Full wwPDB EM Validation Report ⓘ

Oct 1, 2024 – 02:32 pm BST

PDB ID	:	8RS0
EMDB ID	:	EMD-19472
Title	:	Structure of RyR1 in detergent in primed state in complex with nanobody and FKBP
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-24
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

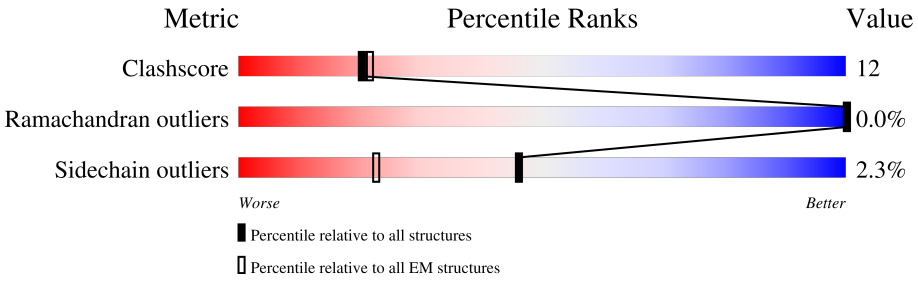
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	107	17% 67% 31% ·
1	D	107	18% 73% 25% ·
1	H	107	19% 70% 28% ·
1	I	107	18% 74% 24% ·
2	B	5027	· 62% 23% · 14%
2	E	5027	· 62% 23% · 14%
2	G	5027	· 63% 23% · 14%
2	J	5027	· 62% 22% · 14%

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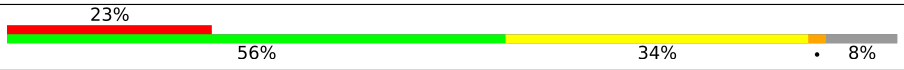
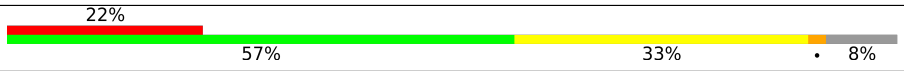
Mol	Chain	Length	Quality of chain
3	C	137	
3	F	137	
3	K	137	
3	M	137	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143570 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	D	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	I	107	Total	C	N	O	S	0	0
			816	514	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	E	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	G	4319	Total	C	N	O	S	1	0
			34149	21751	5887	6284	227		
2	J	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		

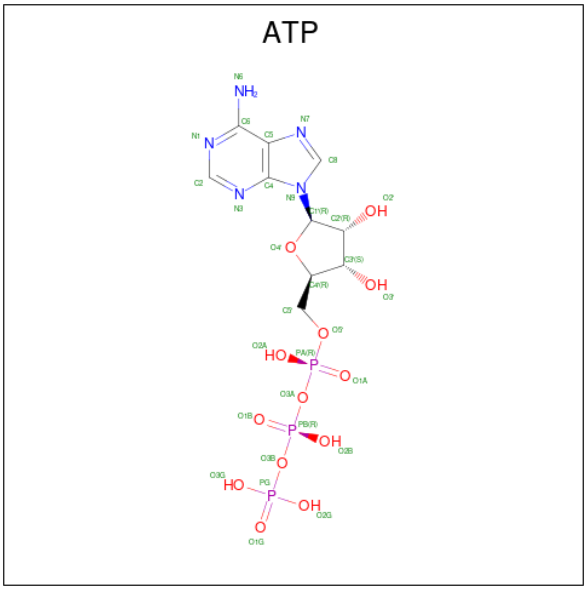
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	F	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	K	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	M	126	Total	C	N	O	S	0	0
			960	591	170	194	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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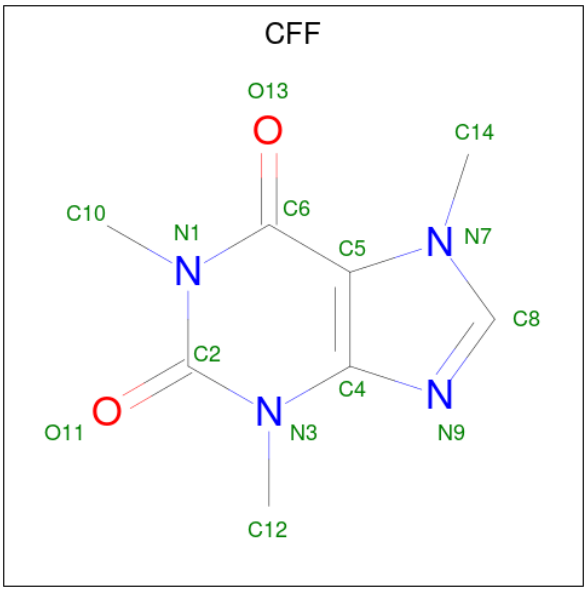
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Ca	0
			1	1	

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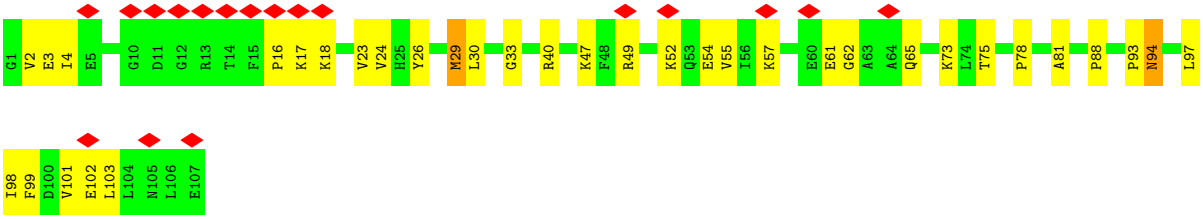
Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Ca 1 1	0
7	G	1	Total Ca 1 1	0
7	J	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

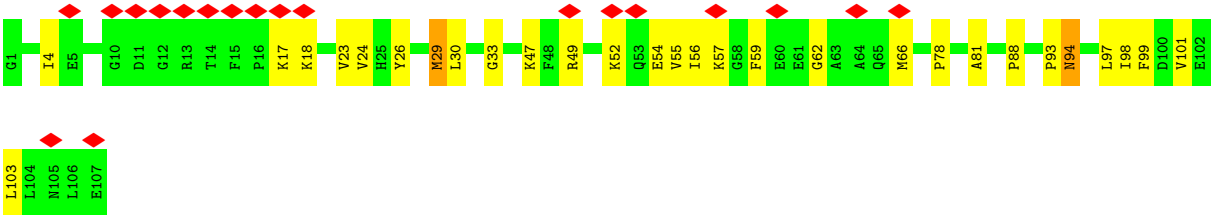
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



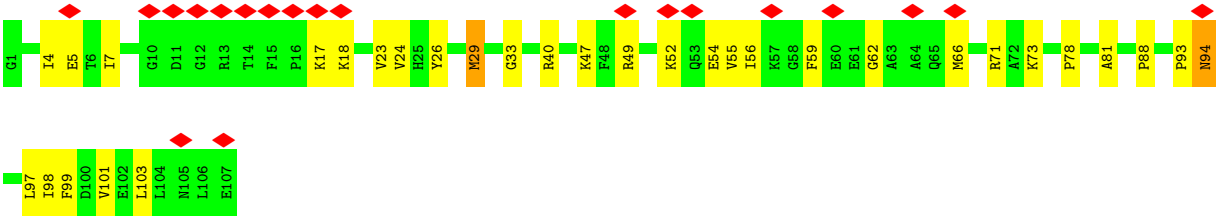
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:



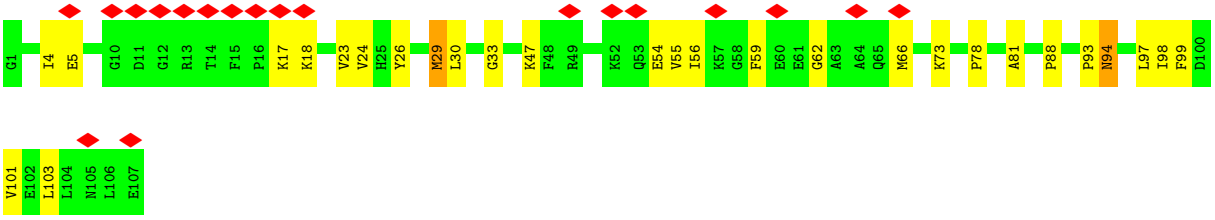
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



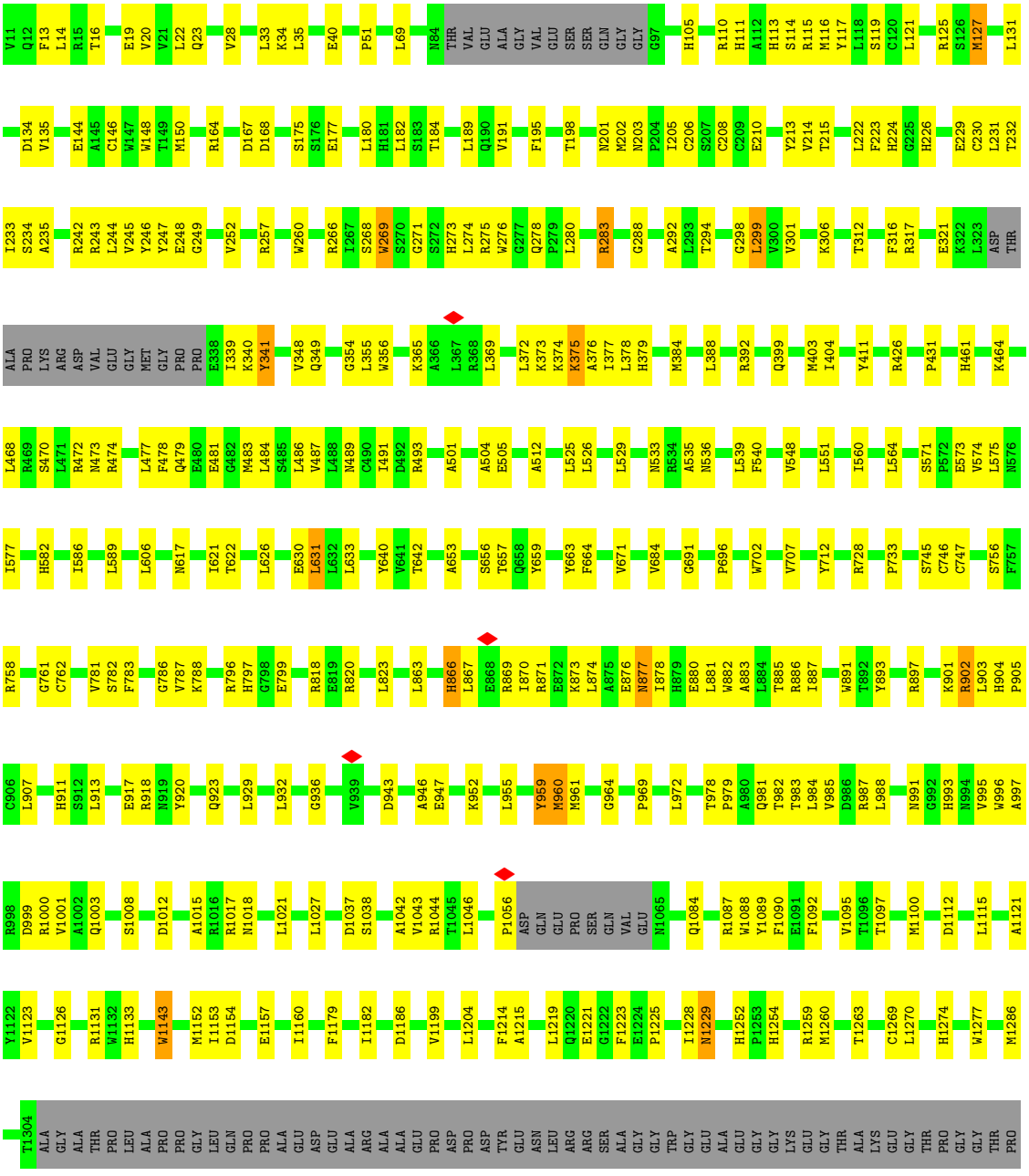
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

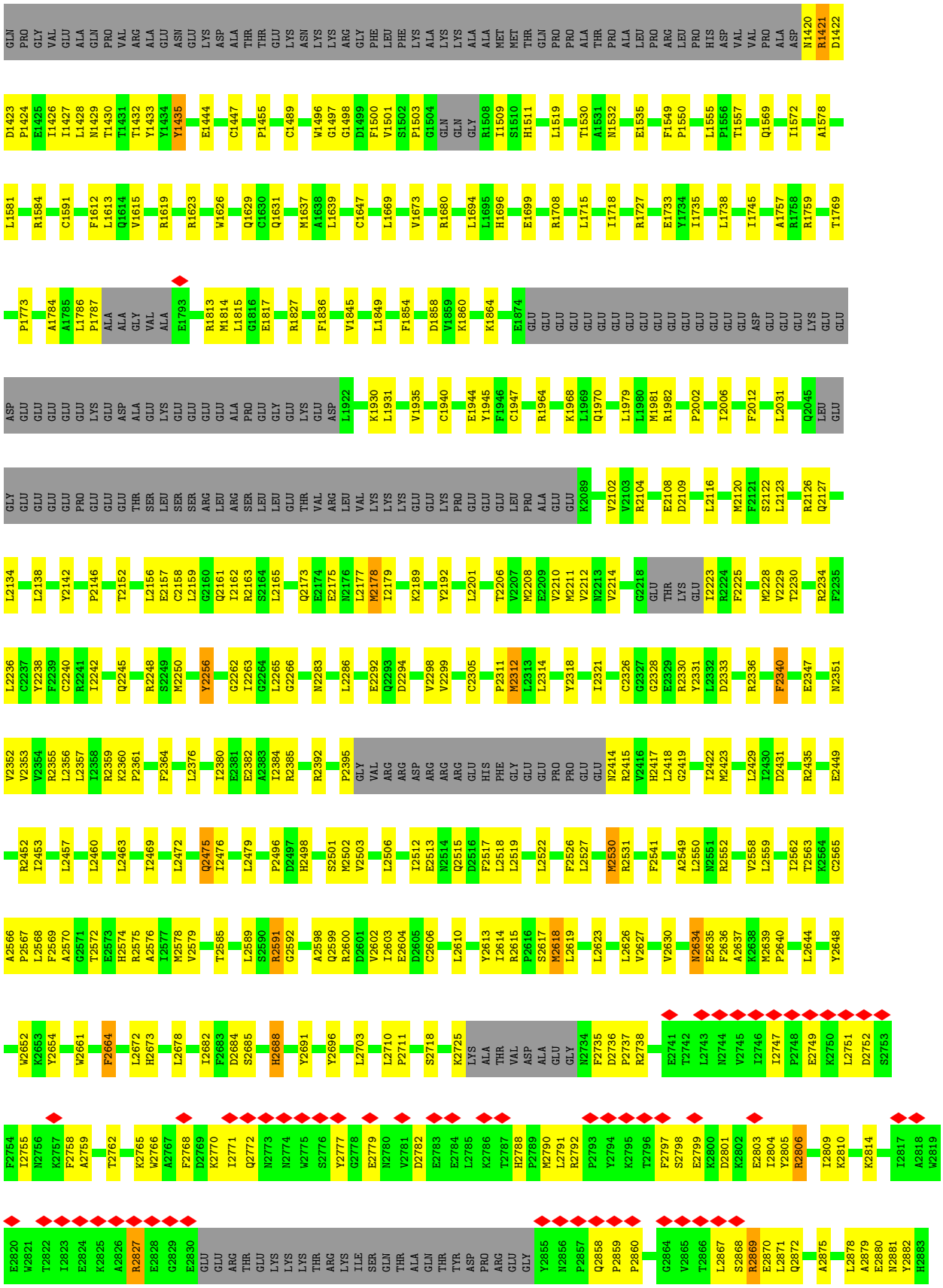
Chain I:

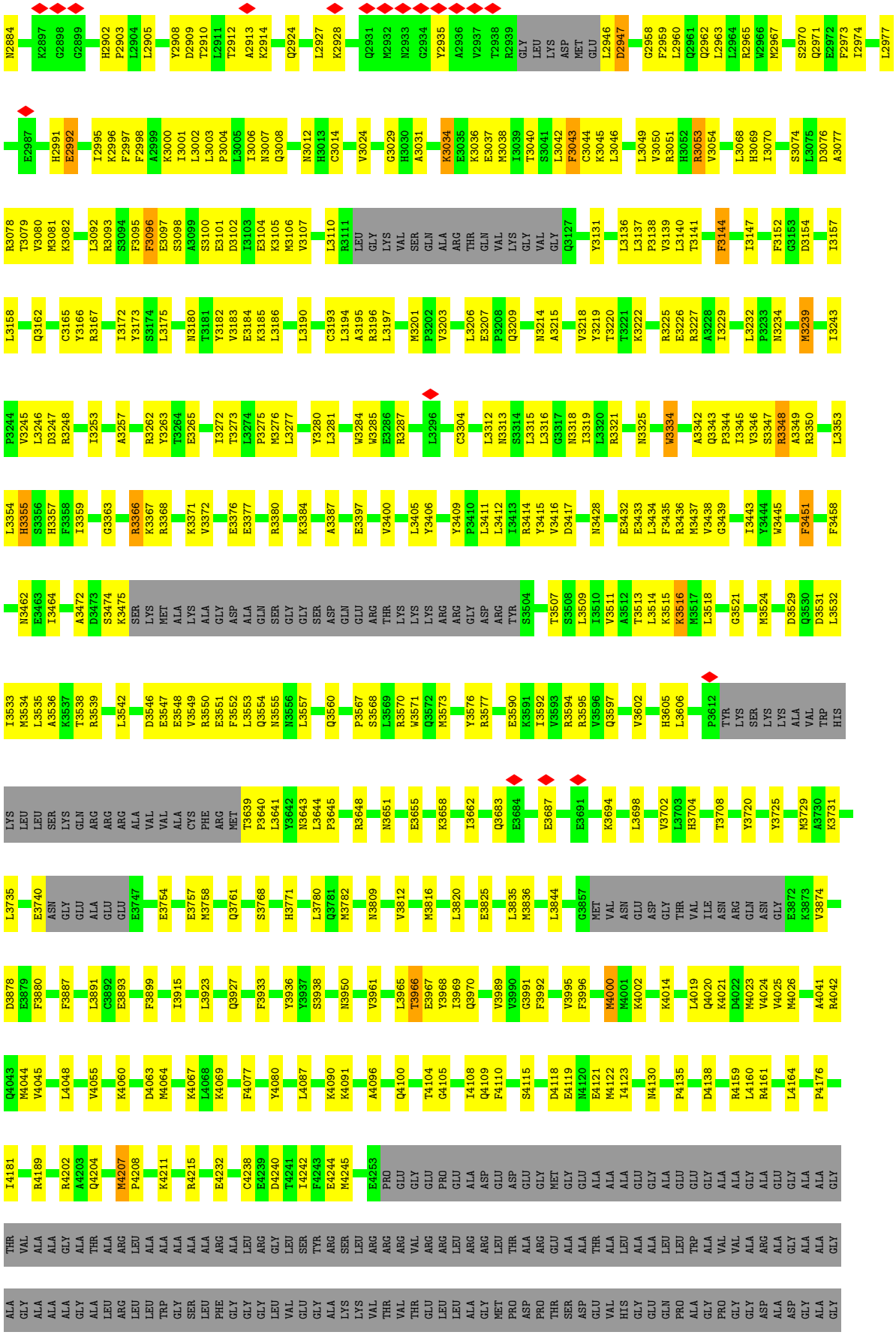


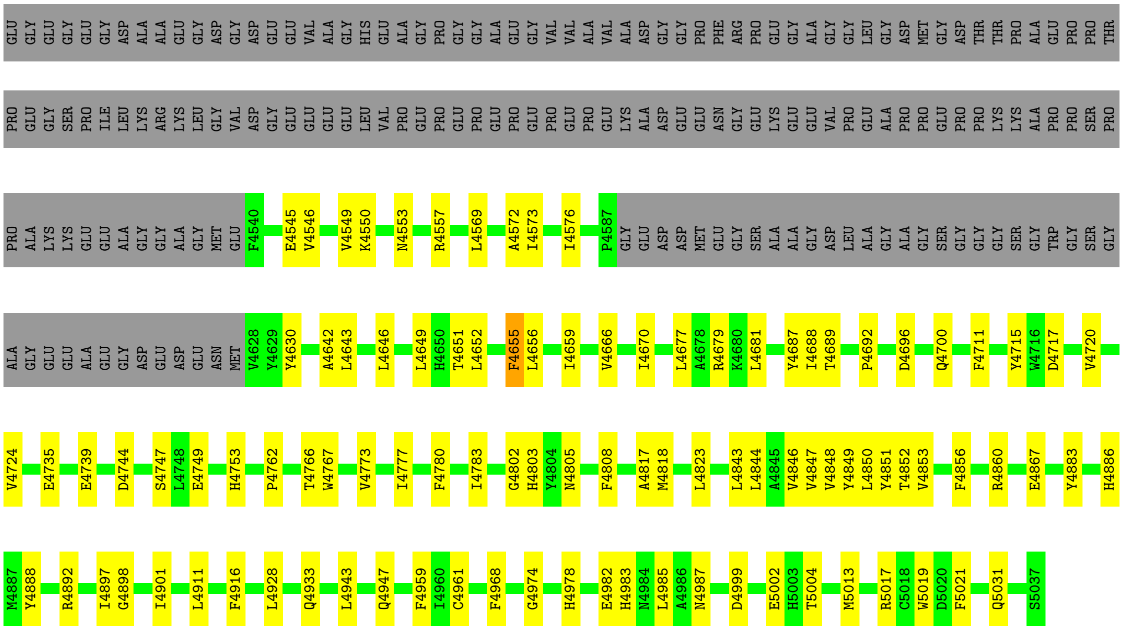
• Molecule 2: Ryanodine receptor 1

Chain B:

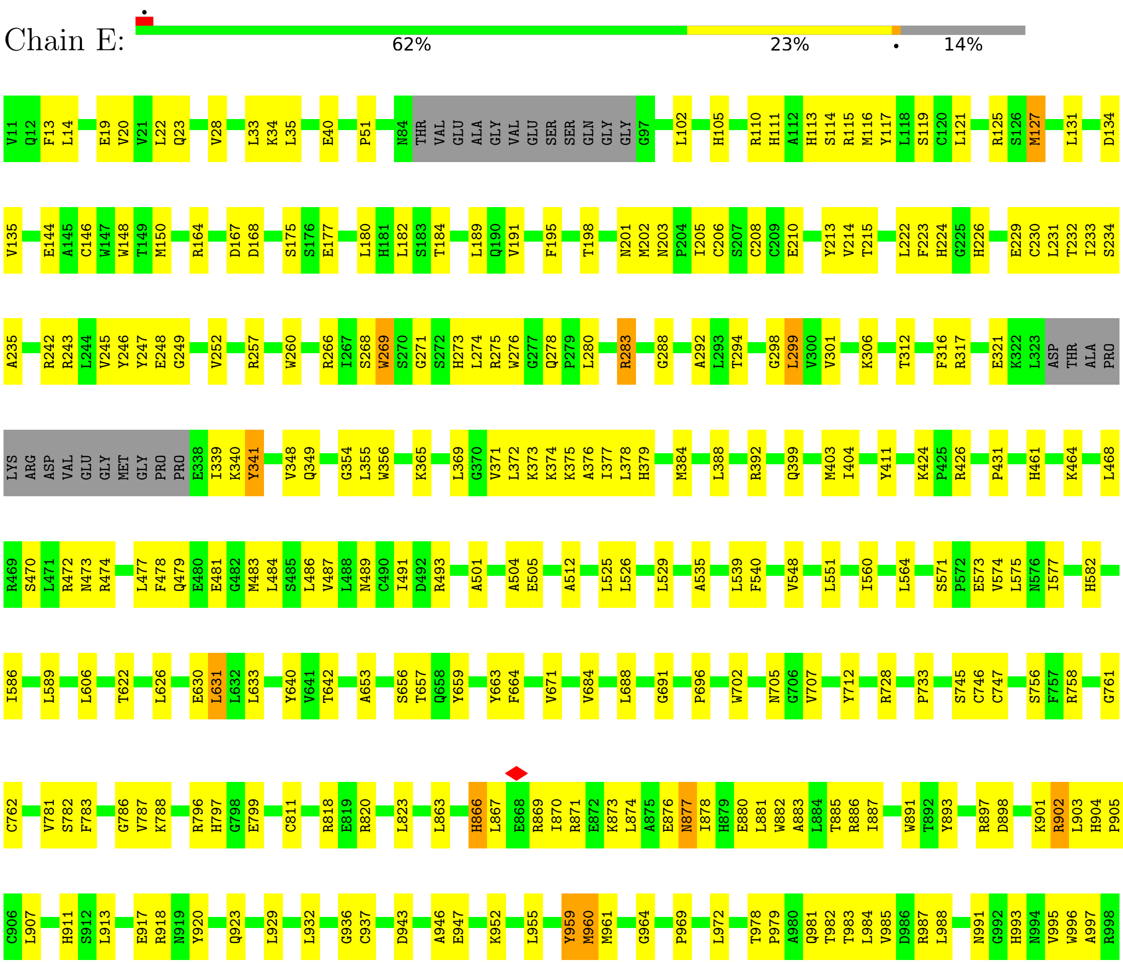


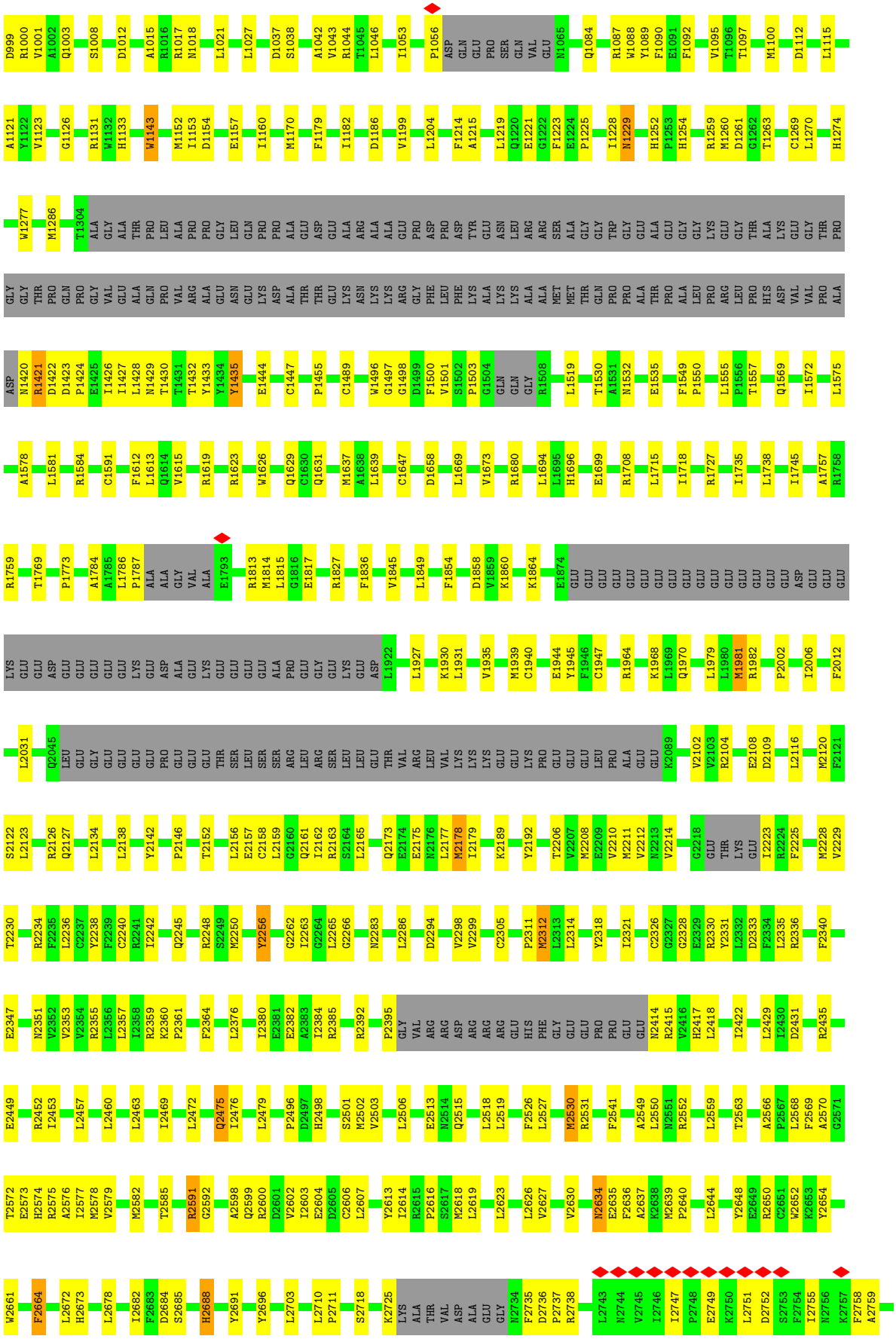


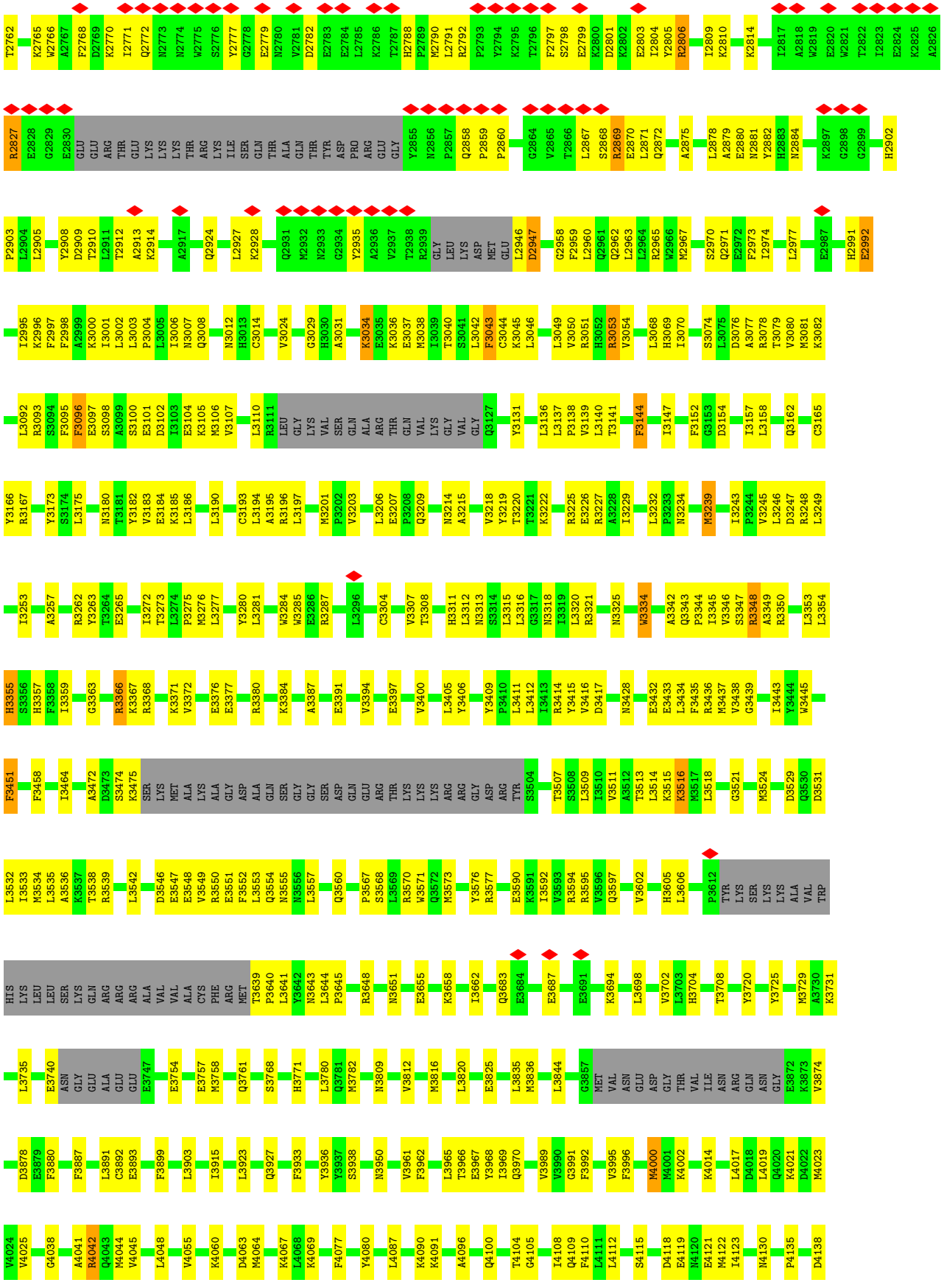


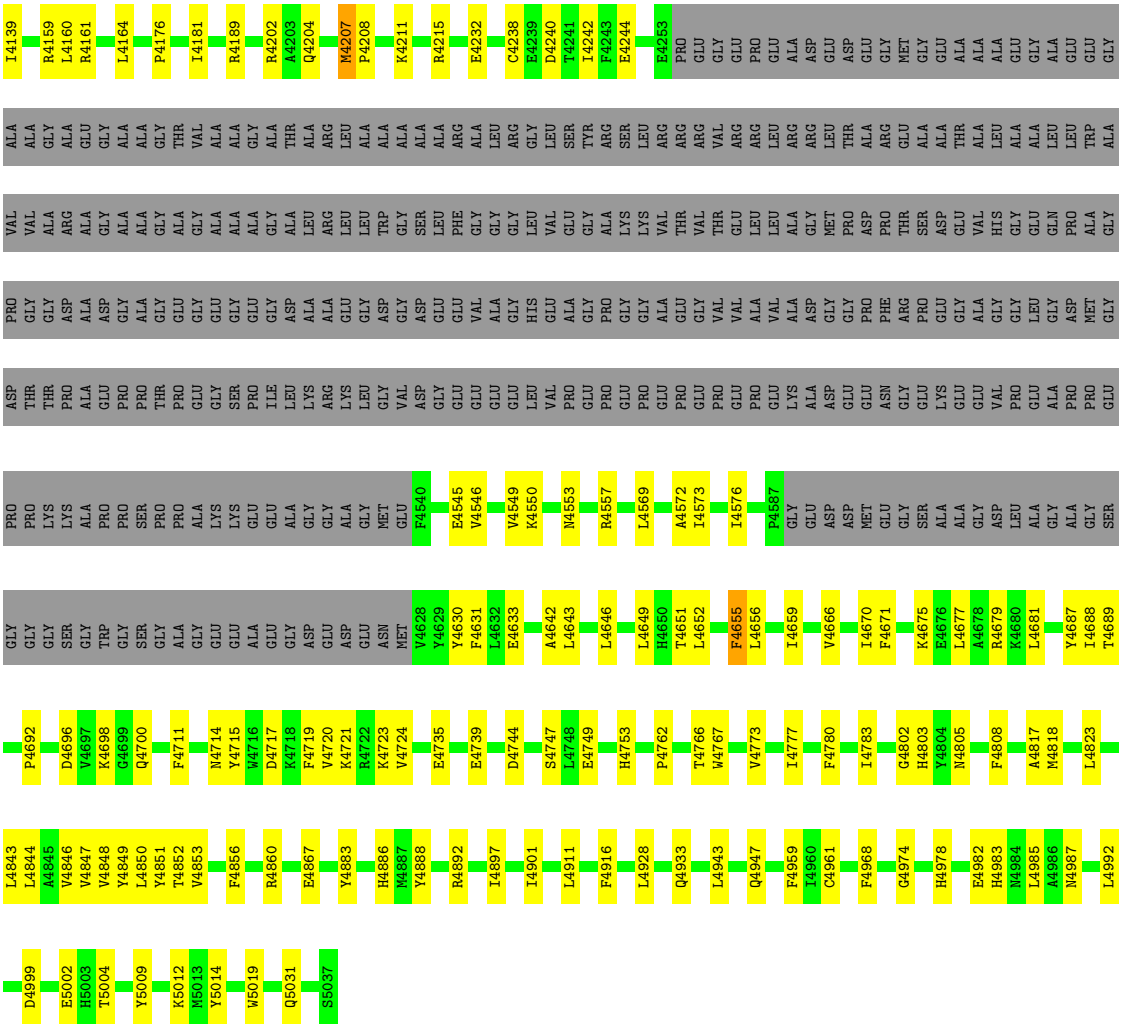


• Molecule 2: Ryanodine receptor 1



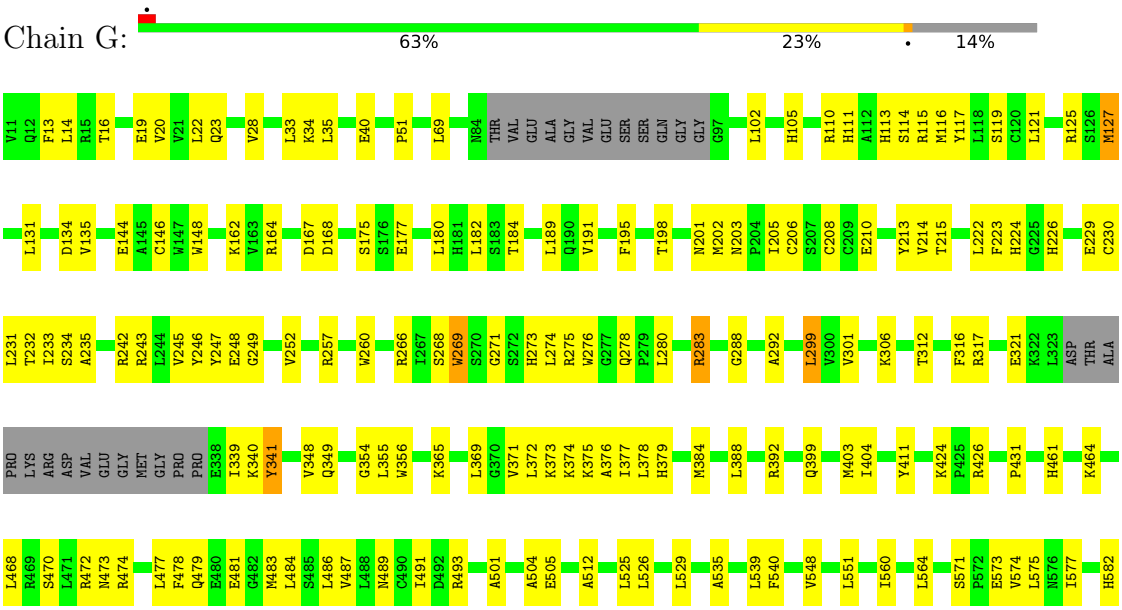


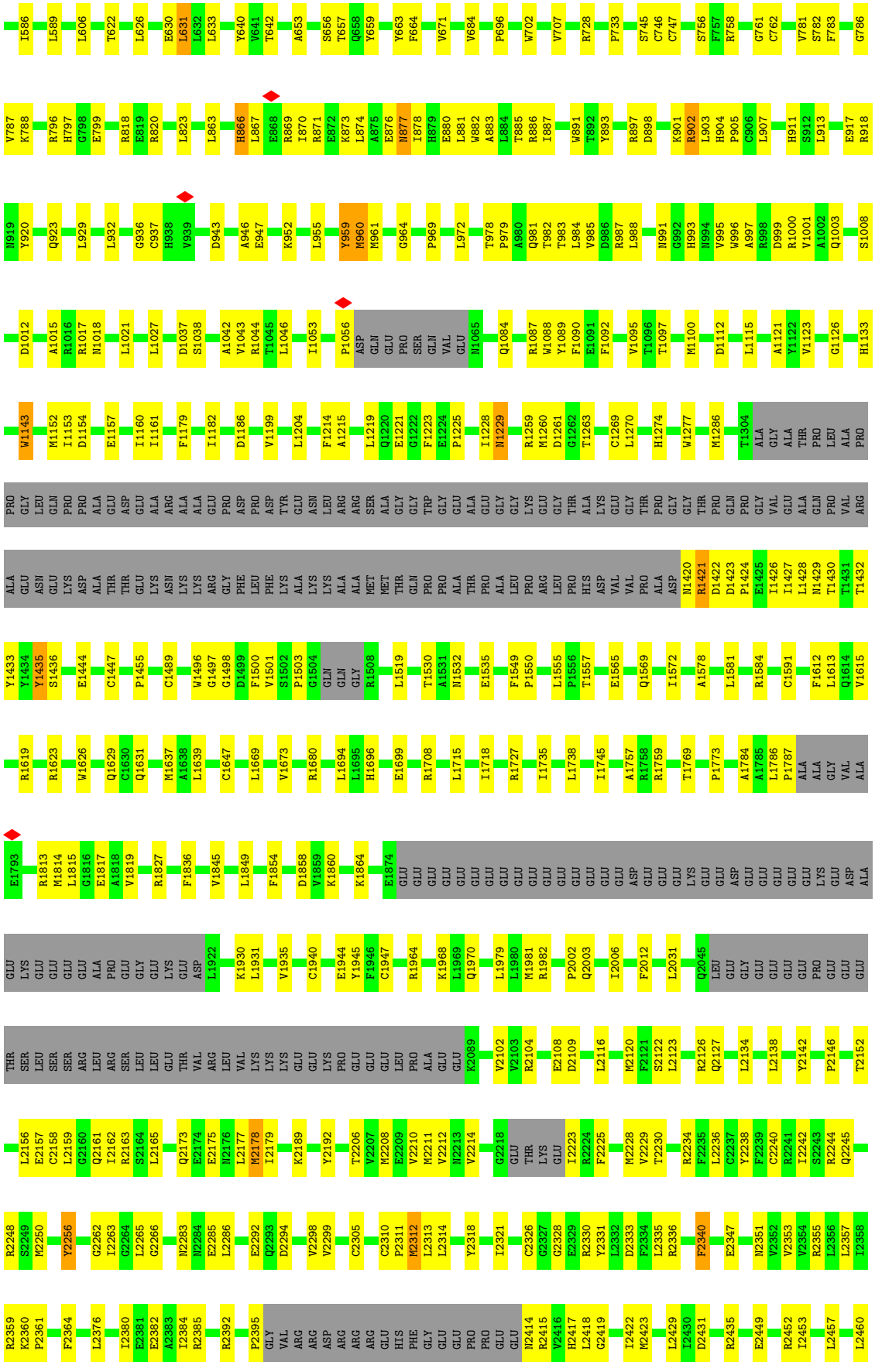


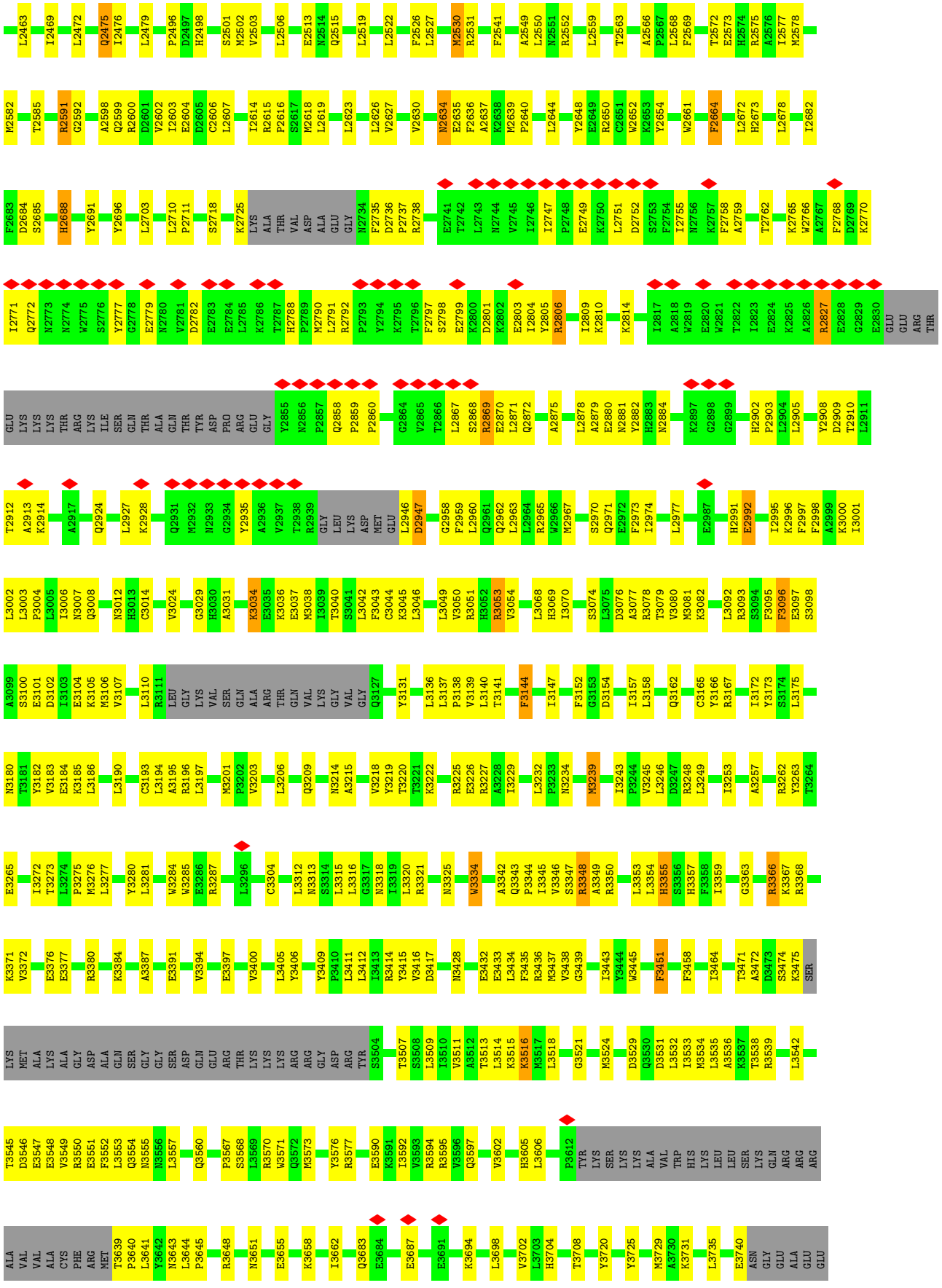


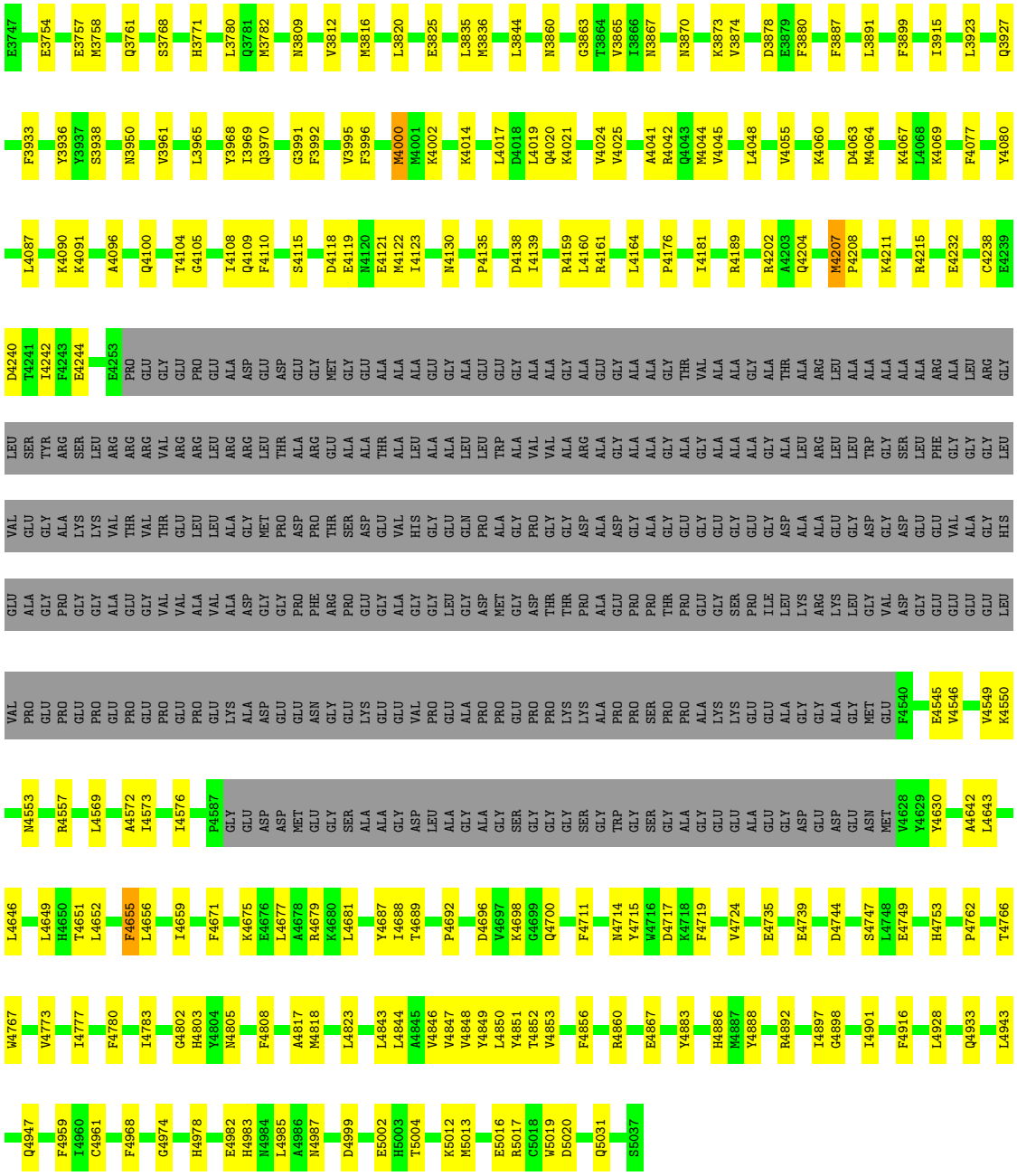
• Molecule 2: Ryanodine receptor 1

Chain G:

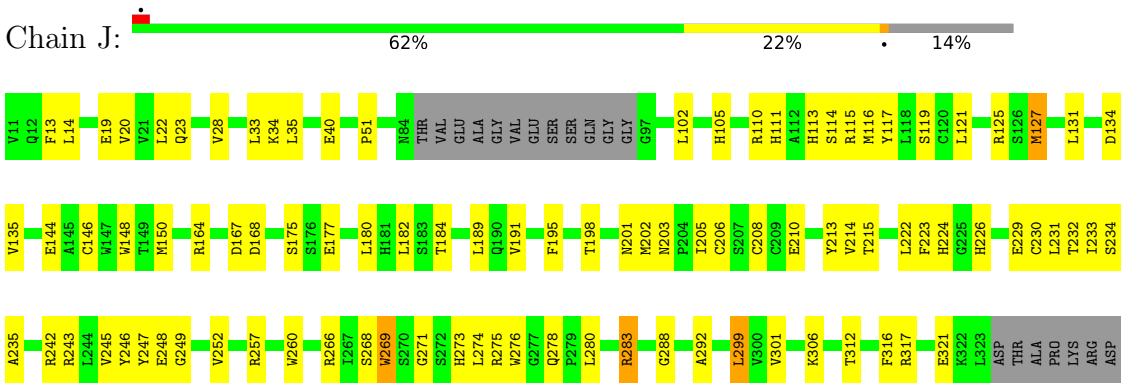


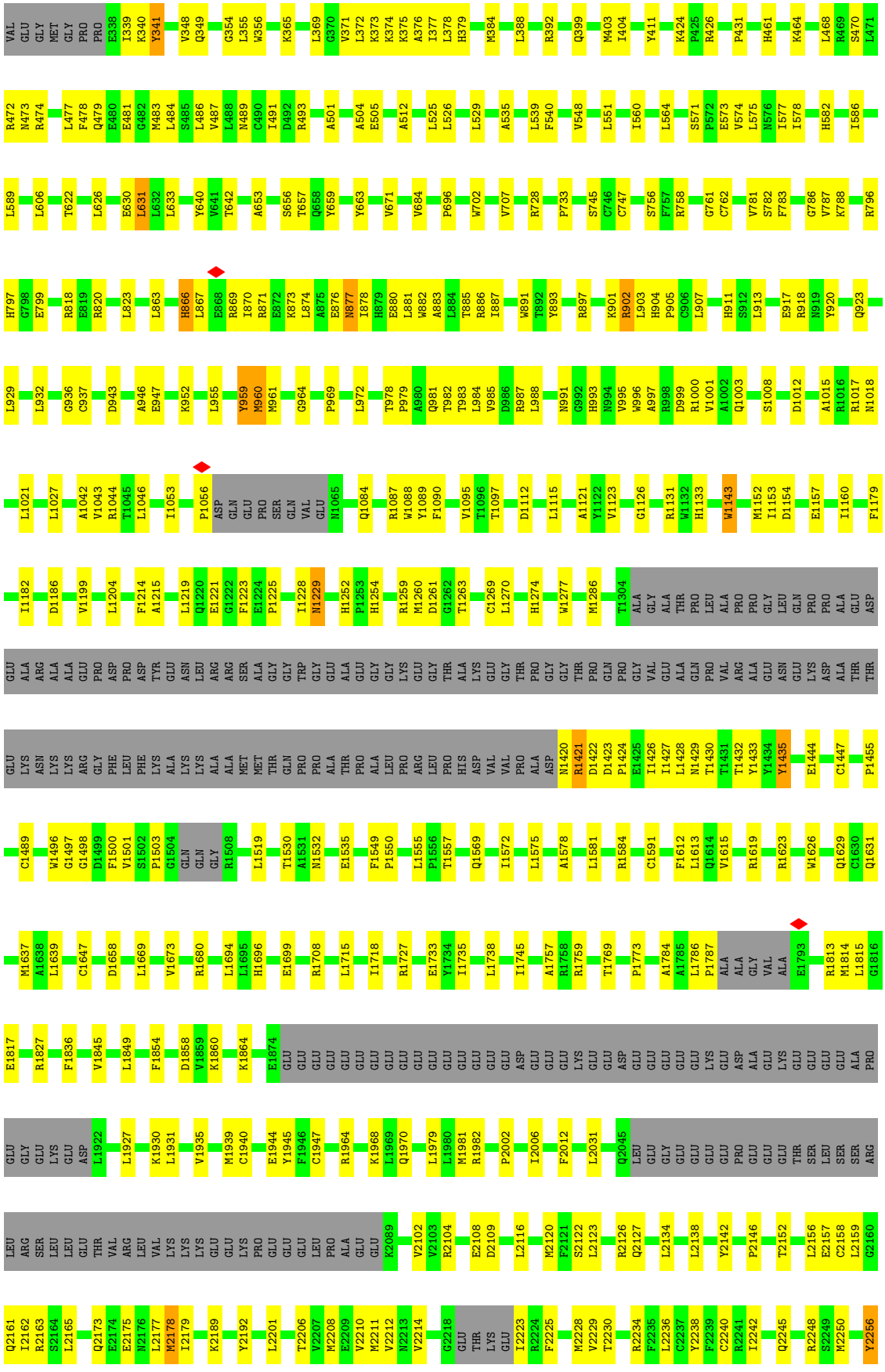


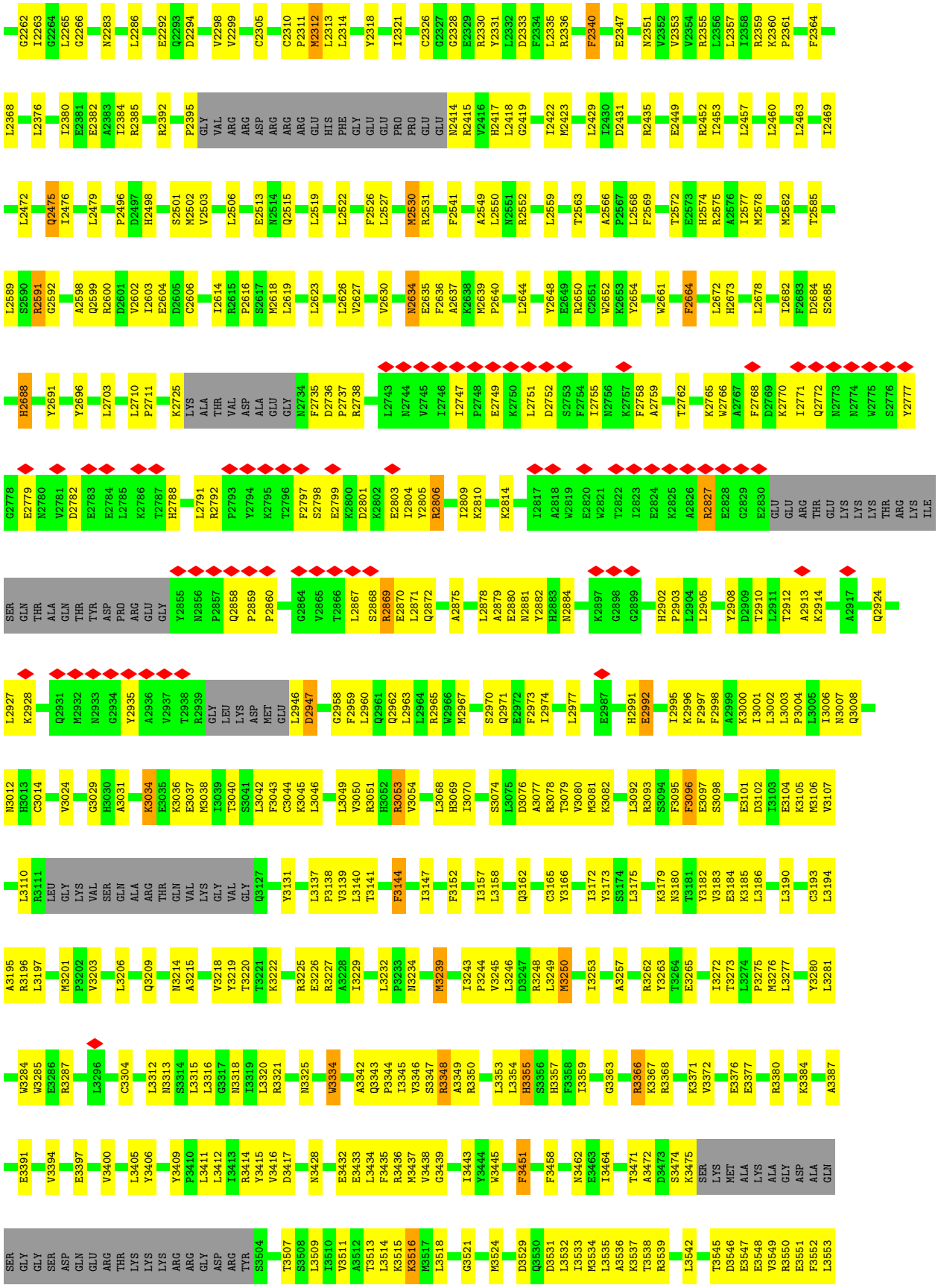


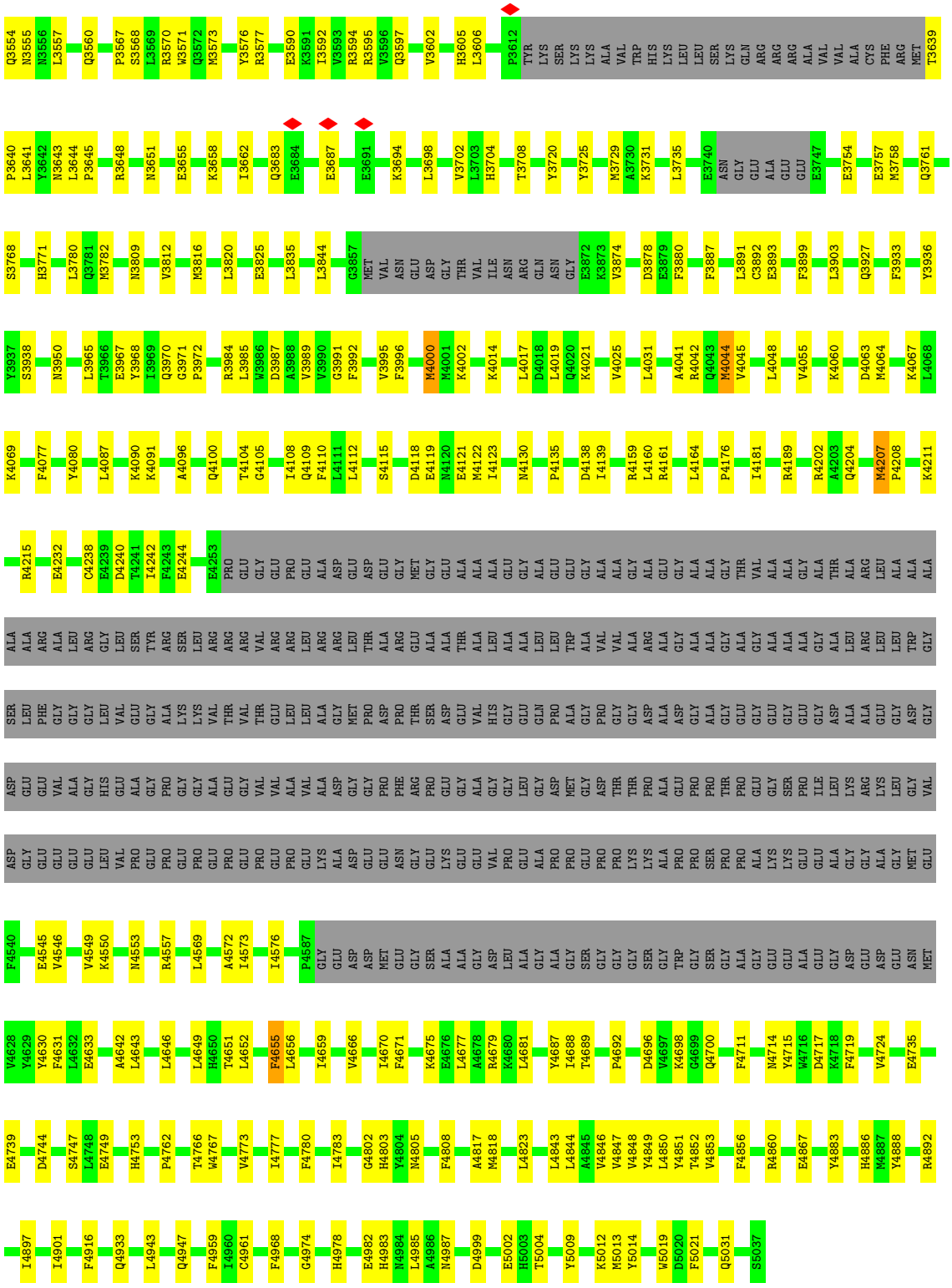


• Molecule 2: Ryanodine receptor 1

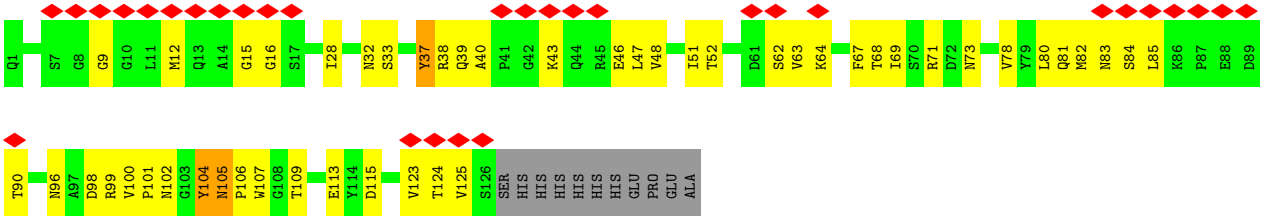






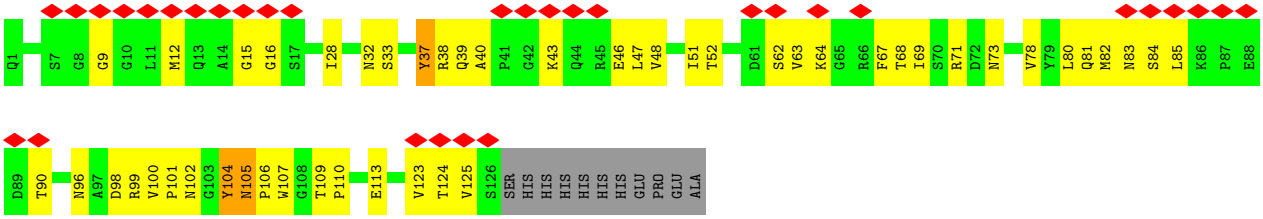


• Molecule 3: Nanobody 9657



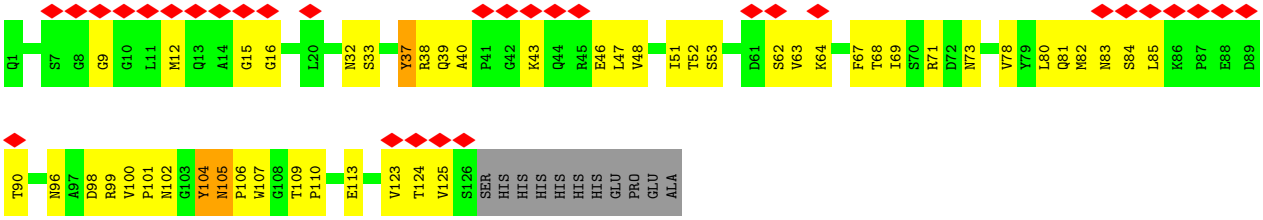
• Molecule 3: Nanobody 9657

Chain F:



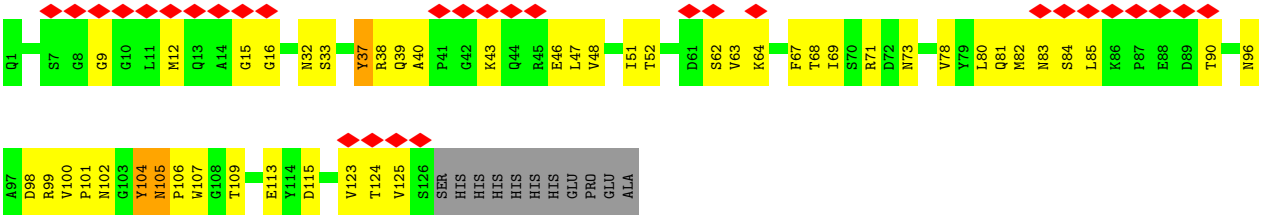
• Molecule 3: Nanobody 9657

Chain K:



• Molecule 3: Nanobody 9657

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.519	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.057	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	500.64, 500.64, 500.64	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/831	0.55	0/1118
1	D	0.27	0/831	0.56	0/1118
1	H	0.27	0/831	0.56	0/1118
1	I	0.27	0/831	0.56	0/1118
2	B	0.25	0/34814	0.50	1/47183 (0.0%)
2	E	0.25	0/34814	0.50	1/47183 (0.0%)
2	G	0.25	0/34921	0.50	1/47329 (0.0%)
2	J	0.25	0/34814	0.50	1/47183 (0.0%)
3	C	0.28	0/979	0.58	0/1329
3	F	0.28	0/979	0.58	0/1329
3	K	0.28	0/979	0.58	0/1329
3	M	0.28	0/979	0.58	0/1329
All	All	0.25	0/146603	0.50	4/198666 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1503	PRO	N-CA-CB	5.74	110.19	103.30
2	J	1503	PRO	N-CA-CB	5.71	110.15	103.30
2	B	1503	PRO	N-CA-CB	5.68	110.11	103.30
2	G	1503	PRO	N-CA-CB	5.66	110.09	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	818	28	0
1	D	816	0	818	23	0
1	H	816	0	818	25	0
1	I	816	0	818	24	0
2	B	34043	0	33446	799	0
2	E	34043	0	33446	803	0
2	G	34149	0	33547	812	0
2	J	34043	0	33446	792	0
3	C	960	0	909	36	0
3	F	960	0	909	41	0
3	K	960	0	909	41	0
3	M	960	0	909	40	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	0	0
5	E	31	0	12	0	0
5	G	31	0	12	0	0
5	J	31	0	12	0	0
6	B	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143570	0	140881	3411	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 12.

All (3411) 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:B:4961:CYS:SG	2:B:4983:HIS:CE1	2.61	0.94
2:G:4961:CYS:SG	2:G:4983:HIS:CE1	2.60	0.93
2:E:4961:CYS:SG	2:E:4983:HIS:CE1	2.60	0.93
3:K:100:VAL:HG22	3:K:105:ASN:HD22	1.34	0.92
2:J:4961:CYS:SG	2:J:4983:HIS:CE1	2.60	0.92
3:M:100:VAL:HG22	3:M:105:ASN:HD22	1.33	0.92
2:B:3207:GLU:HB2	2:B:3246:LEU:HD22	1.51	0.92
2:B:2515:GLN:HA	2:B:2568:LEU:HD21	1.54	0.89
3:C:100:VAL:HG22	3:C:105:ASN:HD22	1.33	0.89
3:F:100:VAL:HG22	3:F:105:ASN:HD22	1.34	0.89
3:K:38:ARG:HH22	3:K:64:LYS:HG2	1.43	0.84
3:M:38:ARG:HH22	3:M:64:LYS:HG2	1.43	0.83
3:C:38:ARG:HH22	3:C:64:LYS:HG2	1.43	0.82
3:F:38:ARG:HH22	3:F:64:LYS:HG2	1.43	0.81
2:B:248:GLU:HB3	2:B:373:LYS:HD3	1.60	0.80
2:E:248:GLU:HA	2:E:372:LEU:HB3	1.65	0.78
2:G:248:GLU:HA	2:G:372:LEU:HB2	1.64	0.77
2:E:247:TYR:HD2	2:E:374:LYS:HB2	1.50	0.76
2:B:3277:LEU:HD13	2:B:3315:LEU:HD22	1.67	0.76
2:G:2974:ILE:HD12	2:G:3053:ARG:HG2	1.68	0.76
2:G:229:GLU:HA	2:G:249:GLY:HA3	1.68	0.76
2:J:2974:ILE:HD12	2:J:3053:ARG:HG2	1.68	0.76
2:E:1422:ASP:HB2	2:E:1427:ILE:HD11	1.68	0.76
2:B:229:GLU:HA	2:B:249:GLY:HA3	1.68	0.75
2:B:1422:ASP:HB2	2:B:1427:ILE:HD11	1.68	0.75
2:B:2974:ILE:HD12	2:B:3053:ARG:HG2	1.68	0.75
2:J:229:GLU:HA	2:J:249:GLY:HA3	1.68	0.75
2:G:1422:ASP:HB2	2:G:1427:ILE:HD11	1.68	0.75
2:E:2974:ILE:HD12	2:E:3053:ARG:HG2	1.68	0.74
2:B:3366:ARG:NH1	2:B:3437:MET:SD	2.60	0.74
2:B:891:TRP:HA	2:B:902:ARG:HB3	1.69	0.74
2:J:404:ILE:HD13	2:J:481:GLU:HG3	1.70	0.74
2:J:959:TYR:HB2	2:J:964:GLY:HA2	1.69	0.74
2:J:891:TRP:HA	2:J:902:ARG:HB3	1.69	0.74
2:J:248:GLU:HB3	2:J:373:LYS:HD3	1.69	0.74
2:G:3366:ARG:NH1	2:G:3437:MET:SD	2.60	0.74
2:E:229:GLU:HA	2:E:249:GLY:HA3	1.68	0.74
2:E:404:ILE:HD13	2:E:481:GLU:HG3	1.70	0.74
2:J:1422:ASP:HB2	2:J:1427:ILE:HD11	1.68	0.74
2:E:3366:ARG:NH1	2:E:3437:MET:SD	2.60	0.73
2:B:959:TYR:HB2	2:B:964:GLY:HA2	1.69	0.73
2:G:959:TYR:HB2	2:G:964:GLY:HA2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:891:TRP:HA	2:G:902:ARG:HB3	1.69	0.73
2:J:3366:ARG:HE	2:J:3367:LYS:HD2	1.54	0.73
2:B:3366:ARG:HE	2:B:3367:LYS:HD2	1.54	0.73
2:G:404:ILE:HD13	2:G:481:GLU:HG3	1.70	0.73
2:E:4852:THR:HG21	2:E:4883:TYR:HA	1.71	0.72
2:G:4715:TYR:HE2	2:G:4717:ASP:HB3	1.53	0.72
2:J:3366:ARG:NH1	2:J:3437:MET:SD	2.60	0.72
2:B:4852:THR:HG21	2:B:4883:TYR:HA	1.71	0.72
2:E:959:TYR:HB2	2:E:964:GLY:HA2	1.69	0.72
2:J:913:LEU:HB3	2:J:917:GLU:HB2	1.72	0.72
2:E:913:LEU:HB3	2:E:917:GLU:HB2	1.72	0.72
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.71	0.72
2:B:247:TYR:HD2	2:B:374:LYS:HB2	1.55	0.72
2:E:891:TRP:HA	2:E:902:ARG:HB3	1.69	0.72
2:B:404:ILE:HD13	2:B:481:GLU:HG3	1.70	0.72
2:G:3320:LEU:HD12	2:G:3357:HIS:CD2	2.25	0.72
2:E:4715:TYR:HE2	2:E:4717:ASP:HB3	1.54	0.72
2:B:3273:THR:HA	2:B:3276:MET:HG2	1.72	0.72
2:J:3277:LEU:HD13	2:J:3315:LEU:HD22	1.71	0.72
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.71	0.71
2:G:4852:THR:HG21	2:G:4883:TYR:HA	1.71	0.71
2:E:3366:ARG:HE	2:E:3367:LYS:HD2	1.54	0.71
2:G:3273:THR:HA	2:G:3276:MET:HG2	1.72	0.71
2:J:3809:ASN:HB3	2:J:3812:VAL:HG22	1.71	0.71
2:J:4715:TYR:HE2	2:J:4717:ASP:HB3	1.55	0.71
2:E:4546:VAL:HG22	2:E:4550:LYS:HE3	1.72	0.70
2:G:2244:ARG:HD3	2:G:3860:ASN:HA	1.73	0.70
2:J:3273:THR:HA	2:J:3276:MET:HG2	1.72	0.70
2:B:913:LEU:HB3	2:B:917:GLU:HB2	1.72	0.70
2:B:3144:PHE:HB2	2:B:3196:ARG:HB3	1.73	0.70
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.71	0.70
2:G:913:LEU:HB3	2:G:917:GLU:HB2	1.72	0.70
2:G:3366:ARG:HE	2:G:3367:LYS:HD2	1.54	0.70
2:E:3144:PHE:HB2	2:E:3196:ARG:HB3	1.73	0.70
2:E:3344:PRO:O	2:E:3348:ARG:NH2	2.25	0.70
2:J:3344:PRO:O	2:J:3348:ARG:NH2	2.25	0.70
2:B:4546:VAL:HG22	2:B:4550:LYS:HE3	1.72	0.70
2:J:4852:THR:HG21	2:J:4883:TYR:HA	1.71	0.70
2:G:3344:PRO:O	2:G:3348:ARG:NH2	2.25	0.70
2:G:4546:VAL:HG22	2:G:4550:LYS:HE3	1.72	0.70
2:E:3273:THR:HA	2:E:3276:MET:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3344:PRO:O	2:B:3348:ARG:NH2	2.25	0.70
2:B:4762:PRO:HD2	2:B:4766:THR:HG21	1.73	0.70
2:J:4762:PRO:HD2	2:J:4766:THR:HG21	1.73	0.70
2:G:3144:PHE:HB2	2:G:3196:ARG:HB3	1.73	0.69
2:J:4546:VAL:HG22	2:J:4550:LYS:HE3	1.72	0.69
2:B:399:GLN:O	2:B:403:MET:HG3	1.92	0.69
2:B:640:TYR:HB3	2:B:1613:LEU:HD11	1.75	0.69
2:B:2321:ILE:HD11	2:B:2418:LEU:HB2	1.74	0.69
2:E:3308:THR:H	2:E:3311:HIS:CD2	2.09	0.69
2:E:4762:PRO:HD2	2:E:4766:THR:HG21	1.73	0.69
2:G:399:GLN:O	2:G:403:MET:HG3	1.92	0.69
2:G:640:TYR:HB3	2:G:1613:LEU:HD11	1.75	0.69
2:G:3870:ASN:HD21	2:G:3873:LYS:HB3	1.57	0.69
2:J:2871:LEU:HG	2:J:2927:LEU:HD21	1.74	0.69
2:E:2321:ILE:HD11	2:E:2418:LEU:HB2	1.74	0.69
2:E:2871:LEU:HG	2:E:2927:LEU:HD21	1.74	0.69
2:J:2788:HIS:HB3	2:J:2791:LEU:HB2	1.75	0.69
2:G:4897:ILE:HG13	2:G:4901:ILE:HD11	1.75	0.69
2:E:4897:ILE:HG13	2:E:4901:ILE:HD11	1.75	0.69
2:J:3144:PHE:HB2	2:J:3196:ARG:HB3	1.73	0.69
2:B:3812:VAL:O	2:B:3816:MET:HG3	1.93	0.68
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.26	0.68
2:E:3812:VAL:O	2:E:3816:MET:HG3	1.93	0.68
2:G:2871:LEU:HG	2:G:2927:LEU:HD21	1.74	0.68
2:J:640:TYR:HB3	2:J:1613:LEU:HD11	1.75	0.68
2:B:2116:LEU:O	2:B:2120:MET:HG2	1.94	0.68
2:B:2871:LEU:HG	2:B:2927:LEU:HD21	1.74	0.68
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.26	0.68
2:E:399:GLN:O	2:E:403:MET:HG3	1.92	0.68
2:J:399:GLN:O	2:J:403:MET:HG3	1.92	0.68
2:B:4897:ILE:HG13	2:B:4901:ILE:HD11	1.75	0.68
2:E:640:TYR:HB3	2:E:1613:LEU:HD11	1.75	0.68
2:J:897:ARG:HD3	2:J:905:PRO:HD3	1.76	0.68
2:J:4897:ILE:HG13	2:J:4901:ILE:HD11	1.75	0.68
2:B:3077:ALA:O	2:B:3081:MET:HG2	1.94	0.68
3:F:71:ARG:NH1	3:F:73:ASN:OD1	2.26	0.68
2:E:3077:ALA:O	2:E:3081:MET:HG2	1.94	0.68
2:J:2116:LEU:O	2:J:2120:MET:HG2	1.94	0.68
2:B:1089:TYR:HD1	2:B:1152:MET:HG2	1.60	0.68
2:G:2321:ILE:HD11	2:G:2418:LEU:HB2	1.74	0.68
2:B:2788:HIS:HB3	2:B:2791:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:MET:HE1	1:H:101:VAL:HG23	1.77	0.67
2:E:2515:GLN:HA	2:E:2568:LEU:HD21	1.75	0.67
2:E:2788:HIS:HB3	2:E:2791:LEU:HB2	1.75	0.67
2:J:2321:ILE:HD11	2:J:2418:LEU:HB2	1.74	0.67
3:K:51:ILE:HG23	3:K:71:ARG:HD2	1.76	0.67
2:G:2116:LEU:O	2:G:2120:MET:HG2	1.94	0.67
2:G:4762:PRO:HD2	2:G:4766:THR:HG21	1.73	0.67
2:J:246:TYR:CG	2:J:373:LYS:HD2	2.30	0.67
2:J:2515:GLN:HA	2:J:2568:LEU:HD21	1.76	0.67
2:J:3262:ARG:HB2	2:J:3265:GLU:HG2	1.76	0.67
2:B:4679:ARG:HE	2:B:5017:ARG:NH2	1.92	0.67
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.26	0.67
2:G:897:ARG:HD3	2:G:905:PRO:HD3	1.76	0.67
2:G:3812:VAL:O	2:G:3816:MET:HG3	1.93	0.67
2:J:3812:VAL:O	2:J:3816:MET:HG3	1.93	0.67
2:J:4176:PRO:O	2:J:4202:ARG:NH2	2.26	0.67
2:E:897:ARG:HD3	2:E:905:PRO:HD3	1.76	0.67
2:G:3262:ARG:HB2	2:G:3265:GLU:HG2	1.76	0.67
2:E:2116:LEU:O	2:E:2120:MET:HG2	1.94	0.67
3:M:51:ILE:HG23	3:M:71:ARG:HD2	1.76	0.67
2:G:1089:TYR:HD1	2:G:1152:MET:HG2	1.60	0.67
2:G:3077:ALA:O	2:G:3081:MET:HG2	1.94	0.67
3:M:71:ARG:NH1	3:M:73:ASN:OD1	2.26	0.67
2:E:1089:TYR:HD1	2:E:1152:MET:HG2	1.60	0.67
2:E:3253:ILE:HG23	2:E:3318:ASN:HD22	1.60	0.67
2:G:2788:HIS:HB3	2:G:2791:LEU:HB2	1.75	0.67
2:J:2513:GLU:N	2:J:2513:GLU:OE2	2.28	0.67
2:J:3077:ALA:O	2:J:3081:MET:HG2	1.94	0.67
2:G:2513:GLU:N	2:G:2513:GLU:OE2	2.29	0.66
3:K:71:ARG:NH1	3:K:73:ASN:OD1	2.26	0.66
3:C:51:ILE:HG23	3:C:71:ARG:HD2	1.76	0.66
2:E:110:ARG:HD3	2:E:115:ARG:HE	1.60	0.66
2:G:248:GLU:HB3	2:G:373:LYS:HD3	1.77	0.66
2:E:3768:SER:HA	2:E:3771:HIS:CD2	2.31	0.66
2:J:110:ARG:HD3	2:J:115:ARG:HE	1.60	0.66
2:J:3433:GLU:HA	2:J:3436:ARG:HD2	1.78	0.66
2:B:3262:ARG:HB2	2:B:3265:GLU:HG2	1.76	0.66
2:G:3433:GLU:HA	2:G:3436:ARG:HD2	1.78	0.66
2:J:3768:SER:HA	2:J:3771:HIS:CD2	2.31	0.66
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.31	0.66
2:G:3768:SER:HA	2:G:3771:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2513:GLU:N	2:B:2513:GLU:OE2	2.29	0.66
2:G:1519:LEU:HD11	2:G:1572:ILE:HD13	1.78	0.66
2:B:897:ARG:HD3	2:B:905:PRO:HD3	1.76	0.66
2:J:247:TYR:HD2	2:J:374:LYS:HB2	1.60	0.66
2:E:2513:GLU:N	2:E:2513:GLU:OE2	2.29	0.65
2:E:2566:ALA:HA	2:E:2569:PHE:HD2	1.59	0.65
2:G:246:TYR:CG	2:G:373:LYS:HD2	2.31	0.65
2:J:1519:LEU:HD11	2:J:1572:ILE:HD13	1.78	0.65
2:B:3031:ALA:O	2:B:3036:LYS:NZ	2.30	0.65
2:E:3262:ARG:HB2	2:E:3265:GLU:HG2	1.76	0.65
2:B:1519:LEU:HD11	2:B:1572:ILE:HD13	1.78	0.65
2:B:3194:LEU:HD13	2:B:3276:MET:SD	2.36	0.65
2:J:3194:LEU:HD13	2:J:3276:MET:SD	2.36	0.65
2:J:1089:TYR:HD1	2:J:1152:MET:HG2	1.60	0.65
2:G:110:ARG:HD3	2:G:115:ARG:HE	1.60	0.65
2:G:3194:LEU:HD13	2:G:3276:MET:SD	2.36	0.65
2:B:3435:PHE:HE2	2:B:3518:LEU:HA	1.62	0.65
2:E:3031:ALA:O	2:E:3036:LYS:NZ	2.30	0.65
2:E:3245:VAL:HG23	2:E:3248:ARG:H	1.61	0.65
2:E:3433:GLU:HA	2:E:3436:ARG:HD2	1.78	0.65
2:J:2263:ILE:HA	2:J:2330:ARG:HH22	1.62	0.65
3:F:51:ILE:HG23	3:F:71:ARG:HD2	1.76	0.65
2:E:3194:LEU:HD13	2:E:3276:MET:SD	2.36	0.65
2:E:3435:PHE:HE2	2:E:3518:LEU:HA	1.62	0.65
2:J:622:THR:HA	2:J:626:LEU:HD13	1.79	0.65
3:M:52:THR:HG21	3:M:102:ASN:HA	1.79	0.65
2:B:110:ARG:HD3	2:B:115:ARG:HE	1.60	0.65
2:G:3031:ALA:O	2:G:3036:LYS:NZ	2.30	0.65
2:J:3594:ARG:NH1	2:J:3594:ARG:HA	2.12	0.65
2:B:2347:GLU:OE1	2:B:2347:GLU:N	2.27	0.64
2:E:1519:LEU:HD11	2:E:1572:ILE:HD13	1.78	0.64
2:E:3594:ARG:NH1	2:E:3594:ARG:HA	2.12	0.64
2:B:3281:LEU:HD12	2:B:3312:LEU:HG	1.79	0.64
2:E:622:THR:HA	2:E:626:LEU:HD13	1.79	0.64
2:G:247:TYR:HD2	2:G:374:LYS:HB2	1.62	0.64
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.79	0.64
2:B:3433:GLU:HA	2:B:3436:ARG:HD2	1.78	0.64
2:E:246:TYR:CG	2:E:373:LYS:HG3	2.33	0.64
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	1.79	0.64
2:G:2263:ILE:HA	2:G:2330:ARG:HH22	1.62	0.64
2:B:3567:PRO:HB2	2:B:3570:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3281:LEU:HD12	2:G:3312:LEU:HG	1.79	0.64
3:C:71:ARG:NH1	3:C:73:ASN:OD1	2.26	0.64
3:F:52:THR:HG21	3:F:102:ASN:HA	1.79	0.64
3:K:52:THR:HG21	3:K:102:ASN:HA	1.79	0.64
2:E:2347:GLU:OE1	2:E:2347:GLU:N	2.27	0.64
2:J:3263:TYR:HE2	2:J:3334:TRP:HD1	1.46	0.64
2:B:3253:ILE:HG23	2:B:3318:ASN:HD22	1.61	0.64
2:J:3031:ALA:O	2:J:3036:LYS:NZ	2.30	0.64
2:B:2518:LEU:HD23	2:B:2568:LEU:HD22	1.78	0.64
2:E:901:LYS:HD3	2:E:903:LEU:HD11	1.79	0.64
2:G:3435:PHE:HE2	2:G:3518:LEU:HA	1.62	0.64
2:B:3594:ARG:NH1	2:B:3594:ARG:HA	2.12	0.64
2:E:3263:TYR:HE2	2:E:3334:TRP:HD1	1.46	0.64
2:G:622:THR:HA	2:G:626:LEU:HD13	1.79	0.64
2:J:3567:PRO:HB2	2:J:3570:ARG:HH21	1.62	0.64
2:B:901:LYS:HD3	2:B:903:LEU:HD11	1.80	0.64
2:E:2575:ARG:HG3	2:E:2578:MET:HG3	1.80	0.64
2:E:2977:LEU:HD11	2:E:2995:ILE:HD13	1.80	0.64
2:G:2566:ALA:HA	2:G:2569:PHE:HD2	1.63	0.64
2:G:3548:GLU:HG2	2:G:3552:PHE:CZ	2.33	0.64
2:B:2263:ILE:HA	2:B:2330:ARG:HH22	1.62	0.63
2:G:3472:ALA:HA	2:G:3475:LYS:HE2	1.80	0.63
2:B:622:THR:HA	2:B:626:LEU:HD13	1.79	0.63
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.63	0.63
2:G:1087:ARG:NH1	2:G:1221:GLU:O	2.31	0.63
2:G:3594:ARG:NH1	2:G:3594:ARG:HA	2.12	0.63
2:J:985:VAL:HG22	2:J:1043:VAL:HG21	1.80	0.63
2:J:3245:VAL:HG23	2:J:3248:ARG:H	1.63	0.63
2:E:205:ILE:H	2:E:205:ILE:HD12	1.64	0.63
2:E:3548:GLU:HG2	2:E:3552:PHE:CZ	2.33	0.63
2:G:1229:ASN:HB3	2:G:1827:ARG:HG3	1.81	0.63
2:G:2630:VAL:HG12	2:G:2682:ILE:HD11	1.81	0.63
2:J:573:GLU:OE1	2:J:573:GLU:N	2.21	0.63
2:B:1087:ARG:NH1	2:B:1221:GLU:O	2.31	0.63
2:B:3263:TYR:HE2	2:B:3334:TRP:HD1	1.46	0.63
2:E:2630:VAL:HG12	2:E:2682:ILE:HD11	1.81	0.63
2:J:2630:VAL:HG12	2:J:2682:ILE:HD11	1.81	0.63
2:J:3253:ILE:HG23	2:J:3318:ASN:HD22	1.61	0.63
2:J:3435:PHE:HE2	2:J:3518:LEU:HA	1.62	0.63
2:J:3472:ALA:HA	2:J:3475:LYS:HE2	1.80	0.63
2:J:4087:LEU:HB3	2:J:4122:MET:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.63	0.63
2:B:1229:ASN:HB3	2:B:1827:ARG:HG3	1.81	0.63
2:B:2977:LEU:HD11	2:B:2995:ILE:HD13	1.80	0.63
2:B:3548:GLU:HG2	2:B:3552:PHE:CZ	2.33	0.63
2:E:985:VAL:HG22	2:E:1043:VAL:HG21	1.80	0.63
2:G:3567:PRO:HB2	2:G:3570:ARG:HH21	1.62	0.63
2:B:985:VAL:HG22	2:B:1043:VAL:HG21	1.80	0.63
2:E:1087:ARG:NH1	2:E:1221:GLU:O	2.32	0.63
2:J:205:ILE:H	2:J:205:ILE:HD12	1.64	0.63
2:J:365:LYS:HE2	2:J:369:LEU:HD21	1.80	0.63
1:D:24:VAL:HG12	1:D:103:LEU:HA	1.81	0.63
2:B:205:ILE:H	2:B:205:ILE:HD12	1.64	0.63
2:B:4087:LEU:HB3	2:B:4122:MET:HB3	1.80	0.63
2:E:981:GLN:O	2:E:985:VAL:HG23	1.99	0.63
2:E:3472:ALA:HA	2:E:3475:LYS:HE2	1.80	0.63
2:E:3567:PRO:HB2	2:E:3570:ARG:HH21	1.62	0.63
2:J:3281:LEU:HD12	2:J:3312:LEU:HG	1.80	0.63
2:G:3590:GLU:O	2:G:3594:ARG:HG2	1.99	0.63
2:B:246:TYR:CG	2:B:373:LYS:HD2	2.34	0.63
2:B:981:GLN:O	2:B:985:VAL:HG23	1.99	0.63
2:B:2630:VAL:HG12	2:B:2682:ILE:HD11	1.81	0.63
2:E:2263:ILE:HA	2:E:2330:ARG:HH22	1.62	0.63
2:J:1087:ARG:NH1	2:J:1221:GLU:O	2.32	0.63
3:C:52:THR:HG21	3:C:102:ASN:HA	1.79	0.63
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.63	0.62
2:G:901:LYS:HD3	2:G:903:LEU:HD11	1.80	0.62
2:G:3245:VAL:HG23	2:G:3248:ARG:H	1.63	0.62
2:J:1229:ASN:HB3	2:J:1827:ARG:HG3	1.81	0.62
2:J:3590:GLU:O	2:J:3594:ARG:HG2	1.99	0.62
2:E:3590:GLU:O	2:E:3594:ARG:HG2	1.99	0.62
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	1.79	0.62
2:E:4087:LEU:HB3	2:E:4122:MET:HB3	1.81	0.62
2:G:3263:TYR:HE2	2:G:3334:TRP:HD1	1.46	0.62
2:J:2902:HIS:HB3	2:J:2905:LEU:HG	1.79	0.62
2:B:2283:ASN:HB3	2:B:2286:LEU:HB2	1.82	0.62
2:G:2977:LEU:HD11	2:G:2995:ILE:HD13	1.80	0.62
2:J:2977:LEU:HD11	2:J:2995:ILE:HD13	1.80	0.62
2:J:3548:GLU:HG2	2:J:3552:PHE:CZ	2.33	0.62
2:B:573:GLU:OE1	2:B:573:GLU:N	2.21	0.62
2:B:1447:CYS:HB3	2:B:1555:LEU:HB3	1.82	0.62
2:J:3359:ILE:H	2:J:3359:ILE:HD12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3590:GLU:O	2:B:3594:ARG:HG2	1.99	0.62
2:E:2283:ASN:HB3	2:E:2286:LEU:HB2	1.82	0.62
2:G:985:VAL:HG22	2:G:1043:VAL:HG21	1.80	0.62
2:J:901:LYS:HD3	2:J:903:LEU:HD11	1.80	0.62
2:B:3472:ALA:HA	2:B:3475:LYS:HE2	1.80	0.62
2:E:1229:ASN:HB3	2:E:1827:ARG:HG3	1.81	0.62
2:E:3568:SER:HA	2:E:3571:TRP:NE1	2.15	0.62
2:E:4090:LYS:HG2	2:E:4123:ILE:HD11	1.82	0.62
2:G:205:ILE:H	2:G:205:ILE:HD12	1.64	0.62
2:G:4091:LYS:HD3	2:G:4091:LYS:N	2.15	0.62
2:J:23:GLN:HE21	2:J:34:LYS:HB3	1.63	0.62
2:G:4087:LEU:HB3	2:G:4122:MET:HB3	1.80	0.62
2:J:4090:LYS:HG2	2:J:4123:ILE:HD11	1.82	0.62
1:H:93:PRO:O	1:H:94:ASN:ND2	2.33	0.62
2:E:3359:ILE:H	2:E:3359:ILE:HD12	1.65	0.62
2:J:952:LYS:H	2:J:969:PRO:HA	1.64	0.62
2:J:3511:VAL:HA	2:J:3515:LYS:HB2	1.81	0.62
1:I:66:MET:HE1	1:I:101:VAL:HG23	1.82	0.61
2:B:3054:VAL:HG11	2:B:3131:TYR:HB2	1.82	0.61
2:B:3511:VAL:HA	2:B:3515:LYS:HB2	1.81	0.61
2:E:3054:VAL:HG11	2:E:3131:TYR:HB2	1.82	0.61
2:B:3350:ARG:HB2	2:B:3353:LEU:HD13	1.81	0.61
2:E:3190:LEU:O	2:E:3194:LEU:HG	2.00	0.61
2:G:3359:ILE:H	2:G:3359:ILE:HD12	1.65	0.61
2:G:3511:VAL:HA	2:G:3515:LYS:HB2	1.81	0.61
2:J:981:GLN:O	2:J:985:VAL:HG23	1.99	0.61
2:J:3568:SER:HA	2:J:3571:TRP:NE1	2.15	0.61
2:B:799:GLU:N	2:B:799:GLU:OE1	2.33	0.61
2:B:4848:VAL:O	2:B:4852:THR:HG23	2.00	0.61
2:G:2515:GLN:HA	2:G:2568:LEU:HD11	1.82	0.61
2:E:1447:CYS:HB3	2:E:1555:LEU:HB3	1.82	0.61
2:E:4091:LYS:HD3	2:E:4091:LYS:N	2.15	0.61
2:G:551:LEU:HD13	2:G:589:LEU:HD11	1.83	0.61
2:G:3190:LEU:O	2:G:3194:LEU:HG	2.01	0.61
2:B:2570:ALA:HB2	2:B:2613:TYR:HB3	1.81	0.61
2:G:2283:ASN:HB3	2:G:2286:LEU:HB2	1.82	0.61
2:G:3384:LYS:HG3	2:G:3387:ALA:H	1.66	0.61
2:G:3568:SER:HA	2:G:3571:TRP:NE1	2.15	0.61
2:J:799:GLU:N	2:J:799:GLU:OE1	2.33	0.61
2:J:3054:VAL:HG11	2:J:3131:TYR:HB2	1.82	0.61
2:E:3384:LYS:HG3	2:E:3387:ALA:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2347:GLU:OE1	2:G:2347:GLU:N	2.27	0.61
2:J:3190:LEU:O	2:J:3194:LEU:HG	2.00	0.61
2:J:3384:LYS:HG3	2:J:3387:ALA:H	1.66	0.61
2:B:551:LEU:HD13	2:B:589:LEU:HD11	1.83	0.61
2:B:2512:ILE:HD13	2:B:2517:PHE:CE2	2.35	0.61
2:B:3359:ILE:H	2:B:3359:ILE:HD12	1.65	0.61
2:B:3568:SER:HA	2:B:3571:TRP:NE1	2.15	0.61
2:E:799:GLU:OE1	2:E:799:GLU:N	2.33	0.61
1:A:17:LYS:HZ2	1:A:18:LYS:HG2	1.66	0.61
2:B:548:VAL:HG21	2:B:582:HIS:HD2	1.66	0.61
2:E:2710:LEU:HD12	2:E:2711:PRO:HD2	1.83	0.61
2:G:799:GLU:N	2:G:799:GLU:OE1	2.33	0.61
2:G:981:GLN:O	2:G:985:VAL:HG23	1.99	0.61
2:G:4090:LYS:HG2	2:G:4123:ILE:HD11	1.82	0.61
2:J:4848:VAL:O	2:J:4852:THR:HG23	2.00	0.61
2:E:2678:LEU:O	2:E:2682:ILE:HG12	2.01	0.61
2:E:3996:PHE:O	2:E:4000:MET:HG2	2.01	0.61
2:G:3350:ARG:HB2	2:G:3353:LEU:HD13	1.81	0.61
1:H:24:VAL:HG12	1:H:103:LEU:HA	1.82	0.60
1:I:24:VAL:HG12	1:I:103:LEU:HA	1.81	0.60
2:E:3350:ARG:HB2	2:E:3353:LEU:HD13	1.82	0.60
2:G:952:LYS:H	2:G:969:PRO:HA	1.64	0.60
2:G:3536:ALA:HB2	2:G:3553:LEU:HD11	1.83	0.60
2:G:4848:VAL:O	2:G:4852:THR:HG23	2.00	0.60
1:A:26:TYR:HB2	1:A:101:VAL:HG12	1.84	0.60
2:B:4849:TYR:O	2:B:4853:VAL:HG23	2.01	0.60
2:E:984:LEU:O	2:E:988:LEU:HD22	2.01	0.60
2:E:3511:VAL:HA	2:E:3515:LYS:HB2	1.81	0.60
2:G:365:LYS:HE2	2:G:369:LEU:HD21	1.83	0.60
2:G:2678:LEU:O	2:G:2682:ILE:HG12	2.01	0.60
2:J:233:ILE:O	2:J:257:ARG:NH1	2.34	0.60
2:J:4867:GLU:OE1	2:J:4867:GLU:N	2.31	0.60
2:B:952:LYS:H	2:B:969:PRO:HA	1.64	0.60
2:B:3190:LEU:O	2:B:3194:LEU:HG	2.00	0.60
2:E:548:VAL:HG21	2:E:582:HIS:HD2	1.66	0.60
2:E:952:LYS:H	2:E:969:PRO:HA	1.64	0.60
2:G:993:HIS:CE1	2:G:1027:LEU:HD11	2.37	0.60
2:J:3350:ARG:HB2	2:J:3353:LEU:HD13	1.81	0.60
1:A:61:GLU:O	1:A:65:GLN:HG3	2.01	0.60
2:B:2710:LEU:HD12	2:B:2711:PRO:HD2	1.83	0.60
2:B:3536:ALA:HB2	2:B:3553:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4090:LYS:HG2	2:B:4123:ILE:HD11	1.82	0.60
2:E:4848:VAL:O	2:E:4852:THR:HG23	2.00	0.60
2:G:3054:VAL:HG11	2:G:3131:TYR:HB2	1.82	0.60
2:J:548:VAL:HG21	2:J:582:HIS:HD2	1.66	0.60
2:J:2283:ASN:HB3	2:J:2286:LEU:HB2	1.82	0.60
2:J:2678:LEU:O	2:J:2682:ILE:HG12	2.01	0.60
2:B:2678:LEU:O	2:B:2682:ILE:HG12	2.01	0.60
2:B:4091:LYS:HD3	2:B:4091:LYS:N	2.15	0.60
2:E:551:LEU:HD13	2:E:589:LEU:HD11	1.83	0.60
2:E:2333:ASP:HA	2:E:2336:ARG:HH11	1.65	0.60
2:G:3368:ARG:O	2:G:3372:VAL:HG23	2.01	0.60
2:J:1447:CYS:HB3	2:J:1555:LEU:HB3	1.82	0.60
2:J:3536:ALA:HB2	2:J:3553:LEU:HD11	1.84	0.60
2:J:4091:LYS:HD3	2:J:4091:LYS:N	2.15	0.60
2:B:993:HIS:CE1	2:B:1027:LEU:HD11	2.36	0.60
2:B:1944:GLU:HG2	2:B:2123:LEU:HD13	1.83	0.60
2:G:984:LEU:O	2:G:988:LEU:HD22	2.01	0.60
2:G:1735:ILE:HD11	2:G:2156:LEU:HD11	1.84	0.60
2:J:2710:LEU:HD12	2:J:2711:PRO:HD2	1.83	0.60
1:A:23:VAL:HG12	1:A:47:LYS:HG2	1.84	0.60
1:H:23:VAL:HG12	1:H:47:LYS:HG2	1.84	0.60
2:B:233:ILE:O	2:B:257:ARG:NH1	2.34	0.60
2:B:2959:PHE:O	2:B:2963:LEU:HG	2.02	0.60
2:G:233:ILE:O	2:G:257:ARG:NH1	2.34	0.60
2:G:3996:PHE:O	2:G:4000:MET:HG2	2.01	0.60
2:J:993:HIS:CE1	2:J:1027:LEU:HD11	2.37	0.60
3:F:38:ARG:NH2	3:F:64:LYS:HG2	2.16	0.60
1:H:17:LYS:HZ2	1:H:18:LYS:HG2	1.66	0.60
1:I:23:VAL:HG12	1:I:47:LYS:HG2	1.84	0.60
2:B:991:ASN:O	2:B:995:VAL:HG23	2.02	0.60
2:E:233:ILE:O	2:E:257:ARG:NH1	2.34	0.60
2:B:3384:LYS:HG3	2:B:3387:ALA:H	1.66	0.60
2:B:4715:TYR:HE2	2:B:4717:ASP:HB3	1.67	0.60
2:E:993:HIS:CE1	2:E:1027:LEU:HD11	2.36	0.60
2:G:2333:ASP:HA	2:G:2336:ARG:HH11	1.65	0.60
2:G:3102:ASP:HA	2:G:3105:LYS:HE2	1.84	0.60
2:J:1115:LEU:HB3	2:J:1123:VAL:HG11	1.84	0.60
2:J:4849:TYR:O	2:J:4853:VAL:HG23	2.01	0.60
2:E:1979:LEU:HD23	2:E:1982:ARG:HH12	1.67	0.60
2:J:551:LEU:HD13	2:J:589:LEU:HD11	1.83	0.60
2:J:1008:SER:HB2	2:J:1017:ARG:HE	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3536:ALA:HB2	2:E:3553:LEU:HD11	1.84	0.59
2:G:2575:ARG:HG3	2:G:2578:MET:HG3	1.83	0.59
2:J:248:GLU:HA	2:J:372:LEU:HB2	1.82	0.59
2:J:991:ASN:O	2:J:995:VAL:HG23	2.02	0.59
2:J:2002:PRO:O	2:J:2006:ILE:HG12	2.02	0.59
2:J:2333:ASP:HA	2:J:2336:ARG:HH11	1.65	0.59
2:J:2959:PHE:O	2:J:2963:LEU:HG	2.02	0.59
2:J:3368:ARG:O	2:J:3372:VAL:HG23	2.01	0.59
2:J:3996:PHE:O	2:J:4000:MET:HG2	2.01	0.59
2:B:984:LEU:O	2:B:988:LEU:HD22	2.01	0.59
2:E:3368:ARG:O	2:E:3372:VAL:HG23	2.01	0.59
2:G:1008:SER:HB2	2:G:1017:ARG:HE	1.67	0.59
2:G:2002:PRO:O	2:G:2006:ILE:HG12	2.02	0.59
2:J:984:LEU:O	2:J:988:LEU:HD22	2.02	0.59
1:D:23:VAL:HG12	1:D:47:LYS:HG2	1.84	0.59
2:B:1860:LYS:HG2	2:B:1864:LYS:HE3	1.84	0.59
2:B:3368:ARG:O	2:B:3372:VAL:HG23	2.02	0.59
2:E:246:TYR:CD1	2:E:373:LYS:HG3	2.37	0.59
2:E:2002:PRO:O	2:E:2006:ILE:HG12	2.02	0.59
2:E:2175:GLU:O	2:E:2179:ILE:HG12	2.02	0.59
2:E:3549:VAL:O	2:E:3553:LEU:HD13	2.02	0.59
2:G:4715:TYR:CE2	2:G:4717:ASP:HB3	2.36	0.59
2:J:2212:VAL:HG22	2:J:2256:TYR:HE1	1.68	0.59
1:H:97:LEU:HB3	1:H:99:PHE:HE2	1.67	0.59
2:B:2962:GLN:OE1	2:B:2965:ARG:NH1	2.36	0.59
2:B:3996:PHE:O	2:B:4000:MET:HG2	2.01	0.59
2:B:4681:LEU:HD12	2:B:4724:VAL:HG21	1.84	0.59
2:B:5017:ARG:HH11	2:B:5019:TRP:HZ2	1.49	0.59
2:E:2212:VAL:HG22	2:E:2256:TYR:HE1	1.68	0.59
2:E:3312:LEU:H	2:E:3312:LEU:HD12	1.67	0.59
2:J:2591:ARG:HA	2:J:2591:ARG:CZ	2.32	0.59
2:J:3549:VAL:O	2:J:3553:LEU:HD13	2.02	0.59
2:E:1008:SER:HB2	2:E:1017:ARG:HE	1.67	0.59
2:E:1944:GLU:HG2	2:E:2123:LEU:HD13	1.83	0.59
2:E:2591:ARG:HA	2:E:2591:ARG:CZ	2.33	0.59
2:J:2175:GLU:O	2:J:2179:ILE:HG12	2.02	0.59
2:B:235:ALA:O	2:B:242:ARG:NH2	2.36	0.59
2:B:1115:LEU:HB3	2:B:1123:VAL:HG11	1.84	0.59
2:B:1979:LEU:HD23	2:B:1982:ARG:HH12	1.67	0.59
2:B:2333:ASP:HA	2:B:2336:ARG:HH11	1.65	0.59
2:G:991:ASN:O	2:G:995:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1619:ARG:HA	2:G:1626:TRP:HA	1.85	0.59
2:G:4849:TYR:O	2:G:4853:VAL:HG23	2.01	0.59
2:J:3102:ASP:HA	2:J:3105:LYS:HE2	1.84	0.59
1:D:93:PRO:O	1:D:94:ASN:ND2	2.33	0.59
1:I:17:LYS:HZ2	1:I:18:LYS:HG2	1.66	0.59
2:B:3246:LEU:HG	2:B:3247:ASP:H	1.66	0.59
2:E:3281:LEU:HD12	2:E:3312:LEU:HG	1.84	0.59
2:G:2710:LEU:HD12	2:G:2711:PRO:HD2	1.83	0.59
2:G:2962:GLN:OE1	2:G:2965:ARG:NH1	2.35	0.59
2:J:1735:ILE:HD11	2:J:2156:LEU:HD11	1.84	0.59
2:J:1979:LEU:HD23	2:J:1982:ARG:HH12	1.67	0.59
2:B:783:PHE:HB2	2:B:787:VAL:HG11	1.85	0.59
2:B:2002:PRO:O	2:B:2006:ILE:HG12	2.02	0.59
2:B:2175:GLU:O	2:B:2179:ILE:HG12	2.02	0.59
2:B:2591:ARG:HA	2:B:2591:ARG:CZ	2.32	0.59
2:B:3050:VAL:HG11	2:B:3068:LEU:HD11	1.85	0.59
2:E:783:PHE:HB2	2:E:787:VAL:HG11	1.85	0.59
2:E:991:ASN:O	2:E:995:VAL:HG23	2.02	0.59
2:G:1447:CYS:HB3	2:G:1555:LEU:HB3	1.82	0.59
2:G:2591:ARG:HA	2:G:2591:ARG:CZ	2.32	0.59
3:K:38:ARG:NH2	3:K:64:LYS:HG2	2.16	0.59
2:B:1497:GLY:HA2	2:B:1500:PHE:HD2	1.68	0.59
2:B:2212:VAL:HG22	2:B:2256:TYR:HE1	1.68	0.59
2:B:2518:LEU:CD2	2:B:2568:LEU:HD22	2.33	0.59
2:B:3102:ASP:HA	2:B:3105:LYS:HE2	1.84	0.59
2:G:548:VAL:HG21	2:G:582:HIS:HD2	1.66	0.59
2:J:1860:LYS:HG2	2:J:1864:LYS:HE3	1.84	0.59
2:J:1944:GLU:HG2	2:J:2123:LEU:HD13	1.83	0.59
2:J:2962:GLN:OE1	2:J:2965:ARG:NH1	2.36	0.59
2:B:3549:VAL:O	2:B:3553:LEU:HD13	2.02	0.59
2:E:1860:LYS:HG2	2:E:1864:LYS:HE3	1.84	0.59
2:E:2959:PHE:O	2:E:2963:LEU:HG	2.02	0.59
2:E:4849:TYR:O	2:E:4853:VAL:HG23	2.01	0.59
2:G:573:GLU:OE1	2:G:573:GLU:N	2.21	0.59
2:J:2347:GLU:OE1	2:J:2347:GLU:N	2.27	0.59
2:E:3050:VAL:HG11	2:E:3068:LEU:HD11	1.85	0.58
2:J:235:ALA:O	2:J:242:ARG:NH2	2.36	0.58
2:E:1115:LEU:HB3	2:E:1123:VAL:HG11	1.84	0.58
2:G:1444:GLU:HG2	2:G:1557:THR:HG21	1.86	0.58
2:G:2175:GLU:O	2:G:2179:ILE:HG12	2.02	0.58
2:G:2212:VAL:HG22	2:G:2256:TYR:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1619:ARG:HA	2:J:1626:TRP:HA	1.85	0.58
3:M:109:THR:O	3:M:113:GLU:HG2	2.03	0.58
2:B:2519:LEU:HD21	2:B:2572:THR:HG21	1.85	0.58
2:B:2563:THR:HG22	2:B:2606:CYS:HA	1.85	0.58
2:B:3312:LEU:H	2:B:3312:LEU:HD12	1.68	0.58
2:E:1735:ILE:HD11	2:E:2156:LEU:HD11	1.84	0.58
2:E:2703:LEU:HD12	2:E:3001:ILE:HD11	1.86	0.58
2:E:2962:GLN:OE1	2:E:2965:ARG:NH1	2.36	0.58
2:G:2959:PHE:O	2:G:2963:LEU:HG	2.02	0.58
2:E:1497:GLY:HA2	2:E:1500:PHE:HD2	1.68	0.58
2:E:4681:LEU:HD12	2:E:4724:VAL:HG21	1.84	0.58
2:G:1115:LEU:HB3	2:G:1123:VAL:HG11	1.84	0.58
2:G:3050:VAL:HG11	2:G:3068:LEU:HD11	1.85	0.58
2:J:3312:LEU:H	2:J:3312:LEU:HD12	1.68	0.58
2:B:1619:ARG:HA	2:B:1626:TRP:HA	1.85	0.58
2:E:1424:PRO:O	2:E:1428:LEU:HG	2.04	0.58
2:G:1944:GLU:HG2	2:G:2123:LEU:HD13	1.83	0.58
2:G:1979:LEU:HD23	2:G:1982:ARG:HH12	1.68	0.58
2:G:3253:ILE:HG23	2:G:3318:ASN:HD22	1.68	0.58
2:G:3549:VAL:O	2:G:3553:LEU:HD13	2.02	0.58
2:J:881:LEU:O	2:J:885:THR:HG23	2.04	0.58
2:J:2575:ARG:HG3	2:J:2578:MET:HG3	1.84	0.58
2:J:3050:VAL:HG11	2:J:3068:LEU:HD11	1.85	0.58
3:K:109:THR:O	3:K:113:GLU:HG2	2.03	0.58
2:B:1735:ILE:HD11	2:B:2156:LEU:HD11	1.84	0.58
2:B:2519:LEU:HA	2:B:2522:LEU:HD12	1.84	0.58
2:J:4681:LEU:HD12	2:J:4724:VAL:HG21	1.84	0.58
2:B:341:TYR:CZ	2:B:392:ARG:HB2	2.38	0.58
2:B:653:ALA:HB3	2:B:656:SER:HB3	1.86	0.58
2:B:2703:LEU:HD12	2:B:3001:ILE:HD11	1.86	0.58
2:E:881:LEU:O	2:E:885:THR:HG23	2.04	0.58
2:G:235:ALA:O	2:G:242:ARG:NH2	2.36	0.58
2:J:341:TYR:CZ	2:J:392:ARG:HB2	2.38	0.58
3:C:109:THR:O	3:C:113:GLU:HG2	2.03	0.58
1:D:17:LYS:HZ2	1:D:18:LYS:HG2	1.67	0.58
2:E:653:ALA:HB3	2:E:656:SER:HB3	1.86	0.58
2:G:3349:ALA:HB1	2:G:3353:LEU:HD22	1.86	0.58
2:J:1497:GLY:HA2	2:J:1500:PHE:HD2	1.68	0.58
2:B:881:LEU:O	2:B:885:THR:HG23	2.04	0.58
2:E:1786:LEU:HD12	2:E:1787:PRO:HD2	1.86	0.58
2:G:783:PHE:HB2	2:G:787:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1860:LYS:HG2	2:G:1864:LYS:HE3	1.84	0.58
2:G:3257:ALA:O	2:G:3325:ASN:ND2	2.37	0.58
2:J:2703:LEU:HD12	2:J:3001:ILE:HD11	1.86	0.58
2:J:3257:ALA:O	2:J:3325:ASN:ND2	2.37	0.58
3:F:109:THR:O	3:F:113:GLU:HG2	2.03	0.58
1:H:17:LYS:NZ	1:H:18:LYS:HG2	2.19	0.58
2:B:1008:SER:HB2	2:B:1017:ARG:HE	1.67	0.58
2:B:1444:GLU:HG2	2:B:1557:THR:HG21	1.86	0.58
2:B:1786:LEU:HD12	2:B:1787:PRO:HD2	1.86	0.58
2:E:110:ARG:NH2	2:E:117:TYR:OH	2.37	0.58
2:E:235:ALA:O	2:E:242:ARG:NH2	2.36	0.58
2:J:110:ARG:NH2	2:J:117:TYR:OH	2.37	0.58
2:J:783:PHE:HB2	2:J:787:VAL:HG11	1.85	0.58
2:B:3349:ALA:HB1	2:B:3353:LEU:HD22	1.86	0.57
2:E:1444:GLU:HG2	2:E:1557:THR:HG21	1.86	0.57
2:E:1619:ARG:HA	2:E:1626:TRP:HA	1.85	0.57
2:E:3102:ASP:HA	2:E:3105:LYS:HE2	1.84	0.57
2:G:341:TYR:CZ	2:G:392:ARG:HB2	2.38	0.57
2:J:3347:SER:HB3	2:J:3348:ARG:NH2	2.19	0.57
3:C:38:ARG:NH2	3:C:64:LYS:HG2	2.16	0.57
2:B:13:PHE:HA	2:B:164:ARG:HA	1.86	0.57
2:B:2518:LEU:O	2:B:2522:LEU:HG	2.04	0.57
2:B:2566:ALA:HA	2:B:2569:PHE:HD2	1.69	0.57
2:E:341:TYR:CZ	2:E:392:ARG:HB2	2.38	0.57
2:G:13:PHE:HA	2:G:164:ARG:HA	1.86	0.57
2:G:881:LEU:O	2:G:885:THR:HG23	2.04	0.57
2:G:1424:PRO:O	2:G:1428:LEU:HG	2.04	0.57
2:J:653:ALA:HB3	2:J:656:SER:HB3	1.86	0.57
2:J:1424:PRO:O	2:J:1428:LEU:HG	2.04	0.57
2:E:882:TRP:CD1	3:F:106:PRO:HB3	2.40	0.57
2:E:3443:ILE:HG12	2:E:3605:HIS:HD2	1.70	0.57
2:G:2779:GLU:HG3	2:G:2792:ARG:HG2	1.86	0.57
2:G:3443:ILE:HG12	2:G:3605:HIS:HD2	1.70	0.57
2:J:1444:GLU:HG2	2:J:1557:THR:HG21	1.86	0.57
2:J:3110:LEU:HD13	2:J:3183:VAL:HG12	1.86	0.57
1:A:17:LYS:NZ	1:A:18:LYS:HG2	2.19	0.57
1:I:93:PRO:O	1:I:94:ASN:ND2	2.33	0.57
2:E:878:ILE:HG21	3:F:107:TRP:NE1	2.20	0.57
2:E:3347:SER:HB3	2:E:3348:ARG:NH2	2.19	0.57
2:G:1497:GLY:HA2	2:G:1500:PHE:HD2	1.68	0.57
2:G:1786:LEU:HD12	2:G:1787:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3347:SER:HB3	2:G:3348:ARG:NH2	2.19	0.57
2:G:4681:LEU:HD12	2:G:4724:VAL:HG21	1.84	0.57
2:J:2779:GLU:HG3	2:J:2792:ARG:HG2	1.86	0.57
3:K:39:GLN:NE2	3:K:40:ALA:O	2.38	0.57
3:M:39:GLN:NE2	3:M:40:ALA:O	2.37	0.57
2:B:1424:PRO:O	2:B:1428:LEU:HG	2.04	0.57
2:B:2779:GLU:HG3	2:B:2792:ARG:HG2	1.86	0.57
2:B:3443:ILE:HG12	2:B:3605:HIS:HD2	1.70	0.57
2:E:13:PHE:HA	2:E:164:ARG:HA	1.86	0.57
2:G:224:HIS:HB3	2:G:229:GLU:HG3	1.86	0.57
2:B:248:GLU:HA	2:B:372:LEU:HB2	1.86	0.57
2:B:3257:ALA:O	2:B:3325:ASN:ND2	2.37	0.57
2:G:355:LEU:HD23	2:G:378:LEU:HB3	1.87	0.57
2:G:2703:LEU:HD12	2:G:3001:ILE:HD11	1.86	0.57
2:J:3443:ILE:HG12	2:J:3605:HIS:HD2	1.70	0.57
3:C:39:GLN:NE2	3:C:40:ALA:O	2.38	0.57
2:B:2766:TRP:O	2:B:2770:LYS:HG2	2.05	0.57
2:E:224:HIS:HB3	2:E:229:GLU:HG3	1.86	0.57
2:G:110:ARG:NH2	2:G:117:TYR:OH	2.37	0.57
2:G:653:ALA:HB3	2:G:656:SER:HB3	1.86	0.57
2:J:684:VAL:HG22	2:J:781:VAL:HG12	1.86	0.57
2:J:2572:THR:HG22	2:J:2575:ARG:HB3	1.87	0.57
2:J:3227:ARG:HB3	2:J:3232:LEU:HB2	1.87	0.57
2:J:3349:ALA:HB1	2:J:3353:LEU:HD22	1.86	0.57
2:B:3347:SER:HB3	2:B:3348:ARG:NH2	2.19	0.57
2:B:4999:ASP:HB2	2:B:5002:GLU:HG2	1.87	0.57
2:E:3227:ARG:HB3	2:E:3232:LEU:HB2	1.87	0.57
2:G:2634:ASN:OD1	2:G:2636:PHE:N	2.37	0.57
2:B:210:GLU:HG3	2:B:213:TYR:HB2	1.87	0.57
2:B:244:LEU:HD13	2:B:375:LYS:HZ1	1.69	0.57
2:B:355:LEU:HD23	2:B:378:LEU:HB3	1.87	0.57
2:E:3257:ALA:O	2:E:3325:ASN:ND2	2.37	0.57
2:E:3349:ALA:HB1	2:E:3353:LEU:HD22	1.86	0.57
2:J:2766:TRP:O	2:J:2770:LYS:HG2	2.05	0.57
3:F:39:GLN:NE2	3:F:40:ALA:O	2.38	0.57
2:B:2991:HIS:O	2:B:2995:ILE:HG13	2.06	0.56
2:B:3110:LEU:HD13	2:B:3183:VAL:HG12	1.86	0.56
2:E:2626:LEU:O	2:E:2630:VAL:HG23	2.05	0.56
2:E:4688:ILE:HG22	2:E:4689:THR:HG23	1.87	0.56
2:G:2766:TRP:O	2:G:2770:LYS:HG2	2.05	0.56
2:G:4999:ASP:HB2	2:G:5002:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:210:GLU:HG3	2:J:213:TYR:HB2	1.87	0.56
3:M:38:ARG:NH2	3:M:64:LYS:HG2	2.16	0.56
2:G:633:LEU:HB3	2:G:1639:LEU:HD11	1.87	0.56
2:G:1947:CYS:SG	2:G:2127:GLN:NE2	2.77	0.56
2:J:224:HIS:HB3	2:J:229:GLU:HG3	1.86	0.56
1:D:97:LEU:HB3	1:D:99:PHE:HE2	1.70	0.56
1:I:17:LYS:NZ	1:I:18:LYS:HG2	2.19	0.56
2:B:633:LEU:HB3	2:B:1639:LEU:HD11	1.87	0.56
2:E:684:VAL:HG22	2:E:781:VAL:HG12	1.87	0.56
2:E:1225:PRO:HG2	2:E:1228:ILE:HD12	1.88	0.56
2:E:2766:TRP:O	2:E:2770:LYS:HG2	2.05	0.56
2:E:2779:GLU:HG3	2:E:2792:ARG:HG2	1.86	0.56
2:E:2991:HIS:O	2:E:2995:ILE:HG13	2.06	0.56
2:G:2575:ARG:HG3	2:G:2578:MET:CG	2.35	0.56
2:G:2626:LEU:O	2:G:2630:VAL:HG23	2.05	0.56
2:J:355:LEU:HD23	2:J:378:LEU:HB3	1.87	0.56
2:J:758:ARG:HH11	2:J:761:GLY:HA2	1.71	0.56
2:B:929:LEU:HA	2:B:932:LEU:HD12	1.87	0.56
2:B:4688:ILE:HG22	2:B:4689:THR:HG23	1.87	0.56
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.39	0.56
2:E:365:LYS:HE2	2:E:369:LEU:HD21	1.87	0.56
2:E:758:ARG:HH11	2:E:761:GLY:HA2	1.71	0.56
2:E:929:LEU:HA	2:E:932:LEU:HD12	1.87	0.56
2:G:210:GLU:HG3	2:G:213:TYR:HB2	1.87	0.56
2:G:878:ILE:HG21	3:M:107:TRP:NE1	2.21	0.56
2:G:2991:HIS:O	2:G:2995:ILE:HG13	2.06	0.56
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.39	0.56
2:J:13:PHE:HA	2:J:164:ARG:HA	1.86	0.56
2:J:1947:CYS:SG	2:J:2127:GLN:NE2	2.77	0.56
1:A:54:GLU:OE2	1:A:54:GLU:N	2.27	0.56
2:B:1225:PRO:HG2	2:B:1228:ILE:HD12	1.87	0.56
2:E:4999:ASP:HB2	2:E:5002:GLU:HG2	1.87	0.56
2:G:758:ARG:HH11	2:G:761:GLY:HA2	1.71	0.56
2:G:3110:LEU:HD13	2:G:3183:VAL:HG12	1.86	0.56
2:J:1786:LEU:HD12	2:J:1787:PRO:HD2	1.86	0.56
2:J:3439:GLY:O	2:J:3443:ILE:HG13	2.06	0.56
2:B:224:HIS:HB3	2:B:229:GLU:HG3	1.86	0.56
2:B:684:VAL:HG22	2:B:781:VAL:HG12	1.87	0.56
2:B:1947:CYS:SG	2:B:2127:GLN:NE2	2.77	0.56
2:B:2626:LEU:O	2:B:2630:VAL:HG23	2.05	0.56
2:E:210:GLU:HG3	2:E:213:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:633:LEU:HB3	2:E:1639:LEU:HD11	1.87	0.56
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.39	0.56
2:J:3547:GLU:O	2:J:3551:GLU:HG2	2.05	0.56
1:A:93:PRO:O	1:A:94:ASN:ND2	2.33	0.56
2:B:2875:ALA:HB2	2:B:2927:LEU:HD22	1.88	0.56
2:B:4715:TYR:CE2	2:B:4717:ASP:HB3	2.39	0.56
2:G:4943:LEU:O	2:G:4947:GLN:HG2	2.06	0.56
2:J:1225:PRO:HG2	2:J:1228:ILE:HD12	1.88	0.56
2:J:4999:ASP:HB2	2:J:5002:GLU:HG2	1.87	0.56
1:D:17:LYS:NZ	1:D:18:LYS:HG2	2.19	0.56
2:B:365:LYS:HE2	2:B:369:LEU:HD21	1.88	0.56
2:E:2575:ARG:HG3	2:E:2578:MET:CG	2.36	0.56
2:G:2498:HIS:O	2:G:2502:MET:HG3	2.06	0.56
2:G:4553:ASN:O	2:G:4557:ARG:HG3	2.06	0.56
2:J:4943:LEU:O	2:J:4947:GLN:HG2	2.06	0.56
2:E:355:LEU:HD23	2:E:378:LEU:HB3	1.87	0.56
2:E:3439:GLY:O	2:E:3443:ILE:HG13	2.06	0.56
2:E:3547:GLU:O	2:E:3551:GLU:HG2	2.05	0.56
2:G:684:VAL:HG22	2:G:781:VAL:HG12	1.87	0.56
2:G:3040:THR:HG21	2:G:3080:VAL:HG11	1.88	0.56
2:G:3547:GLU:O	2:G:3551:GLU:HG2	2.05	0.56
2:J:2575:ARG:HG3	2:J:2578:MET:CG	2.36	0.56
2:B:110:ARG:NH2	2:B:117:TYR:OH	2.37	0.56
2:B:127:MET:SD	2:B:127:MET:N	2.73	0.56
2:B:3040:THR:HG21	2:B:3080:VAL:HG11	1.88	0.56
2:G:2875:ALA:HB2	2:G:2927:LEU:HD22	1.88	0.56
2:G:3227:ARG:HB3	2:G:3232:LEU:HB2	1.87	0.56
2:J:2626:LEU:O	2:J:2630:VAL:HG23	2.05	0.56
2:J:3079:THR:HA	2:J:3082:LYS:HG2	1.88	0.56
2:J:3725:TYR:O	2:J:3729:MET:HG3	2.06	0.56
2:J:4688:ILE:HG22	2:J:4689:THR:HG23	1.87	0.56
2:B:758:ARG:HH11	2:B:761:GLY:HA2	1.71	0.55
2:B:3245:VAL:HG23	2:B:3248:ARG:H	1.71	0.55
2:B:3355:HIS:ND1	2:B:3355:HIS:O	2.40	0.55
2:B:3547:GLU:O	2:B:3551:GLU:HG2	2.05	0.55
2:E:3040:THR:HG21	2:E:3080:VAL:HG11	1.88	0.55
2:E:3110:LEU:HD13	2:E:3183:VAL:HG12	1.86	0.55
2:E:3206:LEU:HB2	2:E:3280:TYR:CE2	2.41	0.55
2:E:5009:TYR:HA	2:E:5012:LYS:HE3	1.87	0.55
2:J:2991:HIS:O	2:J:2995:ILE:HG13	2.06	0.55
2:B:3227:ARG:HB3	2:B:3232:LEU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4553:ASN:O	2:B:4557:ARG:HG3	2.06	0.55
2:E:2572:THR:HA	2:E:2574:HIS:CE1	2.41	0.55
2:G:3206:LEU:HB2	2:G:3280:TYR:HE2	1.72	0.55
2:G:3439:GLY:O	2:G:3443:ILE:HG13	2.06	0.55
2:J:633:LEU:HB3	2:J:1639:LEU:HD11	1.87	0.55
2:J:3040:THR:HG21	2:J:3080:VAL:HG11	1.88	0.55
2:E:920:TYR:HE1	3:F:99:ARG:HE	1.55	0.55
2:E:3592:ILE:HG12	2:E:3595:ARG:HH21	1.72	0.55
2:G:4688:ILE:HG22	2:G:4689:THR:HG23	1.87	0.55
2:J:4749:GLU:HG3	2:J:4753:HIS:CE1	2.42	0.55
2:B:384:MET:N	2:B:384:MET:SD	2.79	0.55
2:B:3206:LEU:HB2	2:B:3280:TYR:CE2	2.41	0.55
2:B:3532:LEU:HD11	2:B:3560:GLN:HB3	1.89	0.55
2:E:2992:GLU:HB2	2:E:2996:LYS:HZ1	1.71	0.55
2:G:2418:LEU:O	2:G:2422:ILE:HG12	2.07	0.55
2:G:3312:LEU:H	2:G:3312:LEU:HD12	1.70	0.55
2:G:3532:LEU:HD11	2:G:3560:GLN:HB3	1.89	0.55
2:G:3725:TYR:O	2:G:3729:MET:HG3	2.06	0.55
2:J:878:ILE:HG21	3:K:107:TRP:NE1	2.20	0.55
2:J:2827:ARG:NH2	2:J:2935:TYR:OH	2.40	0.55
2:J:3355:HIS:ND1	2:J:3355:HIS:O	2.39	0.55
2:J:3532:LEU:HD11	2:J:3560:GLN:HB3	1.89	0.55
2:J:3534:MET:O	2:J:3538:THR:HG23	2.07	0.55
3:K:40:ALA:HB3	3:K:43:LYS:HB2	1.88	0.55
2:B:886:ARG:HH12	2:B:904:HIS:CE1	2.25	0.55
2:B:2498:HIS:O	2:B:2502:MET:HG3	2.06	0.55
2:B:4749:GLU:HG3	2:B:4753:HIS:CE1	2.42	0.55
2:B:5013:MET:HE1	2:B:5021:PHE:HB3	1.88	0.55
2:E:384:MET:N	2:E:384:MET:SD	2.79	0.55
2:E:3532:LEU:HD11	2:E:3560:GLN:HB3	1.89	0.55
2:E:3725:TYR:O	2:E:3729:MET:HG3	2.06	0.55
2:G:1225:PRO:HG2	2:G:1228:ILE:HD12	1.88	0.55
2:G:3507:THR:O	2:G:3511:VAL:HG13	2.07	0.55
2:J:929:LEU:HA	2:J:932:LEU:HD12	1.87	0.55
2:J:2623:LEU:O	2:J:2627:VAL:HG23	2.07	0.55
2:E:2566:ALA:HA	2:E:2569:PHE:CD2	2.39	0.55
2:E:4943:LEU:O	2:E:4947:GLN:HG2	2.06	0.55
2:G:960:MET:SD	2:G:960:MET:N	2.75	0.55
2:G:1084:GLN:NE2	2:G:1186:ASP:O	2.40	0.55
2:J:4553:ASN:O	2:J:4557:ARG:HG3	2.06	0.55
3:M:62:SER:O	3:M:62:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:MET:SD	2:E:127:MET:N	2.73	0.55
2:E:3079:THR:HA	2:E:3082:LYS:HG2	1.88	0.55
2:E:3355:HIS:ND1	2:E:3355:HIS:O	2.39	0.55
2:G:384:MET:N	2:G:384:MET:SD	2.79	0.55
2:G:929:LEU:HA	2:G:932:LEU:HD12	1.87	0.55
2:G:2827:ARG:NH2	2:G:2935:TYR:OH	2.40	0.55
2:G:3206:LEU:HB2	2:G:3280:TYR:CE2	2.41	0.55
2:J:2875:ALA:HB2	2:J:2927:LEU:HD22	1.88	0.55
2:J:4978:HIS:ND1	2:J:4982:GLU:OE1	2.39	0.55
2:B:1087:ARG:HG2	2:B:1154:ASP:OD1	2.07	0.55
2:B:2178:MET:HB2	2:B:2228:MET:HE1	1.89	0.55
2:B:3507:THR:O	2:B:3511:VAL:HG13	2.06	0.55
2:B:4943:LEU:O	2:B:4947:GLN:HG2	2.06	0.55
2:E:1087:ARG:HG2	2:E:1154:ASP:OD1	2.07	0.55
2:G:1087:ARG:HG2	2:G:1154:ASP:OD1	2.07	0.55
2:G:1259:ARG:NH1	2:G:1591:CYS:SG	2.80	0.55
2:G:2623:LEU:O	2:G:2627:VAL:HG23	2.07	0.55
2:J:384:MET:N	2:J:384:MET:SD	2.79	0.55
2:J:2498:HIS:O	2:J:2502:MET:HG3	2.06	0.55
2:J:3592:ILE:HG12	2:J:3595:ARG:HH21	1.72	0.55
1:A:97:LEU:HB3	1:A:99:PHE:HE2	1.72	0.55
2:B:4572:ALA:O	2:B:4576:ILE:HG13	2.07	0.55
2:E:573:GLU:OE1	2:E:573:GLU:N	2.21	0.55
2:E:3207:GLU:HB2	2:E:3246:LEU:CD2	2.37	0.55
2:E:4715:TYR:CE2	2:E:4717:ASP:HB3	2.40	0.55
2:E:4749:GLU:HG3	2:E:4753:HIS:CE1	2.42	0.55
2:G:1940:CYS:O	2:G:1944:GLU:HG3	2.07	0.55
2:G:3079:THR:HA	2:G:3082:LYS:HG2	1.89	0.55
2:G:3355:HIS:ND1	2:G:3355:HIS:O	2.40	0.55
2:G:4867:GLU:OE1	2:G:4867:GLU:N	2.31	0.55
2:J:3206:LEU:HB2	2:J:3280:TYR:CE2	2.42	0.55
2:B:960:MET:HG2	2:B:961:MET:SD	2.47	0.55
2:B:2418:LEU:O	2:B:2422:ILE:HG12	2.07	0.55
2:B:3246:LEU:HG	2:B:3247:ASP:N	2.21	0.55
2:E:248:GLU:OE1	2:E:373:LYS:HE2	2.07	0.55
2:E:886:ARG:HH12	2:E:904:HIS:CE1	2.25	0.55
2:E:1084:GLN:NE2	2:E:1186:ASP:O	2.40	0.55
2:E:2498:HIS:O	2:E:2502:MET:HG3	2.06	0.55
2:E:3534:MET:O	2:E:3538:THR:HG23	2.07	0.55
2:E:3538:THR:O	2:E:3542:LEU:HG	2.07	0.55
2:E:4553:ASN:O	2:E:4557:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3534:MET:O	2:G:3538:THR:HG23	2.07	0.55
2:G:3538:THR:O	2:G:3542:LEU:HG	2.07	0.55
2:J:3206:LEU:HB2	2:J:3280:TYR:HE2	1.72	0.55
2:B:1259:ARG:NH1	2:B:1591:CYS:SG	2.80	0.54
2:B:2827:ARG:NH2	2:B:2935:TYR:OH	2.40	0.54
2:B:3592:ILE:HG12	2:B:3595:ARG:HH21	1.72	0.54
2:B:3725:TYR:O	2:B:3729:MET:HG3	2.06	0.54
2:E:504:ALA:HB2	2:E:512:ALA:HB2	1.89	0.54
2:E:2212:VAL:HG22	2:E:2256:TYR:CE1	2.43	0.54
2:E:3594:ARG:NH1	2:E:3597:GLN:OE1	2.34	0.54
2:G:886:ARG:HH12	2:G:904:HIS:CE1	2.25	0.54
2:G:4572:ALA:O	2:G:4576:ILE:HG13	2.07	0.54
2:J:1087:ARG:HG2	2:J:1154:ASP:OD1	2.07	0.54
2:J:2178:MET:HB2	2:J:2228:MET:HE1	1.88	0.54
2:J:2212:VAL:HG22	2:J:2256:TYR:CE1	2.43	0.54
2:J:3507:THR:O	2:J:3511:VAL:HG13	2.07	0.54
1:I:97:LEU:HB3	1:I:99:PHE:HE2	1.72	0.54
2:B:2518:LEU:HD22	2:B:2565:CYS:HB3	1.89	0.54
2:B:3538:THR:O	2:B:3542:LEU:HG	2.07	0.54
2:E:2875:ALA:HB2	2:E:2927:LEU:HD22	1.88	0.54
2:E:3194:LEU:HA	2:E:3197:LEU:HG	1.90	0.54
2:G:893:TYR:HA	2:G:904:HIS:HB3	1.89	0.54
2:J:1259:ARG:NH1	2:J:1591:CYS:SG	2.80	0.54
2:B:1940:CYS:O	2:B:1944:GLU:HG3	2.07	0.54
2:B:2992:GLU:HB2	2:B:2996:LYS:HZ1	1.71	0.54
2:B:3206:LEU:HB2	2:B:3280:TYR:HE2	1.72	0.54
2:B:3439:GLY:O	2:B:3443:ILE:HG13	2.06	0.54
2:E:2418:LEU:O	2:E:2422:ILE:HG12	2.07	0.54
2:E:2452:ARG:NH2	2:J:177:GLU:OE2	2.41	0.54
2:G:876:GLU:O	2:G:880:GLU:HG3	2.07	0.54
2:G:3277:LEU:HD13	2:G:3315:LEU:HD23	1.89	0.54
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.88	0.54
2:B:504:ALA:HB2	2:B:512:ALA:HB2	1.89	0.54
2:B:2610:LEU:O	2:B:2614:ILE:HG12	2.08	0.54
2:B:2998:PHE:HA	2:B:3002:LEU:HB2	1.90	0.54
2:B:3106:MET:N	2:B:3106:MET:SD	2.80	0.54
2:E:876:GLU:O	2:E:880:GLU:HG3	2.07	0.54
2:E:1699:GLU:HA	2:E:1814:MET:HE1	1.90	0.54
2:E:2827:ARG:NH2	2:E:2935:TYR:OH	2.40	0.54
2:E:2998:PHE:HA	2:E:3002:LEU:HB2	1.90	0.54
2:G:3592:ILE:HG12	2:G:3595:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4749:GLU:HG3	2:G:4753:HIS:CE1	2.42	0.54
2:J:1084:GLN:NE2	2:J:1186:ASP:O	2.40	0.54
2:J:3965:LEU:HA	2:J:3968:TYR:CD2	2.43	0.54
2:J:4572:ALA:O	2:J:4576:ILE:HG13	2.07	0.54
2:B:234:SER:HB2	2:B:242:ARG:HG2	1.89	0.54
2:B:2212:VAL:HG22	2:B:2256:TYR:CE1	2.43	0.54
2:E:3507:THR:O	2:E:3511:VAL:HG13	2.06	0.54
2:G:1970:GLN:NE2	2:G:3641:LEU:O	2.37	0.54
2:G:2749:GLU:HG3	2:G:2752:ASP:HB2	1.90	0.54
2:J:426:ARG:HG3	2:J:431:PRO:HD3	1.90	0.54
2:J:920:TYR:HE1	3:K:99:ARG:HE	1.56	0.54
2:J:2992:GLU:HB2	2:J:2996:LYS:HZ1	1.73	0.54
2:J:2998:PHE:HA	2:J:3002:LEU:HB2	1.90	0.54
2:J:3538:THR:O	2:J:3542:LEU:HG	2.07	0.54
2:B:2623:LEU:O	2:B:2627:VAL:HG23	2.07	0.54
2:B:4867:GLU:OE1	2:B:4867:GLU:N	2.31	0.54
2:E:960:MET:HG2	2:E:961:MET:SD	2.48	0.54
2:J:960:MET:HG2	2:J:961:MET:SD	2.48	0.54
2:J:1699:GLU:HA	2:J:1814:MET:HE1	1.90	0.54
2:B:3079:THR:HA	2:B:3082:LYS:HG2	1.89	0.54
2:E:1259:ARG:NH1	2:E:1591:CYS:SG	2.80	0.54
2:E:3445:TRP:CD1	2:E:3509:LEU:HG	2.43	0.54
2:G:177:GLU:OE2	2:J:2452:ARG:NH2	2.41	0.54
2:G:426:ARG:HG3	2:G:431:PRO:HD3	1.90	0.54
2:G:2123:LEU:O	2:G:2127:GLN:HG2	2.08	0.54
2:G:2238:TYR:O	2:G:2242:ILE:HG12	2.08	0.54
2:J:886:ARG:HH12	2:J:904:HIS:CE1	2.25	0.54
2:J:3445:TRP:CD1	2:J:3509:LEU:HG	2.43	0.54
2:G:960:MET:HG2	2:G:961:MET:SD	2.47	0.54
2:J:877:ASN:O	2:J:881:LEU:HD22	2.08	0.54
2:J:2123:LEU:O	2:J:2127:GLN:HG2	2.08	0.54
2:J:3194:LEU:HA	2:J:3197:LEU:HG	1.90	0.54
2:B:470:SER:HA	2:B:473:ASN:HD21	1.73	0.54
2:B:2749:GLU:HG3	2:B:2752:ASP:HB2	1.90	0.54
2:E:2178:MET:HB2	2:E:2228:MET:HE1	1.89	0.54
2:E:2238:TYR:O	2:E:2242:ILE:HG12	2.08	0.54
2:E:2312:MET:SD	2:E:2312:MET:N	2.79	0.54
2:E:3938:SER:O	2:E:4002:LYS:NZ	2.41	0.54
2:G:470:SER:HA	2:G:473:ASN:HD21	1.73	0.54
2:G:2312:MET:SD	2:G:2312:MET:N	2.79	0.54
2:G:3938:SER:O	2:G:4002:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2634:ASN:OD1	2:J:2636:PHE:N	2.37	0.54
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.88	0.54
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.89	0.54
2:B:1084:GLN:NE2	2:B:1186:ASP:O	2.40	0.54
2:B:2479:LEU:HD23	2:B:2479:LEU:H	1.73	0.54
2:E:877:ASN:O	2:E:881:LEU:HD22	2.08	0.54
2:E:2623:LEU:O	2:E:2627:VAL:HG23	2.07	0.54
2:E:4573:ILE:HG23	2:E:4643:LEU:HD11	1.91	0.54
2:J:3106:MET:N	2:J:3106:MET:SD	2.80	0.54
2:J:4063:ASP:HB2	2:J:4067:LYS:HE3	1.90	0.54
2:B:876:GLU:O	2:B:880:GLU:HG3	2.07	0.53
2:B:877:ASN:O	2:B:881:LEU:HD22	2.08	0.53
2:B:893:TYR:HA	2:B:904:HIS:HB3	1.89	0.53
2:B:1699:GLU:HA	2:B:1814:MET:HE1	1.90	0.53
2:B:2238:TYR:O	2:B:2242:ILE:HG12	2.08	0.53
2:B:3194:LEU:HA	2:B:3197:LEU:HG	1.90	0.53
2:E:2527:LEU:HA	2:E:2530:MET:HG2	1.90	0.53
2:G:2992:GLU:HB2	2:G:2996:LYS:HZ1	1.73	0.53
2:J:2238:TYR:O	2:J:2242:ILE:HG12	2.08	0.53
2:J:3280:TYR:HE1	2:J:3284:TRP:HD1	1.56	0.53
2:B:3280:TYR:CE1	2:B:3284:TRP:HD1	2.27	0.53
2:E:3201:MET:SD	2:E:3203:VAL:HG12	2.48	0.53
2:G:234:SER:HB2	2:G:242:ARG:HG2	1.90	0.53
2:G:877:ASN:O	2:G:881:LEU:HD22	2.08	0.53
2:G:1699:GLU:HA	2:G:1814:MET:HE1	1.90	0.53
2:G:2138:LEU:HD11	2:G:3662:ILE:HD12	1.90	0.53
2:G:3106:MET:N	2:G:3106:MET:SD	2.80	0.53
2:J:2418:LEU:O	2:J:2422:ILE:HG12	2.07	0.53
2:J:2749:GLU:HG3	2:J:2752:ASP:HB2	1.90	0.53
2:B:3201:MET:SD	2:B:3203:VAL:HG12	2.48	0.53
2:E:2123:LEU:O	2:E:2127:GLN:HG2	2.08	0.53
2:E:3093:ARG:O	2:E:3097:GLU:HG2	2.09	0.53
2:E:3106:MET:N	2:E:3106:MET:SD	2.80	0.53
2:E:3376:GLU:OE2	2:E:3380:ARG:NH2	2.39	0.53
2:E:3514:LEU:HD13	2:E:3602:VAL:HG13	1.91	0.53
2:E:4572:ALA:O	2:E:4576:ILE:HG13	2.07	0.53
2:G:2285:GLU:CD	2:G:3860:ASN:HD21	2.12	0.53
2:G:3201:MET:SD	2:G:3203:VAL:HG12	2.48	0.53
2:J:234:SER:HB2	2:J:242:ARG:HG2	1.90	0.53
2:B:206:CYS:HB2	2:B:271:GLY:HA3	1.90	0.53
2:B:426:ARG:HG3	2:B:431:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:ASP:O	2:B:1003:GLN:HG2	2.09	0.53
2:B:2518:LEU:HD21	2:B:2569:PHE:CE2	2.43	0.53
2:E:893:TYR:HA	2:E:904:HIS:HB3	1.89	0.53
2:E:999:ASP:O	2:E:1003:GLN:HG2	2.09	0.53
2:E:4063:ASP:HB2	2:E:4067:LYS:HE3	1.90	0.53
2:E:4867:GLU:OE1	2:E:4867:GLU:N	2.31	0.53
2:G:2178:MET:HB2	2:G:2228:MET:HE1	1.90	0.53
2:G:2527:LEU:HA	2:G:2530:MET:HG2	1.90	0.53
2:G:2736:ASP:OD1	2:G:2736:ASP:N	2.42	0.53
2:G:4573:ILE:HG23	2:G:4643:LEU:HD11	1.91	0.53
2:J:876:GLU:O	2:J:880:GLU:HG3	2.07	0.53
2:J:999:ASP:O	2:J:1003:GLN:HG2	2.09	0.53
2:J:3093:ARG:O	2:J:3097:GLU:HG2	2.09	0.53
2:B:2452:ARG:NH2	2:E:177:GLU:OE2	2.41	0.53
2:E:206:CYS:HB2	2:E:271:GLY:HA3	1.91	0.53
2:E:1947:CYS:SG	2:E:2127:GLN:NE2	2.77	0.53
2:E:2531:ARG:NH1	2:E:2585:THR:HB	2.24	0.53
2:E:2749:GLU:HG3	2:E:2752:ASP:HB2	1.90	0.53
2:G:3376:GLU:OE2	2:G:3380:ARG:NH2	2.39	0.53
2:G:3445:TRP:CD1	2:G:3509:LEU:HG	2.43	0.53
2:J:206:CYS:HB2	2:J:271:GLY:HA3	1.91	0.53
2:J:504:ALA:HB2	2:J:512:ALA:HB2	1.89	0.53
2:J:2792:ARG:NH2	2:J:2798:SER:OG	2.41	0.53
2:E:1569:GLN:HB2	2:E:1572:ILE:HD12	1.91	0.53
2:E:3147:ILE:HG23	2:E:3152:PHE:HB2	1.91	0.53
2:G:206:CYS:HB2	2:G:271:GLY:HA3	1.90	0.53
2:G:2531:ARG:NH1	2:G:2585:THR:HB	2.24	0.53
2:G:3194:LEU:HA	2:G:3197:LEU:HG	1.90	0.53
2:J:470:SER:HA	2:J:473:ASN:HD21	1.73	0.53
2:J:1940:CYS:O	2:J:1944:GLU:HG3	2.07	0.53
2:J:2527:LEU:HA	2:J:2530:MET:HG2	1.90	0.53
2:J:3162:GLN:HG2	2:J:3218:VAL:HG13	1.90	0.53
1:I:54:GLU:OE2	1:I:54:GLU:N	2.27	0.53
2:B:960:MET:SD	2:B:960:MET:N	2.75	0.53
2:B:1569:GLN:HB2	2:B:1572:ILE:HD12	1.91	0.53
2:B:3376:GLU:OE2	2:B:3380:ARG:NH2	2.39	0.53
2:E:3206:LEU:HB2	2:E:3280:TYR:HE2	1.72	0.53
2:E:3835:LEU:HD22	2:E:3880:PHE:HZ	1.74	0.53
2:E:3844:LEU:HD21	2:E:3936:TYR:HB2	1.90	0.53
2:E:4677:LEU:HD23	2:E:4711:PHE:HE1	1.72	0.53
2:G:999:ASP:O	2:G:1003:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2998:PHE:HA	2:G:3002:LEU:HB2	1.90	0.53
2:J:3938:SER:O	2:J:4002:LYS:NZ	2.41	0.53
2:B:1623:ARG:HH11	2:B:1623:ARG:HA	1.74	0.53
2:B:2123:LEU:O	2:B:2127:GLN:HG2	2.08	0.53
2:B:3445:TRP:CD1	2:B:3509:LEU:HG	2.43	0.53
2:B:3534:MET:O	2:B:3538:THR:HG23	2.07	0.53
2:E:234:SER:HB2	2:E:242:ARG:HG2	1.89	0.53
2:E:1940:CYS:O	2:E:1944:GLU:HG3	2.07	0.53
2:E:2616:PRO:HA	2:E:2619:LEU:HD12	1.90	0.53
2:G:1569:GLN:HB2	2:G:1572:ILE:HD12	1.91	0.53
2:G:1708:ARG:NH1	2:G:1836:PHE:O	2.42	0.53
2:G:2479:LEU:HD23	2:G:2479:LEU:H	1.73	0.53
2:G:2566:ALA:HA	2:G:2569:PHE:CD2	2.42	0.53
2:G:3280:TYR:CE1	2:G:3284:TRP:HD1	2.27	0.53
2:B:3008:GLN:O	2:B:3012:ASN:ND2	2.42	0.53
2:B:3938:SER:O	2:B:4002:LYS:NZ	2.41	0.53
2:E:426:ARG:HG3	2:E:431:PRO:HD3	1.90	0.53
2:E:470:SER:HA	2:E:473:ASN:HD21	1.73	0.53
2:E:3008:GLN:O	2:E:3012:ASN:ND2	2.42	0.53
2:G:504:ALA:HB2	2:G:512:ALA:HB2	1.89	0.53
2:J:671:VAL:HG22	2:J:787:VAL:HG23	1.91	0.53
2:J:1708:ARG:NH1	2:J:1836:PHE:O	2.42	0.53
2:J:1970:GLN:NE2	2:J:3641:LEU:O	2.37	0.53
2:J:3201:MET:SD	2:J:3203:VAL:HG12	2.48	0.53
2:B:3835:LEU:HD22	2:B:3880:PHE:HZ	1.74	0.53
2:E:2479:LEU:HD23	2:E:2479:LEU:H	1.73	0.53
2:E:3280:TYR:CE1	2:E:3284:TRP:HD1	2.27	0.53
2:G:2212:VAL:HG22	2:G:2256:TYR:CE1	2.43	0.53
2:J:1569:GLN:HB2	2:J:1572:ILE:HD12	1.91	0.53
2:J:2531:ARG:NH1	2:J:2585:THR:HB	2.24	0.53
2:J:3008:GLN:O	2:J:3012:ASN:ND2	2.42	0.53
2:B:2138:LEU:HD11	2:B:3662:ILE:HD12	1.90	0.52
2:B:3162:GLN:HG2	2:B:3218:VAL:HG13	1.90	0.52
2:B:3844:LEU:HD21	2:B:3936:TYR:HB2	1.90	0.52
2:E:3182:TYR:HA	2:E:3185:LYS:HE3	1.91	0.52
2:G:3008:GLN:O	2:G:3012:ASN:ND2	2.42	0.52
2:G:3076:ASP:O	2:G:3080:VAL:HG23	2.08	0.52
2:G:4104:THR:O	2:G:4108:ILE:HG12	2.09	0.52
2:J:3182:TYR:HA	2:J:3185:LYS:HE3	1.91	0.52
2:J:3280:TYR:CE1	2:J:3284:TRP:HD1	2.27	0.52
2:B:2531:ARG:NH1	2:B:2585:THR:HB	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3147:ILE:HG23	2:B:3152:PHE:HB2	1.91	0.52
2:B:4104:THR:O	2:B:4108:ILE:HG12	2.09	0.52
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.74	0.52
2:G:3093:ARG:O	2:G:3097:GLU:HG2	2.09	0.52
2:G:3891:LEU:HB3	2:G:3899:PHE:CE1	2.45	0.52
3:K:85:LEU:HD13	3:K:125:VAL:HG13	1.91	0.52
2:B:2245:GLN:HG2	2:B:2248:ARG:HH12	1.74	0.52
2:B:3891:LEU:HB3	2:B:3899:PHE:CE1	2.45	0.52
2:E:728:ARG:NH2	2:E:1489:CYS:SG	2.83	0.52
2:E:1623:ARG:HH11	2:E:1623:ARG:HA	1.74	0.52
2:E:3532:LEU:HD12	2:E:3532:LEU:H	1.74	0.52
2:E:4104:THR:O	2:E:4108:ILE:HG12	2.09	0.52
2:G:3835:LEU:HD22	2:G:3880:PHE:HZ	1.74	0.52
2:J:874:LEU:O	2:J:878:ILE:HG12	2.09	0.52
2:J:1727:ARG:NH2	2:J:1773:PRO:O	2.43	0.52
2:J:2265:LEU:HD12	2:J:2265:LEU:H	1.74	0.52
2:J:3076:ASP:O	2:J:3080:VAL:HG23	2.09	0.52
2:B:671:VAL:HG22	2:B:787:VAL:HG23	1.91	0.52
2:B:2312:MET:SD	2:B:2312:MET:N	2.79	0.52
2:B:3076:ASP:O	2:B:3080:VAL:HG23	2.09	0.52
2:B:3215:ALA:HA	2:B:3220:THR:HG21	1.91	0.52
2:E:2245:GLN:HG2	2:E:2248:ARG:HH12	1.73	0.52
2:E:3475:LYS:HD3	2:E:3516:LYS:NZ	2.25	0.52
3:C:85:LEU:HD13	3:C:125:VAL:HG13	1.91	0.52
2:B:40:GLU:O	2:B:114:SER:OG	2.28	0.52
2:B:3093:ARG:O	2:B:3097:GLU:HG2	2.09	0.52
2:E:2619:LEU:O	2:E:2623:LEU:HG	2.09	0.52
2:E:2634:ASN:OD1	2:E:2636:PHE:N	2.37	0.52
2:E:3923:LEU:HB2	2:E:3961:VAL:HG11	1.92	0.52
2:G:2245:GLN:HG2	2:G:2248:ARG:HH12	1.74	0.52
2:J:728:ARG:NH2	2:J:1489:CYS:SG	2.83	0.52
2:J:1854:PHE:HD1	2:J:1858:ASP:HB3	1.74	0.52
2:J:2479:LEU:HD23	2:J:2479:LEU:H	1.74	0.52
2:J:2759:ALA:HB2	2:J:2810:LYS:HZ1	1.74	0.52
2:J:3514:LEU:HD13	2:J:3602:VAL:HG13	1.91	0.52
2:J:4573:ILE:HG23	2:J:4643:LEU:HD11	1.91	0.52
2:B:874:LEU:O	2:B:878:ILE:HG12	2.09	0.52
2:B:2336:ARG:HG2	2:B:2435:ARG:HD3	1.92	0.52
2:B:2960:LEU:HD23	2:B:2963:LEU:HD12	1.92	0.52
2:B:3049:LEU:HA	2:B:3053:ARG:HH21	1.75	0.52
2:B:3280:TYR:HE1	2:B:3284:TRP:HD1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4063:ASP:HB2	2:B:4067:LYS:HE3	1.90	0.52
2:B:4069:LYS:NZ	2:B:4130:ASN:OD1	2.37	0.52
2:B:4573:ILE:HG23	2:B:4643:LEU:HD11	1.91	0.52
2:E:3162:GLN:HG2	2:E:3218:VAL:HG13	1.90	0.52
2:E:3891:LEU:HB3	2:E:3899:PHE:CE1	2.45	0.52
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.52
2:J:3532:LEU:H	2:J:3532:LEU:HD12	1.74	0.52
2:J:3844:LEU:HD21	2:J:3936:TYR:HB2	1.90	0.52
2:B:1708:ARG:NH1	2:B:1836:PHE:O	2.42	0.52
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.75	0.52
2:B:2527:LEU:HA	2:B:2530:MET:HG2	1.90	0.52
2:B:2634:ASN:OD1	2:B:2636:PHE:N	2.37	0.52
2:E:3207:GLU:HB2	2:E:3246:LEU:HD22	1.91	0.52
2:E:3363:GLY:O	2:E:3367:LYS:HG2	2.10	0.52
2:G:40:GLU:O	2:G:114:SER:OG	2.28	0.52
2:G:2189:LYS:HA	2:G:2192:TYR:CZ	2.45	0.52
2:G:2336:ARG:HG2	2:G:2435:ARG:HD3	1.92	0.52
2:G:3049:LEU:HA	2:G:3053:ARG:HH21	1.75	0.52
2:G:3162:GLN:HG2	2:G:3218:VAL:HG13	1.90	0.52
2:G:4063:ASP:HB2	2:G:4067:LYS:HE3	1.90	0.52
2:J:246:TYR:CB	2:J:373:LYS:HD2	2.40	0.52
2:J:882:TRP:CD1	3:K:106:PRO:HB3	2.45	0.52
2:J:893:TYR:HA	2:J:904:HIS:HB3	1.90	0.52
2:J:2245:GLN:HG2	2:J:2248:ARG:HH12	1.74	0.52
2:J:3475:LYS:HD3	2:J:3516:LYS:NZ	2.25	0.52
2:B:3195:ALA:HB2	2:B:3275:PRO:HB3	1.92	0.52
2:E:2792:ARG:NH2	2:E:2798:SER:OG	2.41	0.52
2:E:3076:ASP:O	2:E:3080:VAL:HG23	2.09	0.52
2:G:671:VAL:HG22	2:G:787:VAL:HG23	1.91	0.52
2:G:3514:LEU:HD13	2:G:3602:VAL:HG13	1.91	0.52
2:G:3844:LEU:HD21	2:G:3936:TYR:HB2	1.90	0.52
2:J:1623:ARG:HA	2:J:1623:ARG:HH11	1.74	0.52
2:J:3835:LEU:HD22	2:J:3880:PHE:HZ	1.74	0.52
2:J:3891:LEU:HB3	2:J:3899:PHE:CE1	2.45	0.52
2:E:571:SER:HB2	2:E:574:VAL:HG22	1.92	0.52
2:G:874:LEU:O	2:G:878:ILE:HG12	2.09	0.52
2:G:3754:GLU:O	2:G:3758:MET:HG3	2.10	0.52
2:J:878:ILE:HG13	3:K:107:TRP:HZ2	1.75	0.52
2:J:3147:ILE:HG23	2:J:3152:PHE:HB2	1.91	0.52
1:I:26:TYR:HB2	1:I:101:VAL:HG12	1.92	0.52
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2970:SER:HA	2:B:2973:PHE:CZ	2.45	0.52
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.74	0.52
2:E:2336:ARG:HG2	2:E:2435:ARG:HD3	1.92	0.52
2:E:3962:PHE:O	2:E:3966:THR:HG23	2.09	0.52
2:G:2960:LEU:HD23	2:G:2963:LEU:HD12	1.92	0.52
2:J:4104:THR:O	2:J:4108:ILE:HG12	2.09	0.52
2:J:4715:TYR:CE2	2:J:4717:ASP:HB3	2.40	0.52
2:B:177:GLU:OE2	2:G:2452:ARG:NH2	2.41	0.51
2:B:1970:GLN:NE2	2:B:3641:LEU:O	2.37	0.51
2:B:3363:GLY:O	2:B:3367:LYS:HG2	2.10	0.51
2:E:671:VAL:HG22	2:E:787:VAL:HG23	1.91	0.51
2:E:2138:LEU:HD11	2:E:3662:ILE:HD12	1.90	0.51
2:E:2265:LEU:HD12	2:E:2265:LEU:H	1.74	0.51
2:E:2559:LEU:O	2:E:2563:THR:HG23	2.10	0.51
2:E:2736:ASP:OD1	2:E:2736:ASP:N	2.42	0.51
2:E:3215:ALA:HA	2:E:3220:THR:HG21	1.91	0.51
2:G:728:ARG:NH2	2:G:1489:CYS:SG	2.83	0.51
2:G:2265:LEU:H	2:G:2265:LEU:HD12	1.74	0.51
2:G:2992:GLU:HB2	2:G:2996:LYS:NZ	2.25	0.51
2:G:3147:ILE:HG23	2:G:3152:PHE:HB2	1.91	0.51
2:G:3195:ALA:HB2	2:G:3275:PRO:HB3	1.92	0.51
2:G:3280:TYR:HE1	2:G:3284:TRP:HD1	1.56	0.51
2:J:2138:LEU:HD11	2:J:3662:ILE:HD12	1.90	0.51
2:B:246:TYR:CB	2:B:373:LYS:HD2	2.40	0.51
2:B:3754:GLU:O	2:B:3758:MET:HG3	2.10	0.51
2:E:874:LEU:O	2:E:878:ILE:HG12	2.09	0.51
2:G:1623:ARG:HA	2:G:1623:ARG:HH11	1.74	0.51
2:G:2970:SER:HA	2:G:2973:PHE:CZ	2.45	0.51
2:G:3594:ARG:NH1	2:G:3597:GLN:OE1	2.34	0.51
2:J:210:GLU:HG2	2:J:273:HIS:CE1	2.46	0.51
2:J:4856:PHE:O	2:J:4860:ARG:NH2	2.39	0.51
2:B:728:ARG:NH2	2:B:1489:CYS:SG	2.83	0.51
2:B:3475:LYS:HD3	2:B:3516:LYS:NZ	2.25	0.51
2:B:3532:LEU:H	2:B:3532:LEU:HD12	1.74	0.51
2:E:210:GLU:HG2	2:E:273:HIS:CE1	2.46	0.51
2:E:3535:LEU:HD12	2:E:3539:ARG:HH12	1.76	0.51
2:G:3182:TYR:HA	2:G:3185:LYS:HE3	1.91	0.51
2:J:2336:ARG:HG2	2:J:2435:ARG:HD3	1.92	0.51
2:J:3225:ARG:O	2:J:3229:ILE:HG23	2.11	0.51
3:K:12:MET:HG2	3:K:16:GLY:HA3	1.93	0.51
2:B:231:LEU:O	2:B:260:TRP:NE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2792:ARG:NH2	2:B:2798:SER:OG	2.41	0.51
2:B:4630:TYR:HE1	2:E:4860:ARG:HH22	1.58	0.51
2:E:470:SER:HA	2:E:473:ASN:ND2	2.26	0.51
2:E:1708:ARG:NH1	2:E:1836:PHE:O	2.42	0.51
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.51
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.75	0.51
2:G:210:GLU:HG2	2:G:273:HIS:CE1	2.46	0.51
2:G:2619:LEU:O	2:G:2623:LEU:HG	2.09	0.51
2:G:3532:LEU:H	2:G:3532:LEU:HD12	1.75	0.51
2:G:3535:LEU:O	2:G:3539:ARG:HG2	2.11	0.51
2:J:470:SER:HA	2:J:473:ASN:ND2	2.26	0.51
2:J:2559:LEU:O	2:J:2563:THR:HG23	2.11	0.51
2:J:2992:GLU:HB2	2:J:2996:LYS:NZ	2.25	0.51
2:J:3049:LEU:HA	2:J:3053:ARG:HH21	1.75	0.51
2:J:3535:LEU:O	2:J:3539:ARG:HG2	2.11	0.51
3:F:85:LEU:HD13	3:F:125:VAL:HG13	1.91	0.51
2:B:2644:LEU:HD12	2:B:2648:TYR:HE2	1.76	0.51
2:E:3042:LEU:O	2:E:3046:LEU:HG	2.11	0.51
2:E:3049:LEU:HA	2:E:3053:ARG:HH21	1.75	0.51
2:E:3529:ASP:O	2:E:3533:ILE:HG13	2.11	0.51
2:G:2616:PRO:HA	2:G:2619:LEU:HD12	1.91	0.51
2:G:2644:LEU:HD12	2:G:2648:TYR:HE2	1.76	0.51
2:G:3219:TYR:HE1	2:G:3234:ASN:HA	1.76	0.51
2:J:3363:GLY:O	2:J:3367:LYS:HG2	2.10	0.51
2:J:3754:GLU:O	2:J:3758:MET:HG3	2.10	0.51
3:C:12:MET:HG2	3:C:16:GLY:HA3	1.93	0.51
3:F:12:MET:HG2	3:F:16:GLY:HA3	1.93	0.51
2:B:2189:LYS:HA	2:B:2192:TYR:CZ	2.45	0.51
2:B:3225:ARG:O	2:B:3229:ILE:HG23	2.11	0.51
2:E:878:ILE:HG13	3:F:107:TRP:HZ2	1.74	0.51
2:E:2970:SER:HA	2:E:2973:PHE:CZ	2.45	0.51
2:G:365:LYS:O	2:G:369:LEU:HG	2.10	0.51
2:G:920:TYR:O	2:G:923:GLN:HG2	2.11	0.51
2:G:920:TYR:HE1	3:M:99:ARG:HE	1.59	0.51
2:G:2559:LEU:O	2:G:2563:THR:HG23	2.11	0.51
2:G:4860:ARG:HH22	2:J:4630:TYR:HE1	1.58	0.51
2:J:3529:ASP:O	2:J:3533:ILE:HG13	2.11	0.51
2:J:4569:LEU:HD21	2:J:4649:LEU:HD23	1.93	0.51
2:E:3093:ARG:HA	2:E:3096:PHE:CD1	2.46	0.51
2:G:470:SER:HA	2:G:473:ASN:ND2	2.26	0.51
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:GLY:H	3:F:85:LEU:HB2	1.74	0.51
2:B:1000:ARG:HH12	3:C:115:ASP:H	1.59	0.51
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.74	0.51
2:B:3042:LEU:O	2:B:3046:LEU:HG	2.11	0.51
2:B:3182:TYR:HA	2:B:3185:LYS:HE3	1.91	0.51
2:E:3535:LEU:O	2:E:3539:ARG:HG2	2.11	0.51
2:G:878:ILE:HG13	3:M:107:TRP:HZ2	1.75	0.51
2:G:2682:ILE:HB	2:G:2703:LEU:HD21	1.93	0.51
2:G:3215:ALA:HA	2:G:3220:THR:HG21	1.91	0.51
2:G:3475:LYS:HD3	2:G:3516:LYS:NZ	2.25	0.51
2:J:243:ARG:HA	2:J:301:VAL:HG22	1.93	0.51
2:J:920:TYR:O	2:J:923:GLN:HG2	2.11	0.51
2:J:2189:LYS:HA	2:J:2192:TYR:CZ	2.45	0.51
2:J:2960:LEU:HD23	2:J:2963:LEU:HD12	1.92	0.51
2:J:3215:ALA:HA	2:J:3220:THR:HG21	1.91	0.51
2:J:3535:LEU:HD12	2:J:3539:ARG:HH12	1.76	0.51
3:C:90:THR:HG23	3:C:124:THR:HA	1.93	0.51
3:M:90:THR:HG23	3:M:124:THR:HA	1.93	0.51
1:D:97:LEU:HB3	1:D:99:PHE:CE2	2.46	0.51
1:H:54:GLU:OE2	1:H:54:GLU:N	2.27	0.51
1:I:26:TYR:CB	1:I:101:VAL:HG12	2.41	0.51
2:B:3644:LEU:HD11	2:B:3648:ARG:HD2	1.93	0.51
2:B:4856:PHE:O	2:B:4860:ARG:NH2	2.39	0.51
2:E:2572:THR:HG22	2:E:2575:ARG:HB3	1.93	0.51
2:E:3280:TYR:HE1	2:E:3284:TRP:HD1	1.56	0.51
2:G:3042:LEU:O	2:G:3046:LEU:HG	2.11	0.51
2:J:246:TYR:HE1	2:J:375:LYS:HG2	1.76	0.51
3:M:12:MET:HG2	3:M:16:GLY:HA3	1.93	0.51
3:M:15:GLY:H	3:M:85:LEU:HB2	1.74	0.51
2:B:243:ARG:HA	2:B:301:VAL:HG22	1.93	0.51
2:B:2265:LEU:HD12	2:B:2265:LEU:H	1.74	0.51
2:B:3514:LEU:HD13	2:B:3602:VAL:HG13	1.91	0.51
2:B:3535:LEU:O	2:B:3539:ARG:HG2	2.11	0.51
2:E:3225:ARG:O	2:E:3229:ILE:HG23	2.11	0.51
2:G:233:ILE:HG12	2:G:234:SER:H	1.76	0.51
2:G:571:SER:HB2	2:G:574:VAL:HG22	1.92	0.51
2:G:882:TRP:CD1	3:M:106:PRO:HB3	2.46	0.51
2:G:3698:LEU:O	2:G:3702:VAL:HG12	2.11	0.51
2:J:40:GLU:O	2:J:114:SER:OG	2.28	0.51
2:J:4671:PHE:HD1	2:J:4714:ASN:O	1.94	0.51
3:K:90:THR:HG23	3:K:124:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:SER:HB2	2:B:574:VAL:HG22	1.92	0.50
2:B:3535:LEU:HD12	2:B:3539:ARG:HH12	1.76	0.50
2:B:3594:ARG:NH1	2:B:3597:GLN:OE1	2.34	0.50
2:E:40:GLU:O	2:E:114:SER:OG	2.28	0.50
2:E:243:ARG:HA	2:E:301:VAL:HG22	1.93	0.50
2:E:246:TYR:HE1	2:E:375:LYS:HG2	1.76	0.50
2:E:479:GLN:HE21	2:E:539:LEU:HD11	1.77	0.50
2:E:4189:ARG:HB3	2:E:5031:GLN:HE22	1.76	0.50
2:G:2614:ILE:O	2:G:2650:ARG:NH1	2.41	0.50
2:G:3225:ARG:O	2:G:3229:ILE:HG23	2.11	0.50
2:G:3363:GLY:O	2:G:3367:LYS:HG2	2.10	0.50
2:G:3644:LEU:HD11	2:G:3648:ARG:HD2	1.93	0.50
2:J:2582:MET:HA	2:J:2585:THR:HG22	1.93	0.50
2:J:3195:ALA:HB2	2:J:3275:PRO:HB3	1.92	0.50
2:B:210:GLU:HG2	2:B:273:HIS:CE1	2.46	0.50
2:B:2736:ASP:OD1	2:B:2736:ASP:N	2.42	0.50
2:B:3246:LEU:CG	2:B:3247:ASP:H	2.24	0.50
2:B:3698:LEU:O	2:B:3702:VAL:HG12	2.11	0.50
2:E:2208:MET:O	2:E:2212:VAL:HG23	2.12	0.50
2:E:2582:MET:HA	2:E:2585:THR:HG22	1.93	0.50
2:E:2960:LEU:HD23	2:E:2963:LEU:HD12	1.92	0.50
2:E:4720:VAL:HG13	2:E:4721:LYS:H	1.76	0.50
2:G:3002:LEU:O	2:G:3006:ILE:HG22	2.12	0.50
2:J:233:ILE:HG12	2:J:234:SER:H	1.76	0.50
2:J:365:LYS:O	2:J:369:LEU:HG	2.10	0.50
2:J:2566:ALA:HA	2:J:2569:PHE:HD2	1.76	0.50
3:K:15:GLY:H	3:K:85:LEU:HB2	1.74	0.50
3:M:85:LEU:HD13	3:M:125:VAL:HG13	1.91	0.50
2:B:920:TYR:O	2:B:923:GLN:HG2	2.11	0.50
2:B:2759:ALA:HB2	2:B:2810:LYS:HZ1	1.75	0.50
2:B:4860:ARG:HH22	2:G:4630:TYR:HE1	1.58	0.50
2:E:2644:LEU:HD12	2:E:2648:TYR:HE2	1.76	0.50
2:E:2759:ALA:HB2	2:E:2810:LYS:HZ1	1.75	0.50
2:E:3002:LEU:O	2:E:3006:ILE:HG22	2.12	0.50
2:E:3195:ALA:HB2	2:E:3275:PRO:HB3	1.92	0.50
2:E:3698:LEU:O	2:E:3702:VAL:HG12	2.11	0.50
2:G:243:ARG:HA	2:G:301:VAL:HG22	1.93	0.50
2:G:3535:LEU:HD12	2:G:3539:ARG:HH12	1.76	0.50
2:G:3923:LEU:HB2	2:G:3961:VAL:HG11	1.92	0.50
2:G:4569:LEU:HD21	2:G:4649:LEU:HD23	1.93	0.50
2:J:3042:LEU:O	2:J:3046:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4189:ARG:HB3	2:J:5031:GLN:HE22	1.77	0.50
3:K:62:SER:O	3:K:62:SER:OG	2.24	0.50
2:B:2992:GLU:HB2	2:B:2996:LYS:NZ	2.25	0.50
2:B:3034:LYS:O	2:B:3037:GLU:HG3	2.12	0.50
2:B:3219:TYR:HE1	2:B:3234:ASN:HA	1.76	0.50
2:B:3923:LEU:HB2	2:B:3961:VAL:HG11	1.93	0.50
2:B:4189:ARG:HB3	2:B:5031:GLN:HE22	1.76	0.50
2:E:878:ILE:HG13	3:F:107:TRP:CZ2	2.45	0.50
2:E:2189:LYS:HA	2:E:2192:TYR:CZ	2.45	0.50
2:E:2992:GLU:HB2	2:E:2996:LYS:NZ	2.25	0.50
2:E:3141:THR:HA	2:E:3144:PHE:CD2	2.47	0.50
2:E:3219:TYR:HE1	2:E:3234:ASN:HA	1.76	0.50
2:G:479:GLN:HE21	2:G:539:LEU:HD11	1.76	0.50
2:G:1423:ASP:O	2:G:1427:ILE:HG12	2.12	0.50
2:G:2759:ALA:HB2	2:G:2810:LYS:HZ1	1.76	0.50
2:G:3529:ASP:O	2:G:3533:ILE:HG13	2.11	0.50
2:G:3965:LEU:HA	2:G:3968:TYR:CD2	2.46	0.50
2:G:4545:GLU:O	2:G:4549:VAL:HG13	2.11	0.50
2:J:1423:ASP:O	2:J:1427:ILE:HG12	2.12	0.50
2:J:2109:ASP:HA	2:J:3694:LYS:HD2	1.93	0.50
2:J:2970:SER:HA	2:J:2973:PHE:CZ	2.45	0.50
2:J:3227:ARG:HG2	2:J:3232:LEU:HD12	1.93	0.50
2:J:4545:GLU:O	2:J:4549:VAL:HG13	2.12	0.50
3:F:90:THR:HG23	3:F:124:THR:HA	1.93	0.50
1:D:54:GLU:OE2	1:D:54:GLU:N	2.27	0.50
2:B:470:SER:HA	2:B:473:ASN:ND2	2.26	0.50
2:B:479:GLN:HE21	2:B:539:LEU:HD11	1.76	0.50
2:B:1423:ASP:O	2:B:1427:ILE:HG12	2.12	0.50
2:B:3093:ARG:HA	2:B:3096:PHE:CD1	2.46	0.50
2:E:233:ILE:HG12	2:E:234:SER:H	1.76	0.50
2:E:3644:LEU:HD11	2:E:3648:ARG:HD2	1.93	0.50
2:E:4545:GLU:O	2:E:4549:VAL:HG13	2.12	0.50
2:G:2109:ASP:HA	2:G:3694:LYS:HD2	1.93	0.50
2:G:3227:ARG:HG2	2:G:3232:LEU:HD12	1.93	0.50
2:J:479:GLN:HE21	2:J:539:LEU:HD11	1.76	0.50
2:J:571:SER:HB2	2:J:574:VAL:HG22	1.92	0.50
2:J:2165:LEU:HD13	2:J:2178:MET:HG2	1.94	0.50
2:J:3698:LEU:O	2:J:3702:VAL:HG12	2.11	0.50
2:B:2208:MET:O	2:B:2212:VAL:HG23	2.12	0.50
2:B:2635:GLU:HG3	2:B:2636:PHE:CD2	2.47	0.50
2:B:2682:ILE:HB	2:B:2703:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3966:THR:HG23	2:B:4026:MET:HA	1.92	0.50
2:E:920:TYR:O	2:E:923:GLN:HG2	2.11	0.50
2:E:1970:GLN:NE2	2:E:3641:LEU:O	2.37	0.50
2:G:866:HIS:HE1	2:G:870:ILE:HD12	1.77	0.50
2:G:2635:GLU:HG3	2:G:2636:PHE:CD2	2.47	0.50
2:G:3093:ARG:HA	2:G:3096:PHE:CD1	2.46	0.50
2:G:3141:THR:HA	2:G:3144:PHE:CD2	2.47	0.50
2:J:2380:ILE:O	2:J:2384:ILE:HG13	2.12	0.50
2:J:2457:LEU:HA	2:J:2460:LEU:HD12	1.94	0.50
2:J:3376:GLU:OE2	2:J:3380:ARG:NH2	2.39	0.50
2:B:2576:ALA:HA	2:B:2579:VAL:HB	1.93	0.50
2:B:2879:ALA:HA	2:B:2882:TYR:CD2	2.47	0.50
2:B:3180:ASN:O	2:B:3184:GLU:HG2	2.12	0.50
2:B:4096:ALA:O	2:B:4100:GLN:HG2	2.12	0.50
2:E:1087:ARG:HB3	2:E:1223:PHE:HA	1.94	0.50
2:E:3180:ASN:O	2:E:3184:GLU:HG2	2.12	0.50
2:E:3754:GLU:O	2:E:3758:MET:HG3	2.10	0.50
2:G:246:TYR:HE1	2:G:375:LYS:HG2	1.76	0.50
2:G:2165:LEU:HD13	2:G:2178:MET:HG2	1.93	0.50
2:G:4189:ARG:HB3	2:G:5031:GLN:HE22	1.77	0.50
2:J:127:MET:SD	2:J:127:MET:N	2.73	0.50
2:J:2208:MET:O	2:J:2212:VAL:HG23	2.12	0.50
2:J:2572:THR:HA	2:J:2574:HIS:CE1	2.46	0.50
2:J:2644:LEU:HD12	2:J:2648:TYR:HE2	1.76	0.50
2:J:4105:GLY:O	2:J:4109:GLN:HG2	2.12	0.50
1:D:26:TYR:CB	1:D:101:VAL:HG12	2.42	0.50
2:B:526:LEU:HD11	2:B:540:PHE:HZ	1.77	0.50
2:B:866:HIS:HE1	2:B:870:ILE:HD12	1.76	0.50
2:B:3651:ASN:O	2:B:3655:GLU:HG2	2.12	0.50
2:E:121:LEU:N	2:E:134:ASP:O	2.45	0.50
2:E:365:LYS:O	2:E:369:LEU:HG	2.12	0.50
2:E:501:ALA:O	2:E:505:GLU:HG2	2.12	0.50
2:E:823:LEU:HD11	2:E:1626:TRP:HB3	1.94	0.50
2:E:2635:GLU:HG3	2:E:2636:PHE:CD2	2.47	0.50
2:E:3246:LEU:HD23	2:E:3247:ASP:H	1.77	0.50
2:G:2211:MET:HA	2:G:2214:VAL:HG12	1.94	0.50
2:G:2573:GLU:HB2	2:G:2615:ARG:NH2	2.27	0.50
2:G:2788:HIS:NE2	2:G:2805:TYR:OH	2.38	0.50
2:G:5013:MET:CE	2:G:5020:ASP:HB2	2.42	0.50
2:G:5013:MET:HE3	2:G:5020:ASP:HB2	1.93	0.50
2:J:526:LEU:HD11	2:J:540:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2635:GLU:HG3	2:J:2636:PHE:CD2	2.47	0.50
2:J:3093:ARG:HA	2:J:3096:PHE:CD1	2.46	0.50
2:J:3093:ARG:HA	2:J:3096:PHE:HD1	1.77	0.50
2:B:3093:ARG:HA	2:B:3096:PHE:HD1	1.77	0.50
2:B:3529:ASP:O	2:B:3533:ILE:HG13	2.11	0.50
2:G:2582:MET:HA	2:G:2585:THR:HG22	1.94	0.50
2:G:3180:ASN:O	2:G:3184:GLU:HG2	2.12	0.50
2:J:231:LEU:O	2:J:260:TRP:NE1	2.40	0.50
2:J:1619:ARG:HB3	2:J:1626:TRP:CD2	2.47	0.50
2:J:2364:PHE:HD1	2:J:2429:LEU:HD21	1.75	0.50
2:J:3002:LEU:O	2:J:3006:ILE:HG22	2.12	0.50
2:B:233:ILE:HG12	2:B:234:SER:H	1.76	0.49
2:B:2165:LEU:HD13	2:B:2178:MET:HG2	1.94	0.49
2:B:2211:MET:HA	2:B:2214:VAL:HG12	1.94	0.49
2:B:2415:ARG:HA	2:B:2415:ARG:HH11	1.77	0.49
2:B:2457:LEU:HA	2:B:2460:LEU:HD12	1.94	0.49
2:B:3002:LEU:O	2:B:3006:ILE:HG22	2.12	0.49
2:E:2165:LEU:HD13	2:E:2178:MET:HG2	1.94	0.49
2:E:2879:ALA:HA	2:E:2882:TYR:CD2	2.47	0.49
2:E:3034:LYS:O	2:E:3037:GLU:HG3	2.12	0.49
2:E:3227:ARG:HG2	2:E:3232:LEU:HD12	1.93	0.49
2:E:3406:TYR:HD2	2:E:3464:ILE:HG21	1.77	0.49
2:G:2380:ILE:O	2:G:2384:ILE:HG13	2.12	0.49
2:G:4105:GLY:O	2:G:4109:GLN:HG2	2.12	0.49
2:J:3277:LEU:HB3	2:J:3315:LEU:HD13	1.94	0.49
1:H:97:LEU:HB3	1:H:99:PHE:CE2	2.46	0.49
2:B:3970:GLN:HE21	2:B:5004:THR:HA	1.77	0.49
2:G:501:ALA:O	2:G:505:GLU:HG2	2.12	0.49
2:G:1619:ARG:HB3	2:G:1626:TRP:CD2	2.47	0.49
2:G:2572:THR:HG22	2:G:2575:ARG:HB3	1.94	0.49
2:G:3034:LYS:O	2:G:3037:GLU:HG3	2.12	0.49
2:G:3780:LEU:HD22	2:G:3820:LEU:HD21	1.95	0.49
2:J:2230:THR:O	2:J:2234:ARG:HG3	2.12	0.49
2:J:3034:LYS:O	2:J:3037:GLU:HG3	2.12	0.49
2:J:3219:TYR:HE1	2:J:3234:ASN:HA	1.76	0.49
3:M:37:TYR:HE1	3:M:96:ASN:HB3	1.78	0.49
2:B:3227:ARG:HG2	2:B:3232:LEU:HD12	1.93	0.49
2:B:4569:LEU:HD21	2:B:4649:LEU:HD23	1.93	0.49
2:E:3438:VAL:HB	2:E:3513:THR:HG22	1.94	0.49
2:E:3651:ASN:O	2:E:3655:GLU:HG2	2.12	0.49
2:E:4843:LEU:O	2:E:4847:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:526:LEU:HD11	2:G:540:PHE:HZ	1.76	0.49
2:G:1215:ALA:HA	2:G:1219:LEU:HB3	1.94	0.49
2:G:1260:MET:O	2:G:1263:THR:OG1	2.31	0.49
2:G:2415:ARG:HA	2:G:2415:ARG:HH11	1.77	0.49
2:G:2751:LEU:O	2:G:2755:ILE:HG12	2.13	0.49
2:G:3093:ARG:HA	2:G:3096:PHE:HD1	1.77	0.49
2:G:3531:ASP:O	2:G:3535:LEU:HD23	2.12	0.49
2:J:148:TRP:CZ3	2:J:180:LEU:HG	2.48	0.49
2:J:501:ALA:O	2:J:505:GLU:HG2	2.11	0.49
2:J:823:LEU:HD11	2:J:1626:TRP:HB3	1.94	0.49
2:J:2415:ARG:HA	2:J:2415:ARG:HH11	1.77	0.49
2:J:3438:VAL:HB	2:J:3513:THR:HG22	1.94	0.49
3:C:15:GLY:H	3:C:85:LEU:HB2	1.74	0.49
3:M:63:VAL:O	3:M:63:VAL:HG12	2.13	0.49
2:B:223:PHE:HA	2:B:230:CYS:HA	1.95	0.49
2:B:823:LEU:HD11	2:B:1626:TRP:HB3	1.94	0.49
2:B:1087:ARG:HB3	2:B:1223:PHE:HA	1.94	0.49
2:B:2751:LEU:O	2:B:2755:ILE:HG12	2.13	0.49
2:E:1423:ASP:O	2:E:1427:ILE:HG12	2.12	0.49
2:E:2211:MET:HA	2:E:2214:VAL:HG12	1.94	0.49
2:E:2614:ILE:O	2:E:2650:ARG:NH1	2.41	0.49
2:E:3093:ARG:HA	2:E:3096:PHE:HD1	1.77	0.49
2:E:3531:ASP:O	2:E:3535:LEU:HD23	2.12	0.49
2:E:4569:LEU:HD21	2:E:4649:LEU:HD23	1.93	0.49
2:E:4630:TYR:HE1	2:J:4860:ARG:HH22	1.59	0.49
2:G:2691:TYR:HA	2:G:2696:TYR:CE1	2.47	0.49
2:G:4843:LEU:O	2:G:4847:VAL:HG22	2.13	0.49
2:J:866:HIS:HE1	2:J:870:ILE:HD12	1.77	0.49
2:J:2879:ALA:HA	2:J:2882:TYR:CD2	2.47	0.49
3:F:63:VAL:HG12	3:F:63:VAL:O	2.13	0.49
2:B:501:ALA:O	2:B:505:GLU:HG2	2.12	0.49
2:B:1215:ALA:HA	2:B:1219:LEU:HB3	1.94	0.49
2:B:2567:PRO:HA	2:B:2613:TYR:CD1	2.48	0.49
2:B:3141:THR:HA	2:B:3144:PHE:CD2	2.47	0.49
2:B:4545:GLU:O	2:B:4549:VAL:HG13	2.12	0.49
2:E:1619:ARG:HB3	2:E:1626:TRP:CD2	2.47	0.49
2:E:2380:ILE:O	2:E:2384:ILE:HG13	2.12	0.49
2:E:2475:GLN:NE2	2:E:2476:ILE:O	2.46	0.49
2:E:2682:ILE:HB	2:E:2703:LEU:HD21	1.93	0.49
2:E:2751:LEU:O	2:E:2755:ILE:HG12	2.13	0.49
2:E:3970:GLN:HE21	2:E:5004:THR:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4096:ALA:O	2:E:4100:GLN:HG2	2.12	0.49
2:G:2208:MET:O	2:G:2212:VAL:HG23	2.12	0.49
2:G:2496:PRO:HG3	2:G:2550:LEU:HD23	1.94	0.49
2:G:3651:ASN:O	2:G:3655:GLU:HG2	2.12	0.49
2:J:2211:MET:HA	2:J:2214:VAL:HG12	1.94	0.49
2:J:2431:ASP:HB2	2:J:2501:SER:HB2	1.95	0.49
2:J:3180:ASN:O	2:J:3184:GLU:HG2	2.12	0.49
2:J:3780:LEU:HD22	2:J:3820:LEU:HD21	1.95	0.49
2:B:2496:PRO:HG3	2:B:2550:LEU:HD23	1.94	0.49
2:B:2725:LYS:HZ1	2:B:2737:PRO:HA	1.76	0.49
2:E:2109:ASP:HA	2:E:3694:LYS:HD2	1.93	0.49
2:E:2415:ARG:HA	2:E:2415:ARG:HH11	1.77	0.49
2:E:2869:ARG:HH22	2:E:2946:LEU:HA	1.78	0.49
2:E:2881:ASN:HA	2:E:2884:ASN:ND2	2.28	0.49
2:G:2869:ARG:HH22	2:G:2946:LEU:HA	1.78	0.49
2:G:2881:ASN:HA	2:G:2884:ASN:ND2	2.28	0.49
2:G:3406:TYR:HD2	2:G:3464:ILE:HG21	1.77	0.49
2:G:3438:VAL:HB	2:G:3513:THR:HG22	1.95	0.49
2:J:1087:ARG:HB3	2:J:1223:PHE:HA	1.94	0.49
2:J:3141:THR:HA	2:J:3144:PHE:CD2	2.47	0.49
2:J:3644:LEU:HD11	2:J:3648:ARG:HD2	1.93	0.49
2:J:3970:GLN:NE2	2:J:5004:THR:HA	2.28	0.49
3:K:82:MET:HG3	3:K:84:SER:O	2.13	0.49
1:A:24:VAL:HG12	1:A:103:LEU:HA	1.93	0.49
2:B:349:GLN:HE21	2:B:354:GLY:HA2	1.78	0.49
2:B:3438:VAL:HB	2:B:3513:THR:HG22	1.95	0.49
2:B:3531:ASP:O	2:B:3535:LEU:HD23	2.12	0.49
2:E:148:TRP:CZ3	2:E:180:LEU:HG	2.48	0.49
2:E:866:HIS:HE1	2:E:870:ILE:HD12	1.76	0.49
2:E:4105:GLY:O	2:E:4109:GLN:HG2	2.12	0.49
2:G:148:TRP:CZ3	2:G:180:LEU:HG	2.48	0.49
2:G:2376:LEU:O	2:G:2380:ILE:HG12	2.13	0.49
2:G:2475:GLN:NE2	2:G:2476:ILE:O	2.46	0.49
2:G:2792:ARG:NH2	2:G:2798:SER:OG	2.41	0.49
2:G:3970:GLN:HE21	2:G:5004:THR:HA	1.78	0.49
2:G:4118:ASP:OD1	2:G:4119:GLU:N	2.46	0.49
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	1.95	0.49
2:J:1260:MET:O	2:J:1263:THR:OG1	2.31	0.49
2:J:2376:LEU:O	2:J:2380:ILE:HG12	2.13	0.49
2:J:2881:ASN:HA	2:J:2884:ASN:ND2	2.28	0.49
2:J:2970:SER:O	2:J:2974:ILE:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3406:TYR:HD2	2:J:3464:ILE:HG21	1.77	0.49
2:J:3573:MET:HE2	2:J:3576:TYR:HB3	1.95	0.49
2:J:3651:ASN:O	2:J:3655:GLU:HG2	2.12	0.49
2:J:4096:ALA:O	2:J:4100:GLN:HG2	2.12	0.49
2:J:4677:LEU:HD23	2:J:4711:PHE:HE1	1.77	0.49
1:H:26:TYR:CB	1:H:101:VAL:HG12	2.43	0.49
2:B:2109:ASP:HA	2:B:3694:LYS:HD2	1.93	0.49
2:B:2747:ILE:HG21	2:B:2814:LYS:HE3	1.95	0.49
2:B:3406:TYR:HD2	2:B:3464:ILE:HG21	1.77	0.49
2:B:3573:MET:HE2	2:B:3576:TYR:HB3	1.94	0.49
2:E:2747:ILE:HG21	2:E:2814:LYS:HE3	1.95	0.49
2:E:3051:ARG:NH2	2:E:3098:SER:O	2.46	0.49
2:E:3573:MET:HE2	2:E:3576:TYR:HB3	1.94	0.49
2:G:2431:ASP:HB2	2:G:2501:SER:HB2	1.95	0.49
2:G:2457:LEU:HA	2:G:2460:LEU:HD12	1.94	0.49
2:G:2747:ILE:HG21	2:G:2814:LYS:HE3	1.95	0.49
2:G:2879:ALA:HA	2:G:2882:TYR:CD2	2.47	0.49
2:J:878:ILE:HG13	3:K:107:TRP:CZ2	2.47	0.49
2:J:1215:ALA:HA	2:J:1219:LEU:HB3	1.94	0.49
2:J:2619:LEU:O	2:J:2623:LEU:HG	2.13	0.49
2:J:2751:LEU:O	2:J:2755:ILE:HG12	2.13	0.49
2:J:3531:ASP:O	2:J:3535:LEU:HD23	2.12	0.49
2:J:4843:LEU:O	2:J:4847:VAL:HG22	2.13	0.49
2:J:5009:TYR:HA	2:J:5012:LYS:HE3	1.94	0.49
3:K:37:TYR:HE1	3:K:96:ASN:HB3	1.77	0.49
1:A:78:PRO:HA	1:A:81:ALA:HB3	1.94	0.49
2:B:121:LEU:N	2:B:134:ASP:O	2.45	0.49
2:B:2475:GLN:NE2	2:B:2476:ILE:O	2.46	0.49
2:B:2691:TYR:HA	2:B:2696:TYR:CE1	2.47	0.49
2:B:2881:ASN:HA	2:B:2884:ASN:ND2	2.28	0.49
2:B:3051:ARG:NH2	2:B:3098:SER:O	2.46	0.49
2:E:208:CYS:H	2:E:269:TRP:HH2	1.61	0.49
2:E:882:TRP:CD2	3:F:106:PRO:HG3	2.47	0.49
2:G:371:VAL:CG1	2:G:373:LYS:HG2	2.43	0.49
2:G:863:LEU:HD22	2:G:867:LEU:HD21	1.95	0.49
2:G:1530:THR:HG23	2:G:1535:GLU:H	1.78	0.49
2:G:2230:THR:O	2:G:2234:ARG:HG3	2.12	0.49
2:G:2637:ALA:C	2:G:2640:PRO:HD2	2.33	0.49
2:G:2973:PHE:CD1	2:G:2995:ILE:HG12	2.48	0.49
2:J:1095:VAL:HB	2:J:1199:VAL:HG23	1.95	0.49
2:J:2475:GLN:NE2	2:J:2476:ILE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:PRO:HA	1:H:81:ALA:HB3	1.94	0.49
2:B:148:TRP:CZ3	2:B:180:LEU:HG	2.48	0.49
2:B:1154:ASP:HB3	2:B:1157:GLU:HB2	1.95	0.49
2:B:1619:ARG:HB3	2:B:1626:TRP:CD2	2.47	0.49
2:B:2230:THR:O	2:B:2234:ARG:HG3	2.12	0.49
2:E:526:LEU:HD11	2:E:540:PHE:HZ	1.77	0.49
2:E:1260:MET:O	2:E:1263:THR:OG1	2.31	0.49
2:E:3078:ARG:O	2:E:3082:LYS:HG2	2.13	0.49
2:E:3307:VAL:HA	2:E:3311:HIS:CE1	2.47	0.49
2:E:3316:LEU:HD21	2:E:3345:ILE:HG13	1.95	0.49
2:G:3246:LEU:HD12	2:G:3249:LEU:HD12	1.95	0.49
2:G:3573:MET:SD	2:G:3577:ARG:NH2	2.86	0.49
2:J:349:GLN:HE21	2:J:354:GLY:HA2	1.78	0.49
2:J:2970:SER:HA	2:J:2973:PHE:CE2	2.48	0.49
2:B:208:CYS:H	2:B:269:TRP:HH2	1.61	0.48
2:B:863:LEU:HD22	2:B:867:LEU:HD21	1.95	0.48
2:B:1530:THR:HG23	2:B:1535:GLU:H	1.78	0.48
2:B:2376:LEU:O	2:B:2380:ILE:HG12	2.13	0.48
2:B:2558:VAL:O	2:B:2562:ILE:HG12	2.14	0.48
2:B:2970:SER:HA	2:B:2973:PHE:CE2	2.48	0.48
2:E:349:GLN:HE21	2:E:354:GLY:HA2	1.78	0.48
2:E:2230:THR:O	2:E:2234:ARG:HG3	2.12	0.48
2:E:2431:ASP:HB2	2:E:2501:SER:HB2	1.95	0.48
2:E:2457:LEU:HA	2:E:2460:LEU:HD12	1.94	0.48
2:E:3206:LEU:HD13	2:E:3246:LEU:N	2.28	0.48
2:E:4651:THR:HG21	2:E:4803:HIS:CD2	2.48	0.48
2:J:1530:THR:HG23	2:J:1535:GLU:H	1.78	0.48
2:J:2637:ALA:C	2:J:2640:PRO:HD2	2.33	0.48
2:J:2747:ILE:HG21	2:J:2814:LYS:HE3	1.95	0.48
2:J:3078:ARG:O	2:J:3082:LYS:HG2	2.13	0.48
2:J:4802:GLY:HA2	2:J:4808:PHE:HB2	1.95	0.48
1:D:78:PRO:HA	1:D:81:ALA:HB3	1.94	0.48
2:B:4105:GLY:O	2:B:4109:GLN:HG2	2.12	0.48
2:B:4651:THR:HG21	2:B:4803:HIS:CD2	2.48	0.48
2:E:3573:MET:SD	2:E:3577:ARG:NH2	2.86	0.48
2:E:3780:LEU:HD22	2:E:3820:LEU:HD21	1.95	0.48
2:G:823:LEU:HD11	2:G:1626:TRP:HB3	1.94	0.48
2:G:870:ILE:O	2:G:874:LEU:HG	2.13	0.48
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.48
2:J:2616:PRO:HA	2:J:2619:LEU:HD12	1.94	0.48
2:J:2691:TYR:HA	2:J:2696:TYR:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2973:PHE:CD1	2:J:2995:ILE:HG12	2.48	0.48
2:B:2869:ARG:HH22	2:B:2946:LEU:HA	1.78	0.48
2:B:3315:LEU:O	2:B:3319:ILE:HG13	2.14	0.48
2:E:223:PHE:HA	2:E:230:CYS:HA	1.95	0.48
2:E:2867:LEU:HB2	2:E:2928:LYS:NZ	2.29	0.48
2:E:4118:ASP:OD1	2:E:4119:GLU:N	2.46	0.48
2:J:870:ILE:O	2:J:874:LEU:HG	2.13	0.48
2:J:2682:ILE:HB	2:J:2703:LEU:HD21	1.93	0.48
2:J:2869:ARG:HH22	2:J:2946:LEU:HA	1.78	0.48
2:J:3051:ARG:NH2	2:J:3098:SER:O	2.46	0.48
2:J:3262:ARG:N	2:J:3262:ARG:HD2	2.28	0.48
3:C:63:VAL:O	3:C:63:VAL:HG12	2.13	0.48
3:K:63:VAL:O	3:K:63:VAL:HG12	2.13	0.48
3:M:82:MET:HG3	3:M:84:SER:O	2.13	0.48
1:A:4:ILE:HD11	1:A:62:GLY:HA2	1.96	0.48
1:I:78:PRO:HA	1:I:81:ALA:HB3	1.94	0.48
2:B:733:PRO:HG2	2:B:762:CYS:HB3	1.96	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:2973:PHE:CD1	2:B:2995:ILE:HG12	2.48	0.48
2:B:3573:MET:SD	2:B:3577:ARG:NH2	2.86	0.48
2:G:1087:ARG:HB3	2:G:1223:PHE:HA	1.94	0.48
2:G:2158:CYS:O	2:G:2162:ILE:HG13	2.14	0.48
2:G:2867:LEU:HB2	2:G:2928:LYS:NZ	2.29	0.48
2:J:2788:HIS:NE2	2:J:2805:TYR:OH	2.38	0.48
2:J:4651:THR:HG21	2:J:4803:HIS:CD2	2.48	0.48
2:J:5013:MET:HE1	2:J:5021:PHE:HB3	1.95	0.48
3:C:37:TYR:HE1	3:C:96:ASN:HB3	1.78	0.48
1:A:4:ILE:HG13	1:A:65:GLN:NE2	2.28	0.48
1:D:4:ILE:HD11	1:D:62:GLY:HA2	1.96	0.48
1:I:4:ILE:HD11	1:I:62:GLY:HA2	1.96	0.48
2:B:28:VAL:HG12	2:B:33:LEU:HD23	1.96	0.48
2:B:1735:ILE:HG22	2:B:2142:TYR:HB3	1.95	0.48
2:B:2637:ALA:C	2:B:2640:PRO:HD2	2.33	0.48
2:B:3078:ARG:O	2:B:3082:LYS:HG2	2.13	0.48
2:E:299:LEU:HD21	2:E:377:ILE:HA	1.96	0.48
2:E:1154:ASP:HB3	2:E:1157:GLU:HB2	1.95	0.48
2:E:1623:ARG:HA	2:E:1623:ARG:NH1	2.28	0.48
2:E:2970:SER:HA	2:E:2973:PHE:CE2	2.48	0.48
2:E:3262:ARG:N	2:E:3262:ARG:HD2	2.28	0.48
2:G:121:LEU:N	2:G:134:ASP:O	2.45	0.48
2:G:299:LEU:HD21	2:G:377:ILE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3573:MET:HE2	2:G:3576:TYR:HB3	1.95	0.48
2:J:863:LEU:HD22	2:J:867:LEU:HD21	1.95	0.48
2:J:2158:CYS:O	2:J:2162:ILE:HG13	2.14	0.48
2:J:2496:PRO:HG3	2:J:2550:LEU:HD23	1.93	0.48
3:C:82:MET:HG3	3:C:84:SER:O	2.13	0.48
3:F:37:TYR:HE1	3:F:96:ASN:HB3	1.77	0.48
1:H:4:ILE:HD11	1:H:62:GLY:HA2	1.96	0.48
2:B:2799:GLU:O	2:B:2803:GLU:HG2	2.14	0.48
2:B:3475:LYS:HD3	2:B:3516:LYS:HZ1	1.79	0.48
2:B:3780:LEU:HD22	2:B:3820:LEU:HD21	1.95	0.48
2:E:1426:ILE:HA	2:E:1429:ASN:OD1	2.13	0.48
2:E:2158:CYS:O	2:E:2162:ILE:HG13	2.14	0.48
2:E:2496:PRO:HG3	2:E:2550:LEU:HD23	1.94	0.48
2:E:2637:ALA:C	2:E:2640:PRO:HD2	2.33	0.48
2:E:2691:TYR:HA	2:E:2696:TYR:CE1	2.47	0.48
2:E:2799:GLU:O	2:E:2803:GLU:HG2	2.14	0.48
2:E:2970:SER:O	2:E:2974:ILE:HG23	2.13	0.48
2:E:2973:PHE:CD1	2:E:2995:ILE:HG12	2.48	0.48
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	1.95	0.48
2:G:1154:ASP:HB3	2:G:1157:GLU:HB2	1.95	0.48
2:G:1623:ARG:HA	2:G:1623:ARG:NH1	2.28	0.48
2:G:2970:SER:HA	2:G:2973:PHE:CE2	2.48	0.48
2:G:3051:ARG:NH2	2:G:3098:SER:O	2.46	0.48
2:G:4096:ALA:O	2:G:4100:GLN:HG2	2.12	0.48
2:J:4118:ASP:OD1	2:J:4119:GLU:N	2.46	0.48
2:B:870:ILE:O	2:B:874:LEU:HG	2.14	0.48
2:B:1260:MET:O	2:B:1263:THR:OG1	2.31	0.48
2:B:2626:LEU:HD22	2:B:2640:PRO:HB3	1.95	0.48
2:B:3704:HIS:O	2:B:3708:THR:HG23	2.14	0.48
2:B:4118:ASP:OD1	2:B:4119:GLU:N	2.46	0.48
2:E:369:LEU:HB3	2:E:371:VAL:HG23	1.96	0.48
2:E:3704:HIS:O	2:E:3708:THR:HG23	2.14	0.48
2:E:3836:MET:CE	2:E:3915:ILE:HG23	2.44	0.48
2:G:28:VAL:HG12	2:G:33:LEU:HD23	1.96	0.48
2:G:1735:ILE:HG22	2:G:2142:TYR:HB3	1.95	0.48
2:G:3262:ARG:N	2:G:3262:ARG:HD2	2.28	0.48
2:J:208:CYS:H	2:J:269:TRP:HH2	1.61	0.48
2:B:2431:ASP:HB2	2:B:2501:SER:HB2	1.94	0.48
2:B:2562:ILE:HG23	2:B:2569:PHE:CE2	2.48	0.48
2:B:2970:SER:O	2:B:2974:ILE:HG23	2.13	0.48
2:B:3836:MET:CE	2:B:3915:ILE:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3991:GLY:O	2:B:3995:VAL:HG23	2.13	0.48
2:B:4780:PHE:HA	2:B:4783:ILE:HG22	1.94	0.48
2:B:4843:LEU:O	2:B:4847:VAL:HG22	2.13	0.48
2:E:3354:LEU:HG	2:E:3359:ILE:HD11	1.96	0.48
2:E:3366:ARG:NE	2:E:3367:LYS:HD2	2.26	0.48
2:G:223:PHE:HA	2:G:230:CYS:HA	1.95	0.48
2:G:2626:LEU:HD22	2:G:2640:PRO:HB3	1.96	0.48
2:G:3078:ARG:O	2:G:3082:LYS:HG2	2.13	0.48
2:G:3836:MET:CE	2:G:3915:ILE:HG23	2.44	0.48
2:G:4780:PHE:HA	2:G:4783:ILE:HG22	1.94	0.48
2:J:2376:LEU:HD12	2:J:2376:LEU:H	1.79	0.48
2:J:2566:ALA:HA	2:J:2569:PHE:CD2	2.49	0.48
2:J:3320:LEU:HD23	2:J:3320:LEU:HA	1.74	0.48
3:F:82:MET:HG3	3:F:84:SER:O	2.13	0.48
2:B:2380:ILE:O	2:B:2384:ILE:HG13	2.12	0.48
2:B:3166:TYR:CE1	2:B:3239:MET:HG3	2.49	0.48
2:E:215:THR:HG22	2:E:273:HIS:HA	1.96	0.48
2:E:1215:ALA:HA	2:E:1219:LEU:HB3	1.94	0.48
2:E:3281:LEU:O	2:E:3285:TRP:HB2	2.14	0.48
2:G:1426:ILE:HA	2:G:1429:ASN:OD1	2.13	0.48
2:G:2531:ARG:HH12	2:G:2585:THR:HB	1.79	0.48
2:G:2970:SER:O	2:G:2974:ILE:HG23	2.13	0.48
2:G:3704:HIS:O	2:G:3708:THR:HG23	2.14	0.48
2:G:4064:MET:HE1	2:G:4110:PHE:HD2	1.79	0.48
2:J:1426:ILE:HA	2:J:1429:ASN:OD1	2.13	0.48
2:J:2736:ASP:OD1	2:J:2736:ASP:N	2.42	0.48
2:J:3353:LEU:HG	2:J:3357:HIS:CE1	2.49	0.48
2:J:3573:MET:SD	2:J:3577:ARG:NH2	2.86	0.48
2:J:3991:GLY:O	2:J:3995:VAL:HG23	2.13	0.48
2:B:299:LEU:HD21	2:B:377:ILE:HA	1.96	0.48
2:B:582:HIS:O	2:B:586:ILE:HG13	2.14	0.48
2:B:1089:TYR:CD1	2:B:1152:MET:HG2	2.45	0.48
2:B:1420:ASN:OD1	2:B:1421:ARG:N	2.47	0.48
2:B:2158:CYS:O	2:B:2162:ILE:HG13	2.14	0.48
2:B:3353:LEU:HG	2:B:3357:HIS:CE1	2.49	0.48
2:E:2376:LEU:O	2:E:2380:ILE:HG12	2.13	0.48
2:G:2134:LEU:O	2:G:2138:LEU:HG	2.14	0.48
2:G:2725:LYS:HZ1	2:G:2737:PRO:HA	1.77	0.48
2:G:4651:THR:HG21	2:G:4803:HIS:CD2	2.48	0.48
2:G:4679:ARG:HH21	2:G:5017:ARG:CZ	2.26	0.48
2:J:215:THR:HG22	2:J:273:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1623:ARG:HA	2:J:1623:ARG:NH1	2.28	0.48
2:J:2867:LEU:HB2	2:J:2928:LYS:NZ	2.29	0.48
2:J:3281:LEU:O	2:J:3285:TRP:HB2	2.14	0.48
2:B:215:THR:HG22	2:B:273:HIS:HA	1.96	0.47
2:B:1426:ILE:HA	2:B:1429:ASN:OD1	2.13	0.47
2:B:3044:CYS:SG	2:B:3092:LEU:HB2	2.54	0.47
2:B:3514:LEU:HD12	2:B:3606:LEU:HB2	1.96	0.47
2:B:4679:ARG:NH1	2:B:4715:TYR:OH	2.46	0.47
2:E:630:GLU:HG3	2:E:631:LEU:HD23	1.96	0.47
2:E:3166:TYR:CE1	2:E:3239:MET:HG3	2.49	0.47
2:E:3313:ASN:OD1	2:E:3353:LEU:HD11	2.14	0.47
2:E:4069:LYS:NZ	2:E:4130:ASN:OD1	2.37	0.47
2:G:208:CYS:H	2:G:269:TRP:HH2	1.61	0.47
2:G:582:HIS:O	2:G:586:ILE:HG13	2.14	0.47
2:G:659:TYR:HB2	2:G:1017:ARG:HH22	1.79	0.47
2:G:2869:ARG:NH2	2:G:2947:ASP:H	2.12	0.47
2:J:121:LEU:N	2:J:134:ASP:O	2.45	0.47
2:J:1089:TYR:CD1	2:J:1152:MET:HG2	2.45	0.47
2:J:1154:ASP:HB3	2:J:1157:GLU:HB2	1.95	0.47
2:J:3166:TYR:CE1	2:J:3239:MET:HG3	2.49	0.47
1:I:17:LYS:HG3	1:I:18:LYS:H	1.79	0.47
2:B:630:GLU:HG3	2:B:631:LEU:HD23	1.96	0.47
2:B:2867:LEU:HB2	2:B:2928:LYS:NZ	2.28	0.47
2:B:3051:ARG:NH2	2:B:3102:ASP:HB2	2.30	0.47
2:B:3443:ILE:HG12	2:B:3605:HIS:CD2	2.49	0.47
2:E:404:ILE:HG23	2:E:483:MET:SD	2.54	0.47
2:E:659:TYR:HB2	2:E:1017:ARG:HH22	1.80	0.47
2:E:3044:CYS:SG	2:E:3092:LEU:HB2	2.54	0.47
2:E:3514:LEU:HD12	2:E:3606:LEU:HB2	1.96	0.47
2:E:4749:GLU:HG3	2:E:4753:HIS:NE2	2.29	0.47
2:E:4780:PHE:HA	2:E:4783:ILE:HG22	1.94	0.47
2:G:349:GLN:HE21	2:G:354:GLY:HA2	1.78	0.47
2:G:3044:CYS:SG	2:G:3092:LEU:HB2	2.54	0.47
2:G:4069:LYS:NZ	2:G:4130:ASN:OD1	2.37	0.47
2:J:111:HIS:CE1	2:J:113:HIS:HB3	2.49	0.47
2:J:4780:PHE:HA	2:J:4783:ILE:HG22	1.94	0.47
1:A:17:LYS:HG3	1:A:18:LYS:H	1.79	0.47
2:B:3354:LEU:HG	2:B:3359:ILE:HD11	1.96	0.47
2:B:3970:GLN:NE2	2:B:5004:THR:HA	2.30	0.47
2:E:283:ARG:HE	2:E:288:GLY:HA2	1.80	0.47
2:E:2376:LEU:HD12	2:E:2376:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3970:GLN:NE2	2:E:5004:THR:HA	2.29	0.47
2:G:1274:HIS:HB3	2:G:1277:TRP:HB2	1.97	0.47
2:G:3166:TYR:CE1	2:G:3239:MET:HG3	2.49	0.47
2:G:3991:GLY:O	2:G:3995:VAL:HG23	2.13	0.47
2:J:299:LEU:HD21	2:J:377:ILE:HA	1.96	0.47
2:J:747:CYS:SG	2:J:756:SER:HB2	2.55	0.47
1:D:17:LYS:HG3	1:D:18:LYS:H	1.79	0.47
1:H:17:LYS:HG3	1:H:18:LYS:H	1.79	0.47
2:B:2134:LEU:O	2:B:2138:LEU:HG	2.14	0.47
2:B:2673:HIS:CE1	2:B:2910:THR:HA	2.50	0.47
2:B:2869:ARG:NH2	2:B:2947:ASP:H	2.12	0.47
2:B:3262:ARG:N	2:B:3262:ARG:HD2	2.28	0.47
2:B:3313:ASN:OD1	2:B:3353:LEU:HD11	2.15	0.47
2:E:2788:HIS:NE2	2:E:2805:TYR:OH	2.38	0.47
2:E:3640:PRO:HG2	2:E:3643:ASN:HB2	1.96	0.47
2:G:747:CYS:SG	2:G:756:SER:HB2	2.55	0.47
2:G:818:ARG:NH1	2:G:1027:LEU:O	2.44	0.47
2:G:3970:GLN:NE2	2:G:5004:THR:HA	2.29	0.47
2:J:1735:ILE:HG22	2:J:2142:TYR:HB3	1.95	0.47
2:J:2134:LEU:O	2:J:2138:LEU:HG	2.14	0.47
2:J:3044:CYS:SG	2:J:3092:LEU:HB2	2.54	0.47
2:J:3825:GLU:H	2:J:3825:GLU:CD	2.17	0.47
3:K:71:ARG:HB3	3:K:78:VAL:HG22	1.97	0.47
1:D:26:TYR:HB2	1:D:101:VAL:HG12	1.96	0.47
2:B:4749:GLU:HG3	2:B:4753:HIS:NE2	2.29	0.47
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	1.95	0.47
2:E:582:HIS:O	2:E:586:ILE:HG13	2.14	0.47
2:E:863:LEU:HD22	2:E:867:LEU:HD21	1.95	0.47
2:E:1530:THR:HG23	2:E:1535:GLU:H	1.78	0.47
2:E:2806:ARG:O	2:E:2810:LYS:HG2	2.14	0.47
2:G:111:HIS:CE1	2:G:113:HIS:HB3	2.50	0.47
2:G:1089:TYR:CD1	2:G:1152:MET:HG2	2.45	0.47
2:G:3353:LEU:HG	2:G:3357:HIS:CE1	2.49	0.47
2:G:3475:LYS:HZ1	2:G:3511:VAL:HG21	1.79	0.47
2:J:223:PHE:HA	2:J:230:CYS:HA	1.95	0.47
2:J:2614:ILE:O	2:J:2650:ARG:NH1	2.41	0.47
2:J:2626:LEU:HD22	2:J:2640:PRO:HB3	1.95	0.47
2:E:747:CYS:SG	2:E:756:SER:HB2	2.55	0.47
2:E:870:ILE:O	2:E:874:LEU:HG	2.13	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.47
2:E:1274:HIS:HB3	2:E:1277:TRP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1813:ARG:O	2:E:1817:GLU:HG2	2.15	0.47
2:E:2134:LEU:O	2:E:2138:LEU:HG	2.14	0.47
2:E:2515:GLN:CA	2:E:2568:LEU:HD21	2.44	0.47
2:E:2531:ARG:HH12	2:E:2585:THR:HB	1.79	0.47
2:E:3209:GLN:CD	2:E:3209:GLN:H	2.18	0.47
2:G:2673:HIS:CE1	2:G:2910:THR:HA	2.50	0.47
2:G:2799:GLU:O	2:G:2803:GLU:HG2	2.14	0.47
2:G:2806:ARG:O	2:G:2810:LYS:HG2	2.14	0.47
2:J:404:ILE:HG23	2:J:483:MET:SD	2.54	0.47
2:J:487:VAL:O	2:J:491:ILE:HG13	2.15	0.47
2:J:582:HIS:O	2:J:586:ILE:HG13	2.14	0.47
2:J:863:LEU:HD13	2:J:867:LEU:HD21	1.97	0.47
2:J:3051:ARG:NH2	2:J:3102:ASP:HB2	2.30	0.47
2:J:3704:HIS:O	2:J:3708:THR:HG23	2.14	0.47
2:J:4181:ILE:HG22	2:J:4987:ASN:HB3	1.97	0.47
3:F:71:ARG:HB3	3:F:78:VAL:HG22	1.96	0.47
2:B:365:LYS:O	2:B:369:LEU:HG	2.14	0.47
2:B:404:ILE:HG23	2:B:483:MET:SD	2.54	0.47
2:B:1274:HIS:HB3	2:B:1277:TRP:HB2	1.97	0.47
2:B:1623:ARG:HA	2:B:1623:ARG:NH1	2.28	0.47
2:B:2353:VAL:O	2:B:2357:LEU:HG	2.15	0.47
2:B:2782:ASP:N	2:B:2782:ASP:OD1	2.47	0.47
2:B:3209:GLN:CD	2:B:3209:GLN:H	2.18	0.47
2:B:3280:TYR:HE1	2:B:3284:TRP:CD1	2.33	0.47
2:E:111:HIS:CE1	2:E:113:HIS:HB3	2.50	0.47
2:E:2673:HIS:CE1	2:E:2910:THR:HA	2.50	0.47
2:E:2869:ARG:NH2	2:E:2947:ASP:H	2.12	0.47
2:E:3316:LEU:HD11	2:E:3345:ILE:HG23	1.95	0.47
2:E:3353:LEU:HG	2:E:3357:HIS:CE1	2.49	0.47
2:E:3991:GLY:O	2:E:3995:VAL:HG23	2.14	0.47
2:G:283:ARG:HE	2:G:288:GLY:HA2	1.79	0.47
2:G:733:PRO:HG2	2:G:762:CYS:HB3	1.96	0.47
2:G:3354:LEU:HG	2:G:3359:ILE:HD11	1.96	0.47
2:G:3640:PRO:HG2	2:G:3643:ASN:HB2	1.96	0.47
2:G:4211:LYS:O	2:G:4215:ARG:HG3	2.15	0.47
2:J:28:VAL:HG12	2:J:33:LEU:HD23	1.96	0.47
2:J:246:TYR:CD1	2:J:373:LYS:HB3	2.50	0.47
2:J:799:GLU:OE1	2:J:1623:ARG:NH1	2.48	0.47
2:J:1420:ASN:OD1	2:J:1421:ARG:N	2.47	0.47
2:J:2806:ARG:O	2:J:2810:LYS:HG2	2.14	0.47
2:J:2869:ARG:NH2	2:J:2947:ASP:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3280:TYR:HE1	2:J:3284:TRP:CD1	2.33	0.47
2:J:4211:LYS:O	2:J:4215:ARG:HG3	2.15	0.47
2:B:283:ARG:HE	2:B:288:GLY:HA2	1.79	0.47
2:B:2518:LEU:HD21	2:B:2569:PHE:CZ	2.49	0.47
2:B:3965:LEU:HA	2:B:3968:TYR:CD2	2.50	0.47
2:E:20:VAL:HG12	2:E:22:LEU:H	1.80	0.47
2:E:733:PRO:HG2	2:E:762:CYS:HB3	1.96	0.47
2:E:1420:ASN:OD1	2:E:1421:ARG:N	2.47	0.47
2:E:1735:ILE:HG22	2:E:2142:TYR:HB3	1.95	0.47
2:E:2626:LEU:HD22	2:E:2640:PRO:HB3	1.95	0.47
2:E:2718:SER:OG	2:E:2909:ASP:O	2.25	0.47
2:E:3412:LEU:O	2:E:3416:VAL:HG12	2.15	0.47
2:G:20:VAL:HG12	2:G:22:LEU:H	1.80	0.47
2:G:1420:ASN:OD1	2:G:1421:ARG:N	2.47	0.47
2:G:2225:PHE:O	2:G:2229:VAL:HG23	2.15	0.47
2:G:2592:GLY:O	2:G:2600:ARG:NH1	2.48	0.47
2:G:3209:GLN:CD	2:G:3209:GLN:H	2.18	0.47
2:J:733:PRO:HG2	2:J:762:CYS:HB3	1.96	0.47
2:J:3313:ASN:OD1	2:J:3353:LEU:HD11	2.14	0.47
2:J:4749:GLU:HG3	2:J:4753:HIS:NE2	2.29	0.47
2:B:878:ILE:HG21	3:C:107:TRP:NE1	2.30	0.47
2:B:3197:LEU:O	2:B:3201:MET:HB3	2.15	0.47
2:B:3281:LEU:O	2:B:3285:TRP:HB2	2.14	0.47
2:B:3825:GLU:H	2:B:3825:GLU:CD	2.17	0.47
2:E:3825:GLU:H	2:E:3825:GLU:CD	2.17	0.47
2:G:3281:LEU:O	2:G:3285:TRP:HB2	2.14	0.47
2:J:2469:ILE:HA	2:J:2472:LEU:HG	1.97	0.47
2:J:2531:ARG:HH12	2:J:2585:THR:HB	1.79	0.47
2:J:3412:LEU:O	2:J:3416:VAL:HG12	2.15	0.47
2:B:487:VAL:O	2:B:491:ILE:HG13	2.15	0.47
2:B:747:CYS:SG	2:B:756:SER:HB2	2.55	0.47
2:B:2806:ARG:O	2:B:2810:LYS:HG2	2.14	0.47
2:B:3003:LEU:HB2	2:B:3004:PRO:HD3	1.97	0.47
2:B:3366:ARG:NE	2:B:3367:LYS:HD2	2.26	0.47
2:B:4181:ILE:HG22	2:B:4987:ASN:HB3	1.97	0.47
2:E:317:ARG:NH2	2:E:321:GLU:O	2.48	0.47
2:E:863:LEU:HD13	2:E:867:LEU:HD21	1.97	0.47
2:E:3443:ILE:HG12	2:E:3605:HIS:CD2	2.50	0.47
2:G:215:THR:HG22	2:G:273:HIS:HA	1.96	0.47
2:G:1745:ILE:HD11	2:G:1769:THR:HG23	1.97	0.47
2:G:2809:ILE:H	2:G:2809:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2958:GLY:O	2:G:2962:GLN:HG2	2.15	0.47
2:G:3051:ARG:NH2	2:G:3102:ASP:HB2	2.30	0.47
2:G:3316:LEU:HD21	2:G:3345:ILE:HG13	1.97	0.47
2:G:3475:LYS:HD3	2:G:3516:LYS:HZ1	1.80	0.47
2:J:4064:MET:HE1	2:J:4110:PHE:HD2	1.80	0.47
2:B:2225:PHE:O	2:B:2229:VAL:HG23	2.15	0.46
2:E:2576:ALA:HA	2:E:2579:VAL:HB	1.96	0.46
2:G:317:ARG:NH2	2:G:321:GLU:O	2.48	0.46
2:G:487:VAL:O	2:G:491:ILE:HG13	2.15	0.46
2:G:2152:THR:O	2:G:2156:LEU:HG	2.16	0.46
2:G:3825:GLU:H	2:G:3825:GLU:CD	2.17	0.46
2:J:2152:THR:O	2:J:2156:LEU:HG	2.16	0.46
2:J:3246:LEU:HD13	2:J:3280:TYR:CD2	2.49	0.46
2:J:3246:LEU:HD12	2:J:3249:LEU:HD12	1.97	0.46
2:J:3346:VAL:HG21	2:J:3411:LEU:HB3	1.96	0.46
2:B:111:HIS:CE1	2:B:113:HIS:HB3	2.50	0.46
2:B:659:TYR:HB2	2:B:1017:ARG:HH22	1.79	0.46
2:B:2592:GLY:O	2:B:2600:ARG:NH1	2.48	0.46
2:E:28:VAL:HG12	2:E:33:LEU:HD23	1.96	0.46
2:E:642:THR:HG21	2:E:1615:VAL:HG21	1.98	0.46
2:E:799:GLU:OE1	2:E:1623:ARG:NH1	2.48	0.46
2:E:2867:LEU:HB2	2:E:2928:LYS:HZ3	1.80	0.46
2:G:2469:ILE:HA	2:G:2472:LEU:HG	1.97	0.46
2:G:3197:LEU:O	2:G:3201:MET:HB3	2.15	0.46
2:G:3412:LEU:O	2:G:3416:VAL:HG12	2.15	0.46
2:J:1813:ARG:O	2:J:1817:GLU:HG2	2.15	0.46
2:J:3443:ILE:HG12	2:J:3605:HIS:CD2	2.49	0.46
2:J:4675:LYS:HG3	2:J:4715:TYR:HE1	1.80	0.46
1:I:97:LEU:HB3	1:I:99:PHE:CE2	2.51	0.46
2:B:213:TYR:HA	2:B:340:LYS:HA	1.98	0.46
2:B:642:THR:HG21	2:B:1615:VAL:HG21	1.98	0.46
2:E:487:VAL:O	2:E:491:ILE:HG13	2.15	0.46
2:E:2782:ASP:N	2:E:2782:ASP:OD1	2.47	0.46
2:E:4675:LYS:HG3	2:E:4715:TYR:HE1	1.80	0.46
2:G:213:TYR:HA	2:G:340:LYS:HA	1.97	0.46
2:G:799:GLU:OE1	2:G:1623:ARG:NH1	2.48	0.46
2:G:2294:ASP:O	2:G:2298:VAL:HG12	2.16	0.46
2:G:2376:LEU:H	2:G:2376:LEU:HD12	1.79	0.46
2:G:4181:ILE:HG22	2:G:4987:ASN:HB3	1.97	0.46
2:J:1042:ALA:O	2:J:1046:LEU:HG	2.16	0.46
2:J:2294:ASP:O	2:J:2298:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2353:VAL:O	2:J:2357:LEU:HG	2.15	0.46
2:J:3003:LEU:HB2	2:J:3004:PRO:HD3	1.97	0.46
2:J:3354:LEU:HG	2:J:3359:ILE:HD11	1.96	0.46
2:B:4240:ASP:O	2:B:4244:GLU:HG3	2.16	0.46
2:E:2102:VAL:HG13	2:E:2120:MET:HB2	1.97	0.46
2:E:2104:ARG:O	2:E:2108:GLU:HG2	2.16	0.46
2:E:2152:THR:O	2:E:2156:LEU:HG	2.16	0.46
2:E:2765:LYS:HD3	2:E:2765:LYS:HA	1.67	0.46
2:E:3002:LEU:HD23	2:E:3002:LEU:HA	1.81	0.46
2:E:3346:VAL:HG21	2:E:3411:LEU:HB3	1.96	0.46
2:G:19:GLU:HB3	2:G:205:ILE:HD13	1.98	0.46
2:G:863:LEU:HD13	2:G:867:LEU:HD21	1.97	0.46
2:G:1042:ALA:O	2:G:1046:LEU:HG	2.16	0.46
2:G:1669:LEU:O	2:G:1673:VAL:HG22	2.16	0.46
2:G:1813:ARG:O	2:G:1817:GLU:HG2	2.15	0.46
2:G:1964:ARG:HB3	2:G:1968:LYS:NZ	2.30	0.46
2:G:2782:ASP:N	2:G:2782:ASP:OD1	2.47	0.46
2:G:4749:GLU:HG3	2:G:4753:HIS:NE2	2.29	0.46
2:J:283:ARG:HE	2:J:288:GLY:HA2	1.79	0.46
2:J:1153:ILE:HG13	2:J:1160:ILE:HG12	1.97	0.46
2:J:1669:LEU:O	2:J:1673:VAL:HG22	2.16	0.46
2:J:2225:PHE:O	2:J:2229:VAL:HG23	2.15	0.46
2:J:2328:GLY:HA2	2:J:2331:TYR:HD2	1.81	0.46
2:J:2673:HIS:CE1	2:J:2910:THR:HA	2.50	0.46
2:B:882:TRP:O	2:B:885:THR:OG1	2.28	0.46
2:B:1153:ILE:HG13	2:B:1160:ILE:HG12	1.97	0.46
2:B:2328:GLY:HA2	2:B:2331:TYR:HD2	1.81	0.46
2:B:3412:LEU:O	2:B:3416:VAL:HG12	2.15	0.46
2:B:3640:PRO:HG2	2:B:3643:ASN:HB2	1.96	0.46
2:B:4160:LEU:O	2:B:4164:LEU:HG	2.16	0.46
2:B:4211:LYS:O	2:B:4215:ARG:HG3	2.15	0.46
2:E:1669:LEU:O	2:E:1673:VAL:HG22	2.16	0.46
2:E:1745:ILE:HD11	2:E:1769:THR:HG23	1.97	0.46
2:E:2294:ASP:O	2:E:2298:VAL:HG12	2.16	0.46
2:E:2515:GLN:O	2:E:2519:LEU:HG	2.14	0.46
2:E:3051:ARG:NH2	2:E:3102:ASP:HB2	2.30	0.46
2:E:4160:LEU:O	2:E:4164:LEU:HG	2.16	0.46
2:E:4204:GLN:O	2:E:4207:MET:HB2	2.16	0.46
2:G:630:GLU:HG3	2:G:631:LEU:HD23	1.96	0.46
2:G:3514:LEU:HD12	2:G:3606:LEU:HB2	1.96	0.46
2:G:4160:LEU:O	2:G:4164:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4679:ARG:NH1	2:G:4715:TYR:OH	2.49	0.46
2:J:630:GLU:HG3	2:J:631:LEU:HD23	1.96	0.46
2:J:2312:MET:SD	2:J:2312:MET:N	2.79	0.46
2:J:2592:GLY:O	2:J:2600:ARG:NH1	2.48	0.46
2:J:3428:ASN:O	2:J:3432:GLU:HG2	2.16	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.97	0.46
2:B:247:TYR:CD2	2:B:374:LYS:HB2	2.44	0.46
2:B:317:ARG:NH2	2:B:321:GLU:O	2.48	0.46
2:B:2958:GLY:O	2:B:2962:GLN:HG2	2.15	0.46
2:E:1153:ILE:HG13	2:E:1160:ILE:HG12	1.97	0.46
2:E:1964:ARG:HB3	2:E:1968:LYS:NZ	2.30	0.46
2:E:3548:GLU:HG2	2:E:3552:PHE:CE2	2.51	0.46
2:G:246:TYR:CB	2:G:373:LYS:HD2	2.45	0.46
2:G:478:PHE:HD2	2:G:483:MET:HG3	1.81	0.46
2:G:2328:GLY:HA2	2:G:2331:TYR:HD2	1.81	0.46
2:G:2353:VAL:O	2:G:2357:LEU:HG	2.15	0.46
2:G:2599:GLN:O	2:G:2603:ILE:HG13	2.16	0.46
2:G:4240:ASP:O	2:G:4244:GLU:HG3	2.16	0.46
2:J:642:THR:HG21	2:J:1615:VAL:HG21	1.98	0.46
2:J:1274:HIS:HB3	2:J:1277:TRP:HB2	1.97	0.46
2:J:3197:LEU:O	2:J:3201:MET:HB3	2.15	0.46
2:J:3514:LEU:HD12	2:J:3606:LEU:HB2	1.96	0.46
2:J:4160:LEU:O	2:J:4164:LEU:HG	2.16	0.46
2:B:248:GLU:HA	2:B:372:LEU:CB	2.46	0.46
2:B:799:GLU:OE1	2:B:1623:ARG:NH1	2.48	0.46
2:B:996:TRP:HE1	2:B:1000:ARG:HD2	1.81	0.46
2:B:1745:ILE:HD11	2:B:1769:THR:HG23	1.97	0.46
2:B:1813:ARG:O	2:B:1817:GLU:HG2	2.15	0.46
2:B:1964:ARG:HB3	2:B:1968:LYS:NZ	2.30	0.46
2:B:2376:LEU:HD12	2:B:2376:LEU:H	1.79	0.46
2:B:2531:ARG:HH12	2:B:2585:THR:HB	1.79	0.46
2:B:2696:TYR:HE2	2:B:2997:PHE:HA	1.81	0.46
2:E:996:TRP:HE1	2:E:1000:ARG:HD2	1.81	0.46
2:E:2469:ILE:HA	2:E:2472:LEU:HG	1.97	0.46
2:G:863:LEU:HD13	2:G:867:LEU:HD11	1.98	0.46
2:G:3428:ASN:O	2:G:3432:GLU:HG2	2.16	0.46
2:G:3969:ILE:O	2:G:3970:GLN:C	2.54	0.46
2:J:20:VAL:HG12	2:J:22:LEU:H	1.80	0.46
2:J:659:TYR:HB2	2:J:1017:ARG:HH22	1.79	0.46
2:J:2799:GLU:O	2:J:2803:GLU:HG2	2.14	0.46
2:J:2881:ASN:HA	2:J:2884:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2958:GLY:O	2:J:2962:GLN:HG2	2.15	0.46
2:J:3366:ARG:NE	2:J:3367:LYS:HD2	2.26	0.46
2:J:3405:LEU:HD13	2:J:3451:PHE:HZ	1.81	0.46
3:K:38:ARG:HD3	3:K:48:VAL:HG22	1.98	0.46
2:B:19:GLU:HB3	2:B:205:ILE:HD13	1.98	0.46
2:B:20:VAL:HG12	2:B:22:LEU:H	1.80	0.46
2:B:316:PHE:HE2	2:B:348:VAL:HG22	1.81	0.46
2:B:478:PHE:HD2	2:B:483:MET:HG3	1.81	0.46
2:B:696:PRO:HG2	2:B:1612:PHE:HE2	1.81	0.46
2:B:820:ARG:HG2	2:B:820:ARG:HH11	1.81	0.46
2:B:1042:ALA:O	2:B:1046:LEU:HG	2.16	0.46
2:B:2152:THR:O	2:B:2156:LEU:HG	2.16	0.46
2:B:3346:VAL:HG21	2:B:3411:LEU:HB3	1.96	0.46
2:E:1260:MET:HB2	2:E:1269:CYS:SG	2.56	0.46
2:E:2599:GLN:O	2:E:2603:ILE:HG13	2.16	0.46
2:E:3277:LEU:HD13	2:E:3315:LEU:HD13	1.96	0.46
2:G:404:ILE:HG23	2:G:483:MET:SD	2.54	0.46
2:G:642:THR:HG21	2:G:1615:VAL:HG21	1.98	0.46
2:G:2104:ARG:O	2:G:2108:GLU:HG2	2.16	0.46
2:G:3757:GLU:O	2:G:3761:GLN:HG2	2.16	0.46
2:J:317:ARG:NH2	2:J:321:GLU:O	2.48	0.46
2:J:478:PHE:HD2	2:J:483:MET:HG3	1.81	0.46
2:J:1964:ARG:HB3	2:J:1968:LYS:NZ	2.30	0.46
2:J:3342:ALA:HA	2:J:3345:ILE:HG22	1.98	0.46
2:J:3548:GLU:HG2	2:J:3552:PHE:CE2	2.51	0.46
2:J:3757:GLU:O	2:J:3761:GLN:HG2	2.16	0.46
3:C:71:ARG:HB3	3:C:78:VAL:HG22	1.97	0.46
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.97	0.46
1:H:88:PRO:HB2	2:G:1680:ARG:HH12	1.81	0.46
2:B:863:LEU:HD13	2:B:867:LEU:HD11	1.98	0.46
2:B:1260:MET:HB2	2:B:1269:CYS:SG	2.56	0.46
2:E:2225:PHE:O	2:E:2229:VAL:HG23	2.15	0.46
2:E:2353:VAL:O	2:E:2357:LEU:HG	2.15	0.46
2:E:2696:TYR:HE2	2:E:2997:PHE:HA	1.81	0.46
2:E:2809:ILE:H	2:E:2809:ILE:HD12	1.80	0.46
2:E:2881:ASN:HA	2:E:2884:ASN:HD21	1.81	0.46
2:E:2958:GLY:O	2:E:2962:GLN:HG2	2.15	0.46
2:E:3405:LEU:HD13	2:E:3451:PHE:HZ	1.81	0.46
2:G:231:LEU:O	2:G:260:TRP:NE1	2.40	0.46
2:G:316:PHE:HE2	2:G:348:VAL:HG22	1.81	0.46
2:G:1498:GLY:HA2	2:G:1501:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3003:LEU:HB2	2:G:3004:PRO:HD3	1.97	0.46
2:G:3346:VAL:HG21	2:G:3411:LEU:HB3	1.96	0.46
2:J:960:MET:SD	2:J:960:MET:N	2.75	0.46
2:J:1745:ILE:HD11	2:J:1769:THR:HG23	1.97	0.46
2:J:1927:LEU:HD23	2:J:1939:MET:HE1	1.98	0.46
2:J:2809:ILE:H	2:J:2809:ILE:HD12	1.80	0.46
2:J:3173:TYR:CG	2:J:3243:ILE:HG12	2.51	0.46
2:J:3475:LYS:HZ1	2:J:3511:VAL:HG21	1.80	0.46
2:J:3639:THR:N	2:J:3640:PRO:HD2	2.31	0.46
2:B:3969:ILE:O	2:B:3970:GLN:C	2.55	0.46
2:B:4238:CYS:O	2:B:4242:ILE:HG13	2.16	0.46
2:E:231:LEU:O	2:E:260:TRP:NE1	2.40	0.46
2:E:3197:LEU:O	2:E:3201:MET:HB3	2.15	0.46
2:E:3342:ALA:HA	2:E:3345:ILE:HG22	1.98	0.46
2:E:4112:LEU:HD12	2:E:4112:LEU:HA	1.84	0.46
2:E:4181:ILE:HG22	2:E:4987:ASN:HB3	1.97	0.46
2:E:4856:PHE:O	2:E:4860:ARG:NH2	2.39	0.46
2:G:797:HIS:HA	2:G:1619:ARG:HH22	1.81	0.46
2:G:2607:LEU:HD23	2:G:2607:LEU:HA	1.83	0.46
2:G:3137:LEU:HB3	2:G:3138:PRO:HD3	1.98	0.46
2:G:3313:ASN:OD1	2:G:3353:LEU:HD11	2.14	0.46
2:G:3443:ILE:HG12	2:G:3605:HIS:CD2	2.49	0.46
2:J:2688:HIS:ND1	2:J:2688:HIS:N	2.63	0.46
2:J:3640:PRO:HG2	2:J:3643:ASN:HB2	1.96	0.46
2:J:4240:ASP:O	2:J:4244:GLU:HG3	2.16	0.46
3:M:71:ARG:HB3	3:M:78:VAL:HG22	1.96	0.46
2:B:1669:LEU:O	2:B:1673:VAL:HG22	2.16	0.45
2:B:2104:ARG:O	2:B:2108:GLU:HG2	2.16	0.45
2:B:3034:LYS:O	2:B:3038:MET:HG2	2.16	0.45
2:B:3342:ALA:HA	2:B:3345:ILE:HG22	1.98	0.45
2:B:3475:LYS:HZ1	2:B:3511:VAL:HG21	1.81	0.45
2:E:210:GLU:H	2:E:273:HIS:CE1	2.34	0.45
2:E:818:ARG:NH1	2:E:1027:LEU:O	2.44	0.45
2:E:863:LEU:HD13	2:E:867:LEU:HD11	1.98	0.45
2:E:1042:ALA:O	2:E:1046:LEU:HG	2.16	0.45
2:E:2592:GLY:O	2:E:2600:ARG:NH1	2.48	0.45
2:E:3003:LEU:HB2	2:E:3004:PRO:HD3	1.97	0.45
2:E:3969:ILE:O	2:E:3970:GLN:C	2.55	0.45
2:E:4240:ASP:O	2:E:4244:GLU:HG3	2.16	0.45
2:E:4735:GLU:O	2:E:4739:GLU:HG2	2.17	0.45
2:G:820:ARG:HG2	2:G:820:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:873:LYS:NZ	2:G:947:GLU:OE1	2.48	0.45
2:G:3276:MET:O	2:G:3280:TYR:HB2	2.16	0.45
2:G:3280:TYR:HE1	2:G:3284:TRP:CD1	2.33	0.45
2:G:3554:GLN:O	2:G:3557:LEU:HD23	2.16	0.45
2:G:3639:THR:N	2:G:3640:PRO:HD2	2.31	0.45
2:J:210:GLU:H	2:J:273:HIS:CE1	2.34	0.45
2:J:818:ARG:NH1	2:J:1027:LEU:O	2.44	0.45
2:J:1260:MET:HB2	2:J:1269:CYS:SG	2.56	0.45
2:J:3209:GLN:CD	2:J:3209:GLN:H	2.18	0.45
2:B:210:GLU:H	2:B:273:HIS:CE1	2.35	0.45
2:B:2240:CYS:SG	2:B:2250:MET:HG3	2.57	0.45
2:B:2294:ASP:O	2:B:2298:VAL:HG12	2.16	0.45
2:B:2463:LEU:HD11	2:B:2506:LEU:HD13	1.98	0.45
2:B:2469:ILE:HA	2:B:2472:LEU:HG	1.97	0.45
2:B:2502:MET:HB2	2:B:2502:MET:HE3	1.66	0.45
2:B:2809:ILE:H	2:B:2809:ILE:HD12	1.80	0.45
2:B:2881:ASN:HA	2:B:2884:ASN:HD21	1.81	0.45
2:B:4207:MET:CE	2:B:4208:PRO:HD2	2.46	0.45
2:B:4651:THR:HG21	2:B:4803:HIS:NE2	2.31	0.45
2:E:3157:ILE:HG22	2:E:3162:GLN:OE1	2.16	0.45
2:G:996:TRP:HE1	2:G:1000:ARG:HD2	1.81	0.45
2:G:1153:ILE:HG13	2:G:1160:ILE:HG12	1.97	0.45
2:G:2463:LEU:HD11	2:G:2506:LEU:HD13	1.98	0.45
2:G:2765:LYS:HA	2:G:2765:LYS:HD3	1.67	0.45
2:G:4064:MET:HE1	2:G:4110:PHE:CD2	2.51	0.45
2:G:4856:PHE:O	2:G:4860:ARG:NH2	2.39	0.45
2:J:863:LEU:HD13	2:J:867:LEU:HD11	1.98	0.45
2:J:2104:ARG:O	2:J:2108:GLU:HG2	2.16	0.45
2:J:2463:LEU:HD11	2:J:2506:LEU:HD13	1.98	0.45
2:J:3034:LYS:O	2:J:3038:MET:HG2	2.16	0.45
2:J:3157:ILE:HG22	2:J:3162:GLN:OE1	2.16	0.45
2:J:3244:PRO:HB2	2:J:3248:ARG:HB3	1.98	0.45
2:J:4090:LYS:HG3	2:J:4121:GLU:HB3	1.98	0.45
2:J:4204:GLN:O	2:J:4207:MET:HB2	2.16	0.45
1:H:29:MET:SD	1:H:33:GLY:HA2	2.57	0.45
2:B:292:ALA:HB2	2:B:312:THR:HG22	1.98	0.45
2:B:818:ARG:NH1	2:B:1027:LEU:O	2.44	0.45
2:B:4204:GLN:O	2:B:4207:MET:HB2	2.16	0.45
2:E:372:LEU:HG	2:E:374:LYS:NZ	2.32	0.45
2:E:1089:TYR:CD1	2:E:1152:MET:HG2	2.45	0.45
2:E:3475:LYS:HZ1	2:E:3511:VAL:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3757:GLU:O	2:E:3761:GLN:HG2	2.16	0.45
2:G:878:ILE:HG13	3:M:107:TRP:CZ2	2.50	0.45
2:G:3405:LEU:HD13	2:G:3451:PHE:HZ	1.81	0.45
2:G:3887:PHE:O	2:G:3891:LEU:HG	2.17	0.45
2:G:4238:CYS:O	2:G:4242:ILE:HG13	2.16	0.45
2:J:213:TYR:HA	2:J:340:LYS:HA	1.97	0.45
2:J:3107:VAL:HG12	2:J:3175:LEU:HD11	1.98	0.45
2:J:3140:LEU:HD12	2:J:3140:LEU:O	2.16	0.45
2:J:3887:PHE:O	2:J:3891:LEU:HG	2.17	0.45
3:C:9:GLY:HA3	3:C:123:VAL:HG22	1.99	0.45
1:D:57:LYS:HE2	1:D:57:LYS:HB2	1.75	0.45
2:B:2566:ALA:HA	2:B:2569:PHE:CD2	2.49	0.45
2:B:2599:GLN:O	2:B:2603:ILE:HG13	2.16	0.45
2:B:3137:LEU:HB3	2:B:3138:PRO:HD3	1.98	0.45
2:B:3548:GLU:HG2	2:B:3552:PHE:CE2	2.51	0.45
2:B:3554:GLN:O	2:B:3557:LEU:HD23	2.16	0.45
2:B:4696:ASP:O	2:B:4700:GLN:HG2	2.17	0.45
2:E:213:TYR:HA	2:E:340:LYS:HA	1.97	0.45
2:E:820:ARG:HH11	2:E:820:ARG:HG2	1.81	0.45
2:E:2463:LEU:HD11	2:E:2506:LEU:HD13	1.99	0.45
2:E:3034:LYS:O	2:E:3038:MET:HG2	2.16	0.45
2:E:3140:LEU:HD12	2:E:3140:LEU:O	2.16	0.45
2:E:3475:LYS:HD3	2:E:3516:LYS:HZ1	1.80	0.45
2:E:4064:MET:HE1	2:E:4110:PHE:HD2	1.81	0.45
2:E:4211:LYS:O	2:E:4215:ARG:HG3	2.15	0.45
2:G:3342:ALA:HA	2:G:3345:ILE:HG22	1.98	0.45
2:G:4204:GLN:O	2:G:4207:MET:HB2	2.16	0.45
2:G:4675:LYS:HG3	2:G:4715:TYR:HE1	1.81	0.45
2:J:2240:CYS:SG	2:J:2250:MET:HG3	2.57	0.45
2:J:2696:TYR:HE2	2:J:2997:PHE:HA	1.81	0.45
2:J:2782:ASP:N	2:J:2782:ASP:OD1	2.47	0.45
2:J:3276:MET:O	2:J:3280:TYR:HB2	2.16	0.45
2:J:3927:GLN:HB2	2:J:3992:PHE:CE2	2.52	0.45
1:D:29:MET:SD	1:D:33:GLY:HA2	2.57	0.45
1:I:29:MET:SD	1:I:33:GLY:HA2	2.57	0.45
2:B:863:LEU:HD13	2:B:867:LEU:HD21	1.97	0.45
2:B:1455:PRO:HG3	2:B:1549:PHE:HE1	1.82	0.45
2:B:2568:LEU:C	2:B:2568:LEU:HD23	2.37	0.45
2:B:3140:LEU:HD12	2:B:3140:LEU:O	2.16	0.45
2:B:3276:MET:O	2:B:3280:TYR:HB2	2.16	0.45
2:B:3757:GLU:O	2:B:3761:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4048:LEU:HD22	2:B:4055:VAL:HG21	1.99	0.45
2:B:4064:MET:HE1	2:B:4110:PHE:CD2	2.52	0.45
2:B:4090:LYS:HG3	2:B:4121:GLU:HB3	1.98	0.45
2:B:4735:GLU:O	2:B:4739:GLU:HG2	2.17	0.45
2:B:4744:ASP:HB3	2:B:4747:SER:HB3	1.99	0.45
2:E:3194:LEU:HD21	2:E:3272:ILE:HG23	1.98	0.45
2:E:3887:PHE:O	2:E:3891:LEU:HG	2.17	0.45
2:E:3927:GLN:HB2	2:E:3992:PHE:CE2	2.52	0.45
2:G:226:HIS:CD2	2:G:226:HIS:N	2.85	0.45
2:G:1260:MET:HB2	2:G:1269:CYS:SG	2.56	0.45
2:G:2515:GLN:CA	2:G:2568:LEU:HD11	2.46	0.45
2:J:292:ALA:HB2	2:J:312:THR:HG22	1.98	0.45
2:J:3104:GLU:HA	2:J:3107:VAL:HG22	1.98	0.45
2:J:4207:MET:CE	2:J:4208:PRO:HD2	2.46	0.45
2:J:4651:THR:HG21	2:J:4803:HIS:NE2	2.31	0.45
3:C:38:ARG:HD3	3:C:48:VAL:HG22	1.98	0.45
2:B:1179:PHE:HB2	2:B:1182:ILE:HD11	1.98	0.45
2:B:2102:VAL:HG13	2:B:2120:MET:HB2	1.97	0.45
2:B:3405:LEU:HG	2:B:3409:TYR:CE1	2.51	0.45
2:B:4232:GLU:HG2	2:B:5019:TRP:NE1	2.32	0.45
2:E:226:HIS:CD2	2:E:226:HIS:N	2.85	0.45
2:E:573:GLU:O	2:E:577:ILE:HG22	2.17	0.45
2:E:2240:CYS:SG	2:E:2250:MET:HG3	2.57	0.45
2:E:2688:HIS:ND1	2:E:2688:HIS:N	2.63	0.45
2:E:4207:MET:CE	2:E:4208:PRO:HD2	2.46	0.45
2:E:4720:VAL:O	2:E:4723:LYS:N	2.50	0.45
2:G:2102:VAL:HG13	2:G:2120:MET:HB2	1.97	0.45
2:G:2236:LEU:HD22	2:G:2250:MET:SD	2.57	0.45
2:G:2240:CYS:SG	2:G:2250:MET:HG3	2.57	0.45
2:G:2299:VAL:HG12	2:G:2360:LYS:HD2	1.99	0.45
2:G:2881:ASN:HA	2:G:2884:ASN:HD21	1.81	0.45
2:G:4207:MET:CE	2:G:4208:PRO:HD2	2.46	0.45
2:J:696:PRO:HG2	2:J:1612:PHE:HE2	1.81	0.45
2:J:2262:GLY:O	2:J:2266:GLY:N	2.47	0.45
2:J:4115:SER:HB2	2:J:4123:ILE:HG21	1.98	0.45
2:J:4238:CYS:O	2:J:4242:ILE:HG13	2.16	0.45
1:D:55:VAL:HA	2:E:1784:ALA:HA	1.99	0.45
2:B:873:LYS:NZ	2:B:947:GLU:OE1	2.49	0.45
2:B:1694:LEU:HD11	2:B:1718:ILE:HD11	1.99	0.45
2:B:3428:ASN:O	2:B:3432:GLU:HG2	2.16	0.45
2:B:3639:THR:N	2:B:3640:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4064:MET:HE1	2:B:4110:PHE:HD2	1.81	0.45
2:E:276:TRP:CE2	2:E:339:ILE:HG12	2.52	0.45
2:E:1455:PRO:HG3	2:E:1549:PHE:HE1	1.82	0.45
2:E:4048:LEU:HD22	2:E:4055:VAL:HG21	1.99	0.45
2:E:4064:MET:HE1	2:E:4110:PHE:CD2	2.52	0.45
2:E:4232:GLU:HG2	2:E:5019:TRP:NE1	2.32	0.45
2:E:4238:CYS:O	2:E:4242:ILE:HG13	2.16	0.45
2:G:993:HIS:HE1	2:G:1027:LEU:HD11	1.78	0.45
2:G:1455:PRO:HG3	2:G:1549:PHE:HE1	1.82	0.45
2:G:2503:VAL:HG21	2:G:2526:PHE:HZ	1.82	0.45
2:G:2867:LEU:HB2	2:G:2928:LYS:HZ3	1.82	0.45
2:G:3034:LYS:O	2:G:3038:MET:HG2	2.16	0.45
2:G:3107:VAL:HG12	2:G:3175:LEU:HD11	1.98	0.45
2:G:3316:LEU:HD11	2:G:3345:ILE:HG23	1.99	0.45
2:J:276:TRP:CE2	2:J:339:ILE:HG12	2.52	0.45
2:J:316:PHE:HE2	2:J:348:VAL:HG22	1.81	0.45
2:J:797:HIS:HA	2:J:1619:ARG:HH22	1.81	0.45
2:J:3405:LEU:HG	2:J:3409:TYR:CE1	2.51	0.45
2:J:4064:MET:HE1	2:J:4110:PHE:CD2	2.52	0.45
3:C:68:THR:OG1	3:C:81:GLN:HB3	2.17	0.45
2:B:1214:PHE:CZ	2:B:1225:PRO:HD3	2.52	0.45
2:B:1498:GLY:HA2	2:B:1501:VAL:HG12	1.98	0.45
2:B:2619:LEU:O	2:B:2623:LEU:HG	2.17	0.45
2:B:2725:LYS:NZ	2:B:2736:ASP:O	2.50	0.45
2:E:2012:PHE:CZ	2:E:2031:LEU:HD23	2.52	0.45
2:E:2691:TYR:CD2	2:E:2996:LYS:HD2	2.52	0.45
2:E:3104:GLU:HA	2:E:3107:VAL:HG22	1.98	0.45
2:E:3137:LEU:HB3	2:E:3138:PRO:HD3	1.98	0.45
2:E:3280:TYR:HE1	2:E:3284:TRP:CD1	2.33	0.45
2:E:3639:THR:N	2:E:3640:PRO:HD2	2.31	0.45
2:E:4696:ASP:O	2:E:4700:GLN:HG2	2.17	0.45
2:G:210:GLU:H	2:G:273:HIS:CE1	2.35	0.45
2:G:246:TYR:CD1	2:G:373:LYS:HB3	2.51	0.45
2:G:484:LEU:HD11	2:G:540:PHE:HE1	1.82	0.45
2:G:551:LEU:HD23	2:G:560:ILE:HG13	1.99	0.45
2:G:1179:PHE:HB2	2:G:1182:ILE:HD11	1.99	0.45
2:G:2575:ARG:HH11	2:G:2577:ILE:HG23	1.82	0.45
2:G:4696:ASP:O	2:G:4700:GLN:HG2	2.17	0.45
2:J:484:LEU:HD11	2:J:540:PHE:HE1	1.82	0.45
2:J:551:LEU:HD23	2:J:560:ILE:HG13	1.99	0.45
2:J:1435:TYR:CZ	2:J:1550:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1575:LEU:HD23	2:J:1575:LEU:HA	1.82	0.45
2:J:2157:GLU:O	2:J:2161:GLN:HG3	2.17	0.45
2:J:2299:VAL:HG12	2:J:2360:LYS:HD2	1.98	0.45
2:J:2599:GLN:O	2:J:2603:ILE:HG13	2.16	0.45
2:J:3377:GLU:HA	2:J:3380:ARG:HG2	1.99	0.45
3:K:68:THR:OG1	3:K:81:GLN:HB3	2.17	0.45
1:A:29:MET:SD	1:A:33:GLY:HA2	2.57	0.45
2:B:35:LEU:HG	2:B:51:PRO:HA	1.98	0.45
2:B:1930:LYS:HD2	2:B:1931:LEU:N	2.32	0.45
2:B:2654:TYR:HB2	2:B:2661:TRP:HE3	1.82	0.45
2:B:2691:TYR:CD2	2:B:2996:LYS:HD2	2.52	0.45
2:E:478:PHE:HD2	2:E:483:MET:HG3	1.81	0.45
2:E:2236:LEU:HD22	2:E:2250:MET:SD	2.57	0.45
2:E:3276:MET:O	2:E:3280:TYR:HB2	2.16	0.45
2:E:3428:ASN:O	2:E:3432:GLU:HG2	2.16	0.45
2:E:4090:LYS:HG3	2:E:4121:GLU:HB3	1.98	0.45
2:E:4115:SER:HB2	2:E:4123:ILE:HG21	1.98	0.45
2:E:4651:THR:HG21	2:E:4803:HIS:NE2	2.31	0.45
2:E:4671:PHE:HD1	2:E:4714:ASN:O	2.00	0.45
2:E:4744:ASP:HB3	2:E:4747:SER:HB3	1.99	0.45
2:E:4959:PHE:CD1	2:E:4985:LEU:HD11	2.52	0.45
2:G:374:LYS:O	2:G:375:LYS:C	2.53	0.45
2:G:489:ASN:OD1	2:G:493:ARG:NH1	2.50	0.45
2:G:2157:GLU:O	2:G:2161:GLN:HG3	2.17	0.45
2:G:3024:VAL:HG13	2:G:3029:GLY:HA2	1.99	0.45
2:G:3377:GLU:HA	2:G:3380:ARG:HG2	1.99	0.45
2:G:3405:LEU:HG	2:G:3409:TYR:CE1	2.52	0.45
2:G:3754:GLU:HG3	2:G:4719:PHE:CZ	2.52	0.45
2:J:35:LEU:HG	2:J:51:PRO:HA	1.98	0.45
2:J:993:HIS:HE1	2:J:1027:LEU:HD11	1.79	0.45
2:J:996:TRP:HE1	2:J:1000:ARG:HD2	1.81	0.45
2:J:1455:PRO:HG3	2:J:1549:PHE:HE1	1.82	0.45
2:J:2102:VAL:HG13	2:J:2120:MET:HB2	1.97	0.45
2:J:3137:LEU:HB3	2:J:3138:PRO:HD3	1.98	0.45
2:J:3194:LEU:HD21	2:J:3272:ILE:HG23	1.98	0.45
3:M:38:ARG:HD3	3:M:48:VAL:HG22	1.98	0.45
2:B:184:THR:HG22	2:B:189:LEU:HD13	1.99	0.45
2:B:797:HIS:HA	2:B:1619:ARG:HH22	1.82	0.45
2:B:876:GLU:HA	2:B:876:GLU:OE1	2.17	0.45
2:B:2688:HIS:ND1	2:B:2688:HIS:N	2.63	0.45
2:B:2960:LEU:HD13	2:B:3038:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:GLU:HB3	2:E:205:ILE:HD13	1.98	0.45
2:E:1694:LEU:HD11	2:E:1718:ILE:HD11	1.99	0.45
2:E:2328:GLY:HA2	2:E:2331:TYR:HD2	1.81	0.45
2:E:3965:LEU:HA	2:E:3968:TYR:CD2	2.52	0.45
2:G:276:TRP:CE2	2:G:339:ILE:HG12	2.51	0.45
2:G:2691:TYR:CD2	2:G:2996:LYS:HD2	2.52	0.45
2:G:2696:TYR:HE2	2:G:2997:PHE:HA	1.81	0.45
2:G:4090:LYS:HG3	2:G:4121:GLU:HB3	1.98	0.45
2:G:4651:THR:HG21	2:G:4803:HIS:NE2	2.31	0.45
2:J:573:GLU:O	2:J:577:ILE:HG22	2.17	0.45
2:J:820:ARG:HG2	2:J:820:ARG:HH11	1.81	0.45
2:J:1214:PHE:CZ	2:J:1225:PRO:HD3	2.52	0.45
2:J:2549:ALA:HA	2:J:2552:ARG:NH1	2.32	0.45
2:J:2672:LEU:HD12	2:J:2672:LEU:HA	1.81	0.45
2:J:2725:LYS:NZ	2:J:2736:ASP:O	2.50	0.45
2:J:2924:GLN:O	2:J:2928:LYS:HG2	2.17	0.45
2:J:3024:VAL:HG13	2:J:3029:GLY:HA2	1.99	0.45
2:J:3316:LEU:HD11	2:J:3345:ILE:HG23	1.99	0.45
2:J:3554:GLN:O	2:J:3557:LEU:HD23	2.16	0.45
3:C:69:ILE:HB	3:C:80:LEU:HD13	1.99	0.45
3:F:38:ARG:HD3	3:F:48:VAL:HG22	1.98	0.45
1:H:5:GLU:HB2	1:H:73:LYS:HE2	1.99	0.44
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.99	0.44
2:E:489:ASN:OD1	2:E:493:ARG:NH1	2.50	0.44
2:E:797:HIS:HA	2:E:1619:ARG:HH22	1.81	0.44
2:E:876:GLU:OE1	2:E:876:GLU:HA	2.17	0.44
2:E:2570:ALA:HA	2:E:2613:TYR:O	2.17	0.44
2:E:2725:LYS:NZ	2:E:2736:ASP:O	2.50	0.44
2:E:3377:GLU:HA	2:E:3380:ARG:HG2	1.99	0.44
2:E:4021:LYS:O	2:E:4025:VAL:HG23	2.17	0.44
2:E:4679:ARG:NH1	2:E:4715:TYR:OH	2.50	0.44
2:G:127:MET:SD	2:G:127:MET:N	2.73	0.44
2:G:292:ALA:HB2	2:G:312:THR:HG22	1.98	0.44
2:G:1214:PHE:CZ	2:G:1225:PRO:HD3	2.52	0.44
2:G:3104:GLU:HA	2:G:3107:VAL:HG22	1.98	0.44
2:G:3140:LEU:HD12	2:G:3140:LEU:O	2.16	0.44
2:G:3865:VAL:HG22	2:G:3867:ASN:H	1.81	0.44
2:G:4048:LEU:HD22	2:G:4055:VAL:HG21	1.99	0.44
2:J:1498:GLY:HA2	2:J:1501:VAL:HG12	1.98	0.44
2:J:2880:GLU:HB2	2:J:2908:TYR:CD2	2.52	0.44
3:F:68:THR:OG1	3:F:81:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:GLY:HA3	3:M:123:VAL:HG22	1.99	0.44
1:A:24:VAL:HG12	1:A:102:GLU:O	2.17	0.44
2:B:489:ASN:OD1	2:B:493:ARG:NH1	2.50	0.44
2:B:2012:PHE:CZ	2:B:2031:LEU:HD23	2.52	0.44
2:B:2604:GLU:HG2	2:B:2639:MET:HG3	2.00	0.44
2:B:3107:VAL:HG12	2:B:3175:LEU:HD11	1.98	0.44
2:B:3194:LEU:HD21	2:B:3272:ILE:HG23	1.98	0.44
2:E:525:LEU:O	2:E:529:LEU:HG	2.17	0.44
2:E:1018:ASN:OD1	2:E:1021:LEU:N	2.51	0.44
2:E:1435:TYR:CZ	2:E:1550:PRO:HB3	2.52	0.44
2:E:1930:LYS:HD2	2:E:1931:LEU:N	2.32	0.44
2:E:2549:ALA:HA	2:E:2552:ARG:NH1	2.32	0.44
2:E:2654:TYR:HB2	2:E:2661:TRP:HE3	1.82	0.44
2:E:2924:GLN:O	2:E:2928:LYS:HG2	2.17	0.44
2:E:3397:GLU:O	2:E:3400:VAL:HG12	2.18	0.44
2:E:3405:LEU:HG	2:E:3409:TYR:CE1	2.51	0.44
2:G:35:LEU:HG	2:G:51:PRO:HA	1.98	0.44
2:G:2262:GLY:O	2:G:2266:GLY:N	2.47	0.44
2:G:2858:GLN:HB2	2:G:2859:PRO:HD3	2.00	0.44
2:G:3157:ILE:HG22	2:G:3162:GLN:OE1	2.17	0.44
2:G:3548:GLU:HG2	2:G:3552:PHE:CE2	2.51	0.44
2:G:5017:ARG:NH1	2:G:5019:TRP:HZ2	2.15	0.44
2:J:1694:LEU:HD11	2:J:1718:ILE:HD11	1.99	0.44
2:J:4232:GLU:HG2	2:J:5019:TRP:NE1	2.32	0.44
3:K:69:ILE:HB	3:K:80:LEU:HD13	1.99	0.44
2:B:276:TRP:CE2	2:B:339:ILE:HG12	2.52	0.44
2:B:551:LEU:HD23	2:B:560:ILE:HG13	1.99	0.44
2:B:3887:PHE:O	2:B:3891:LEU:HG	2.17	0.44
2:E:2880:GLU:HB2	2:E:2908:TYR:CD2	2.53	0.44
2:G:696:PRO:HG2	2:G:1612:PHE:HE2	1.81	0.44
2:G:1694:LEU:HD11	2:G:1718:ILE:HD11	1.99	0.44
2:G:1930:LYS:HD2	2:G:1931:LEU:N	2.32	0.44
2:G:2138:LEU:HD12	2:G:3658:LYS:HG3	1.99	0.44
2:G:3567:PRO:O	2:G:3570:ARG:HB3	2.17	0.44
2:G:3731:LYS:NZ	2:G:3735:LEU:HD21	2.32	0.44
2:G:4115:SER:HB2	2:G:4123:ILE:HG21	1.98	0.44
2:J:3051:ARG:HH22	2:J:3102:ASP:HB2	1.83	0.44
3:M:68:THR:OG1	3:M:81:GLN:HB3	2.17	0.44
2:B:3024:VAL:HG13	2:B:3029:GLY:HA2	1.99	0.44
2:B:3377:GLU:HA	2:B:3380:ARG:HG2	1.99	0.44
2:B:3405:LEU:HD13	2:B:3451:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3836:MET:HE1	2:B:3915:ILE:HG23	1.99	0.44
2:B:3927:GLN:HB2	2:B:3992:PHE:CE2	2.52	0.44
2:B:4115:SER:HB2	2:B:4123:ILE:HG21	1.98	0.44
2:B:4652:LEU:O	2:B:4656:LEU:HG	2.18	0.44
2:E:696:PRO:HG2	2:E:1612:PHE:HE2	1.81	0.44
2:E:2157:GLU:O	2:E:2161:GLN:HG3	2.17	0.44
2:E:2960:LEU:HD13	2:E:3038:MET:HG3	2.00	0.44
2:G:184:THR:HG22	2:G:189:LEU:HD13	1.99	0.44
2:G:3194:LEU:HD21	2:G:3272:ILE:HG23	1.98	0.44
2:G:3366:ARG:NE	2:G:3367:LYS:HD2	2.26	0.44
2:G:3927:GLN:HB2	2:G:3992:PHE:CE2	2.52	0.44
2:G:5012:LYS:HE2	2:G:5016:GLU:OE2	2.16	0.44
2:J:525:LEU:O	2:J:529:LEU:HG	2.17	0.44
2:J:3971:GLY:O	2:J:3972:PRO:C	2.56	0.44
2:J:4696:ASP:O	2:J:4700:GLN:HG2	2.16	0.44
1:H:98:ILE:HD12	1:H:98:ILE:N	2.33	0.44
2:B:573:GLU:O	2:B:577:ILE:HG22	2.17	0.44
2:B:2503:VAL:HG21	2:B:2526:PHE:HZ	1.82	0.44
2:B:2718:SER:OG	2:B:2909:ASP:O	2.25	0.44
2:B:3157:ILE:HG22	2:B:3162:GLN:OE1	2.17	0.44
2:B:4021:LYS:O	2:B:4025:VAL:HG23	2.18	0.44
2:B:4959:PHE:CD1	2:B:4985:LEU:HD11	2.52	0.44
2:E:292:ALA:HB2	2:E:312:THR:HG22	1.98	0.44
2:E:316:PHE:HE2	2:E:348:VAL:HG22	1.81	0.44
2:E:2672:LEU:HD12	2:E:2672:LEU:HA	1.81	0.44
2:E:3107:VAL:HG12	2:E:3175:LEU:HD11	1.98	0.44
2:E:3874:VAL:HG21	2:E:3950:ASN:ND2	2.33	0.44
2:E:4021:LYS:HD3	2:E:4138:ASP:HB3	2.00	0.44
2:E:4911:LEU:HD23	2:E:4911:LEU:HA	1.85	0.44
2:G:573:GLU:O	2:G:577:ILE:HG22	2.17	0.44
2:G:876:GLU:OE1	2:G:876:GLU:HA	2.17	0.44
2:G:972:LEU:HB2	2:G:1044:ARG:HE	1.83	0.44
2:G:2012:PHE:CZ	2:G:2031:LEU:HD23	2.52	0.44
2:G:4021:LYS:O	2:G:4025:VAL:HG23	2.18	0.44
2:J:2330:ARG:HE	2:J:2330:ARG:HB2	1.68	0.44
2:J:2503:VAL:HG21	2:J:2526:PHE:HZ	1.82	0.44
2:J:3014:CYS:SG	2:J:3074:SER:HB3	2.58	0.44
2:J:3537:LYS:HE2	2:J:3537:LYS:HB3	1.85	0.44
2:J:3731:LYS:NZ	2:J:3735:LEU:HD21	2.32	0.44
2:J:3754:GLU:HG3	2:J:4719:PHE:CZ	2.53	0.44
2:J:4735:GLU:O	2:J:4739:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4959:PHE:CD1	2:J:4985:LEU:HD11	2.52	0.44
1:A:26:TYR:CB	1:A:101:VAL:HG12	2.46	0.44
1:I:98:ILE:N	1:I:98:ILE:HD12	2.32	0.44
2:B:2236:LEU:HD22	2:B:2250:MET:SD	2.57	0.44
2:B:2768:PHE:O	2:B:2772:GLN:HG2	2.18	0.44
2:B:3397:GLU:O	2:B:3400:VAL:HG12	2.18	0.44
2:E:1214:PHE:CZ	2:E:1225:PRO:HD3	2.52	0.44
2:E:2138:LEU:HD12	2:E:3658:LYS:HG3	1.99	0.44
2:E:2449:GLU:O	2:E:2453:ILE:HG12	2.17	0.44
2:G:525:LEU:O	2:G:529:LEU:HG	2.17	0.44
2:G:887:ILE:HD13	2:G:959:TYR:HB3	2.00	0.44
2:G:2359:ARG:HD3	2:G:2359:ARG:HA	1.82	0.44
2:G:2967:MET:CE	2:G:3045:LYS:HB3	2.48	0.44
2:G:3051:ARG:HH22	2:G:3102:ASP:HB2	1.83	0.44
2:J:135:VAL:HG21	2:J:191:VAL:HG22	2.00	0.44
2:J:371:VAL:HG12	2:J:373:LYS:HG2	1.98	0.44
2:J:371:VAL:CG1	2:J:373:LYS:HG2	2.47	0.44
2:J:882:TRP:CD2	3:K:106:PRO:HG3	2.52	0.44
2:J:2012:PHE:CZ	2:J:2031:LEU:HD23	2.52	0.44
2:J:2236:LEU:HD22	2:J:2250:MET:SD	2.57	0.44
2:J:2967:MET:CE	2:J:3045:LYS:HB3	2.48	0.44
2:J:3244:PRO:HG2	2:J:3249:LEU:HD23	1.98	0.44
2:J:3644:LEU:HD12	2:J:3645:PRO:HD2	1.99	0.44
2:J:4048:LEU:HD22	2:J:4055:VAL:HG21	1.99	0.44
2:J:4698:LYS:HE3	2:J:4698:LYS:HB2	1.84	0.44
2:J:4744:ASP:HB3	2:J:4747:SER:HB3	1.99	0.44
1:D:66:MET:HE2	1:D:66:MET:HB3	1.71	0.44
2:B:474:ARG:O	2:B:478:PHE:HD1	2.01	0.44
2:B:920:TYR:HE1	3:C:99:ARG:HE	1.65	0.44
2:B:2575:ARG:O	2:B:2579:VAL:HG23	2.17	0.44
2:B:2880:GLU:HB2	2:B:2908:TYR:CD2	2.53	0.44
2:B:3092:LEU:O	2:B:3095:PHE:HB3	2.18	0.44
2:B:3731:LYS:NZ	2:B:3735:LEU:HD21	2.32	0.44
2:E:35:LEU:HG	2:E:51:PRO:HA	1.98	0.44
2:E:2563:THR:HG22	2:E:2606:CYS:HA	2.00	0.44
2:E:3014:CYS:SG	2:E:3074:SER:HB3	2.58	0.44
2:G:2880:GLU:HB2	2:G:2908:TYR:CD2	2.53	0.44
2:G:3014:CYS:SG	2:G:3074:SER:HB3	2.58	0.44
2:G:3246:LEU:HD13	2:G:3280:TYR:CD2	2.53	0.44
2:J:882:TRP:CZ2	3:K:104:TYR:HB2	2.53	0.44
2:J:3284:TRP:CZ3	2:J:3287:ARG:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3874:VAL:HG21	2:J:3950:ASN:ND2	2.33	0.44
3:F:9:GLY:HA3	3:F:123:VAL:HG22	1.99	0.44
2:B:1018:ASN:OD1	2:B:1021:LEU:N	2.51	0.44
2:B:2157:GLU:O	2:B:2161:GLN:HG3	2.17	0.44
2:B:2788:HIS:NE2	2:B:2805:TYR:OH	2.38	0.44
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.99	0.44
2:E:2503:VAL:HG21	2:E:2526:PHE:HZ	1.82	0.44
2:E:2518:LEU:HD21	2:E:2569:PHE:CZ	2.52	0.44
2:E:2967:MET:CE	2:E:3045:LYS:HB3	2.48	0.44
2:G:2688:HIS:ND1	2:G:2688:HIS:N	2.63	0.44
2:G:2768:PHE:O	2:G:2772:GLN:HG2	2.18	0.44
2:G:2960:LEU:HD13	2:G:3038:MET:HG3	2.00	0.44
2:G:3284:TRP:CZ3	2:G:3287:ARG:HD3	2.53	0.44
2:G:4652:LEU:O	2:G:4656:LEU:HG	2.18	0.44
2:G:4735:GLU:O	2:G:4739:GLU:HG2	2.17	0.44
2:G:4817:ALA:HA	2:G:4823:LEU:HB3	2.00	0.44
2:J:19:GLU:HB3	2:J:205:ILE:HD13	1.98	0.44
2:J:489:ASN:OD1	2:J:493:ARG:NH1	2.50	0.44
2:J:873:LYS:NZ	2:J:947:GLU:OE1	2.48	0.44
2:J:2691:TYR:CD2	2:J:2996:LYS:HD2	2.52	0.44
2:J:3475:LYS:HD3	2:J:3516:LYS:HZ1	1.81	0.44
2:J:4652:LEU:O	2:J:4656:LEU:HG	2.18	0.44
1:H:56:ILE:HG13	1:H:59:PHE:HB2	2.00	0.44
1:I:56:ILE:HG13	1:I:59:PHE:HB2	2.00	0.44
2:B:226:HIS:CD2	2:B:226:HIS:N	2.85	0.44
2:B:2777:TYR:HB2	2:B:2791:LEU:O	2.18	0.44
2:B:2924:GLN:O	2:B:2928:LYS:HG2	2.17	0.44
2:B:3874:VAL:HG21	2:B:3950:ASN:ND2	2.33	0.44
2:B:3996:PHE:HZ	2:B:4019:LEU:HG	1.83	0.44
2:E:2607:LEU:HD23	2:E:2607:LEU:HA	1.83	0.44
2:E:2768:PHE:O	2:E:2772:GLN:HG2	2.18	0.44
2:E:3098:SER:O	2:E:3101:GLU:HG3	2.18	0.44
2:G:135:VAL:HG21	2:G:191:VAL:HG22	2.00	0.44
2:G:1435:TYR:CZ	2:G:1550:PRO:HB3	2.52	0.44
2:G:4671:PHE:HD1	2:G:4714:ASN:O	2.01	0.44
2:J:1433:TYR:CE1	2:J:1578:ALA:HB2	2.53	0.44
2:J:2960:LEU:HD13	2:J:3038:MET:HG3	1.99	0.44
2:J:4021:LYS:O	2:J:4025:VAL:HG23	2.18	0.44
2:J:4069:LYS:NZ	2:J:4130:ASN:OD1	2.37	0.44
2:B:2858:GLN:HB2	2:B:2859:PRO:HD3	2.00	0.43
2:B:3567:PRO:O	2:B:3570:ARG:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD23	2:E:560:ILE:HG13	1.99	0.43
2:E:1179:PHE:HB2	2:E:1182:ILE:HD11	1.99	0.43
2:E:1433:TYR:CE1	2:E:1578:ALA:HB2	2.53	0.43
2:E:1498:GLY:HA2	2:E:1501:VAL:HG12	1.98	0.43
2:G:1121:ALA:HB1	2:G:1123:VAL:HG13	2.01	0.43
2:G:3996:PHE:HZ	2:G:4019:LEU:HG	1.83	0.43
2:G:4744:ASP:HB3	2:G:4747:SER:HB3	1.98	0.43
2:G:4959:PHE:CD1	2:G:4985:LEU:HD11	2.52	0.43
2:J:1815:LEU:HD22	2:J:1845:VAL:HG21	1.99	0.43
2:J:1930:LYS:HD2	2:J:1931:LEU:N	2.32	0.43
2:J:2684:ASP:OD1	2:J:2685:SER:N	2.51	0.43
2:J:2858:GLN:HB2	2:J:2859:PRO:HD3	2.00	0.43
2:J:3567:PRO:O	2:J:3570:ARG:HB3	2.17	0.43
3:K:32:ASN:ND2	3:K:101:PRO:HB3	2.33	0.43
3:M:69:ILE:HB	3:M:80:LEU:HD13	1.99	0.43
1:D:56:ILE:HG13	1:D:59:PHE:HB2	2.00	0.43
2:B:887:ILE:HD13	2:B:959:TYR:HB3	2.00	0.43
2:B:2262:GLY:O	2:B:2266:GLY:N	2.47	0.43
2:B:2967:MET:CE	2:B:3045:LYS:HB3	2.48	0.43
2:B:3014:CYS:SG	2:B:3074:SER:HB3	2.58	0.43
2:B:3414:ARG:NH2	2:B:3474:SER:O	2.51	0.43
2:E:3458:PHE:CE2	2:E:3464:ILE:HG13	2.54	0.43
2:E:3554:GLN:O	2:E:3557:LEU:HD23	2.16	0.43
2:E:4642:ALA:O	2:E:4646:LEU:HD23	2.18	0.43
2:G:663:TYR:CE1	2:G:745:SER:HB3	2.53	0.43
2:G:1000:ARG:NH2	2:G:1003:GLN:HG3	2.34	0.43
2:G:2563:THR:HG22	2:G:2606:CYS:HA	2.00	0.43
2:G:2725:LYS:NZ	2:G:2736:ASP:O	2.50	0.43
2:G:2870[B]:GLU:CD	2:G:2870[B]:GLU:H	2.22	0.43
2:G:3092:LEU:O	2:G:3095:PHE:HB3	2.18	0.43
2:G:4698:LYS:HE3	2:G:4698:LYS:HB2	1.84	0.43
2:J:201:ASN:ND2	2:J:203:ASN:HD21	2.17	0.43
2:J:3594:ARG:NH1	2:J:3597:GLN:OE1	2.34	0.43
2:B:1426:ILE:O	2:B:1430:THR:HB	2.18	0.43
2:B:2138:LEU:HD12	2:B:3658:LYS:HG3	1.99	0.43
2:B:3458:PHE:CE2	2:B:3464:ILE:HG13	2.54	0.43
2:E:201:ASN:ND2	2:E:203:ASN:HD21	2.17	0.43
2:E:972:LEU:HB2	2:E:1044:ARG:HE	1.83	0.43
2:E:1738:LEU:HB2	2:E:2146:PRO:HD3	2.00	0.43
2:E:2604:GLU:HG2	2:E:2639:MET:HG3	2.00	0.43
2:E:2777:TYR:HB2	2:E:2791:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3024:VAL:HG13	2:E:3029:GLY:HA2	1.99	0.43
2:E:3284:TRP:CZ3	2:E:3287:ARG:HD3	2.53	0.43
2:E:3644:LEU:HD12	2:E:3645:PRO:HD2	1.99	0.43
2:E:3731:LYS:NZ	2:E:3735:LEU:HD21	2.32	0.43
2:G:882:TRP:CD2	3:M:106:PRO:HG3	2.53	0.43
2:G:882:TRP:O	2:G:885:THR:OG1	2.28	0.43
2:G:2654:TYR:HB2	2:G:2661:TRP:HE3	1.82	0.43
2:G:2768:PHE:HA	2:G:2771:ILE:HG22	2.00	0.43
2:G:3414:ARG:NH2	2:G:3474:SER:O	2.51	0.43
2:G:3874:VAL:HG21	2:G:3950:ASN:ND2	2.33	0.43
2:J:876:GLU:HA	2:J:876:GLU:OE1	2.17	0.43
2:J:1581:LEU:HD12	2:J:1584:ARG:HE	1.84	0.43
2:J:2449:GLU:O	2:J:2453:ILE:HG12	2.17	0.43
2:J:3996:PHE:HZ	2:J:4019:LEU:HG	1.83	0.43
3:C:32:ASN:OD1	3:C:33:SER:N	2.51	0.43
3:M:32:ASN:ND2	3:M:101:PRO:HB3	2.33	0.43
1:I:5:GLU:HB2	1:I:73:LYS:HE2	2.01	0.43
2:B:1000:ARG:NH2	2:B:1003:GLN:HG3	2.33	0.43
2:B:2449:GLU:O	2:B:2453:ILE:HG12	2.17	0.43
2:B:2878:LEU:HG	2:B:2882:TYR:CZ	2.53	0.43
2:B:3098:SER:O	2:B:3101:GLU:HG3	2.18	0.43
2:B:3284:TRP:CZ3	2:B:3287:ARG:HD3	2.53	0.43
2:B:3644:LEU:HD12	2:B:3645:PRO:HD2	1.99	0.43
2:B:4677:LEU:HD23	2:B:4711:PHE:HE1	1.84	0.43
2:E:2684:ASP:OD1	2:E:2685:SER:N	2.51	0.43
2:E:3567:PRO:O	2:E:3570:ARG:HB3	2.17	0.43
2:G:144:GLU:HG3	2:G:175:SER:HB2	2.01	0.43
2:G:1426:ILE:O	2:G:1430:THR:HB	2.18	0.43
2:G:2449:GLU:O	2:G:2453:ILE:HG12	2.17	0.43
2:G:2573:GLU:HB2	2:G:2615:ARG:HH21	1.82	0.43
2:G:2777:TYR:HB2	2:G:2791:LEU:O	2.18	0.43
2:G:2924:GLN:O	2:G:2928:LYS:HG2	2.17	0.43
2:G:2971:GLN:HA	2:G:2974:ILE:HG12	2.00	0.43
2:G:3644:LEU:HD12	2:G:3645:PRO:HD2	1.99	0.43
2:J:663:TYR:CE1	2:J:745:SER:HB3	2.53	0.43
2:J:1000:ARG:NH2	2:J:1003:GLN:HG3	2.33	0.43
2:J:3397:GLU:O	2:J:3400:VAL:HG12	2.18	0.43
2:J:3414:ARG:NH2	2:J:3474:SER:O	2.51	0.43
2:J:4021:LYS:HD3	2:J:4138:ASP:HB3	2.00	0.43
3:F:62:SER:O	3:F:62:SER:OG	2.24	0.43
3:F:69:ILE:HB	3:F:80:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:85:LEU:HD23	3:K:85:LEU:HA	1.92	0.43
2:B:135:VAL:HG21	2:B:191:VAL:HG22	2.00	0.43
2:B:484:LEU:HD11	2:B:540:PHE:HE1	1.82	0.43
2:B:1097:THR:HG23	2:B:1143:TRP:CD1	2.54	0.43
2:B:1435:TYR:CZ	2:B:1550:PRO:HB3	2.52	0.43
2:B:2299:VAL:HG12	2:B:2360:LYS:HD2	1.98	0.43
2:B:2318:TYR:HA	2:B:2395:PRO:HA	2.01	0.43
2:B:2549:ALA:HA	2:B:2552:ARG:NH1	2.33	0.43
2:B:2575:ARG:HG3	2:B:2578:MET:HG3	2.00	0.43
2:B:2870[B]:GLU:H	2:B:2870[B]:GLU:CD	2.22	0.43
2:B:3222:LYS:HB3	2:B:3226:GLU:HB3	2.00	0.43
2:B:4911:LEU:HD23	2:B:4911:LEU:HA	1.85	0.43
2:E:184:THR:HG22	2:E:189:LEU:HD13	1.99	0.43
2:E:663:TYR:CE1	2:E:745:SER:HB3	2.53	0.43
2:E:1012:ASP:HB3	2:E:1015:ALA:HB3	2.00	0.43
2:E:1575:LEU:HD23	2:E:1575:LEU:HA	1.82	0.43
2:E:2299:VAL:HG12	2:E:2360:LYS:HD2	1.99	0.43
2:E:3051:ARG:HH22	2:E:3102:ASP:HB2	1.83	0.43
2:G:232:THR:HG21	2:G:252:VAL:HG11	2.01	0.43
2:G:1433:TYR:CE1	2:G:1578:ALA:HB2	2.53	0.43
2:G:2604:GLU:HG2	2:G:2639:MET:HG3	2.00	0.43
2:G:2635:GLU:HG3	2:G:2636:PHE:HD2	1.83	0.43
2:G:4642:ALA:O	2:G:4646:LEU:HD23	2.18	0.43
2:J:232:THR:HG21	2:J:252:VAL:HG11	2.01	0.43
2:J:1012:ASP:HB3	2:J:1015:ALA:HB3	2.00	0.43
2:J:1179:PHE:HB2	2:J:1182:ILE:HD11	1.98	0.43
2:J:2318:TYR:HA	2:J:2395:PRO:HA	2.01	0.43
2:J:2768:PHE:O	2:J:2772:GLN:HG2	2.18	0.43
2:J:4112:LEU:HD12	2:J:4112:LEU:HA	1.84	0.43
3:C:64:LYS:N	3:C:64:LYS:HD2	2.33	0.43
3:K:9:GLY:HA3	3:K:123:VAL:HG22	1.99	0.43
3:M:46:GLU:HG3	3:M:62:SER:HB2	2.00	0.43
3:M:64:LYS:HD2	3:M:64:LYS:N	2.33	0.43
2:B:144:GLU:HG3	2:B:175:SER:HB2	2.00	0.43
2:B:972:LEU:HB2	2:B:1044:ARG:HE	1.83	0.43
2:B:1012:ASP:HB3	2:B:1015:ALA:HB3	2.00	0.43
2:B:1121:ALA:HB1	2:B:1123:VAL:HG13	2.00	0.43
2:B:1433:TYR:CE1	2:B:1578:ALA:HB2	2.53	0.43
2:B:1738:LEU:HB2	2:B:2146:PRO:HD3	2.00	0.43
2:B:2515:GLN:O	2:B:2519:LEU:HG	2.19	0.43
2:B:3104:GLU:HA	2:B:3107:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4720:VAL:O	2:B:4724:VAL:HG23	2.19	0.43
2:E:484:LEU:HD11	2:E:540:PHE:HE1	1.82	0.43
2:E:978:THR:O	2:E:982:THR:HG23	2.19	0.43
2:E:993:HIS:HE1	2:E:1027:LEU:HD11	1.78	0.43
2:E:2318:TYR:HA	2:E:2395:PRO:HA	2.01	0.43
2:E:2573:GLU:HA	2:E:2576:ALA:HB2	1.99	0.43
2:E:2870[B]:GLU:H	2:E:2870[B]:GLU:CD	2.22	0.43
2:E:3996:PHE:HZ	2:E:4019:LEU:HG	1.83	0.43
2:G:201:ASN:ND2	2:G:203:ASN:HD21	2.17	0.43
2:G:1496:TRP:CE2	2:G:1498:GLY:HA3	2.54	0.43
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.99	0.43
2:G:2223:ILE:HG21	2:G:2229:VAL:HG21	2.00	0.43
2:G:2867:LEU:HD23	2:G:2868:SER:O	2.18	0.43
2:J:245:VAL:HG13	2:J:376:ALA:HB3	2.01	0.43
2:J:2138:LEU:HD12	2:J:3658:LYS:HG3	1.99	0.43
2:J:2223:ILE:HG21	2:J:2229:VAL:HG21	2.01	0.43
3:F:64:LYS:N	3:F:64:LYS:HD2	2.33	0.43
2:B:119:SER:HA	2:B:146:CYS:HA	2.00	0.43
2:B:2684:ASP:OD1	2:B:2685:SER:N	2.51	0.43
2:B:2768:PHE:HA	2:B:2771:ILE:HG22	2.00	0.43
2:B:3417:ASP:OD1	2:B:3516:LYS:HG2	2.19	0.43
2:E:144:GLU:HG3	2:E:175:SER:HB2	2.01	0.43
2:E:2502:MET:HE3	2:E:2502:MET:HB2	1.66	0.43
2:E:2878:LEU:HG	2:E:2882:TYR:CZ	2.53	0.43
2:E:3836:MET:HE1	2:E:3915:ILE:HG23	2.00	0.43
2:E:4652:LEU:O	2:E:4656:LEU:HG	2.18	0.43
2:G:878:ILE:HG21	3:M:107:TRP:HE1	1.83	0.43
2:G:1097:THR:HG23	2:G:1143:TRP:CD1	2.54	0.43
2:G:2318:TYR:HA	2:G:2395:PRO:HA	2.01	0.43
2:G:2878:LEU:HG	2:G:2882:TYR:CZ	2.53	0.43
2:G:4021:LYS:HD3	2:G:4138:ASP:HB3	2.00	0.43
2:J:184:THR:HG22	2:J:189:LEU:HD13	1.99	0.43
2:J:1115:LEU:HD23	2:J:1123:VAL:HG11	2.01	0.43
2:J:2589:LEU:HD23	2:J:2589:LEU:HA	1.87	0.43
2:J:2635:GLU:HG3	2:J:2636:PHE:HD2	1.83	0.43
2:J:2654:TYR:HB2	2:J:2661:TRP:HE3	1.82	0.43
2:J:2768:PHE:HA	2:J:2771:ILE:HG22	2.00	0.43
2:J:2878:LEU:HG	2:J:2882:TYR:CZ	2.53	0.43
2:J:3206:LEU:HD13	2:J:3246:LEU:N	2.34	0.43
2:J:3458:PHE:CE2	2:J:3464:ILE:HG13	2.54	0.43
2:J:4888:TYR:O	2:J:4892:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:O	3:C:62:SER:HB3	2.19	0.43
1:I:55:VAL:HA	2:J:1784:ALA:HA	2.00	0.43
2:B:525:LEU:O	2:B:529:LEU:HG	2.17	0.43
2:B:663:TYR:CE1	2:B:745:SER:HB3	2.53	0.43
2:B:867:LEU:O	2:B:871:ARG:HB3	2.19	0.43
2:B:2672:LEU:HD12	2:B:2672:LEU:HA	1.81	0.43
2:B:4642:ALA:O	2:B:4646:LEU:HD23	2.19	0.43
2:E:245:VAL:HG13	2:E:376:ALA:HB3	2.01	0.43
2:E:2858:GLN:HB2	2:E:2859:PRO:HD3	1.99	0.43
2:E:3354:LEU:HD11	2:E:3434:LEU:HD22	2.01	0.43
2:E:3414:ARG:NH2	2:E:3474:SER:O	2.51	0.43
2:G:882:TRP:CZ2	3:M:104:TYR:HB2	2.54	0.43
2:G:2003:GLN:NE2	2:G:3863:GLY:HA3	2.34	0.43
2:G:2549:ALA:HA	2:G:2552:ARG:NH1	2.32	0.43
2:G:2575:ARG:NH1	2:G:2577:ILE:HG23	2.34	0.43
2:G:3354:LEU:HD11	2:G:3434:LEU:HD22	2.01	0.43
2:G:3458:PHE:CE2	2:G:3464:ILE:HG13	2.54	0.43
2:J:867:LEU:O	2:J:871:ARG:HB3	2.19	0.43
2:J:1496:TRP:CE2	2:J:1498:GLY:HA3	2.54	0.43
2:J:2867:LEU:HD23	2:J:2868:SER:O	2.18	0.43
2:J:2971:GLN:HA	2:J:2974:ILE:HG12	2.00	0.43
2:J:3098:SER:O	2:J:3101:GLU:HG3	2.18	0.43
2:J:3222:LYS:HD2	2:J:3226:GLU:CD	2.39	0.43
2:J:3222:LYS:HB3	2:J:3226:GLU:HB3	2.00	0.43
2:J:4817:ALA:HA	2:J:4823:LEU:HB3	2.00	0.43
1:D:98:ILE:N	1:D:98:ILE:HD12	2.34	0.43
1:H:7:ILE:HD12	1:H:71:ARG:HG2	2.01	0.43
2:B:131:LEU:HD13	2:B:195:PHE:HD2	1.84	0.43
2:B:1092:PHE:HE2	2:B:1100:MET:HE3	1.84	0.43
2:B:1694:LEU:HD13	2:B:1715:LEU:HD12	2.01	0.43
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	2.00	0.43
2:B:2206:THR:O	2:B:2210:VAL:HG23	2.19	0.43
2:B:2765:LYS:NZ	2:B:2860:PRO:HA	2.34	0.43
2:B:2996:LYS:O	2:B:3000:LYS:HG2	2.19	0.43
2:B:4021:LYS:HD3	2:B:4138:ASP:HB3	2.00	0.43
2:B:4846:VAL:O	2:B:4850:LEU:HG	2.19	0.43
2:E:135:VAL:HG21	2:E:191:VAL:HG22	2.00	0.43
2:E:474:ARG:O	2:E:478:PHE:HD1	2.01	0.43
2:E:1121:ALA:HB1	2:E:1123:VAL:HG13	2.00	0.43
2:E:1426:ILE:O	2:E:1430:THR:HB	2.18	0.43
2:E:1581:LEU:HD12	2:E:1584:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3367:LYS:O	2:E:3371:LYS:HG2	2.19	0.43
2:E:3754:GLU:HG3	2:E:4719:PHE:CZ	2.54	0.43
2:E:3989:VAL:HG13	2:E:4023:MET:HE2	2.01	0.43
2:G:796:ARG:HD3	2:G:1619:ARG:HH12	1.84	0.43
2:G:1012:ASP:HB3	2:G:1015:ALA:HB3	2.00	0.43
2:G:1115:LEU:HD23	2:G:1123:VAL:HG11	2.01	0.43
2:G:2765:LYS:NZ	2:G:2860:PRO:HA	2.34	0.43
2:G:3222:LYS:HD2	2:G:3226:GLU:CD	2.39	0.43
2:G:3346:VAL:HB	2:G:3411:LEU:HD22	2.01	0.43
2:G:3397:GLU:O	2:G:3400:VAL:HG12	2.18	0.43
2:J:2563:THR:HG22	2:J:2606:CYS:HA	2.00	0.43
2:J:2870[B]:GLU:H	2:J:2870[B]:GLU:CD	2.22	0.43
2:J:3511:VAL:HG12	2:J:3515:LYS:HD2	2.01	0.43
2:J:4679:ARG:NH1	2:J:4715:TYR:OH	2.51	0.43
3:C:32:ASN:ND2	3:C:101:PRO:HB3	2.33	0.43
3:M:32:ASN:OD1	3:M:33:SER:N	2.51	0.43
1:A:88:PRO:HB2	2:B:1680:ARG:HH12	1.84	0.43
2:B:294:THR:N	2:B:298:GLY:O	2.39	0.43
2:B:878:ILE:HG13	3:C:107:TRP:HZ2	1.84	0.43
2:B:3511:VAL:HG12	2:B:3515:LYS:HD2	2.01	0.43
2:E:232:THR:HG21	2:E:252:VAL:HG11	2.01	0.43
2:E:786:GLY:H	2:E:1631:GLN:HA	1.84	0.43
2:E:873:LYS:NZ	2:E:947:GLU:OE1	2.48	0.43
2:E:3222:LYS:HB3	2:E:3226:GLU:HB3	2.00	0.43
2:E:3878:ASP:OD1	2:E:3878:ASP:N	2.52	0.43
2:E:4817:ALA:HA	2:E:4823:LEU:HB3	2.00	0.43
2:G:474:ARG:O	2:G:478:PHE:HD1	2.01	0.43
2:G:1152:MET:HE2	2:G:1161:ILE:HB	2.01	0.43
2:G:2159:LEU:O	2:G:2163:ARG:HG3	2.19	0.43
2:G:2515:GLN:O	2:G:2519:LEU:HG	2.19	0.43
2:G:2684:ASP:OD1	2:G:2685:SER:N	2.51	0.43
2:G:3511:VAL:HG12	2:G:3515:LYS:HD2	2.01	0.43
2:G:4677:LEU:HD23	2:G:4711:PHE:HE1	1.84	0.43
2:G:4888:TYR:O	2:G:4892:ARG:HD3	2.18	0.43
2:J:707:VAL:HG23	2:J:782:SER:OG	2.19	0.43
2:J:887:ILE:HD13	2:J:959:TYR:HB3	2.00	0.43
2:J:979:PRO:O	2:J:983:THR:HG23	2.19	0.43
2:J:1018:ASN:OD1	2:J:1021:LEU:N	2.51	0.43
2:J:1738:LEU:HB2	2:J:2146:PRO:HD3	2.00	0.43
2:J:2604:GLU:HG2	2:J:2639:MET:HG3	2.00	0.43
2:J:3354:LEU:HD11	2:J:3434:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:32:ASN:OD1	3:F:33:SER:N	2.51	0.43
3:F:46:GLU:HG3	3:F:62:SER:HB2	2.00	0.43
3:F:47:LEU:O	3:F:62:SER:HB3	2.19	0.43
3:K:64:LYS:N	3:K:64:LYS:HD2	2.33	0.43
2:B:232:THR:HG21	2:B:252:VAL:HG11	2.01	0.42
2:B:993:HIS:HE1	2:B:1027:LEU:HD11	1.78	0.42
2:B:2618:MET:SD	2:B:2618:MET:N	2.91	0.42
2:B:3051:ARG:HH22	2:B:3102:ASP:HB2	1.83	0.42
2:B:3222:LYS:HD2	2:B:3226:GLU:CD	2.39	0.42
2:B:3346:VAL:HB	2:B:3411:LEU:HD22	2.01	0.42
2:B:3354:LEU:HD11	2:B:3434:LEU:HD22	2.01	0.42
2:E:887:ILE:HD13	2:E:959:TYR:HB3	2.00	0.42
2:E:1432:THR:HG23	2:E:1572:ILE:HG23	2.01	0.42
2:E:2867:LEU:HD23	2:E:2868:SER:O	2.18	0.42
2:E:4846:VAL:O	2:E:4850:LEU:HG	2.19	0.42
2:G:786:GLY:H	2:G:1631:GLN:HA	1.84	0.42
2:G:1018:ASN:OD1	2:G:1021:LEU:N	2.51	0.42
2:G:2206:THR:O	2:G:2210:VAL:HG23	2.19	0.42
2:G:2230:THR:HG22	2:G:2234:ARG:HH11	1.83	0.42
2:G:3367:LYS:O	2:G:3371:LYS:HG2	2.19	0.42
2:G:4232:GLU:HG2	2:G:5019:TRP:NE1	2.34	0.42
2:G:4818:MET:N	2:G:4818:MET:SD	2.92	0.42
2:J:978:THR:O	2:J:982:THR:HG23	2.19	0.42
2:J:1097:THR:HG23	2:J:1143:TRP:CD1	2.54	0.42
2:J:2515:GLN:O	2:J:2519:LEU:HG	2.19	0.42
2:J:2777:TYR:HB2	2:J:2791:LEU:O	2.18	0.42
2:J:3521:GLY:HA2	2:J:3524:MET:SD	2.59	0.42
2:J:4642:ALA:O	2:J:4646:LEU:HD23	2.19	0.42
3:K:47:LEU:O	3:K:62:SER:HB3	2.19	0.42
2:B:1432:THR:HG23	2:B:1572:ILE:HG23	2.01	0.42
2:B:4014:LYS:HG2	2:B:4135:PRO:HB3	2.01	0.42
2:B:4805:ASN:HB3	2:B:4808:PHE:CD2	2.54	0.42
2:E:248:GLU:O	2:E:372:LEU:HD23	2.19	0.42
2:E:424:LYS:HE2	2:E:424:LYS:HB2	1.92	0.42
2:E:468:LEU:O	2:E:472:ARG:HG2	2.19	0.42
2:E:979:PRO:O	2:E:983:THR:HG23	2.19	0.42
2:E:2768:PHE:HA	2:E:2771:ILE:HG22	2.00	0.42
2:E:3511:VAL:HG12	2:E:3515:LYS:HD2	2.01	0.42
2:G:1694:LEU:HD13	2:G:1715:LEU:HD12	2.01	0.42
2:G:3098:SER:O	2:G:3101:GLU:HG3	2.18	0.42
2:G:3157:ILE:HG23	2:G:3165:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:144:GLU:HG3	2:J:175:SER:HB2	2.01	0.42
2:J:275:ARG:HB3	2:J:278:GLN:HB2	2.01	0.42
2:J:3367:LYS:O	2:J:3371:LYS:HG2	2.19	0.42
2:J:4818:MET:N	2:J:4818:MET:SD	2.92	0.42
2:B:978:THR:O	2:B:982:THR:HG23	2.19	0.42
2:B:979:PRO:O	2:B:983:THR:HG23	2.19	0.42
2:B:2654:TYR:HB2	2:B:2661:TRP:CE3	2.55	0.42
2:B:2867:LEU:HD23	2:B:2868:SER:O	2.18	0.42
2:E:349:GLN:HB2	2:E:356:TRP:CZ3	2.54	0.42
2:E:2765:LYS:NZ	2:E:2860:PRO:HA	2.34	0.42
2:E:2971:GLN:HA	2:E:2974:ILE:HG12	2.00	0.42
2:E:3092:LEU:O	2:E:3095:PHE:HB3	2.18	0.42
2:E:4818:MET:N	2:E:4818:MET:SD	2.92	0.42
2:G:131:LEU:HD13	2:G:195:PHE:HD2	1.84	0.42
2:G:978:THR:O	2:G:982:THR:HG23	2.19	0.42
2:G:2312:MET:CE	2:G:2312:MET:H	2.32	0.42
2:G:2359:ARG:O	2:G:2361:PRO:HD3	2.19	0.42
2:G:2575:ARG:O	2:G:2578:MET:HG3	2.19	0.42
2:G:3521:GLY:HA2	2:G:3524:MET:SD	2.60	0.42
2:J:2159:LEU:O	2:J:2163:ARG:HG3	2.19	0.42
2:J:2765:LYS:NZ	2:J:2860:PRO:HA	2.34	0.42
3:K:53:SER:H	3:K:53:SER:HG	1.62	0.42
1:D:88:PRO:HB2	2:E:1680:ARG:HH12	1.84	0.42
2:B:182:LEU:HD13	2:B:198:THR:HG21	2.02	0.42
2:B:535:ALA:O	2:B:539:LEU:HG	2.19	0.42
2:B:707:VAL:HG23	2:B:782:SER:OG	2.19	0.42
2:B:1581:LEU:HD12	2:B:1584:ARG:HE	1.84	0.42
2:B:2312:MET:H	2:B:2312:MET:CE	2.32	0.42
2:B:2359:ARG:O	2:B:2361:PRO:HD3	2.19	0.42
2:E:371:VAL:HG12	2:E:373:LYS:H	1.85	0.42
2:E:372:LEU:HD12	2:E:372:LEU:HA	1.81	0.42
2:E:548:VAL:HA	2:E:551:LEU:HG	2.02	0.42
2:E:707:VAL:HG23	2:E:782:SER:OG	2.19	0.42
2:E:2654:TYR:HB2	2:E:2661:TRP:CE3	2.55	0.42
2:E:2790:MET:O	2:E:2792:ARG:NE	2.52	0.42
2:E:4888:TYR:O	2:E:4892:ARG:HD3	2.18	0.42
2:G:275:ARG:HB3	2:G:278:GLN:HB2	2.01	0.42
2:G:548:VAL:HA	2:G:551:LEU:HG	2.02	0.42
2:G:3222:LYS:HB3	2:G:3226:GLU:HB3	2.00	0.42
2:G:4232:GLU:HG2	2:G:5019:TRP:HE1	1.84	0.42
2:J:226:HIS:CD2	2:J:226:HIS:N	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:535:ALA:O	2:J:539:LEU:HG	2.19	0.42
2:J:1931:LEU:HD22	2:J:1935:VAL:HG11	2.00	0.42
2:J:2206:THR:O	2:J:2210:VAL:HG23	2.19	0.42
2:J:2351:ASN:O	2:J:2355:ARG:HG3	2.19	0.42
3:K:46:GLU:HG3	3:K:62:SER:HB2	2.00	0.42
3:M:63:VAL:HA	3:M:67:PHE:HE2	1.85	0.42
2:B:468:LEU:O	2:B:472:ARG:HG2	2.19	0.42
2:B:2159:LEU:O	2:B:2163:ARG:HG3	2.19	0.42
2:B:2971:GLN:HA	2:B:2974:ILE:HG12	2.00	0.42
2:B:3316:LEU:HD11	2:B:3345:ILE:HG23	2.01	0.42
2:B:3367:LYS:O	2:B:3371:LYS:HG2	2.19	0.42
2:B:4818:MET:N	2:B:4818:MET:SD	2.92	0.42
2:B:4888:TYR:O	2:B:4892:ARG:HD3	2.18	0.42
2:E:14:LEU:HD13	2:E:202:MET:HG2	2.02	0.42
2:E:943:ASP:HB2	2:E:946:ALA:HB3	2.02	0.42
2:E:1000:ARG:NH2	2:E:1003:GLN:HG3	2.33	0.42
2:E:1261:ASP:N	2:E:1261:ASP:OD1	2.53	0.42
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	2.00	0.42
2:E:2351:ASN:O	2:E:2355:ARG:HG3	2.20	0.42
2:G:707:VAL:HG23	2:G:782:SER:OG	2.19	0.42
2:G:867:LEU:O	2:G:871:ARG:HB3	2.19	0.42
2:G:1738:LEU:HB2	2:G:2146:PRO:HD3	2.00	0.42
2:G:1757:ALA:O	2:G:1759:ARG:HD2	2.20	0.42
2:G:2541:PHE:N	2:G:2541:PHE:CD1	2.87	0.42
2:G:2801:ASP:HA	2:G:2804:ILE:HG12	2.01	0.42
2:J:548:VAL:HG21	2:J:582:HIS:CD2	2.52	0.42
2:J:972:LEU:HB2	2:J:1044:ARG:HE	1.83	0.42
2:J:1757:ALA:O	2:J:1759:ARG:HD2	2.20	0.42
2:J:3007:ASN:OD1	2:J:3070:ILE:HG13	2.19	0.42
2:J:3092:LEU:O	2:J:3095:PHE:HB3	2.18	0.42
3:F:32:ASN:ND2	3:F:101:PRO:HB3	2.33	0.42
1:H:17:LYS:HG3	1:H:18:LYS:N	2.35	0.42
2:B:201:ASN:ND2	2:B:203:ASN:HD21	2.17	0.42
2:B:943:ASP:HB2	2:B:946:ALA:HB3	2.02	0.42
2:B:1496:TRP:CE2	2:B:1498:GLY:HA3	2.54	0.42
2:B:2725:LYS:HE3	2:B:2735:PHE:CE1	2.55	0.42
2:B:2902:HIS:CG	2:B:2903:PRO:HD2	2.55	0.42
2:B:3157:ILE:HG23	2:B:3165:CYS:SG	2.59	0.42
2:B:3343:GLN:HB3	2:B:3344:PRO:HD3	2.02	0.42
2:B:4817:ALA:HA	2:B:4823:LEU:HB3	2.00	0.42
2:E:131:LEU:HD13	2:E:195:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:LEU:HD13	2:E:198:THR:HG21	2.02	0.42
2:E:535:ALA:O	2:E:539:LEU:HG	2.19	0.42
2:E:657:THR:HB	2:E:1021:LEU:HG	2.02	0.42
2:E:1115:LEU:HD23	2:E:1123:VAL:HG11	2.01	0.42
2:E:2165:LEU:HD11	2:E:2177:LEU:HB3	2.02	0.42
2:E:2173:GLN:O	2:E:2177:LEU:HD23	2.20	0.42
2:E:2223:ILE:HG21	2:E:2229:VAL:HG21	2.00	0.42
2:E:2359:ARG:O	2:E:2361:PRO:HD3	2.19	0.42
2:E:2640:PRO:O	2:E:2644:LEU:HD23	2.20	0.42
2:E:3417:ASP:OD1	2:E:3516:LYS:HG2	2.19	0.42
2:E:4852:THR:HG22	2:E:4886:HIS:CG	2.55	0.42
2:G:1432:THR:HG23	2:G:1572:ILE:HG23	2.02	0.42
2:J:131:LEU:HD13	2:J:195:PHE:HD2	1.84	0.42
2:J:468:LEU:O	2:J:472:ARG:HG2	2.19	0.42
2:J:474:ARG:O	2:J:478:PHE:HD1	2.01	0.42
2:J:943:ASP:HB2	2:J:946:ALA:HB3	2.02	0.42
2:J:1426:ILE:O	2:J:1430:THR:HB	2.19	0.42
2:J:1432:THR:HG23	2:J:1572:ILE:HG23	2.01	0.42
2:J:2996:LYS:O	2:J:3000:LYS:HG2	2.19	0.42
2:J:4060:LYS:HA	2:J:4063:ASP:OD2	2.20	0.42
2:J:4805:ASN:HB3	2:J:4808:PHE:CD2	2.54	0.42
2:J:4852:THR:HG22	2:J:4886:HIS:CG	2.55	0.42
3:F:83:ASN:OD1	3:F:83:ASN:N	2.53	0.42
3:K:32:ASN:OD1	3:K:33:SER:N	2.51	0.42
1:I:17:LYS:HG3	1:I:18:LYS:N	2.35	0.42
2:B:14:LEU:HD13	2:B:202:MET:HG2	2.02	0.42
2:B:786:GLY:H	2:B:1631:GLN:HA	1.84	0.42
2:B:796:ARG:HD3	2:B:1619:ARG:HH12	1.84	0.42
2:B:2173:GLN:O	2:B:2177:LEU:HD23	2.20	0.42
2:B:2598:ALA:O	2:B:2602:VAL:HG23	2.20	0.42
2:B:2640:PRO:O	2:B:2644:LEU:HD23	2.20	0.42
2:B:3154:ASP:N	2:B:3154:ASP:OD1	2.53	0.42
2:E:867:LEU:O	2:E:871:ARG:HB3	2.19	0.42
2:E:1496:TRP:CE2	2:E:1498:GLY:HA3	2.54	0.42
2:E:2725:LYS:HE3	2:E:2735:PHE:CE1	2.55	0.42
2:E:2765:LYS:HZ2	2:E:2860:PRO:HA	1.85	0.42
2:E:3154:ASP:OD1	2:E:3154:ASP:N	2.53	0.42
2:G:245:VAL:HG13	2:G:376:ALA:HB3	2.01	0.42
2:G:2640:PRO:O	2:G:2644:LEU:HD23	2.20	0.42
2:G:2996:LYS:O	2:G:3000:LYS:HG2	2.19	0.42
2:J:119:SER:HA	2:J:146:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:461:HIS:HA	2:J:464:LYS:HE3	2.02	0.42
2:J:551:LEU:HD11	2:J:564:LEU:HD22	2.02	0.42
2:J:2312:MET:H	2:J:2312:MET:CE	2.31	0.42
2:J:2541:PHE:N	2:J:2541:PHE:CD1	2.87	0.42
2:J:3538:THR:OG1	2:J:3539:ARG:NH1	2.53	0.42
1:A:98:ILE:N	1:A:98:ILE:HD12	2.34	0.42
2:B:144:GLU:OE2	2:G:2452:ARG:HD2	2.20	0.42
2:B:245:VAL:HG13	2:B:376:ALA:HB3	2.01	0.42
2:B:883:ALA:O	2:B:887:ILE:HG13	2.20	0.42
2:B:2292:GLU:H	2:B:2292:GLU:CD	2.21	0.42
2:B:2664:PHE:CD1	2:B:2664:PHE:N	2.88	0.42
2:B:3002:LEU:HD23	2:B:3002:LEU:HA	1.81	0.42
2:B:3567:PRO:CB	2:B:3570:ARG:HH21	2.32	0.42
2:B:3735:LEU:O	2:B:3740:GLU:N	2.53	0.42
2:B:4677:LEU:HD12	2:B:4677:LEU:HA	1.91	0.42
2:E:1097:THR:HG23	2:E:1143:TRP:CD1	2.54	0.42
2:E:1694:LEU:HD13	2:E:1715:LEU:HD12	2.01	0.42
2:E:2122:SER:O	2:E:2126:ARG:HG3	2.20	0.42
2:E:2159:LEU:O	2:E:2163:ARG:HG3	2.19	0.42
2:E:2206:THR:O	2:E:2210:VAL:HG23	2.19	0.42
2:E:2312:MET:H	2:E:2312:MET:CE	2.32	0.42
2:E:2996:LYS:O	2:E:3000:LYS:HG2	2.19	0.42
2:E:3343:GLN:HB3	2:E:3344:PRO:HD3	2.02	0.42
2:E:3346:VAL:HB	2:E:3411:LEU:HD22	2.01	0.42
2:E:4655:PHE:O	2:E:4659:ILE:HG12	2.20	0.42
2:G:266:ARG:NE	2:G:268:SER:O	2.53	0.42
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	2.00	0.42
2:G:2330:ARG:HE	2:G:2330:ARG:HB2	1.68	0.42
2:G:2351:ASN:O	2:G:2355:ARG:HG3	2.19	0.42
2:G:3078:ARG:HG2	2:G:3152:PHE:CE1	2.55	0.42
2:J:349:GLN:HB2	2:J:356:TRP:CZ3	2.54	0.42
2:J:464:LYS:HE3	2:J:464:LYS:HB3	1.93	0.42
2:J:657:THR:HB	2:J:1021:LEU:HG	2.02	0.42
2:J:786:GLY:H	2:J:1631:GLN:HA	1.84	0.42
2:J:2359:ARG:O	2:J:2361:PRO:HD3	2.19	0.42
2:J:3250:MET:CE	2:J:3315:LEU:HD21	2.50	0.42
2:J:3771:HIS:CG	2:J:3812:VAL:HG12	2.55	0.42
2:J:3878:ASP:N	2:J:3878:ASP:OD1	2.52	0.42
3:C:46:GLU:HG3	3:C:62:SER:HB2	2.00	0.42
3:F:85:LEU:HD23	3:F:85:LEU:HA	1.92	0.42
2:B:266:ARG:NE	2:B:268:SER:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:HB2	2:B:356:TRP:CZ3	2.54	0.42
2:B:464:LYS:O	2:B:468:LEU:HG	2.20	0.42
2:B:911:HIS:HE1	2:B:918:ARG:NE	2.18	0.42
2:B:1115:LEU:HD23	2:B:1123:VAL:HG11	2.01	0.42
2:B:3136:LEU:O	2:B:3140:LEU:HB3	2.20	0.42
2:B:3521:GLY:HA2	2:B:3524:MET:SD	2.59	0.42
2:B:3771:HIS:CG	2:B:3812:VAL:HG12	2.55	0.42
2:B:3893:GLU:HA	2:B:3967:GLU:OE2	2.19	0.42
2:B:4852:THR:HG22	2:B:4886:HIS:CG	2.55	0.42
2:E:119:SER:HA	2:E:146:CYS:HA	2.00	0.42
2:E:551:LEU:HD11	2:E:564:LEU:HD22	2.02	0.42
2:E:1037:ASP:OD1	2:E:1038:SER:N	2.52	0.42
2:E:2230:THR:HG22	2:E:2234:ARG:HH11	1.83	0.42
2:E:2311:PRO:O	2:E:2314:LEU:HG	2.20	0.42
2:E:3007:ASN:OD1	2:E:3070:ILE:HG13	2.19	0.42
2:E:3157:ILE:HG23	2:E:3165:CYS:SG	2.59	0.42
2:E:3222:LYS:HD2	2:E:3226:GLU:CD	2.39	0.42
2:E:3320:LEU:HD23	2:E:3320:LEU:HA	1.74	0.42
2:E:4805:ASN:HB3	2:E:4808:PHE:CD2	2.54	0.42
2:E:4852:THR:HG21	2:E:4883:TYR:HD1	1.85	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.00	0.42
2:G:883:ALA:O	2:G:887:ILE:HG13	2.20	0.42
2:G:3069:HIS:CD2	2:G:3139:VAL:HA	2.55	0.42
2:G:3546:ASP:O	2:G:3550:ARG:HG3	2.19	0.42
2:G:3878:ASP:N	2:G:3878:ASP:OD1	2.52	0.42
2:G:4928:LEU:HD23	2:G:4928:LEU:HA	1.89	0.42
2:J:411:TYR:HB2	2:J:486:LEU:HD21	2.02	0.42
2:J:2230:THR:HG22	2:J:2234:ARG:HH11	1.83	0.42
2:J:2725:LYS:HE3	2:J:2735:PHE:CE1	2.55	0.42
2:J:3257:ALA:HB1	2:J:3321:ARG:HB3	2.02	0.42
2:J:3316:LEU:HD21	2:J:3345:ILE:HG13	2.02	0.42
2:J:3546:ASP:O	2:J:3550:ARG:HG3	2.19	0.42
2:J:4846:VAL:O	2:J:4850:LEU:HG	2.19	0.42
3:K:83:ASN:OD1	3:K:83:ASN:N	2.53	0.42
3:K:104:TYR:HD1	3:K:106:PRO:HD3	1.85	0.42
3:M:47:LEU:O	3:M:62:SER:HB3	2.19	0.42
1:A:40:ARG:H	1:A:40:ARG:HG2	1.72	0.42
2:B:167:ASP:OD1	2:B:168:ASP:N	2.53	0.42
2:B:548:VAL:HA	2:B:551:LEU:HG	2.02	0.42
2:B:984:LEU:HA	2:B:987:ARG:NH1	2.35	0.42
2:B:2223:ILE:HG21	2:B:2229:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2351:ASN:O	2:B:2355:ARG:HG3	2.20	0.42
2:B:2559:LEU:O	2:B:2563:THR:HG23	2.20	0.42
2:B:2635:GLU:HG3	2:B:2636:PHE:HD2	1.84	0.42
2:B:2737:PRO:HB2	2:B:2884:ASN:HB2	2.02	0.42
2:B:3172:ILE:HD11	2:B:3190:LEU:HB3	2.02	0.42
2:B:3535:LEU:CD1	2:B:3539:ARG:HH12	2.33	0.42
2:B:4687:TYR:HE1	2:B:4692:PRO:HG3	1.85	0.42
2:E:167:ASP:OD1	2:E:168:ASP:N	2.53	0.42
2:E:266:ARG:NE	2:E:268:SER:O	2.53	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HB2	2.02	0.42
2:E:984:LEU:HA	2:E:987:ARG:NH1	2.35	0.42
2:E:1757:ALA:O	2:E:1759:ARG:HD2	2.20	0.42
2:E:2801:ASP:HA	2:E:2804:ILE:HG12	2.01	0.42
2:E:2905:LEU:HD23	2:E:2905:LEU:HA	1.93	0.42
2:E:3043:PHE:CD1	2:E:3043:PHE:C	2.93	0.42
2:E:3246:LEU:HA	2:E:3249:LEU:HG	2.02	0.42
2:E:3735:LEU:O	2:E:3740:GLU:N	2.53	0.42
2:E:4687:TYR:HE1	2:E:4692:PRO:HG3	1.85	0.42
2:G:461:HIS:HA	2:G:464:LYS:HE3	2.02	0.42
2:G:468:LEU:O	2:G:472:ARG:HG2	2.19	0.42
2:G:535:ALA:O	2:G:539:LEU:HG	2.20	0.42
2:G:3007:ASN:OD1	2:G:3070:ILE:HG13	2.19	0.42
2:G:3049:LEU:HA	2:G:3053:ARG:NH2	2.35	0.42
2:G:3206:LEU:HD13	2:G:3246:LEU:N	2.35	0.42
2:G:4014:LYS:HG2	2:G:4135:PRO:HB3	2.01	0.42
2:G:4852:THR:HG22	2:G:4886:HIS:CG	2.55	0.42
2:J:548:VAL:HA	2:J:551:LEU:HG	2.02	0.42
2:J:883:ALA:O	2:J:887:ILE:HG13	2.20	0.42
2:J:2598:ALA:O	2:J:2602:VAL:HG23	2.20	0.42
2:J:3069:HIS:CD2	2:J:3139:VAL:HA	2.55	0.42
2:J:4687:TYR:HE1	2:J:4692:PRO:HG3	1.85	0.42
2:J:4773:VAL:O	2:J:4777:ILE:HG13	2.20	0.42
1:I:73:LYS:HE2	1:I:73:LYS:HB3	1.92	0.41
2:B:214:VAL:HG13	2:B:274:LEU:HB2	2.02	0.41
2:B:664:PHE:CE1	2:B:746:CYS:HB2	2.55	0.41
2:B:1088:TRP:HB2	2:B:1153:ILE:HG22	2.02	0.41
2:B:2122:SER:O	2:B:2126:ARG:HG3	2.20	0.41
2:B:2652:TRP:CD1	2:B:2652:TRP:C	2.93	0.41
2:B:3186:LEU:HG	2:B:3190:LEU:HD21	2.02	0.41
2:B:3878:ASP:OD1	2:B:3878:ASP:N	2.52	0.41
2:B:4968:PHE:O	2:B:4974:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:461:HIS:HA	2:E:464:LYS:HE3	2.02	0.41
2:E:796:ARG:HD3	2:E:1619:ARG:HH12	1.84	0.41
2:E:2452:ARG:HD2	2:J:144:GLU:OE2	2.19	0.41
2:E:2652:TRP:CD1	2:E:2652:TRP:C	2.93	0.41
2:E:2902:HIS:CG	2:E:2903:PRO:HD2	2.55	0.41
2:E:3078:ARG:HG2	2:E:3152:PHE:CE1	2.55	0.41
2:E:3257:ALA:HB1	2:E:3321:ARG:HB3	2.02	0.41
2:E:3538:THR:OG1	2:E:3539:ARG:NH1	2.53	0.41
2:E:3546:ASP:O	2:E:3550:ARG:HG3	2.19	0.41
2:E:3771:HIS:CG	2:E:3812:VAL:HG12	2.55	0.41
2:E:4038:GLY:O	2:E:4042:ARG:NE	2.46	0.41
2:G:943:ASP:HB2	2:G:946:ALA:HB3	2.02	0.41
2:G:997:ALA:O	2:G:1001:VAL:HG23	2.20	0.41
2:G:1261:ASP:N	2:G:1261:ASP:OD1	2.53	0.41
2:G:2122:SER:O	2:G:2126:ARG:HG3	2.20	0.41
2:G:2654:TYR:HB2	2:G:2661:TRP:CE3	2.55	0.41
2:G:2725:LYS:HE3	2:G:2735:PHE:CE1	2.55	0.41
2:G:3172:ILE:HD11	2:G:3190:LEU:HB3	2.02	0.41
2:G:4041:ALA:O	2:G:4045:VAL:HG23	2.20	0.41
2:G:4060:LYS:HA	2:G:4063:ASP:OD2	2.20	0.41
2:J:464:LYS:O	2:J:468:LEU:HG	2.20	0.41
2:J:1090:PHE:HB2	2:J:1204:LEU:HA	2.02	0.41
2:J:3049:LEU:HA	2:J:3053:ARG:NH2	2.35	0.41
2:J:3078:ARG:HG2	2:J:3152:PHE:CE1	2.55	0.41
2:J:3157:ILE:HG23	2:J:3165:CYS:SG	2.59	0.41
2:J:3316:LEU:HD13	2:J:3316:LEU:HA	1.95	0.41
2:J:3346:VAL:HB	2:J:3411:LEU:HD22	2.01	0.41
2:J:4655:PHE:O	2:J:4659:ILE:HG12	2.20	0.41
1:A:2:VAL:HA	1:A:75:THR:O	2.20	0.41
2:B:1037:ASP:OD1	2:B:1038:SER:N	2.52	0.41
2:B:2230:THR:HG22	2:B:2234:ARG:HH11	1.83	0.41
2:B:3007:ASN:OD1	2:B:3070:ILE:HG13	2.19	0.41
2:B:3043:PHE:CD1	2:B:3043:PHE:C	2.93	0.41
2:B:3257:ALA:HB1	2:B:3321:ARG:HB3	2.02	0.41
2:E:688:LEU:HD12	2:E:688:LEU:HA	1.87	0.41
2:E:911:HIS:HB2	2:E:913:LEU:HG	2.02	0.41
2:E:2598:ALA:O	2:E:2602:VAL:HG23	2.20	0.41
2:G:979:PRO:O	2:G:983:THR:HG23	2.19	0.41
2:G:1581:LEU:HD12	2:G:1584:ARG:HE	1.83	0.41
2:G:3735:LEU:O	2:G:3740:GLU:N	2.53	0.41
2:G:4546:VAL:HA	2:G:4549:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4805:ASN:HB3	2:G:4808:PHE:CD2	2.54	0.41
2:J:266:ARG:NE	2:J:268:SER:O	2.53	0.41
2:J:796:ARG:HD3	2:J:1619:ARG:HH12	1.84	0.41
2:J:2522:LEU:HD11	2:J:2569:PHE:CE1	2.54	0.41
2:J:2652:TRP:CD1	2:J:2652:TRP:C	2.93	0.41
2:J:2801:ASP:HA	2:J:2804:ILE:HG12	2.01	0.41
3:C:104:TYR:HD1	3:C:106:PRO:HD3	1.85	0.41
3:K:63:VAL:HA	3:K:67:PHE:HE2	1.85	0.41
2:B:461:HIS:HA	2:B:464:LYS:HE3	2.02	0.41
2:B:911:HIS:HB2	2:B:913:LEU:HG	2.02	0.41
2:B:3069:HIS:CD2	2:B:3139:VAL:HA	2.55	0.41
2:B:4245:MET:HE3	2:B:4245:MET:HB3	1.91	0.41
2:E:214:VAL:HG13	2:E:274:LEU:HB2	2.02	0.41
2:E:575:LEU:HD13	2:E:606:LEU:HA	2.02	0.41
2:E:2123:LEU:HD12	2:E:2123:LEU:HA	1.91	0.41
2:E:3069:HIS:CD2	2:E:3139:VAL:HA	2.55	0.41
2:E:3683:GLN:O	2:E:3687:GLU:HB2	2.21	0.41
2:E:4014:LYS:HG2	2:E:4135:PRO:HB3	2.01	0.41
2:E:4041:ALA:O	2:E:4045:VAL:HG23	2.20	0.41
2:G:144:GLU:OE2	2:J:2452:ARG:HD2	2.19	0.41
2:G:182:LEU:HD13	2:G:198:THR:HG21	2.02	0.41
2:G:1037:ASP:OD1	2:G:1038:SER:N	2.52	0.41
2:G:2664:PHE:CD1	2:G:2664:PHE:N	2.88	0.41
2:G:2737:PRO:HB2	2:G:2884:ASN:HB2	2.02	0.41
2:G:3257:ALA:HB1	2:G:3321:ARG:HB3	2.02	0.41
2:G:3417:ASP:OD1	2:G:3516:LYS:HG2	2.19	0.41
2:G:4687:TYR:HE1	2:G:4692:PRO:HG3	1.85	0.41
2:J:167:ASP:OD1	2:J:168:ASP:N	2.53	0.41
2:J:182:LEU:HD13	2:J:198:THR:HG21	2.02	0.41
2:J:788:LYS:HG2	2:J:1629:GLN:HB2	2.02	0.41
2:J:1121:ALA:HB1	2:J:1123:VAL:HG13	2.00	0.41
2:J:1694:LEU:HD13	2:J:1715:LEU:HD12	2.01	0.41
2:J:2640:PRO:O	2:J:2644:LEU:HD23	2.20	0.41
2:J:2758:PHE:O	2:J:2762:THR:HG23	2.21	0.41
2:J:2902:HIS:CG	2:J:2903:PRO:HD2	2.55	0.41
2:J:3417:ASP:OD1	2:J:3516:LYS:HG2	2.19	0.41
2:J:3592:ILE:HG12	2:J:3595:ARG:NH2	2.35	0.41
2:J:4014:LYS:HG2	2:J:4135:PRO:HB3	2.01	0.41
2:J:4017:LEU:HD22	2:J:4139:ILE:HG21	2.03	0.41
2:J:4031:LEU:HD13	2:J:4044:MET:HE3	2.03	0.41
3:C:28:ILE:HD12	3:C:28:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:63:VAL:HA	3:F:67:PHE:HE2	1.85	0.41
1:I:88:PRO:HB2	2:J:1680:ARG:HH12	1.85	0.41
2:B:3078:ARG:HG2	2:B:3152:PHE:CE1	2.55	0.41
2:B:3546:ASP:O	2:B:3550:ARG:HG3	2.19	0.41
2:B:4060:LYS:HA	2:B:4063:ASP:OD2	2.20	0.41
2:B:4655:PHE:O	2:B:4659:ILE:HG12	2.20	0.41
2:B:4773:VAL:O	2:B:4777:ILE:HG13	2.20	0.41
2:B:4928:LEU:HD23	2:B:4928:LEU:HA	1.89	0.41
2:E:882:TRP:CZ2	3:F:104:TYR:HB2	2.55	0.41
2:E:911:HIS:HE1	2:E:918:ARG:NE	2.18	0.41
2:E:936:GLY:HA3	2:E:1056:PRO:HB3	2.01	0.41
2:E:937:CYS:HB3	2:E:1053:ILE:HB	2.02	0.41
2:E:1927:LEU:HD23	2:E:1939:MET:HE1	2.03	0.41
2:E:3521:GLY:HA2	2:E:3524:MET:SD	2.60	0.41
2:E:4060:LYS:HA	2:E:4063:ASP:OD2	2.20	0.41
2:E:4698:LYS:HE3	2:E:4698:LYS:HB2	1.84	0.41
2:G:14:LEU:HD13	2:G:202:MET:HG2	2.02	0.41
2:G:904:HIS:CD2	2:G:907:LEU:H	2.39	0.41
2:G:984:LEU:HA	2:G:987:ARG:NH1	2.35	0.41
2:G:2173:GLN:O	2:G:2177:LEU:HD23	2.20	0.41
2:G:2598:ALA:O	2:G:2602:VAL:HG23	2.20	0.41
2:G:2902:HIS:CG	2:G:2903:PRO:HD2	2.55	0.41
2:G:3836:MET:HE3	2:G:3915:ILE:HG23	2.02	0.41
2:G:4232:GLU:HG2	2:G:5019:TRP:CD1	2.56	0.41
2:G:4773:VAL:O	2:G:4777:ILE:HG13	2.20	0.41
2:G:4851:TYR:HD1	2:G:4916:PHE:CE1	2.39	0.41
2:G:4968:PHE:O	2:G:4974:GLY:HA3	2.20	0.41
2:J:984:LEU:HA	2:J:987:ARG:NH1	2.35	0.41
2:J:997:ALA:O	2:J:1001:VAL:HG23	2.20	0.41
2:J:2173:GLN:O	2:J:2177:LEU:HD23	2.20	0.41
2:J:2737:PRO:HB2	2:J:2884:ASN:HB2	2.02	0.41
2:J:4852:THR:HG21	2:J:4883:TYR:HD1	1.85	0.41
3:M:104:TYR:HD1	3:M:106:PRO:HD3	1.85	0.41
2:B:657:THR:HB	2:B:1021:LEU:HG	2.02	0.41
2:B:904:HIS:CD2	2:B:907:LEU:H	2.39	0.41
2:B:2452:ARG:HD2	2:E:144:GLU:OE2	2.19	0.41
2:B:2589:LEU:HD23	2:B:2589:LEU:HA	1.87	0.41
2:B:2615:ARG:HD2	2:B:2664:PHE:HA	2.01	0.41
2:B:3193:CYS:O	2:B:3197:LEU:HG	2.21	0.41
2:B:3683:GLN:O	2:B:3687:GLU:HB2	2.21	0.41
2:E:866:HIS:ND1	2:E:870:ILE:HB	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1088:TRP:HB2	2:E:1153:ILE:HG22	2.02	0.41
2:E:1092:PHE:HE2	2:E:1100:MET:HE3	1.86	0.41
2:E:1849:LEU:HG	2:E:1945:TYR:CE2	2.56	0.41
2:E:2737:PRO:HB2	2:E:2884:ASN:HB2	2.02	0.41
2:E:4968:PHE:O	2:E:4974:GLY:HA3	2.20	0.41
2:G:162:LYS:NZ	2:J:3987:ASP:OD2	2.49	0.41
2:G:167:ASP:OD1	2:G:168:ASP:N	2.53	0.41
2:G:349:GLN:HB2	2:G:356:TRP:CZ3	2.54	0.41
2:G:371:VAL:HG11	2:G:373:LYS:HG2	2.02	0.41
2:G:464:LYS:O	2:G:468:LEU:HG	2.20	0.41
2:G:657:THR:HB	2:G:1021:LEU:HG	2.02	0.41
2:G:911:HIS:HE1	2:G:918:ARG:NE	2.18	0.41
2:G:1088:TRP:HB2	2:G:1153:ILE:HG22	2.02	0.41
2:G:1090:PHE:HB2	2:G:1204:LEU:HA	2.02	0.41
2:G:2292:GLU:H	2:G:2292:GLU:CD	2.21	0.41
2:G:2340:PHE:HB2	2:G:2435:ARG:HE	1.86	0.41
2:G:2382:GLU:HA	2:G:2385:ARG:NE	2.36	0.41
2:G:2718:SER:OG	2:G:2909:ASP:O	2.25	0.41
2:G:2790:MET:O	2:G:2792:ARG:NE	2.52	0.41
2:G:2947:ASP:OD1	2:G:2947:ASP:N	2.54	0.41
2:G:3173:TYR:CG	2:G:3243:ILE:HG12	2.56	0.41
2:G:3193:CYS:O	2:G:3197:LEU:HG	2.21	0.41
2:G:3343:GLN:HB3	2:G:3344:PRO:HD3	2.02	0.41
2:G:3535:LEU:CD1	2:G:3539:ARG:HH12	2.33	0.41
2:G:3567:PRO:CB	2:G:3570:ARG:HH21	2.32	0.41
2:G:3771:HIS:CG	2:G:3812:VAL:HG12	2.55	0.41
2:J:102:LEU:HD21	2:J:105:HIS:CE1	2.56	0.41
2:J:214:VAL:HG13	2:J:274:LEU:HB2	2.02	0.41
2:J:3172:ILE:HD11	2:J:3190:LEU:HB3	2.02	0.41
2:J:3179:LYS:HE3	2:J:3179:LYS:HB3	1.95	0.41
2:J:3391:GLU:HA	2:J:3394:VAL:HG22	2.03	0.41
3:F:104:TYR:HD1	3:F:106:PRO:HD3	1.85	0.41
1:A:73:LYS:HB3	1:A:73:LYS:HE2	1.86	0.41
2:B:575:LEU:HD13	2:B:606:LEU:HA	2.02	0.41
2:B:997:ALA:O	2:B:1001:VAL:HG23	2.20	0.41
2:B:1637:MET:HG3	2:B:1696:HIS:ND1	2.36	0.41
2:B:2519:LEU:HD11	2:B:2572:THR:HG23	2.03	0.41
2:B:3049:LEU:HA	2:B:3053:ARG:NH2	2.35	0.41
2:E:705:ASN:N	2:E:705:ASN:HD22	2.19	0.41
2:E:997:ALA:O	2:E:1001:VAL:HG23	2.20	0.41
2:E:2479:LEU:HD22	2:E:2541:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:222:LEU:HB3	2:G:388:LEU:HD12	2.02	0.41
2:G:575:LEU:HD13	2:G:606:LEU:HA	2.02	0.41
2:G:1000:ARG:HH12	3:M:115:ASP:H	1.69	0.41
2:G:2311:PRO:O	2:G:2314:LEU:HG	2.20	0.41
2:G:3354:LEU:HD13	2:G:3415:TYR:HE2	1.86	0.41
2:J:473:ASN:O	2:J:477:LEU:HG	2.21	0.41
2:J:575:LEU:HD13	2:J:606:LEU:HA	2.02	0.41
2:J:904:HIS:CD2	2:J:907:LEU:H	2.39	0.41
2:J:2311:PRO:O	2:J:2314:LEU:HG	2.20	0.41
2:J:2368:LEU:HD23	2:J:2368:LEU:HA	1.88	0.41
2:J:4851:TYR:HD1	2:J:4916:PHE:CE1	2.39	0.41
2:B:222:LEU:HB3	2:B:388:LEU:HD12	2.02	0.41
2:B:473:ASN:O	2:B:477:LEU:HG	2.21	0.41
2:B:1757:ALA:O	2:B:1759:ARG:HD2	2.20	0.41
2:B:1849:LEU:HG	2:B:1945:TYR:CE2	2.56	0.41
2:B:2382:GLU:HA	2:B:2385:ARG:NE	2.35	0.41
2:B:4041:ALA:O	2:B:4045:VAL:HG23	2.20	0.41
2:E:102:LEU:HD21	2:E:105:HIS:CE1	2.56	0.41
2:E:275:ARG:HB3	2:E:278:GLN:HB2	2.01	0.41
2:E:898:ASP:O	2:E:902:ARG:N	2.54	0.41
2:E:1090:PHE:HB2	2:E:1204:LEU:HA	2.02	0.41
2:E:1658:ASP:N	2:E:1658:ASP:OD1	2.54	0.41
2:E:2262:GLY:O	2:E:2266:GLY:N	2.47	0.41
2:E:3186:LEU:HG	2:E:3190:LEU:HD21	2.02	0.41
2:E:3567:PRO:CB	2:E:3570:ARG:HH21	2.32	0.41
2:G:162:LYS:HG3	2:J:3984:ARG:HH22	1.86	0.41
2:G:788:LYS:HG2	2:G:1629:GLN:HB2	2.02	0.41
2:G:2165:LEU:HD11	2:G:2177:LEU:HB3	2.02	0.41
2:G:2575:ARG:NH1	2:G:2578:MET:HB3	2.36	0.41
2:G:3100:SER:HB3	2:G:3167:ARG:HE	1.85	0.41
2:G:3186:LEU:HG	2:G:3190:LEU:HD21	2.02	0.41
2:G:3316:LEU:O	2:G:3320:LEU:HG	2.20	0.41
2:G:4017:LEU:HD22	2:G:4139:ILE:HG21	2.03	0.41
2:G:4846:VAL:O	2:G:4850:LEU:HG	2.19	0.41
2:J:14:LEU:HD13	2:J:202:MET:HG2	2.02	0.41
2:J:222:LEU:HB3	2:J:388:LEU:HD12	2.02	0.41
2:J:878:ILE:HG21	3:K:107:TRP:HE1	1.85	0.41
2:J:936:GLY:HA3	2:J:1056:PRO:HB3	2.02	0.41
2:J:1126:GLY:HA3	2:J:1143:TRP:CE3	2.56	0.41
2:J:1658:ASP:N	2:J:1658:ASP:OD1	2.54	0.41
2:J:2292:GLU:H	2:J:2292:GLU:CD	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2414:ASN:HB2	2:J:2417:HIS:CE1	2.56	0.41
2:J:2672:LEU:HD11	2:J:2711:PRO:HD2	2.03	0.41
2:J:4546:VAL:HA	2:J:4549:VAL:HG22	2.03	0.41
3:C:83:ASN:OD1	3:C:83:ASN:N	2.53	0.41
1:H:88:PRO:HB2	2:G:1680:ARG:NH1	2.36	0.41
2:B:232:THR:OG1	2:B:248:GLU:HG2	2.21	0.41
2:B:2311:PRO:O	2:B:2314:LEU:HG	2.20	0.41
2:B:2758:PHE:O	2:B:2762:THR:HG23	2.21	0.41
2:B:2765:LYS:HD3	2:B:2765:LYS:HA	1.67	0.41
2:B:2871:LEU:HD11	2:B:2927:LEU:HD11	2.03	0.41
2:B:3552:PHE:HA	2:B:3555:ASN:OD1	2.21	0.41
2:E:411:TYR:HB2	2:E:486:LEU:HD21	2.02	0.41
2:E:664:PHE:CE1	2:E:746:CYS:HB2	2.56	0.41
2:E:883:ALA:O	2:E:887:ILE:HG13	2.20	0.41
2:E:2414:ASN:HB2	2:E:2417:HIS:CE1	2.56	0.41
2:E:2758:PHE:O	2:E:2762:THR:HG23	2.20	0.41
2:E:2871:LEU:HD11	2:E:2927:LEU:HD11	2.03	0.41
2:E:3347:SER:HB2	2:E:3414:ARG:HG3	2.03	0.41
2:G:473:ASN:O	2:G:477:LEU:HG	2.21	0.41
2:G:866:HIS:CD2	2:G:869:ARG:HH21	2.39	0.41
2:G:1126:GLY:HA3	2:G:1143:TRP:CE3	2.56	0.41
2:G:2285:GLU:H	2:G:2285:GLU:HG2	1.69	0.41
2:G:2522:LEU:HD11	2:G:2569:PHE:CE1	2.55	0.41
2:G:2672:LEU:HD12	2:G:2672:LEU:HA	1.81	0.41
2:G:3347:SER:HB2	2:G:3414:ARG:HG3	2.03	0.41
2:G:3545:THR:O	2:G:3549:VAL:HG13	2.21	0.41
2:G:3592:ILE:HG12	2:G:3595:ARG:NH2	2.35	0.41
2:G:3592:ILE:HA	2:G:3595:ARG:HE	1.86	0.41
2:G:3809:ASN:HB3	2:G:3812:VAL:CG2	2.48	0.41
2:J:1849:LEU:HG	2:J:1945:TYR:CE2	2.56	0.41
2:J:2359:ARG:HD3	2:J:2359:ARG:HA	1.82	0.41
2:J:2479:LEU:HD22	2:J:2541:PHE:HZ	1.86	0.41
2:J:2654:TYR:HB2	2:J:2661:TRP:CE3	2.55	0.41
1:A:17:LYS:HG3	1:A:18:LYS:N	2.35	0.41
2:B:275:ARG:HB3	2:B:278:GLN:HB2	2.02	0.41
2:B:551:LEU:HD11	2:B:564:LEU:HD22	2.02	0.41
2:B:866:HIS:CD2	2:B:869:ARG:HH21	2.39	0.41
2:B:1090:PHE:HB2	2:B:1204:LEU:HA	2.02	0.41
2:B:2165:LEU:HD11	2:B:2177:LEU:HB3	2.02	0.41
2:B:2419:GLY:O	2:B:2423:MET:HG2	2.21	0.41
2:B:2617:SER:OG	2:B:2618:MET:SD	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2790:MET:O	2:B:2792:ARG:NE	2.52	0.41
2:B:3354:LEU:HD13	2:B:3415:TYR:HE2	1.86	0.41
2:B:3835:LEU:HD22	2:B:3880:PHE:CZ	2.56	0.41
2:B:4852:THR:HG21	2:B:4883:TYR:HD1	1.85	0.41
2:E:1126:GLY:HA3	2:E:1143:TRP:CE3	2.56	0.41
2:E:1637:MET:HG3	2:E:1696:HIS:ND1	2.36	0.41
2:E:2382:GLU:HA	2:E:2385:ARG:NE	2.36	0.41
2:E:2664:PHE:N	2:E:2664:PHE:CD1	2.88	0.41
2:E:3214:ASN:HB2	2:E:3304:CYS:HB3	2.02	0.41
2:E:3391:GLU:HA	2:E:3394:VAL:HG22	2.03	0.41
2:E:4773:VAL:O	2:E:4777:ILE:HG13	2.20	0.41
2:E:4851:TYR:HD1	2:E:4916:PHE:CE1	2.39	0.41
2:E:4992:LEU:HD13	2:E:5014:TYR:CZ	2.56	0.41
2:G:214:VAL:HG13	2:G:274:LEU:HB2	2.02	0.41
2:G:548:VAL:HG21	2:G:582:HIS:CD2	2.52	0.41
2:G:551:LEU:HD11	2:G:564:LEU:HD22	2.02	0.41
2:G:1637:MET:HG3	2:G:1696:HIS:ND1	2.36	0.41
2:G:1849:LEU:HG	2:G:1945:TYR:CE2	2.56	0.41
2:G:1931:LEU:HD13	2:G:1935:VAL:HG12	2.03	0.41
2:G:2331:TYR:O	2:G:2335:LEU:HG	2.21	0.41
2:G:2414:ASN:HB2	2:G:2417:HIS:CE1	2.56	0.41
2:G:2652:TRP:CD1	2:G:2652:TRP:C	2.93	0.41
2:G:2672:LEU:HD11	2:G:2711:PRO:HD2	2.03	0.41
2:G:2912:THR:OG1	2:G:2913:ALA:N	2.54	0.41
2:G:3214:ASN:HB2	2:G:3304:CYS:HB3	2.02	0.41
2:G:3316:LEU:HD13	2:G:3316:LEU:HA	1.92	0.41
2:G:3391:GLU:HA	2:G:3394:VAL:HG22	2.03	0.41
2:G:3683:GLN:O	2:G:3687:GLU:HB2	2.21	0.41
2:G:4852:THR:HG21	2:G:4883:TYR:HD1	1.85	0.41
2:J:911:HIS:HE1	2:J:918:ARG:NE	2.18	0.41
2:J:911:HIS:HB2	2:J:913:LEU:HG	2.02	0.41
2:J:1252:HIS:CE1	2:J:1254:HIS:HB2	2.56	0.41
2:J:2122:SER:O	2:J:2126:ARG:HG3	2.20	0.41
2:J:2165:LEU:HD11	2:J:2177:LEU:HB3	2.02	0.41
2:J:2515:GLN:CA	2:J:2568:LEU:HD21	2.48	0.41
2:J:2566:ALA:O	2:J:2569:PHE:HB2	2.21	0.41
2:J:2664:PHE:CD1	2:J:2664:PHE:N	2.88	0.41
2:J:2947:ASP:OD1	2:J:2947:ASP:N	2.54	0.41
2:J:3343:GLN:HB3	2:J:3344:PRO:HD3	2.02	0.41
2:J:3354:LEU:HD13	2:J:3415:TYR:HE2	1.86	0.41
2:J:3552:PHE:HA	2:J:3555:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3683:GLN:O	2:J:3687:GLU:HB2	2.21	0.41
2:J:4041:ALA:O	2:J:4045:VAL:HG23	2.20	0.41
2:J:4968:PHE:O	2:J:4974:GLY:HA3	2.20	0.41
3:C:63:VAL:HA	3:C:67:PHE:HE2	1.85	0.41
3:C:85:LEU:HD23	3:C:85:LEU:HA	1.92	0.41
3:C:101:PRO:O	3:C:104:TYR:N	2.48	0.41
3:F:109:THR:OG1	3:F:110:PRO:HD3	2.21	0.41
3:M:101:PRO:O	3:M:104:TYR:N	2.48	0.41
1:D:17:LYS:HG3	1:D:18:LYS:N	2.35	0.41
1:D:49:ARG:HB2	1:D:52:LYS:HG2	2.03	0.41
1:I:88:PRO:HB2	2:J:1680:ARG:NH1	2.36	0.41
2:B:214:VAL:HA	2:B:341:TYR:CD2	2.56	0.41
2:B:411:TYR:HB2	2:B:486:LEU:HD21	2.02	0.41
2:B:866:HIS:ND1	2:B:870:ILE:HB	2.36	0.41
2:B:1126:GLY:HA3	2:B:1143:TRP:CE3	2.56	0.41
2:B:2562:ILE:HG23	2:B:2569:PHE:CZ	2.56	0.41
2:E:222:LEU:HB3	2:E:388:LEU:HD12	2.02	0.41
2:E:464:LYS:O	2:E:468:LEU:HG	2.20	0.41
2:E:691:GLY:HA3	2:E:712:TYR:CD1	2.56	0.41
2:E:866:HIS:CD2	2:E:869:ARG:HH21	2.39	0.41
2:E:878:ILE:HG21	3:F:107:TRP:CE2	2.55	0.41
2:E:1131:ARG:HB2	2:E:1179:PHE:CZ	2.56	0.41
2:E:3100:SER:HB3	2:E:3167:ARG:HE	1.85	0.41
2:E:3193:CYS:O	2:E:3197:LEU:HG	2.21	0.41
2:E:3893:GLU:HA	2:E:3967:GLU:OE2	2.21	0.41
2:E:4017:LEU:HD22	2:E:4139:ILE:HG21	2.03	0.41
2:G:102:LEU:HD21	2:G:105:HIS:CE1	2.56	0.41
2:G:424:LYS:HE2	2:G:424:LYS:HB2	1.92	0.41
2:G:911:HIS:HB2	2:G:913:LEU:HG	2.02	0.41
2:G:3552:PHE:HA	2:G:3555:ASN:OD1	2.21	0.41
2:J:575:LEU:HA	2:J:578:ILE:HG12	2.03	0.41
2:J:937:CYS:HB3	2:J:1053:ILE:HB	2.02	0.41
2:J:2340:PHE:HB2	2:J:2435:ARG:HE	1.86	0.41
2:J:3137:LEU:HD12	2:J:3137:LEU:HA	1.91	0.41
2:J:3535:LEU:CD1	2:J:3539:ARG:HH12	2.33	0.41
2:J:4666:VAL:O	2:J:4670:ILE:HG12	2.21	0.41
1:H:49:ARG:HB2	1:H:52:LYS:HG2	2.03	0.40
1:I:29:MET:HG3	1:I:30:LEU:O	2.21	0.40
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.04	0.40
2:B:691:GLY:HA3	2:B:712:TYR:CD1	2.56	0.40
2:B:788:LYS:HG2	2:B:1629:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2479:LEU:HD22	2:B:2541:PHE:HZ	1.86	0.40
2:B:2801:ASP:HA	2:B:2804:ILE:HG12	2.01	0.40
2:B:2947:ASP:OD1	2:B:2947:ASP:N	2.54	0.40
2:B:3173:TYR:CG	2:B:3243:ILE:HG12	2.56	0.40
2:B:3277:LEU:HB3	2:B:3315:LEU:HD13	2.03	0.40
2:B:3354:LEU:HD13	2:B:3415:TYR:CE2	2.57	0.40
2:B:3592:ILE:HA	2:B:3595:ARG:HE	1.86	0.40
2:B:4851:TYR:HD1	2:B:4916:PHE:CE1	2.39	0.40
2:E:105:HIS:O	2:E:150:MET:HG2	2.22	0.40
2:E:232:THR:OG1	2:E:248:GLU:HG2	2.21	0.40
2:E:294:THR:N	2:E:298:GLY:O	2.39	0.40
2:E:473:ASN:O	2:E:477:LEU:HG	2.21	0.40
2:E:2575:ARG:NH1	2:E:2577:ILE:HG23	2.36	0.40
2:E:2947:ASP:OD1	2:E:2947:ASP:N	2.54	0.40
2:E:3535:LEU:CD1	2:E:3539:ARG:HH12	2.33	0.40
2:G:2419:GLY:O	2:G:2423:MET:HG2	2.21	0.40
2:G:2566:ALA:O	2:G:2569:PHE:HB2	2.21	0.40
2:G:3136:LEU:O	2:G:3140:LEU:HB3	2.20	0.40
2:G:3471:THR:O	2:G:3475:LYS:HG3	2.21	0.40
2:J:866:HIS:ND1	2:J:870:ILE:HB	2.36	0.40
2:J:1131:ARG:HB2	2:J:1179:PHE:CZ	2.56	0.40
2:J:1261:ASP:N	2:J:1261:ASP:OD1	2.53	0.40
2:J:2382:GLU:HA	2:J:2385:ARG:NE	2.35	0.40
2:J:2871:LEU:HD11	2:J:2927:LEU:HD11	2.03	0.40
2:J:3193:CYS:O	2:J:3197:LEU:HG	2.21	0.40
2:J:3592:ILE:HA	2:J:3595:ARG:HE	1.86	0.40
3:F:28:ILE:HD12	3:F:28:ILE:HA	1.93	0.40
1:A:49:ARG:HB2	1:A:52:LYS:HG2	2.03	0.40
1:A:57:LYS:HB2	1:A:57:LYS:HE2	1.75	0.40
1:H:26:TYR:HB2	1:H:101:VAL:HG12	2.03	0.40
2:B:936:GLY:HA3	2:B:1056:PRO:HB3	2.01	0.40
2:B:1252:HIS:CE1	2:B:1254:HIS:HB2	2.56	0.40
2:B:1733:GLU:HG2	2:B:2201:LEU:HD23	2.03	0.40
2:B:2359:ARG:HD3	2:B:2359:ARG:HA	1.82	0.40
2:B:3100:SER:HB3	2:B:3167:ARG:HE	1.85	0.40
2:B:3137:LEU:HD12	2:B:3137:LEU:HA	1.91	0.40
2:B:4546:VAL:HA	2:B:4549:VAL:HG22	2.03	0.40
2:B:4898:GLY:HA2	2:B:4901:ILE:HD12	2.03	0.40
2:E:664:PHE:HB3	2:E:811:CYS:SG	2.62	0.40
2:E:3173:TYR:CG	2:E:3243:ILE:HG12	2.56	0.40
2:E:3354:LEU:HD13	2:E:3415:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4666:VAL:O	2:E:4670:ILE:HG12	2.21	0.40
2:E:4928:LEU:HA	2:E:4928:LEU:HD23	1.89	0.40
2:G:16:THR:HA	2:G:69:LEU:HD22	2.04	0.40
2:G:664:PHE:CE1	2:G:746:CYS:HB2	2.55	0.40
2:G:4655:PHE:O	2:G:4659:ILE:HG12	2.20	0.40
2:G:4847:VAL:O	2:G:4851:TYR:HD2	2.04	0.40
2:G:4898:GLY:HA2	2:G:4901:ILE:HD12	2.03	0.40
2:J:1637:MET:HG3	2:J:1696:HIS:ND1	2.36	0.40
2:J:2912:THR:OG1	2:J:2913:ALA:N	2.54	0.40
2:J:3985:LEU:O	2:J:3989:VAL:HG23	2.21	0.40
3:K:109:THR:OG1	3:K:110:PRO:HD3	2.21	0.40
1:A:16:PRO:HG3	1:A:103:LEU:HD21	2.03	0.40
1:H:40:ARG:H	1:H:40:ARG:HG2	1.72	0.40
2:B:105:HIS:O	2:B:150:MET:HG2	2.22	0.40
2:B:617:ASN:O	2:B:621:ILE:HG13	2.22	0.40
2:B:2352:VAL:O	2:B:2356:LEU:HG	2.22	0.40
2:B:2414:ASN:HB2	2:B:2417:HIS:CE1	2.56	0.40
2:B:3214:ASN:HB2	2:B:3304:CYS:HB3	2.03	0.40
2:B:3347:SER:HB2	2:B:3414:ARG:HG3	2.03	0.40
2:B:3989:VAL:HG13	2:B:4023:MET:HE2	2.03	0.40
2:E:548:VAL:HG21	2:E:582:HIS:CD2	2.52	0.40
2:E:904:HIS:CD2	2:E:907:LEU:H	2.39	0.40
2:E:960:MET:SD	2:E:960:MET:N	2.75	0.40
2:E:2331:TYR:O	2:E:2335:LEU:HG	2.21	0.40
2:E:2575:ARG:O	2:E:2578:MET:HG3	2.21	0.40
2:E:3136:LEU:O	2:E:3140:LEU:HB3	2.20	0.40
2:E:3552:PHE:HA	2:E:3555:ASN:OD1	2.21	0.40
2:G:411:TYR:HB2	2:G:486:LEU:HD21	2.02	0.40
2:G:898:ASP:O	2:G:902:ARG:N	2.54	0.40
2:G:936:GLY:HA3	2:G:1056:PRO:HB3	2.01	0.40
2:G:937:CYS:HB3	2:G:1053:ILE:HB	2.02	0.40
2:G:1092:PHE:HE2	2:G:1100:MET:HE3	1.86	0.40
2:G:2310:CYS:SG	2:G:2313:LEU:HB2	2.62	0.40
2:G:2758:PHE:O	2:G:2762:THR:HG23	2.20	0.40
2:G:3246:LEU:HD22	2:G:3280:TYR:CE2	2.56	0.40
2:G:4020:GLN:O	2:G:4024:VAL:HG23	2.21	0.40
2:J:866:HIS:CD2	2:J:869:ARG:HH21	2.39	0.40
2:J:2575:ARG:NH1	2:J:2577:ILE:HG23	2.37	0.40
2:J:3186:LEU:HG	2:J:3190:LEU:HD21	2.02	0.40
2:J:3347:SER:HB2	2:J:3414:ARG:HG3	2.03	0.40
2:J:3545:THR:O	2:J:3549:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3731:LYS:HZ2	2:J:3735:LEU:HD21	1.86	0.40
1:A:29:MET:HG3	1:A:30:LEU:O	2.21	0.40
2:B:1509:ILE:HG22	2:B:1511:HIS:H	1.86	0.40
2:B:2340:PHE:HB2	2:B:2435:ARG:HE	1.86	0.40
2:B:2867:LEU:HB2	2:B:2928:LYS:HZ3	1.84	0.40
2:B:2912:THR:OG1	2:B:2913:ALA:N	2.54	0.40
2:B:3462:ASN:HB2	2:B:3464:ILE:HG12	2.04	0.40
2:B:4020:GLN:O	2:B:4024:VAL:HG23	2.21	0.40
2:B:4666:VAL:O	2:B:4670:ILE:HG12	2.22	0.40
2:E:1252:HIS:CE1	2:E:1254:HIS:HB2	2.56	0.40
2:E:1981:MET:CE	2:E:1981:MET:HA	2.52	0.40
2:E:3285:TRP:CD1	2:E:3312:LEU:HD11	2.56	0.40
2:G:2479:LEU:HD22	2:G:2541:PHE:HZ	1.86	0.40
2:G:2578:MET:HE2	2:G:2578:MET:HB2	2.01	0.40
2:G:4048:LEU:HD23	2:G:4048:LEU:HA	1.88	0.40
2:J:2331:TYR:O	2:J:2335:LEU:HG	2.21	0.40
2:J:3462:ASN:HB2	2:J:3464:ILE:HG12	2.04	0.40
2:J:3471:THR:O	2:J:3475:LYS:HG3	2.21	0.40
2:J:3892:CYS:SG	2:J:3903:LEU:HD12	2.62	0.40
3:M:83:ASN:OD1	3:M:83:ASN:N	2.53	0.40
1:A:3:GLU:HB2	1:A:75:THR:HB	2.02	0.40
1:D:29:MET:HG3	1:D:30:LEU:O	2.21	0.40
2:B:16:THR:HA	2:B:69:LEU:HD22	2.04	0.40
2:B:1131:ARG:HB2	2:B:1179:PHE:CZ	2.56	0.40
2:B:1931:LEU:HD13	2:B:1935:VAL:HG12	2.03	0.40
2:B:2541:PHE:N	2:B:2541:PHE:CD1	2.87	0.40
2:E:2626:LEU:CD2	2:E:2640:PRO:HB3	2.51	0.40
2:E:2912:THR:OG1	2:E:2913:ALA:N	2.54	0.40
2:E:3835:LEU:HD22	2:E:3880:PHE:CZ	2.56	0.40
2:E:3892:CYS:SG	2:E:3903:LEU:HD12	2.62	0.40
2:E:4631:PHE:CE2	2:E:4633:GLU:HB2	2.57	0.40
2:G:866:HIS:ND1	2:G:870:ILE:HB	2.36	0.40
2:G:1436:SER:OG	2:G:1565:GLU:HB2	2.22	0.40
2:G:1815:LEU:O	2:G:1819:VAL:HG23	2.22	0.40
2:G:2871:LEU:HD11	2:G:2927:LEU:HD11	2.03	0.40
2:G:3154:ASP:OD1	2:G:3154:ASP:N	2.53	0.40
2:J:105:HIS:O	2:J:150:MET:HG2	2.22	0.40
2:J:424:LYS:HE2	2:J:424:LYS:HB2	1.92	0.40
2:J:1088:TRP:HB2	2:J:1153:ILE:HG22	2.03	0.40
2:J:1733:GLU:HG2	2:J:2201:LEU:HD23	2.03	0.40
2:J:2310:CYS:SG	2:J:2313:LEU:HB2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2419:GLY:O	2:J:2423:MET:HG2	2.21	0.40
2:J:2575:ARG:NH1	2:J:2578:MET:HB3	2.37	0.40
2:J:2575:ARG:O	2:J:2578:MET:HG3	2.21	0.40
2:J:3214:ASN:HB2	2:J:3304:CYS:HB3	2.02	0.40
2:J:3893:GLU:HA	2:J:3967:GLU:OE2	2.21	0.40
2:J:4631:PHE:CE2	2:J:4633:GLU:HB2	2.57	0.40
2:J:4847:VAL:O	2:J:4851:TYR:HD2	2.04	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	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	I	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	B	4264/5027 (85%)	4160 (98%)	103 (2%)	1 (0%)	100	100
2	E	4264/5027 (85%)	4162 (98%)	102 (2%)	0	100	100
2	G	4280/5027 (85%)	4175 (98%)	105 (2%)	0	100	100
2	J	4264/5027 (85%)	4161 (98%)	103 (2%)	0	100	100
3	C	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	F	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	K	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	M	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
All	All	17988/21084 (85%)	17529 (97%)	458 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	D	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	H	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	I	87/88 (99%)	85 (98%)	2 (2%)	45	68
2	B	3662/4270 (86%)	3580 (98%)	82 (2%)	47	69
2	E	3662/4270 (86%)	3581 (98%)	81 (2%)	47	69
2	G	3674/4270 (86%)	3594 (98%)	80 (2%)	47	69
2	J	3662/4270 (86%)	3580 (98%)	82 (2%)	47	69
3	C	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	F	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	K	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	M	103/114 (90%)	99 (96%)	4 (4%)	27	55
All	All	15420/17888 (86%)	15071 (98%)	349 (2%)	46	68

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	94	ASN
1	D	29	MET
1	D	94	ASN
1	H	29	MET
1	H	94	ASN
1	I	29	MET
1	I	94	ASN
2	B	116	MET
2	B	125	ARG

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Mol	Chain	Res	Type
2	B	127	MET
2	B	269	TRP
2	B	280	LEU
2	B	283	ARG
2	B	299	LEU
2	B	306	LYS
2	B	341	TYR
2	B	379	HIS
2	B	631	LEU
2	B	702	TRP
2	B	866	HIS
2	B	877	ASN
2	B	902	ARG
2	B	955	LEU
2	B	959	TYR
2	B	960	MET
2	B	1112	ASP
2	B	1133	HIS
2	B	1143	TRP
2	B	1229	ASN
2	B	1270	LEU
2	B	1286	MET
2	B	1421	ARG
2	B	1435	TYR
2	B	1532	ASN
2	B	1647	CYS
2	B	1981	MET
2	B	2178	MET
2	B	2256	TYR
2	B	2305	CYS
2	B	2312	MET
2	B	2326	CYS
2	B	2340	PHE
2	B	2392	ARG
2	B	2475	GLN
2	B	2530	MET
2	B	2574	HIS
2	B	2591	ARG
2	B	2618	MET
2	B	2634	ASN
2	B	2664	PHE
2	B	2688	HIS

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Mol	Chain	Res	Type
2	B	2738	ARG
2	B	2797	PHE
2	B	2806	ARG
2	B	2827	ARG
2	B	2869	ARG
2	B	2872	GLN
2	B	2914	LYS
2	B	2947	ASP
2	B	2992	GLU
2	B	3034	LYS
2	B	3043	PHE
2	B	3053	ARG
2	B	3096	PHE
2	B	3144	PHE
2	B	3158	LEU
2	B	3239	MET
2	B	3334	TRP
2	B	3348	ARG
2	B	3355	HIS
2	B	3366	ARG
2	B	3451	PHE
2	B	3516	LYS
2	B	3720	TYR
2	B	3782	MET
2	B	3933	PHE
2	B	3966	THR
2	B	4000	MET
2	B	4042	ARG
2	B	4044	MET
2	B	4077	PHE
2	B	4080	TYR
2	B	4159	ARG
2	B	4161	ARG
2	B	4207	MET
2	B	4655	PHE
2	B	4767	TRP
2	B	4844	LEU
2	B	4933	GLN
2	E	116	MET
2	E	125	ARG
2	E	127	MET
2	E	269	TRP

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Mol	Chain	Res	Type
2	E	280	LEU
2	E	283	ARG
2	E	299	LEU
2	E	306	LYS
2	E	341	TYR
2	E	379	HIS
2	E	631	LEU
2	E	702	TRP
2	E	866	HIS
2	E	877	ASN
2	E	902	ARG
2	E	955	LEU
2	E	959	TYR
2	E	960	MET
2	E	1112	ASP
2	E	1133	HIS
2	E	1143	TRP
2	E	1170	MET
2	E	1229	ASN
2	E	1270	LEU
2	E	1286	MET
2	E	1421	ARG
2	E	1435	TYR
2	E	1532	ASN
2	E	1647	CYS
2	E	1981	MET
2	E	2178	MET
2	E	2256	TYR
2	E	2305	CYS
2	E	2312	MET
2	E	2326	CYS
2	E	2340	PHE
2	E	2392	ARG
2	E	2475	GLN
2	E	2530	MET
2	E	2591	ARG
2	E	2618	MET
2	E	2634	ASN
2	E	2664	PHE
2	E	2688	HIS
2	E	2738	ARG
2	E	2797	PHE

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Mol	Chain	Res	Type
2	E	2806	ARG
2	E	2827	ARG
2	E	2869	ARG
2	E	2872	GLN
2	E	2914	LYS
2	E	2947	ASP
2	E	2992	GLU
2	E	3034	LYS
2	E	3043	PHE
2	E	3053	ARG
2	E	3096	PHE
2	E	3144	PHE
2	E	3158	LEU
2	E	3239	MET
2	E	3334	TRP
2	E	3348	ARG
2	E	3355	HIS
2	E	3366	ARG
2	E	3451	PHE
2	E	3516	LYS
2	E	3720	TYR
2	E	3782	MET
2	E	3933	PHE
2	E	4000	MET
2	E	4042	ARG
2	E	4044	MET
2	E	4077	PHE
2	E	4080	TYR
2	E	4159	ARG
2	E	4161	ARG
2	E	4207	MET
2	E	4655	PHE
2	E	4767	TRP
2	E	4844	LEU
2	E	4933	GLN
2	G	116	MET
2	G	125	ARG
2	G	127	MET
2	G	269	TRP
2	G	280	LEU
2	G	283	ARG
2	G	299	LEU

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Mol	Chain	Res	Type
2	G	306	LYS
2	G	341	TYR
2	G	379	HIS
2	G	631	LEU
2	G	702	TRP
2	G	866	HIS
2	G	877	ASN
2	G	902	ARG
2	G	955	LEU
2	G	959	TYR
2	G	960	MET
2	G	1112	ASP
2	G	1133	HIS
2	G	1143	TRP
2	G	1229	ASN
2	G	1270	LEU
2	G	1286	MET
2	G	1421	ARG
2	G	1435	TYR
2	G	1532	ASN
2	G	1647	CYS
2	G	1981	MET
2	G	2178	MET
2	G	2256	TYR
2	G	2305	CYS
2	G	2312	MET
2	G	2326	CYS
2	G	2340	PHE
2	G	2392	ARG
2	G	2475	GLN
2	G	2530	MET
2	G	2591	ARG
2	G	2618	MET
2	G	2634	ASN
2	G	2664	PHE
2	G	2688	HIS
2	G	2738	ARG
2	G	2797	PHE
2	G	2806	ARG
2	G	2827	ARG
2	G	2869	ARG
2	G	2872	GLN

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Mol	Chain	Res	Type
2	G	2914	LYS
2	G	2947	ASP
2	G	2992	GLU
2	G	3034	LYS
2	G	3043	PHE
2	G	3053	ARG
2	G	3096	PHE
2	G	3144	PHE
2	G	3158	LEU
2	G	3239	MET
2	G	3334	TRP
2	G	3348	ARG
2	G	3355	HIS
2	G	3366	ARG
2	G	3451	PHE
2	G	3516	LYS
2	G	3720	TYR
2	G	3782	MET
2	G	3933	PHE
2	G	4000	MET
2	G	4042	ARG
2	G	4044	MET
2	G	4077	PHE
2	G	4080	TYR
2	G	4159	ARG
2	G	4161	ARG
2	G	4207	MET
2	G	4655	PHE
2	G	4767	TRP
2	G	4844	LEU
2	G	4933	GLN
2	J	116	MET
2	J	125	ARG
2	J	127	MET
2	J	269	TRP
2	J	280	LEU
2	J	283	ARG
2	J	299	LEU
2	J	306	LYS
2	J	341	TYR
2	J	379	HIS
2	J	631	LEU

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Mol	Chain	Res	Type
2	J	702	TRP
2	J	866	HIS
2	J	877	ASN
2	J	902	ARG
2	J	955	LEU
2	J	959	TYR
2	J	960	MET
2	J	1112	ASP
2	J	1133	HIS
2	J	1143	TRP
2	J	1229	ASN
2	J	1270	LEU
2	J	1286	MET
2	J	1421	ARG
2	J	1435	TYR
2	J	1532	ASN
2	J	1647	CYS
2	J	1981	MET
2	J	2178	MET
2	J	2256	TYR
2	J	2305	CYS
2	J	2312	MET
2	J	2326	CYS
2	J	2340	PHE
2	J	2392	ARG
2	J	2475	GLN
2	J	2530	MET
2	J	2591	ARG
2	J	2618	MET
2	J	2634	ASN
2	J	2664	PHE
2	J	2688	HIS
2	J	2738	ARG
2	J	2797	PHE
2	J	2806	ARG
2	J	2827	ARG
2	J	2869	ARG
2	J	2872	GLN
2	J	2914	LYS
2	J	2947	ASP
2	J	2992	GLU
2	J	3034	LYS

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Mol	Chain	Res	Type
2	J	3043	PHE
2	J	3053	ARG
2	J	3096	PHE
2	J	3144	PHE
2	J	3158	LEU
2	J	3239	MET
2	J	3250	MET
2	J	3334	TRP
2	J	3348	ARG
2	J	3355	HIS
2	J	3366	ARG
2	J	3451	PHE
2	J	3516	LYS
2	J	3720	TYR
2	J	3782	MET
2	J	3933	PHE
2	J	4000	MET
2	J	4042	ARG
2	J	4044	MET
2	J	4077	PHE
2	J	4080	TYR
2	J	4159	ARG
2	J	4161	ARG
2	J	4207	MET
2	J	4655	PHE
2	J	4767	TRP
2	J	4844	LEU
2	J	4933	GLN
2	J	5014	TYR
3	C	37	TYR
3	C	98	ASP
3	C	104	TYR
3	C	105	ASN
3	F	37	TYR
3	F	98	ASP
3	F	104	TYR
3	F	105	ASN
3	K	37	TYR
3	K	98	ASP
3	K	104	TYR
3	K	105	ASN
3	M	37	TYR

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Mol	Chain	Res	Type
3	M	98	ASP
3	M	104	TYR
3	M	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	65	GLN
1	H	25	HIS
1	I	25	HIS
2	B	23	GLN
2	B	203	ASN
2	B	273	HIS
2	B	879	HIS
2	B	904	HIS
2	B	1220	GLN
2	B	1300	HIS
2	B	3318	ASN
2	B	3605	HIS
2	B	3960	GLN
2	B	3970	GLN
2	E	23	GLN
2	E	203	ASN
2	E	273	HIS
2	E	879	HIS
2	E	904	HIS
2	E	1300	HIS
2	E	2574	HIS
2	E	3311	HIS
2	E	3318	ASN
2	E	3605	HIS
2	E	3960	GLN
2	E	3970	GLN
2	E	4714	ASN
2	G	23	GLN
2	G	203	ASN
2	G	273	HIS
2	G	879	HIS
2	G	1300	HIS
2	G	2574	HIS
2	G	3318	ASN

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Mol	Chain	Res	Type
2	G	3605	HIS
2	G	3860	ASN
2	G	3870	ASN
2	G	3960	GLN
2	G	3970	GLN
2	J	23	GLN
2	J	203	ASN
2	J	273	HIS
2	J	879	HIS
2	J	904	HIS
2	J	1220	GLN
2	J	1300	HIS
2	J	3318	ASN
2	J	3605	HIS
3	C	105	ASN
3	F	105	ASN
3	K	105	ASN
3	M	105	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CFF	E	5103	-	8,15,15	2.39	3 (37%)	8,23,23	1.18	1 (12%)
6	CFF	G	5103	-	8,15,15	2.40	3 (37%)	8,23,23	1.16	1 (12%)
6	CFF	J	5103	-	8,15,15	2.40	3 (37%)	8,23,23	1.18	1 (12%)
5	ATP	E	5102	-	26,33,33	0.59	0	31,52,52	0.81	2 (6%)
5	ATP	B	5102	-	26,33,33	0.59	0	31,52,52	0.81	2 (6%)
6	CFF	B	5103	-	8,15,15	2.39	3 (37%)	8,23,23	1.16	1 (12%)
5	ATP	G	5102	-	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
5	ATP	J	5102	-	26,33,33	0.60	0	31,52,52	0.81	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	E	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	J	5103	-	-	-	0/2/2/2
5	ATP	E	5102	-	-	7/18/38/38	0/3/3/3
5	ATP	B	5102	-	-	7/18/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
5	ATP	G	5102	-	-	7/18/38/38	0/3/3/3
5	ATP	J	5102	-	-	7/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5103	CFF	C5-C4	4.57	1.45	1.39
6	J	5103	CFF	C5-C4	4.49	1.45	1.39
6	G	5103	CFF	C5-C4	4.47	1.45	1.39
6	E	5103	CFF	C5-C4	4.46	1.45	1.39
6	G	5103	CFF	C5-C6	4.35	1.48	1.41
6	J	5103	CFF	C5-C6	4.34	1.48	1.41
6	E	5103	CFF	C5-C6	4.34	1.48	1.41
6	B	5103	CFF	C5-C6	4.30	1.48	1.41
6	E	5103	CFF	C6-N1	2.29	1.41	1.38
6	J	5103	CFF	C6-N1	2.28	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5103	CFF	C6-N1	2.27	1.41	1.38
6	B	5103	CFF	C6-N1	2.12	1.41	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	5102	ATP	C5-C6-N6	2.29	123.84	120.35
6	J	5103	CFF	C5-C6-N1	-2.28	115.77	118.20
5	B	5102	ATP	C5-C6-N6	2.27	123.80	120.35
5	E	5102	ATP	C5-C6-N6	2.27	123.80	120.35
5	J	5102	ATP	C5-C6-N6	2.27	123.80	120.35
6	B	5103	CFF	C5-C6-N1	-2.25	115.80	118.20
6	G	5103	CFF	C5-C6-N1	-2.24	115.81	118.20
6	E	5103	CFF	C5-C6-N1	-2.24	115.81	118.20
5	J	5102	ATP	PB-O3B-PG	2.03	139.80	132.83
5	E	5102	ATP	PB-O3B-PG	2.02	139.77	132.83
5	B	5102	ATP	PB-O3B-PG	2.01	139.74	132.83
5	G	5102	ATP	PB-O3B-PG	2.01	139.74	132.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	PB-O3B-PG-O2G
5	B	5102	ATP	C5'-O5'-PA-O3A
5	E	5102	ATP	PB-O3B-PG-O2G
5	E	5102	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	PB-O3B-PG-O2G
5	G	5102	ATP	C5'-O5'-PA-O3A
5	J	5102	ATP	PB-O3B-PG-O2G
5	J	5102	ATP	C5'-O5'-PA-O3A
5	B	5102	ATP	O4'-C4'-C5'-O5'
5	E	5102	ATP	O4'-C4'-C5'-O5'
5	G	5102	ATP	O4'-C4'-C5'-O5'
5	J	5102	ATP	O4'-C4'-C5'-O5'
5	B	5102	ATP	C3'-C4'-C5'-O5'
5	E	5102	ATP	C3'-C4'-C5'-O5'
5	G	5102	ATP	C3'-C4'-C5'-O5'
5	J	5102	ATP	C3'-C4'-C5'-O5'
5	B	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O1A
5	G	5102	ATP	C5'-O5'-PA-O1A

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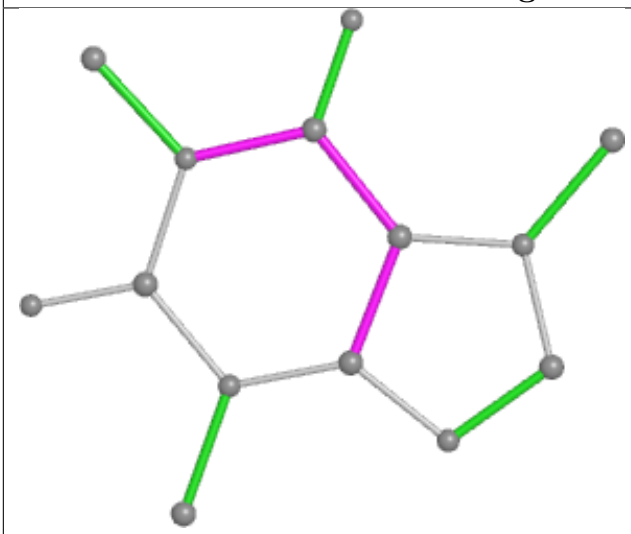
Mol	Chain	Res	Type	Atoms
5	J	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	PB-O3B-PG-O1G
5	E	5102	ATP	PB-O3B-PG-O1G
5	G	5102	ATP	PB-O3B-PG-O1G
5	J	5102	ATP	PB-O3B-PG-O1G
5	B	5102	ATP	PB-O3B-PG-O3G
5	E	5102	ATP	PB-O3B-PG-O3G
5	G	5102	ATP	PB-O3B-PG-O3G
5	J	5102	ATP	PB-O3B-PG-O3G

There are no ring outliers.

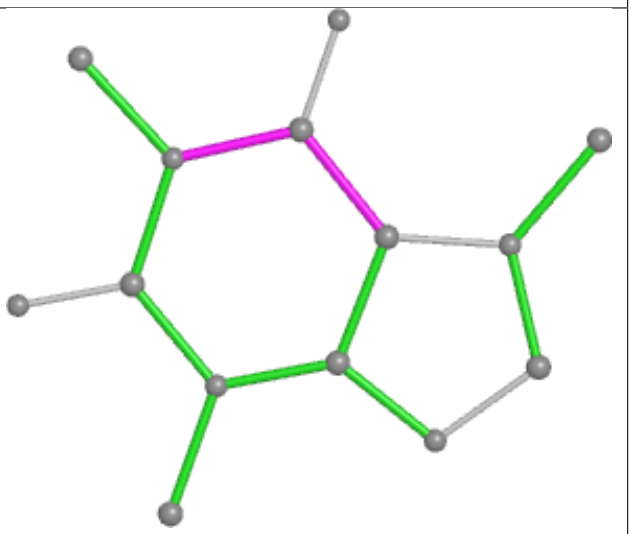
No monomer is involved in short contacts.

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 then 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.

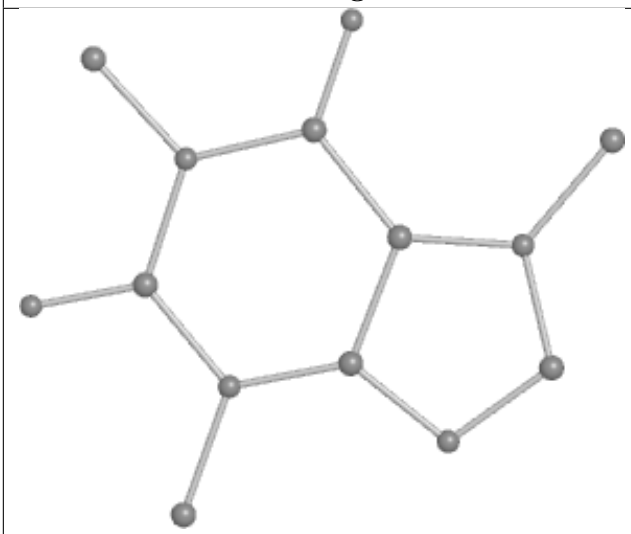
Ligand CFF E 5103



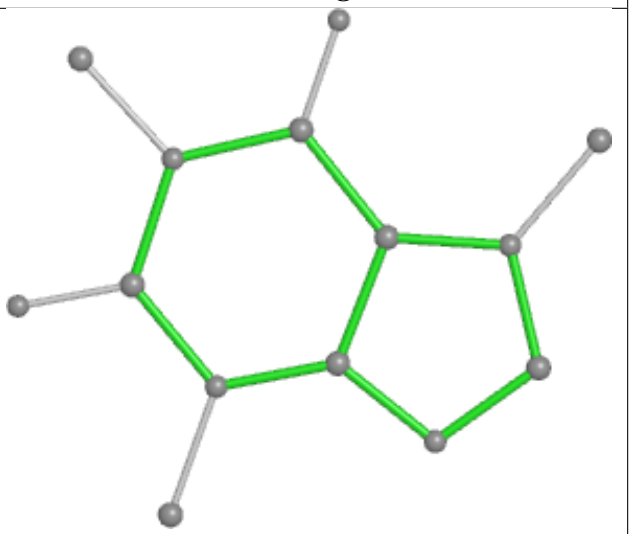
Bond lengths



Bond angles

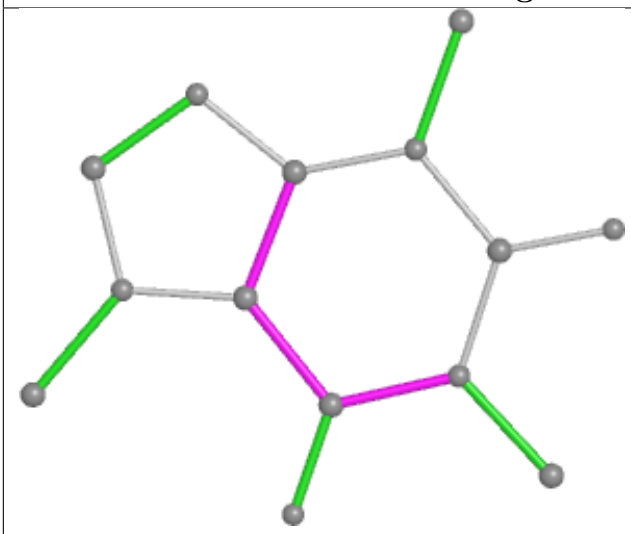


Torsions

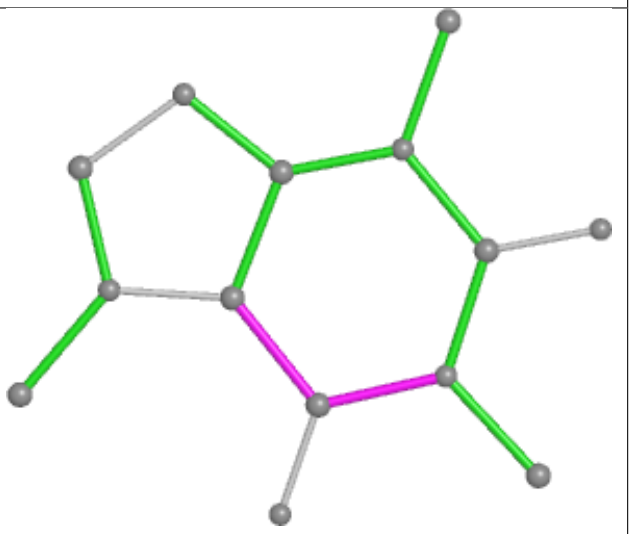


Rings

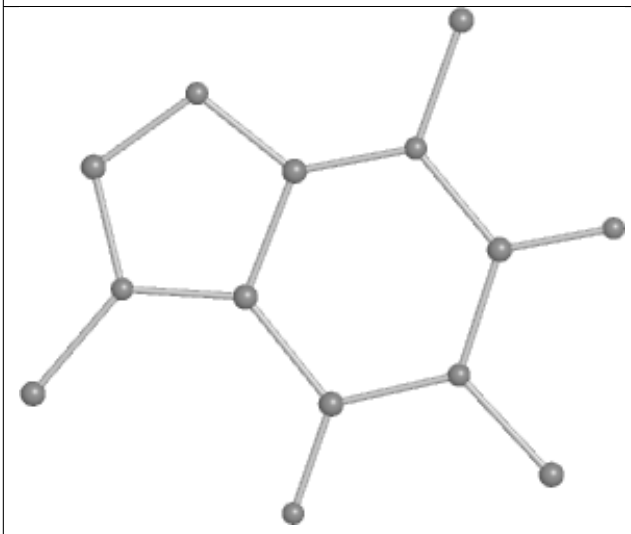
Ligand CFF G 5103



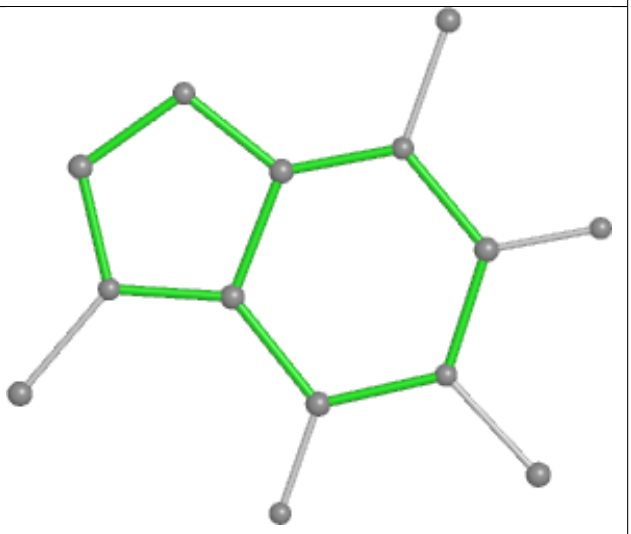
Bond lengths



Bond angles

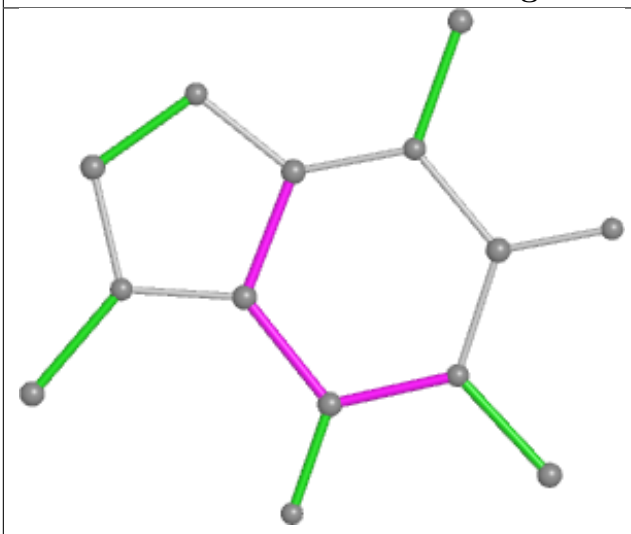


Torsions

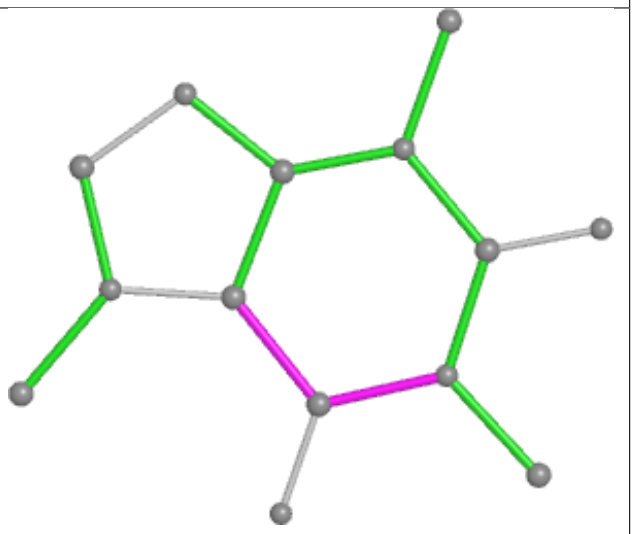


Rings

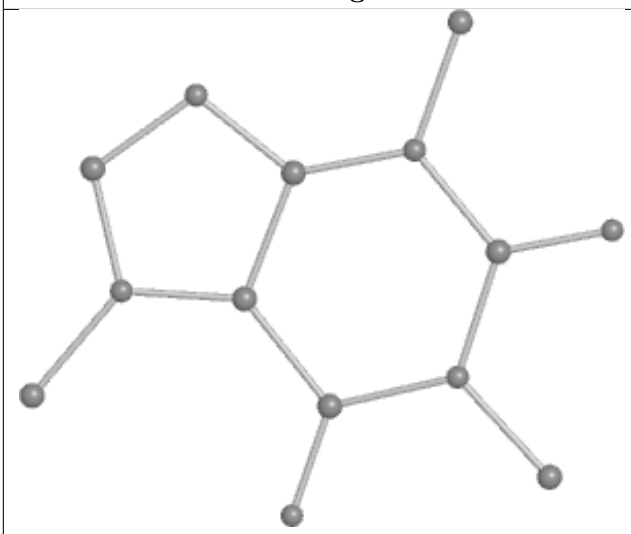
Ligand CFF J 5103



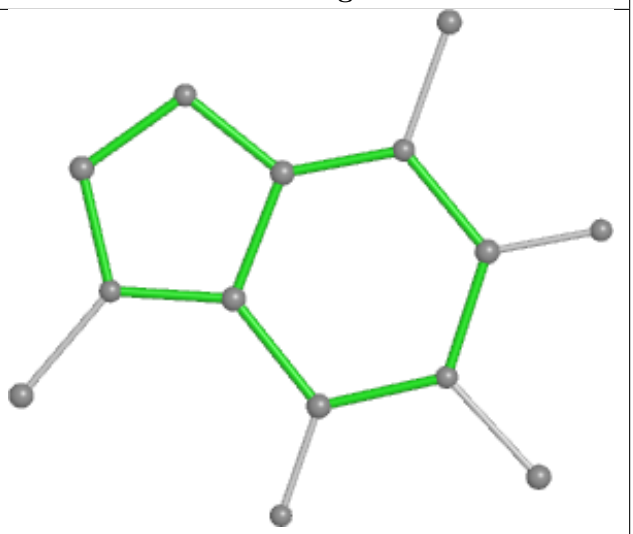
Bond lengths



Bond angles

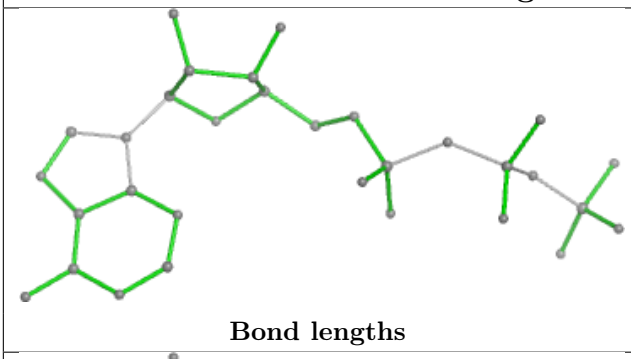


Torsions

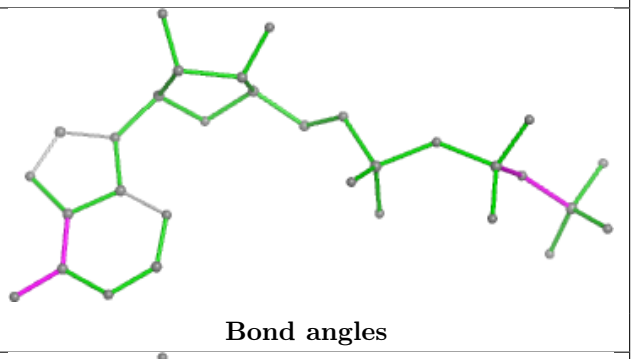


Rings

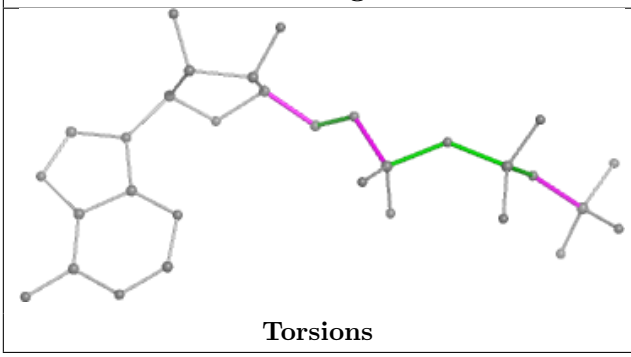
Ligand ATP E 5102



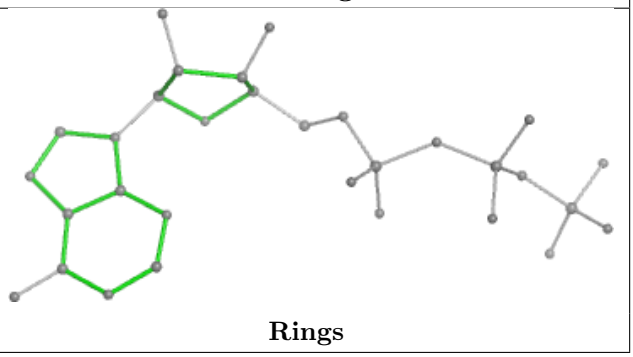
Bond lengths



Bond angles

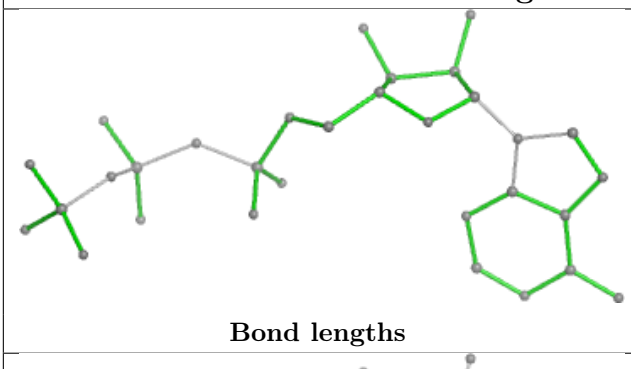


Torsions

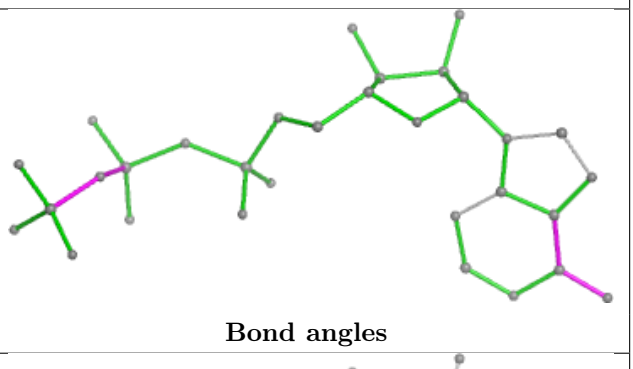


Rings

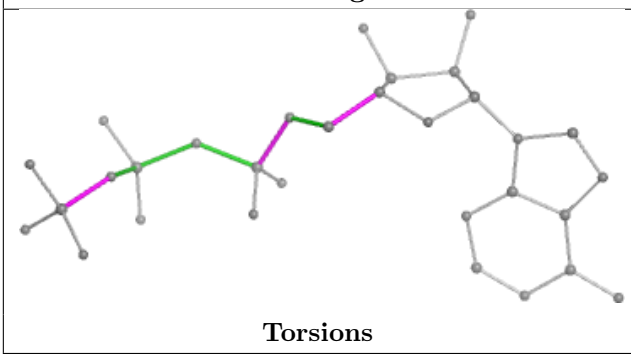
Ligand ATP B 5102



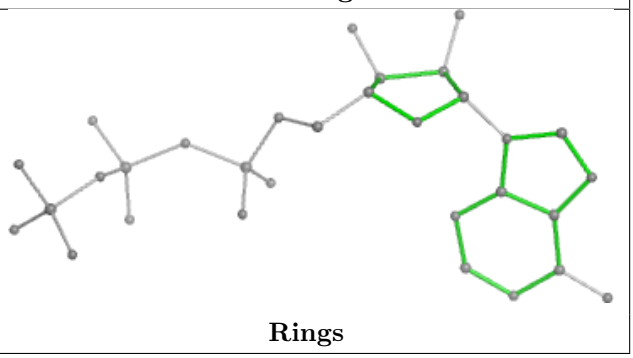
Bond lengths



Bond angles

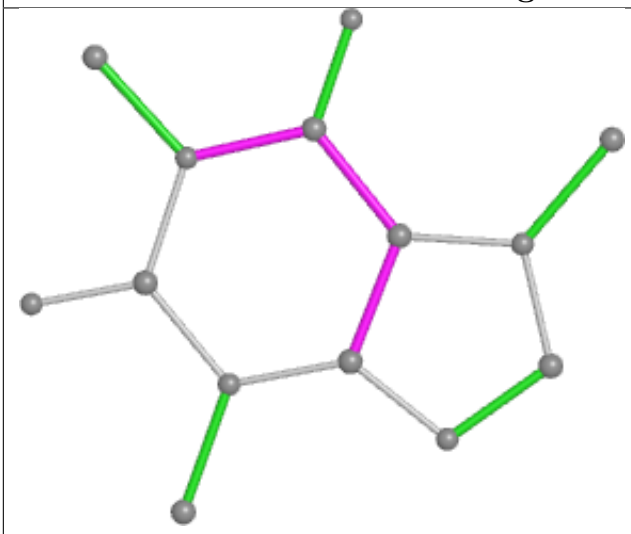


Torsions

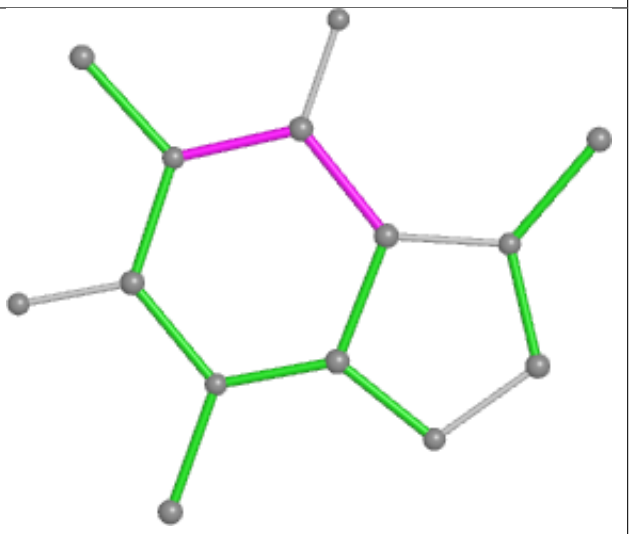


Rings

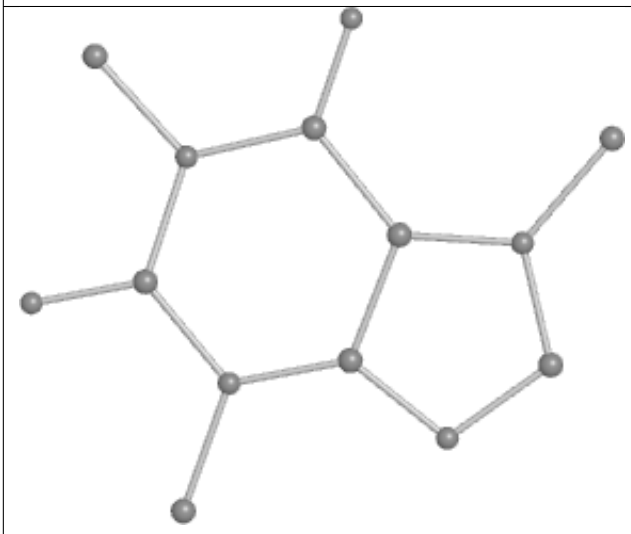
Ligand CFF B 5103



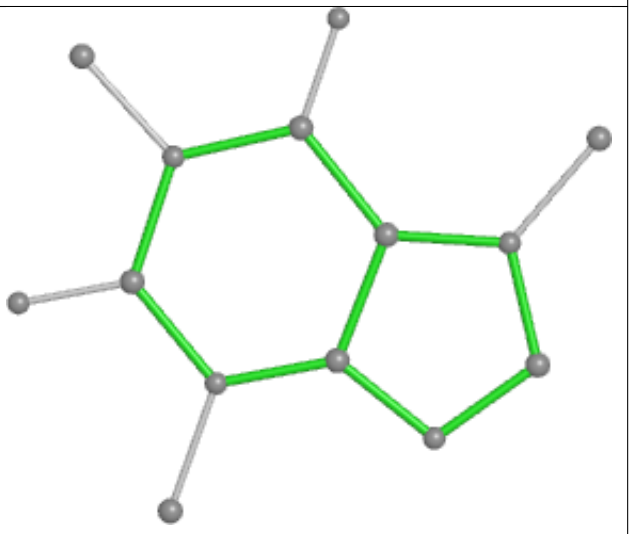
Bond lengths



Bond angles

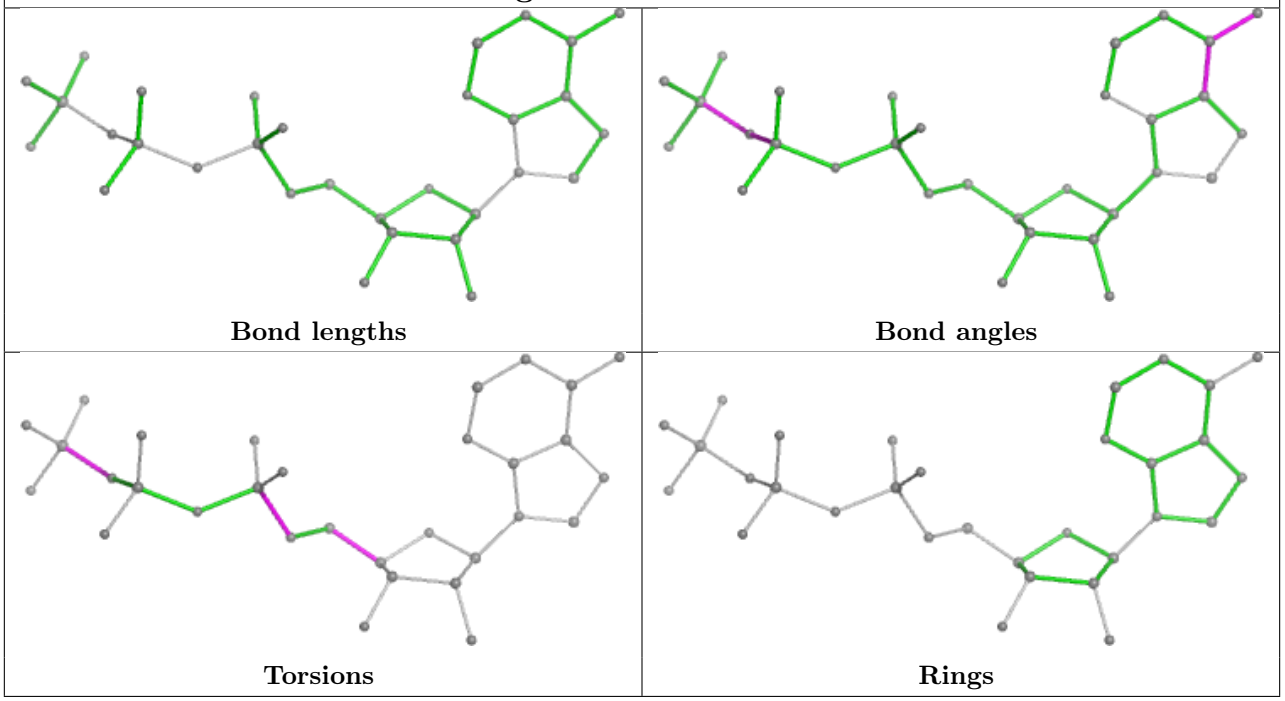


Torsions

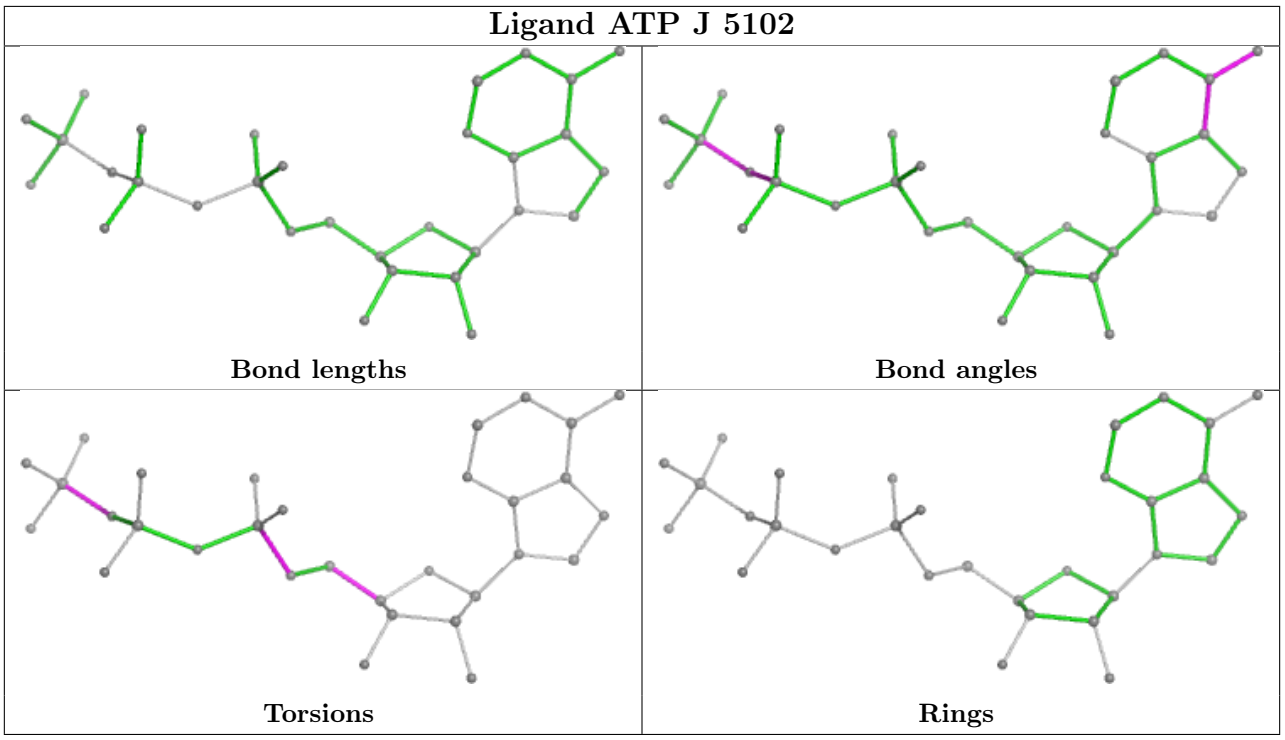


Rings

Ligand ATP G 5102



Ligand ATP J 5102



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.

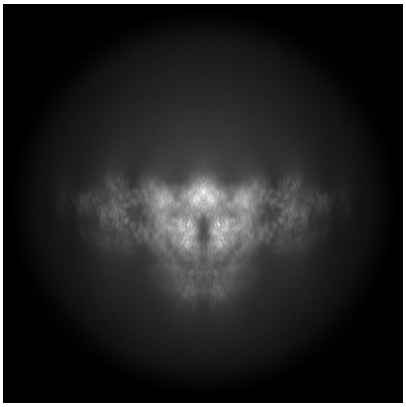
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19472. These allow visual inspection of the internal detail of the map and identification of artifacts.

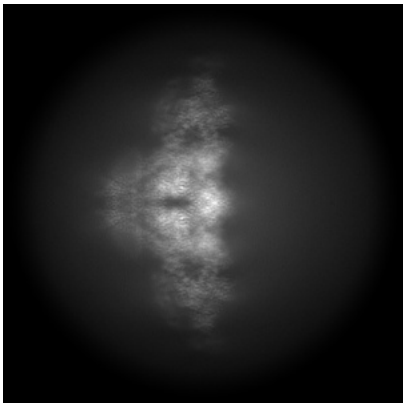
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

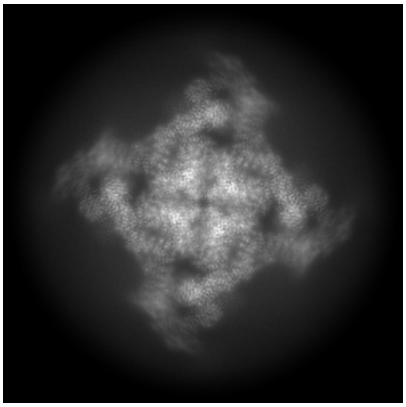
6.1.1 Primary map



X



Y



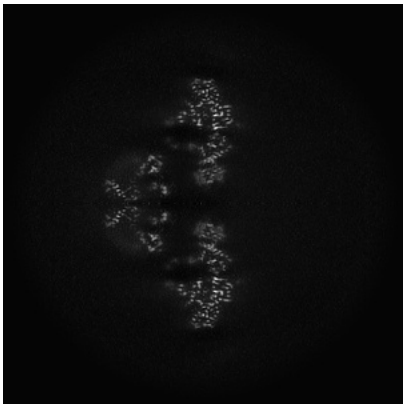
Z

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

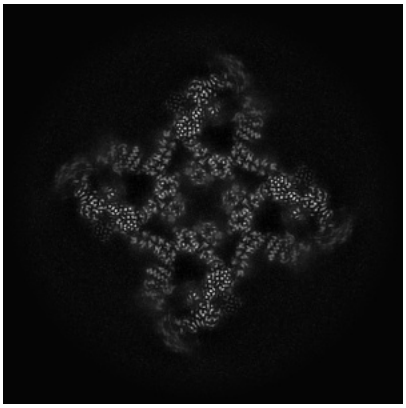
6.2 Central slices

6.2.1 Primary map

X Index: 168



Y Index: 168

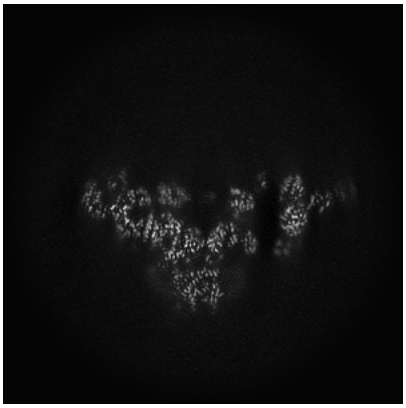


Z Index: 168

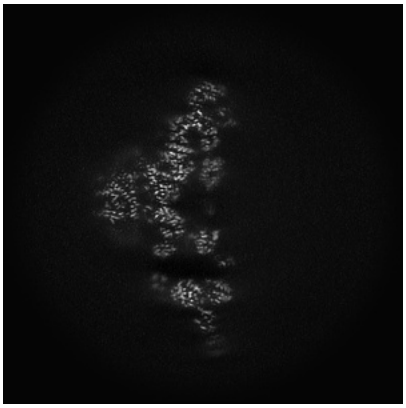
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

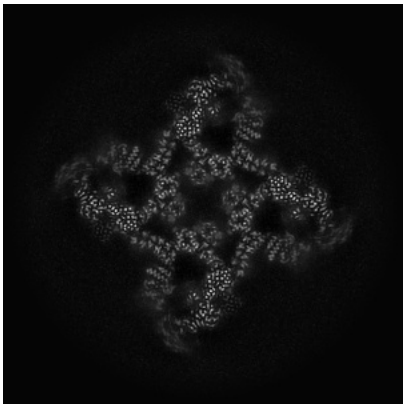
6.3.1 Primary map



X Index: 178



Y Index: 178

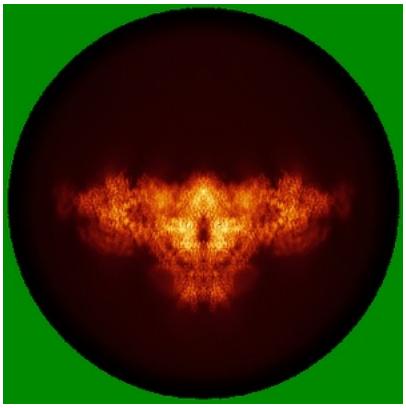


Z Index: 168

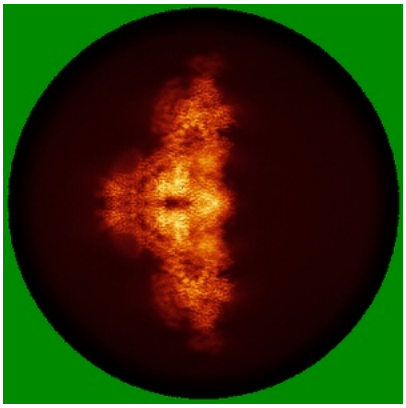
The images above show the largest variance slices of the map in three orthogonal directions.

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

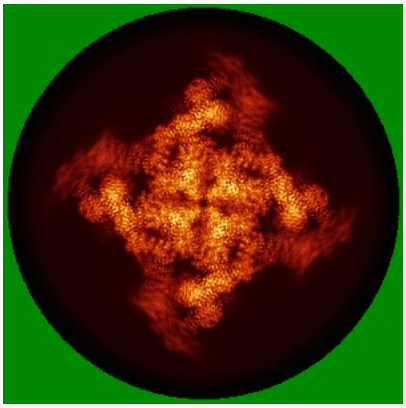
6.4.1 Primary map



X



Y

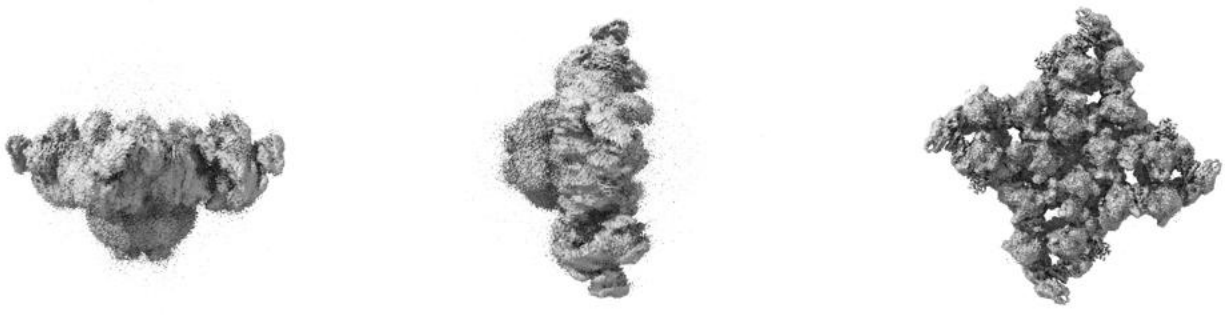


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

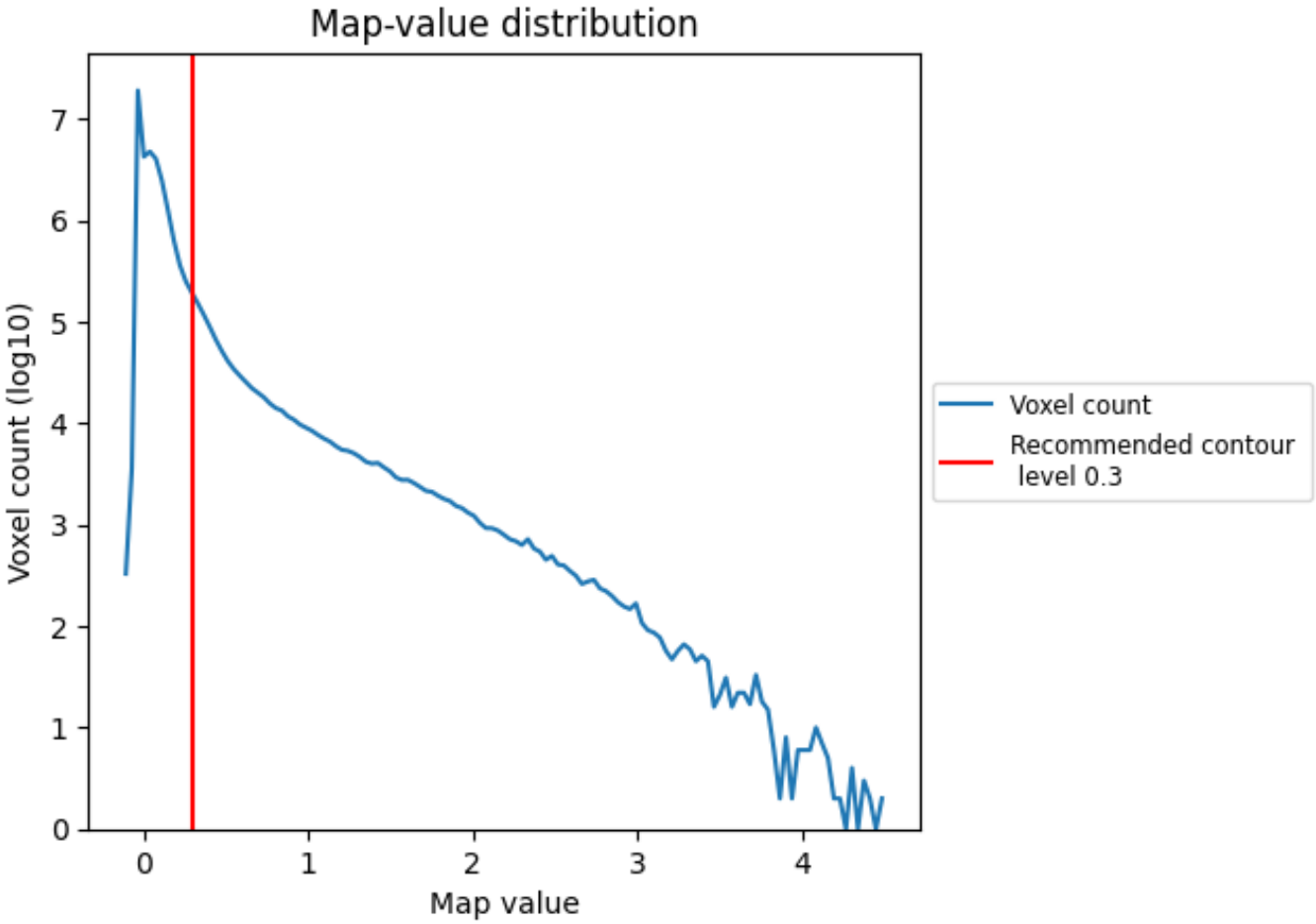
6.6 Mask visualisation (i)

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

7 Map analysis

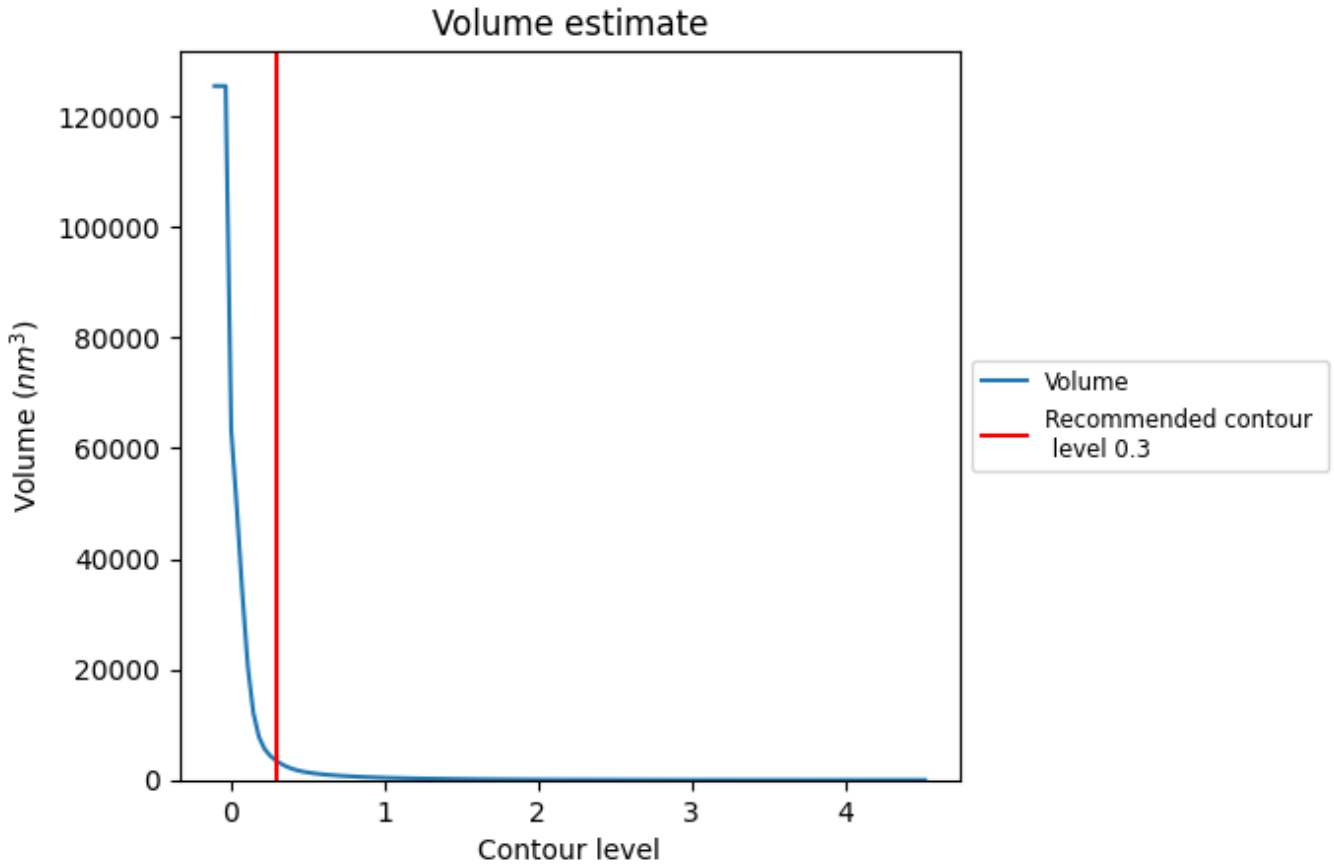
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

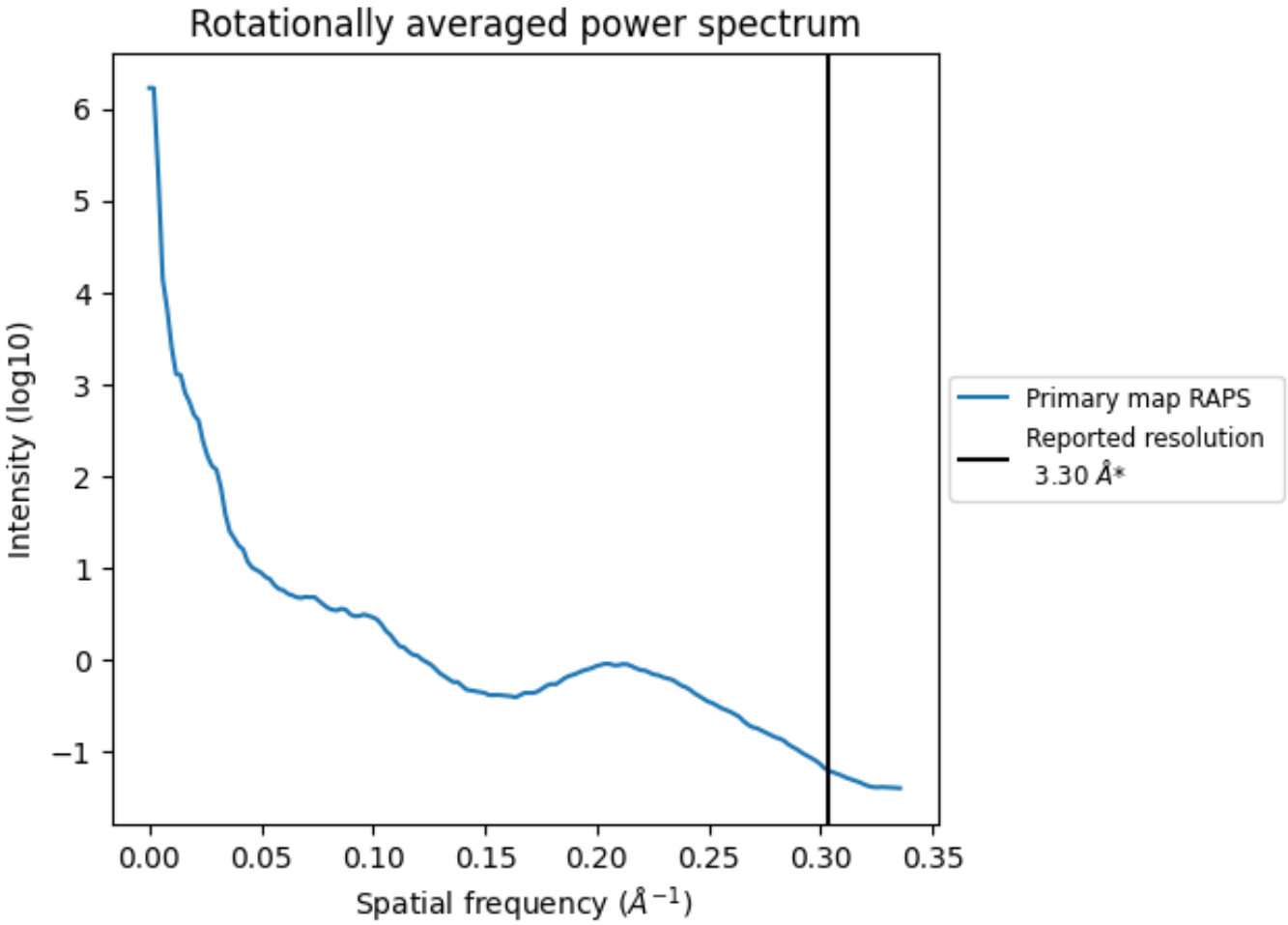
7.2 Volume estimate



The volume at the recommended contour level is 3395 nm^3; this corresponds to an approximate mass of 3067 kDa.

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

7.3 Rotationally averaged power spectrum (i)

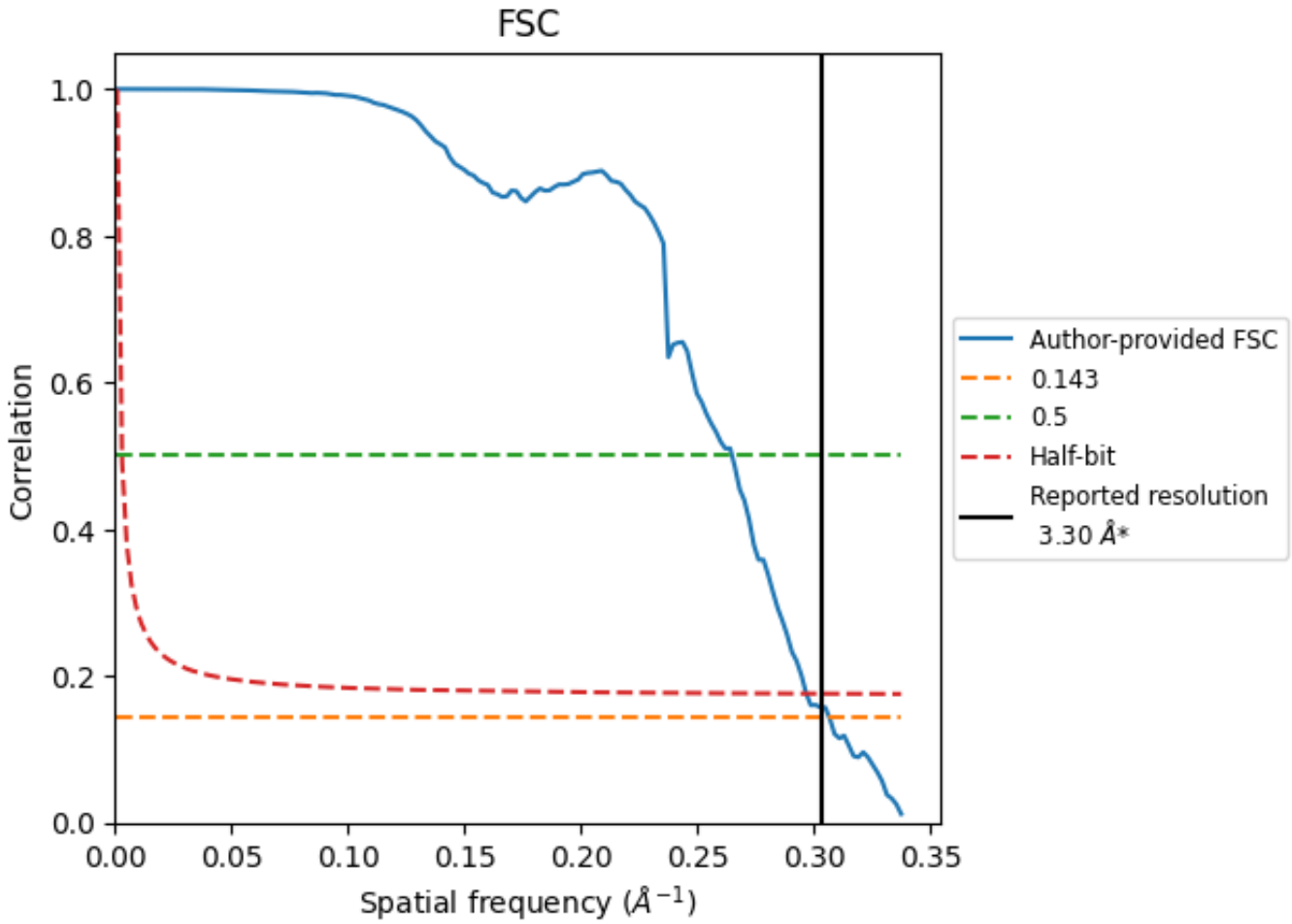


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

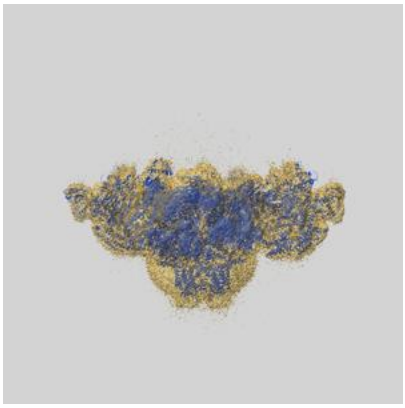
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.78	3.37
Unmasked-calculated*	-	-	-

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

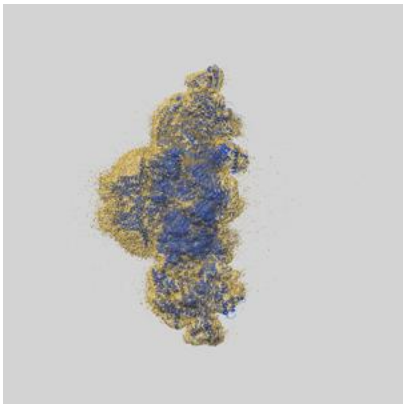
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19472 and PDB model 8RS0. Per-residue inclusion information can be found in section 3 on page 8.

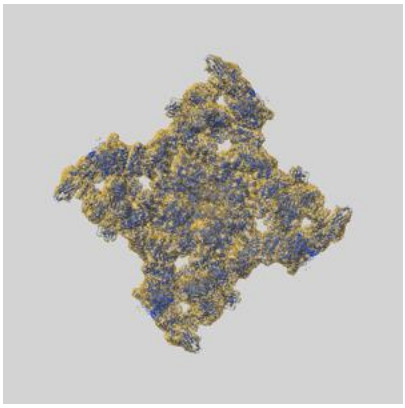
9.1 Map-model overlay



X



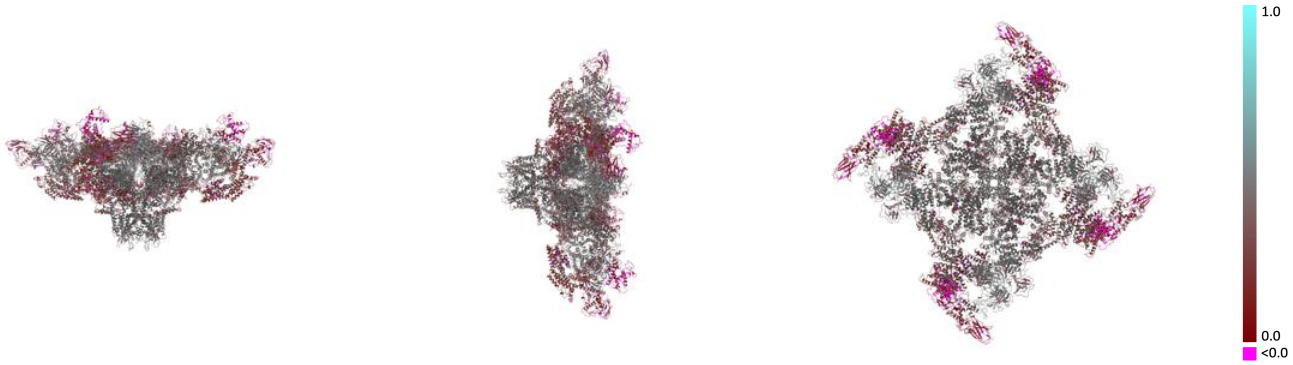
Y



Z

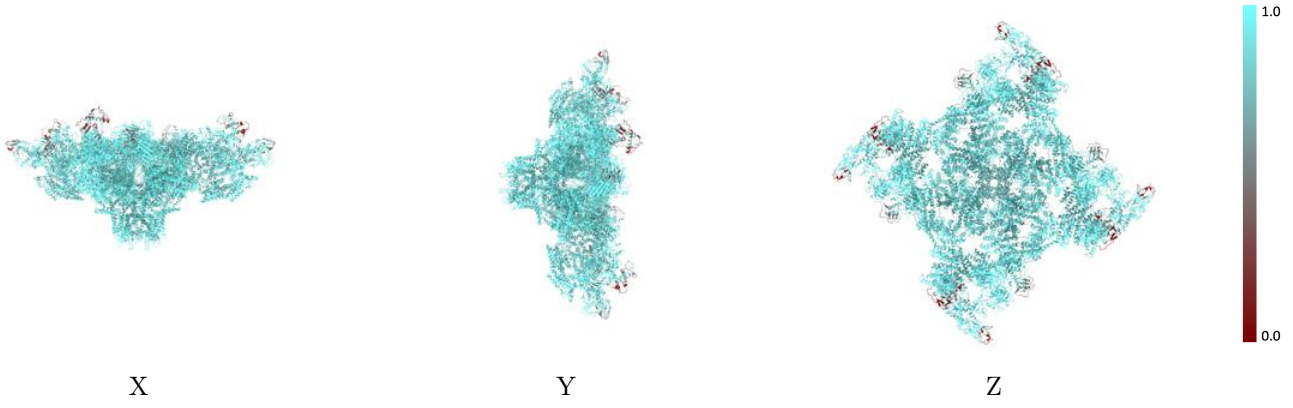
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



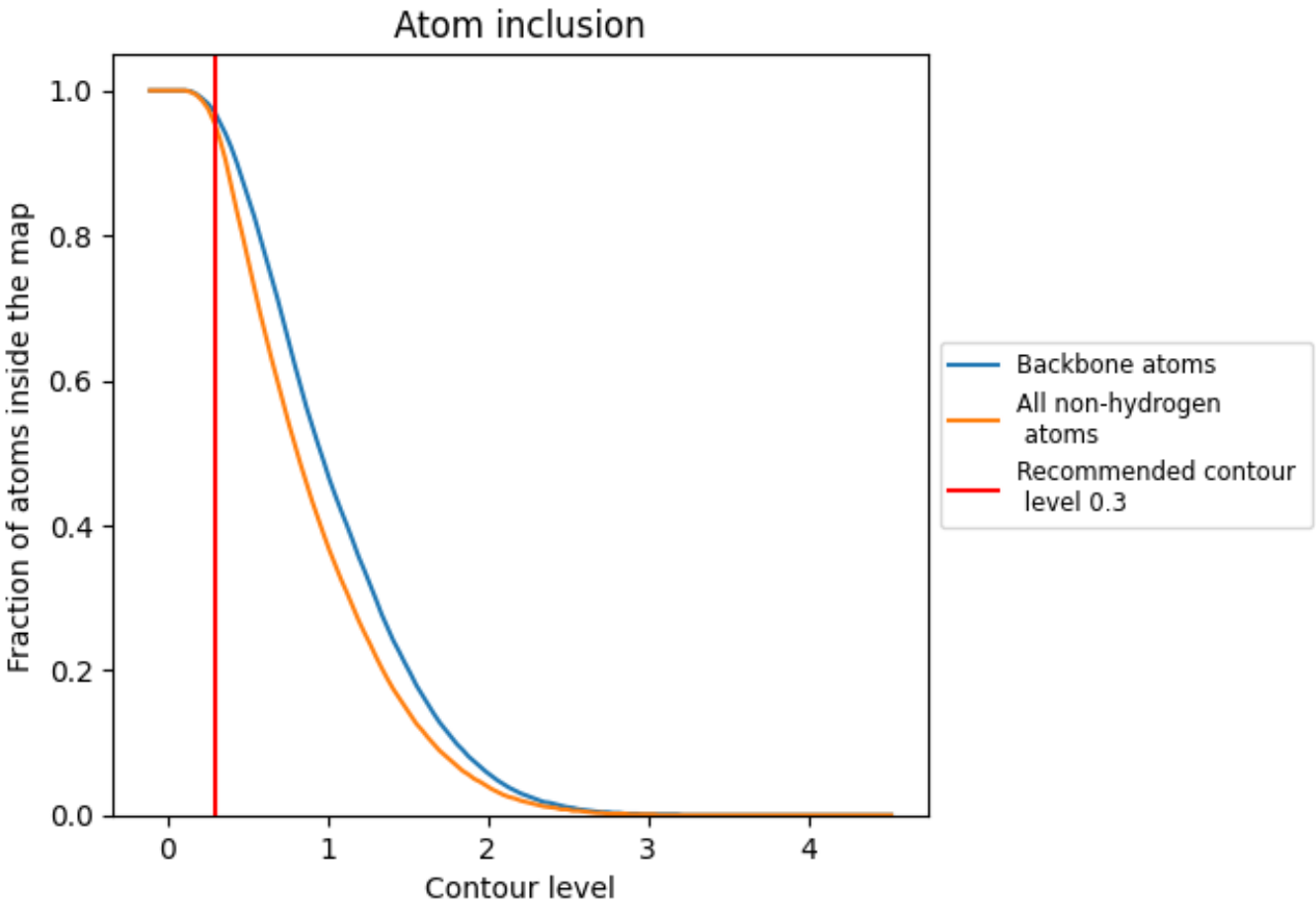
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.3560
A	0.6870	0.3860
B	0.9670	0.3620
C	0.6930	0.1320
D	0.6890	0.3950
E	0.9670	0.3620
F	0.6880	0.1320
G	0.9670	0.3610
H	0.6880	0.3920
I	0.6850	0.3940
J	0.9670	0.3620
K	0.6880	0.1340
M	0.6910	0.1310