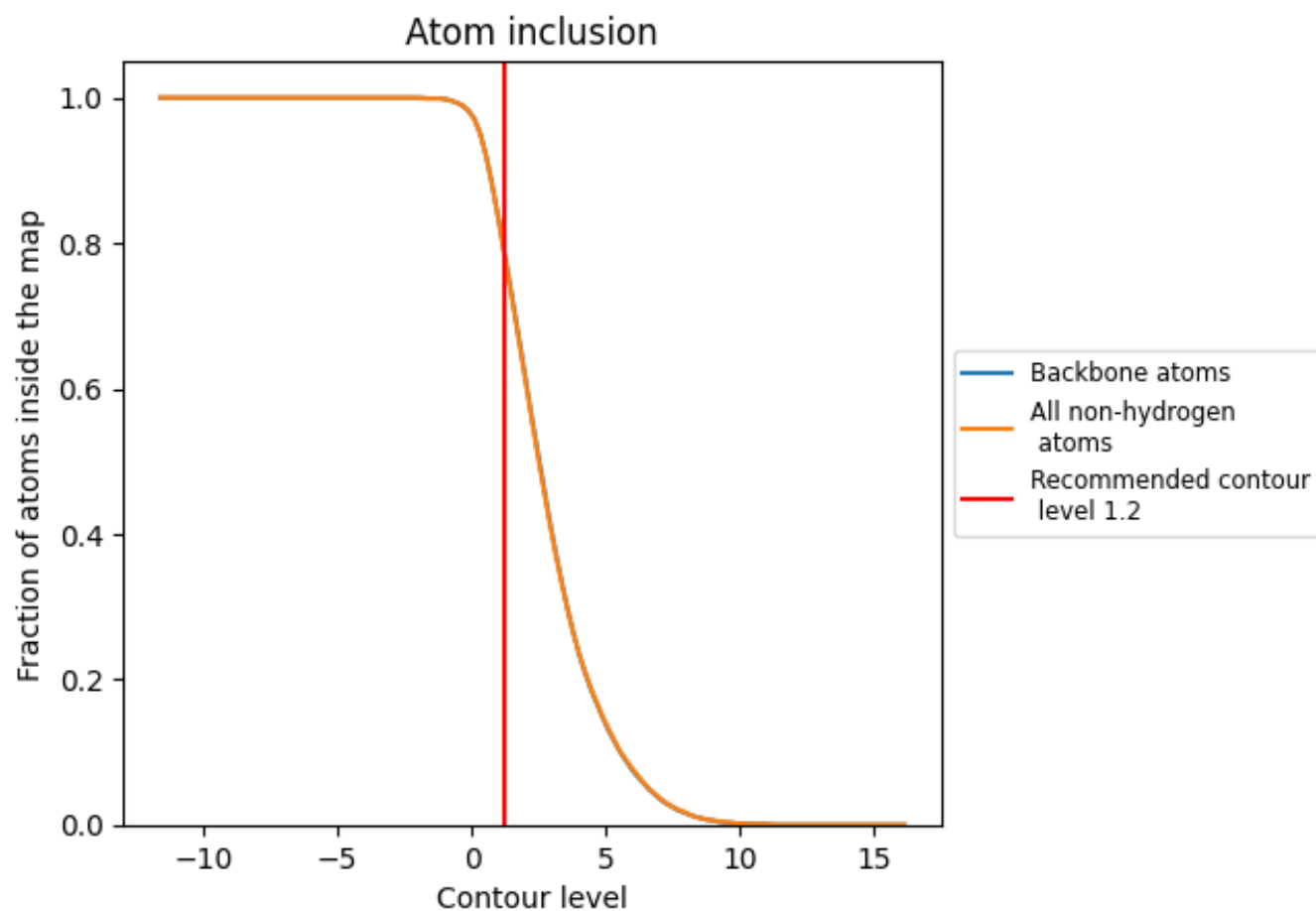
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7910</div>	<div><div></div>0.5570</div>
A	<div><div></div>0.7320</div>	<div><div></div>0.5290</div>
C	<div><div></div>0.8840</div>	<div><div></div>0.5980</div>
E	<div><div></div>0.7310</div>	<div><div></div>0.5300</div>
G	<div><div></div>0.8830</div>	<div><div></div>0.5950</div>
I	<div><div></div>0.7320</div>	<div><div></div>0.5290</div>
K	<div><div></div>0.8840</div>	<div><div></div>0.5960</div>
M	<div><div></div>0.7310</div>	<div><div></div>0.5300</div>
O	<div><div></div>0.8840</div>	<div><div></div>0.5960</div>
Q	<div><div></div>0.7320</div>	<div><div></div>0.5300</div>
S	<div><div></div>0.8840</div>	<div><div></div>0.5980</div>
U	<div><div></div>0.7300</div>	<div><div></div>0.5300</div>
X	<div><div></div>0.8840</div>	<div><div></div>0.5970</div>

1.0

0.0

<0.0