Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 03:00 PM JST

PDB ID	:	8XLF
EMDB ID	:	EMD-38447
Title	:	Structure of chimeric RyR
Authors	:	Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on	:	2023-12-25
Resolution	:	3.62 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:

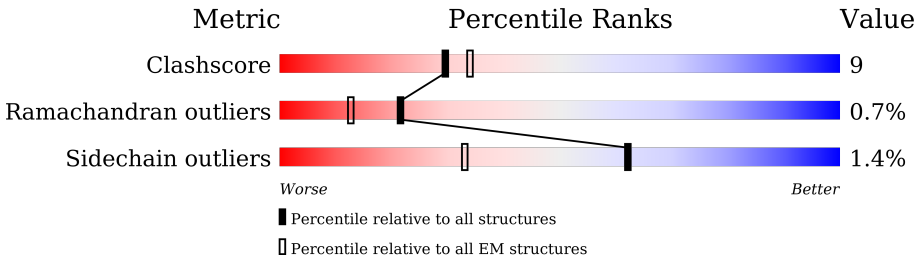
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.62 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	5037	63% 14% • 22%
1	B	5037	63% 14% • 22%
1	C	5037	63% 14% • 22%
1	D	5037	63% 14% • 22%
2	I	148	81% 12% • 6%
2	J	148	82% 11% • 6%
2	K	148	81% 12% • 6%
2	L	148	82% 11% • 6%

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Mol	Chain	Length	Quality of chain
3	E	107	84% 16%
3	F	107	86% 14%
3	G	107	88% 12%
3	H	107	88% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 118944 atoms, of which 88 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	B	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	C	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		
1	D	3916	Total	C	N	O	S	0	0
			27821	17738	4950	4957	176		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	ILE	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	ILE	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	ILE	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	ILE	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	I	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	J	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
2	K	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
3	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

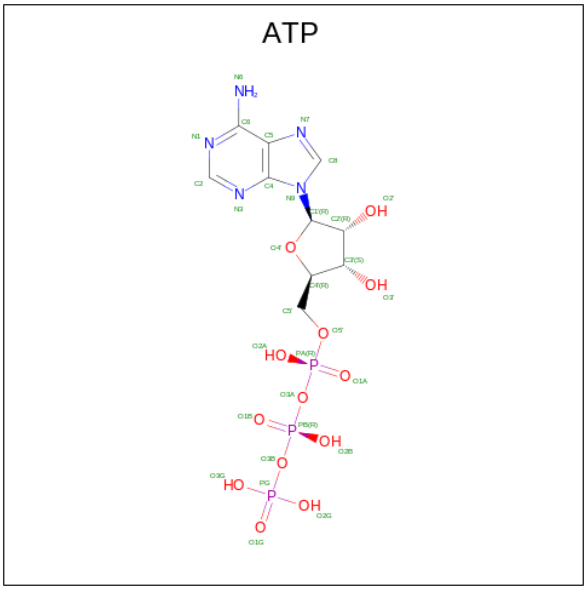
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0
5	C	1	Total Zn 1 1	0
5	D	1	Total Zn 1 1	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C H N O P 43 10 12 5 13 3	0

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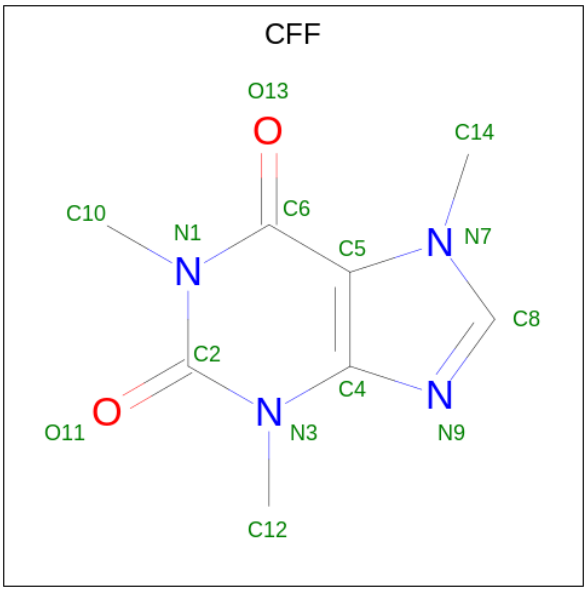
Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



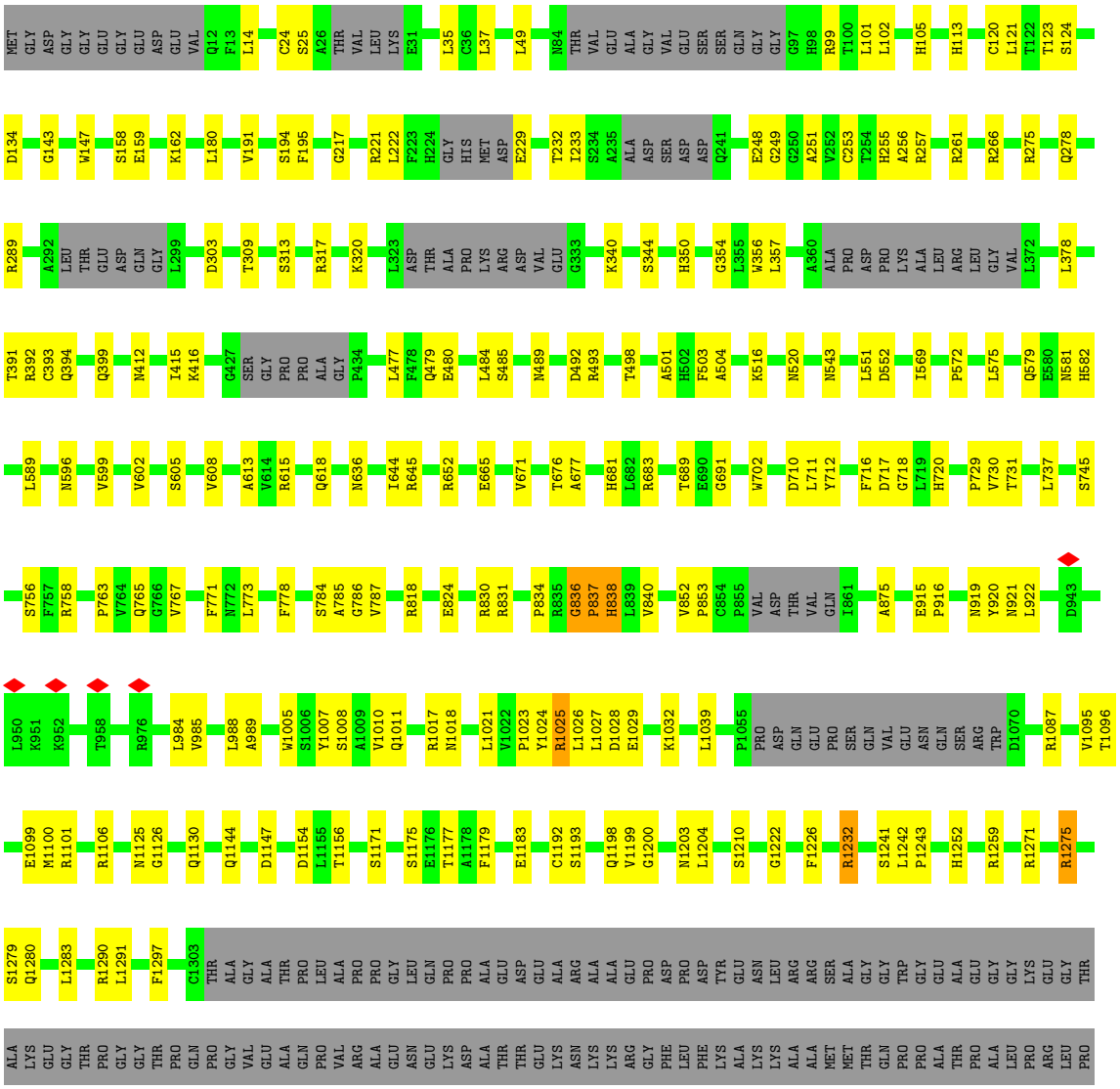
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
7	D	1	Total	C	H	N	O	0
			24	8	10	4	2	

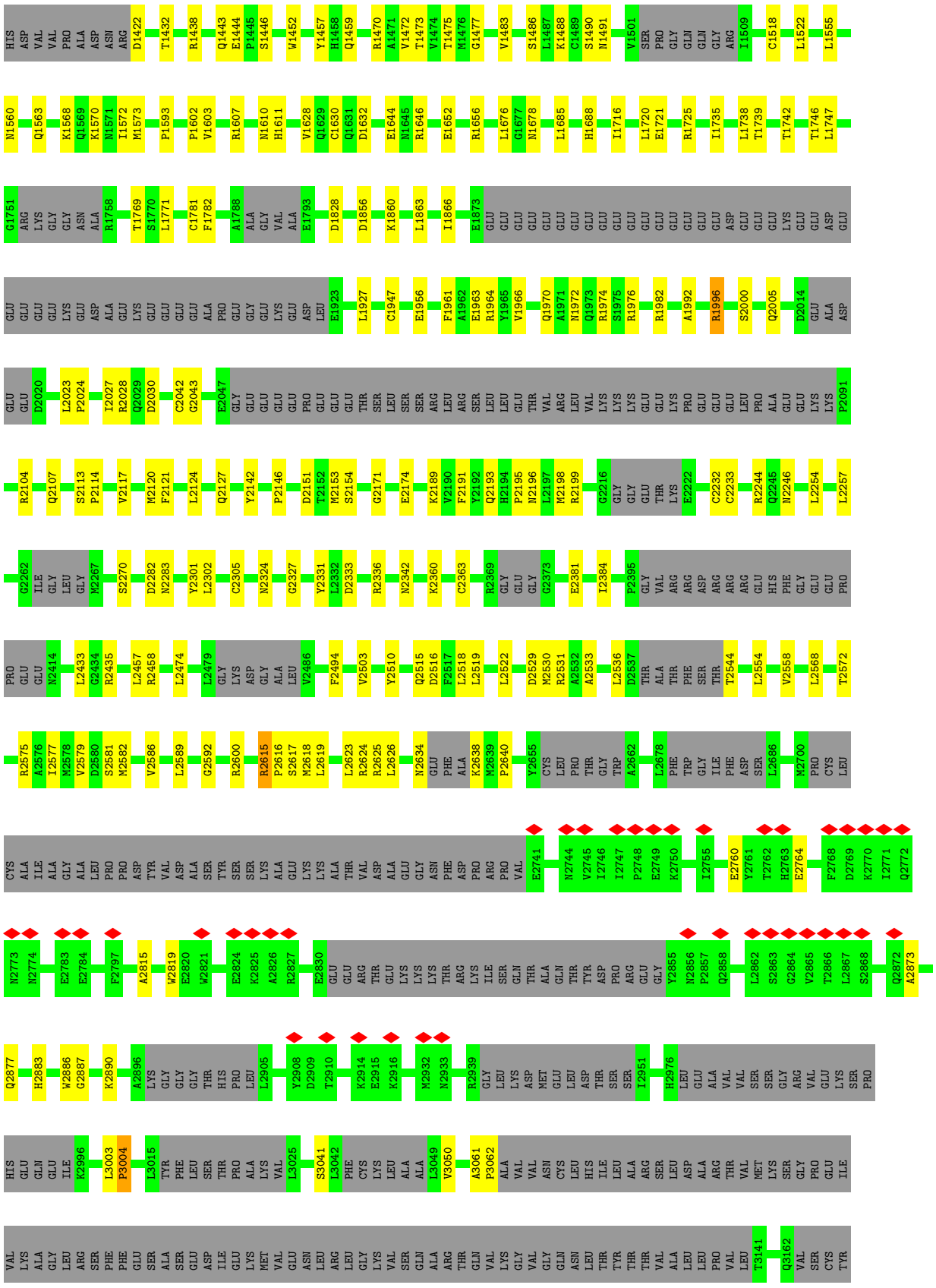
3 Residue-property plots (i)

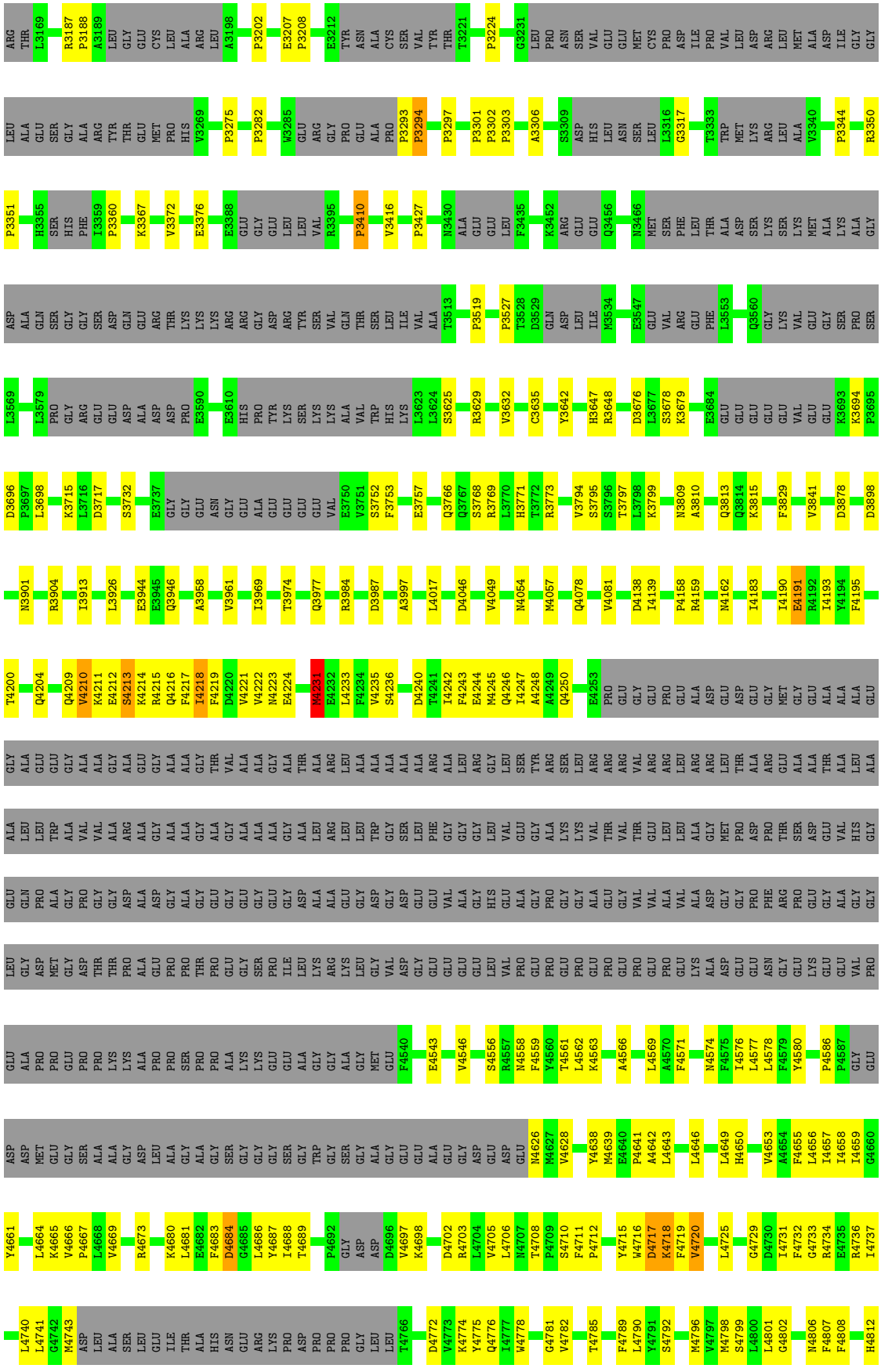
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

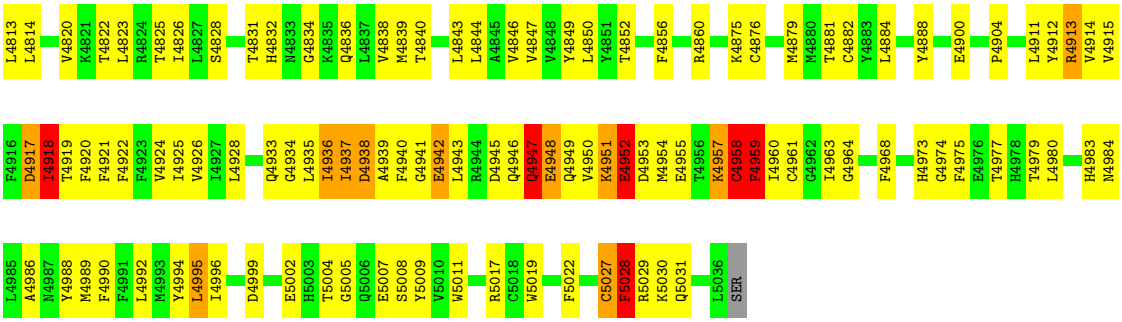
- Molecule 1: Ryanodine receptor 1

Chain A:



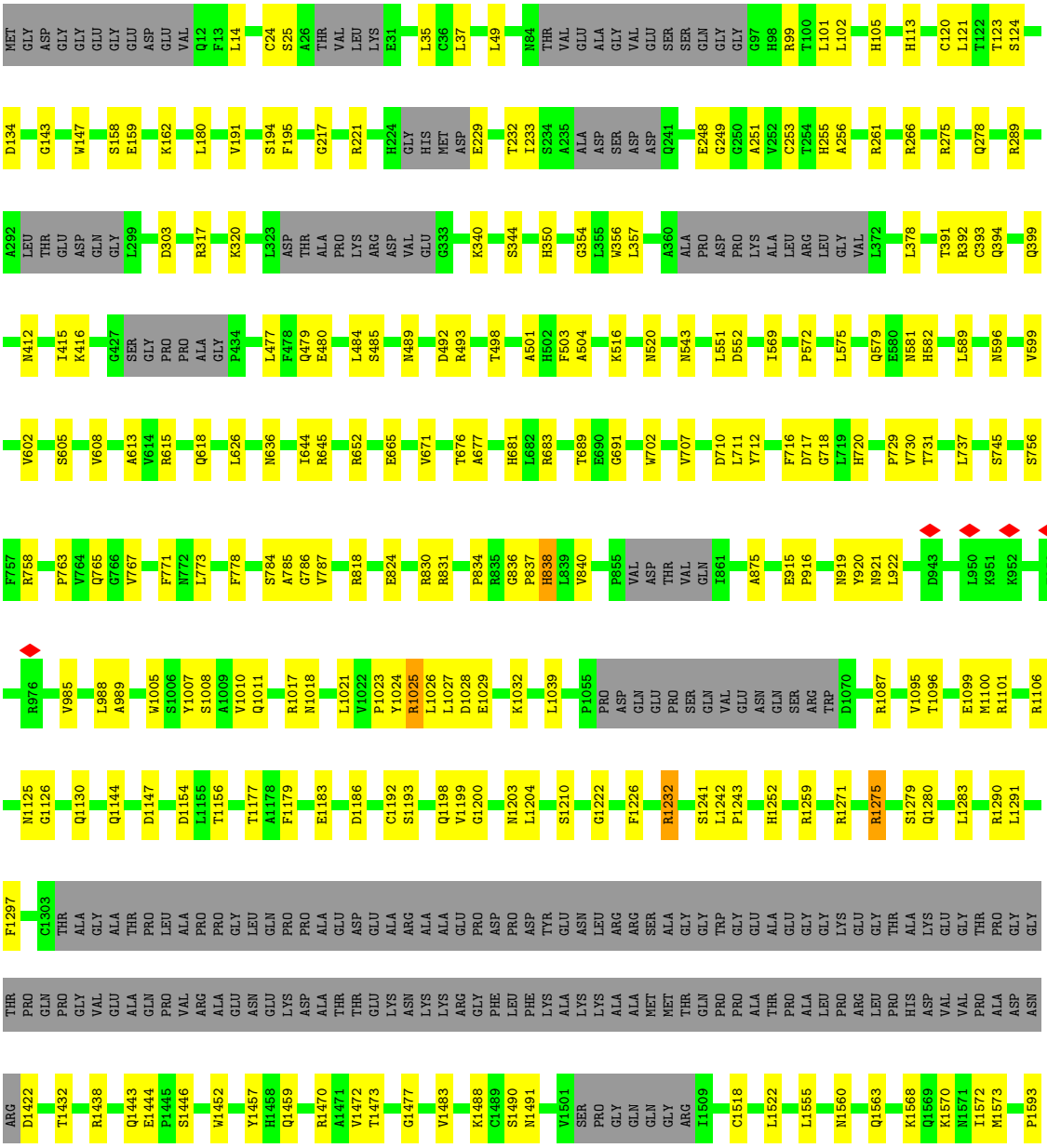


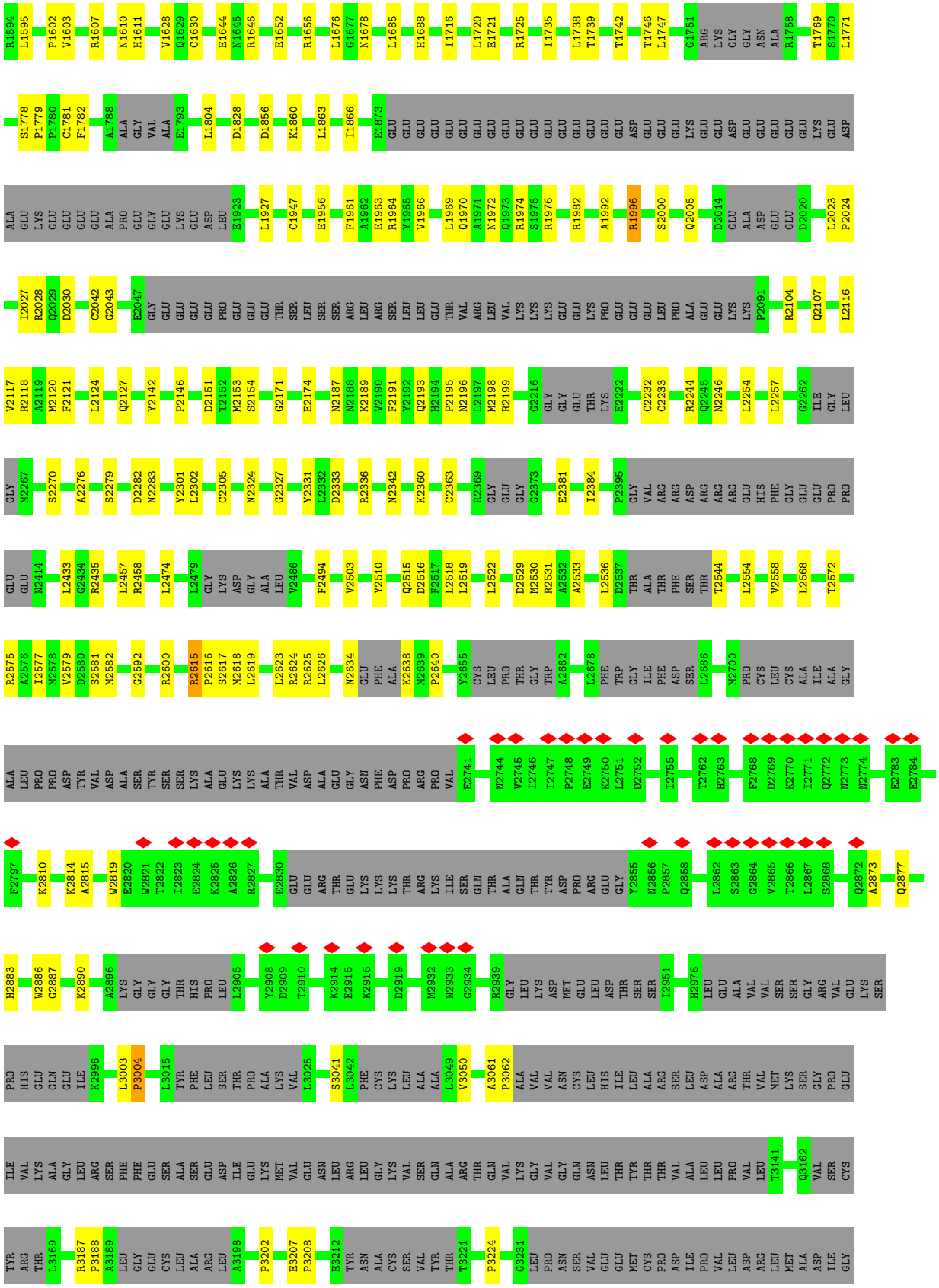


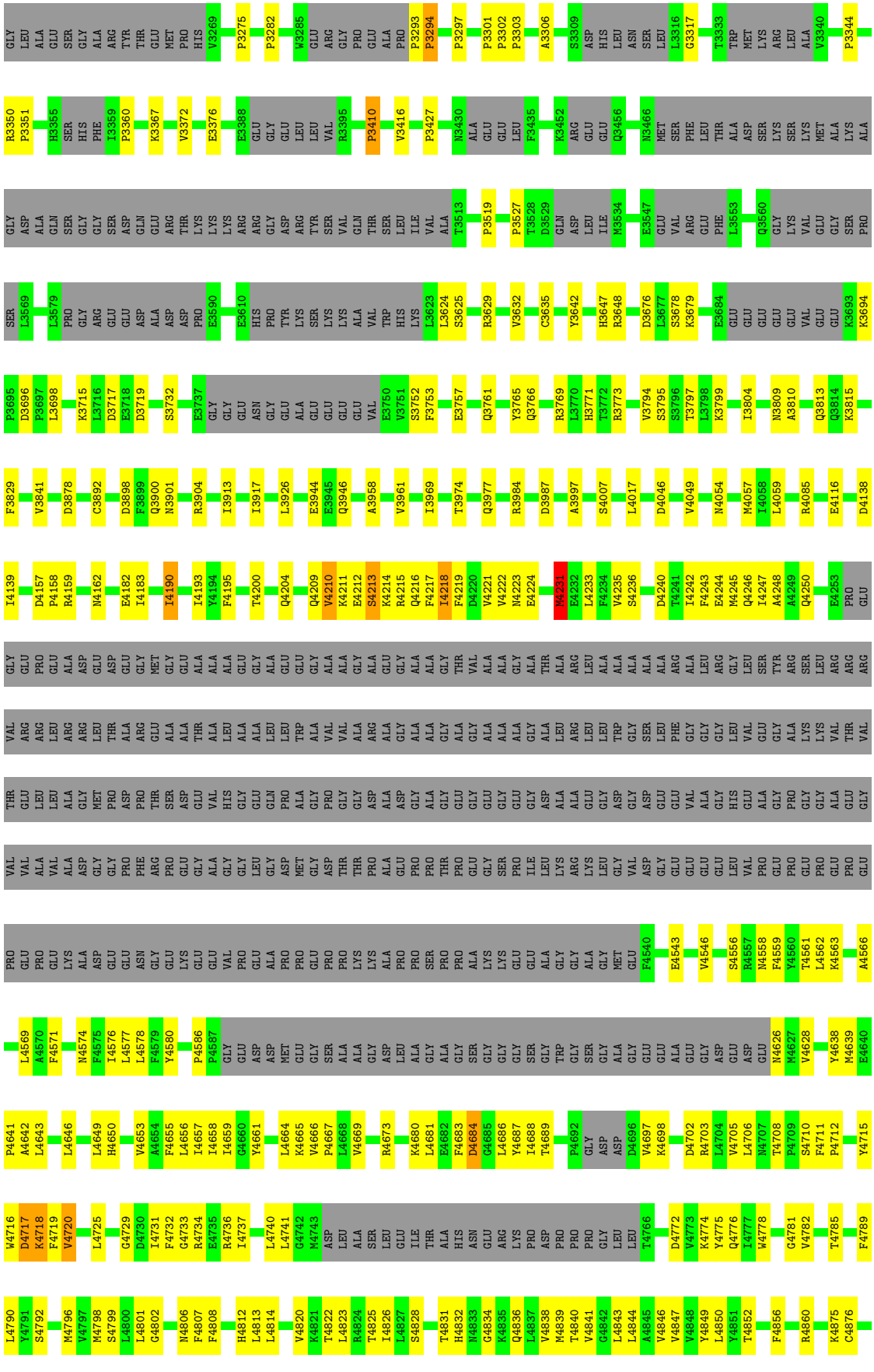


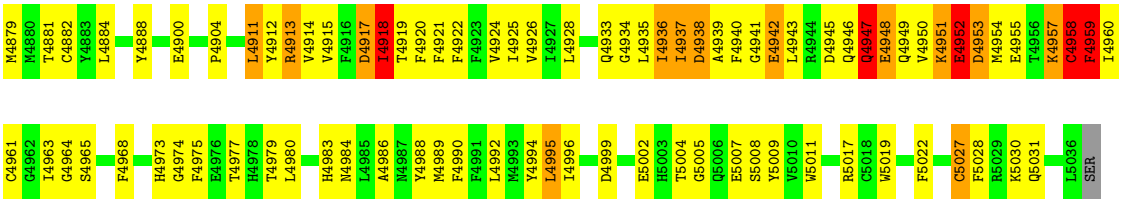
• Molecule 1: Ryanodine receptor 1

Chain B:



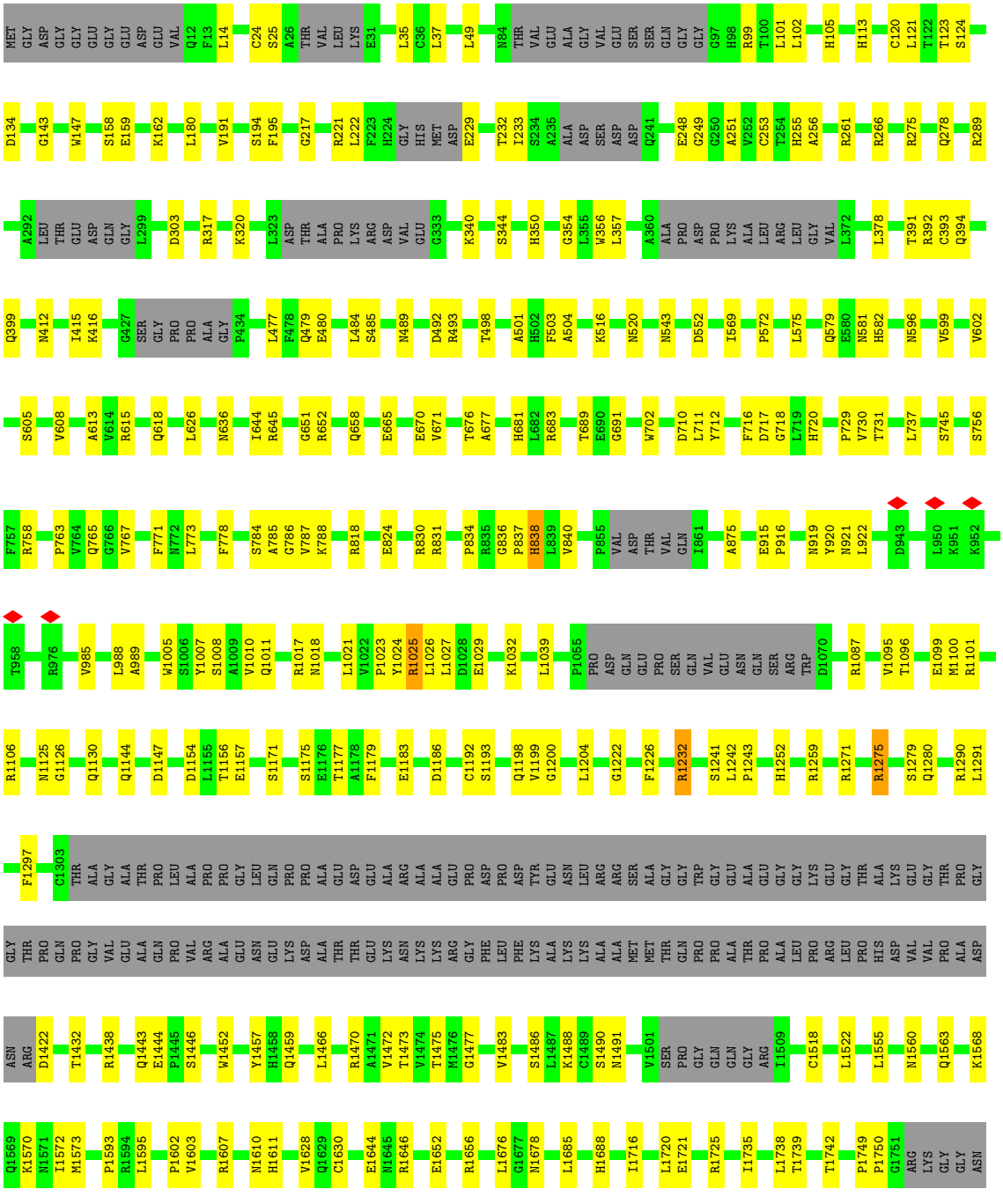


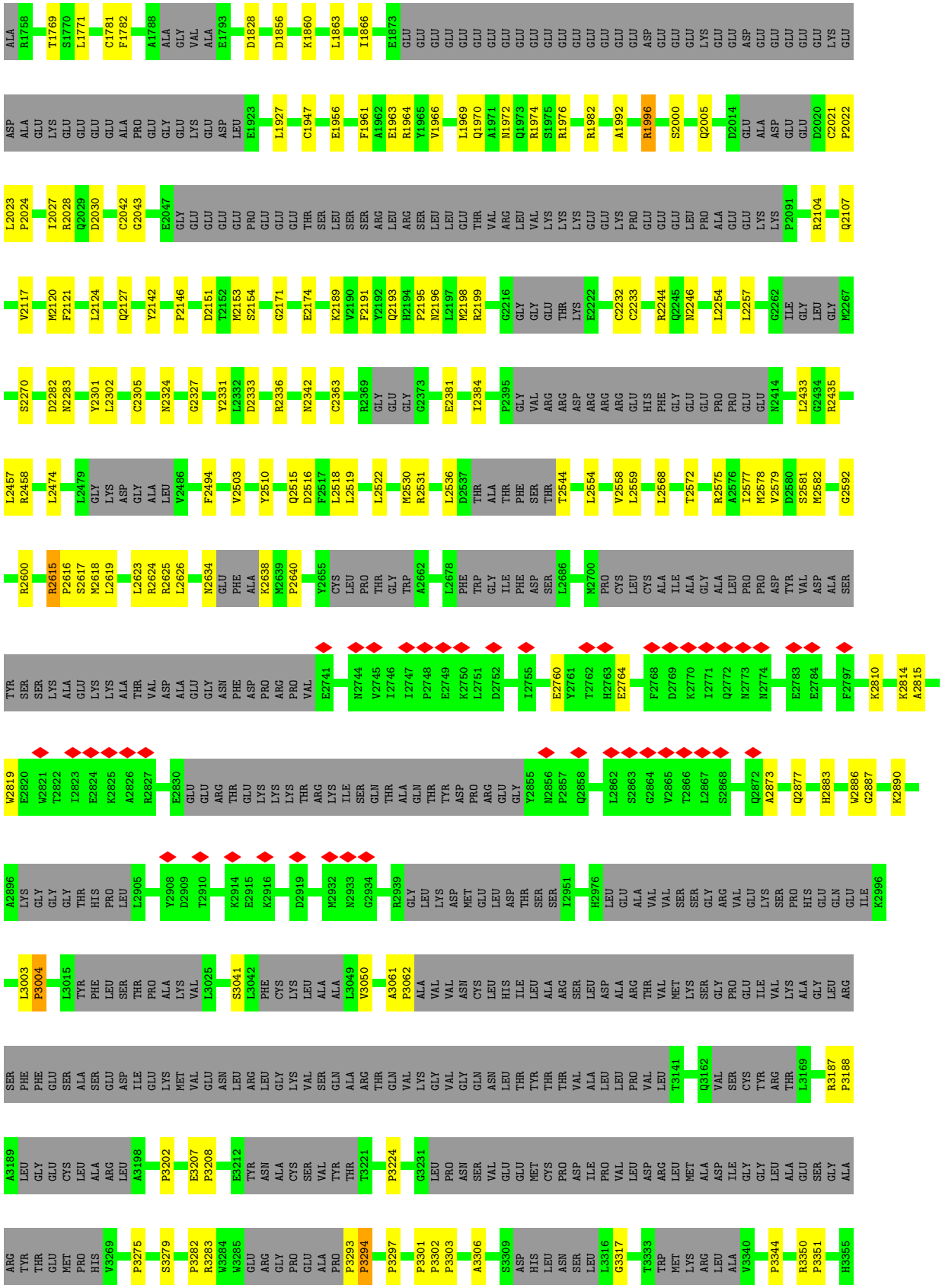


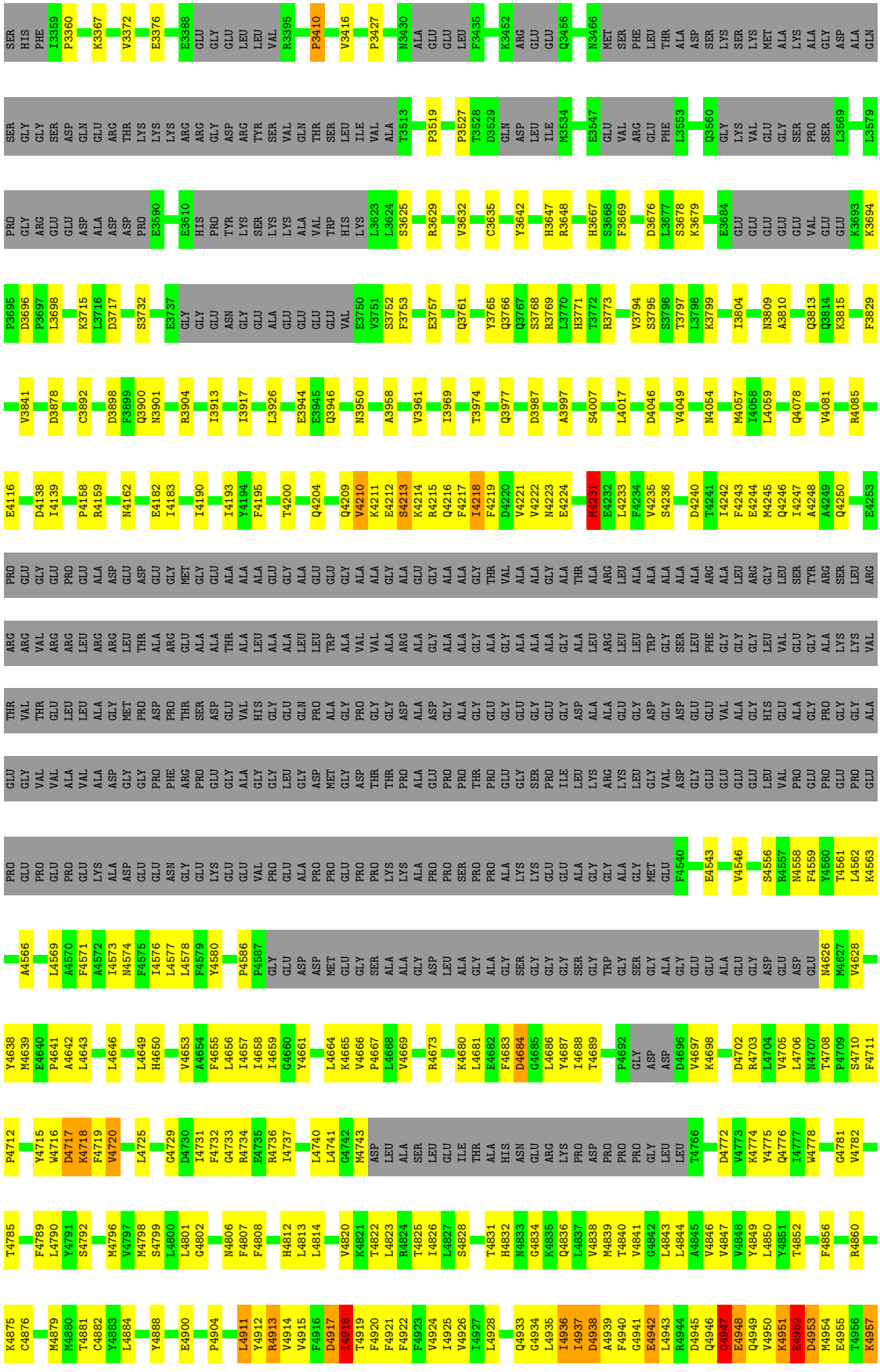


• Molecule 1: Ryanodine receptor 1

Chain C:

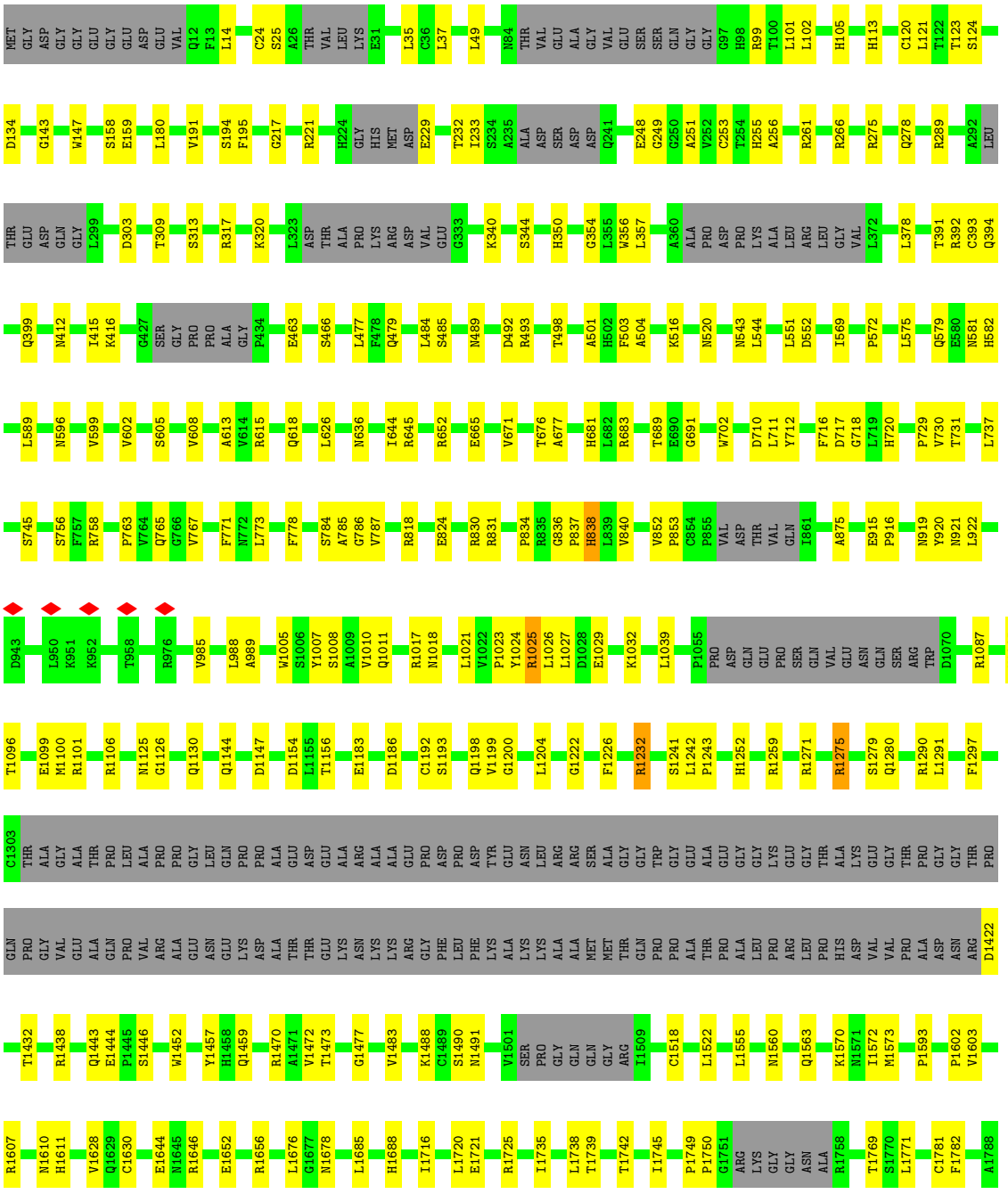


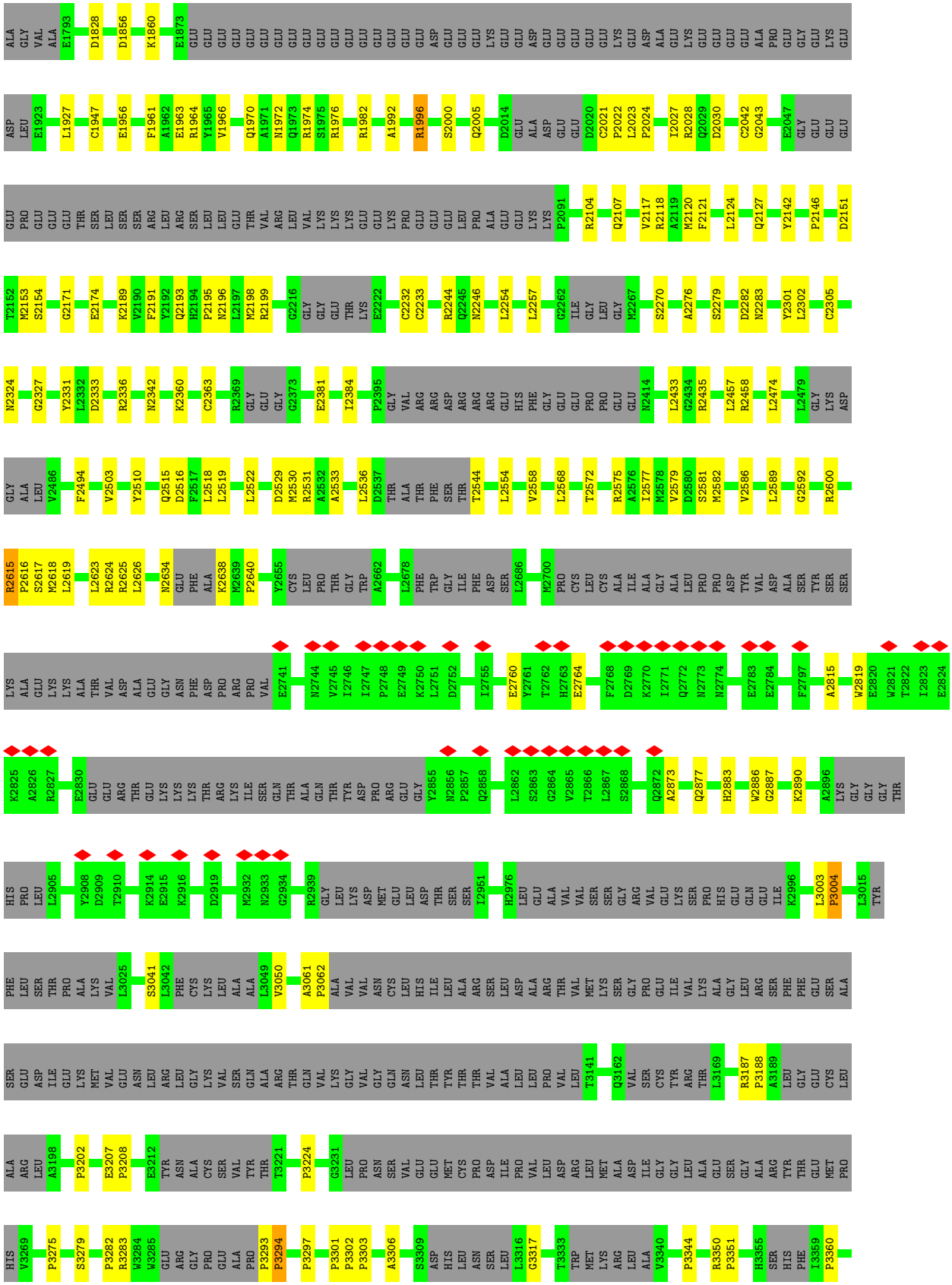


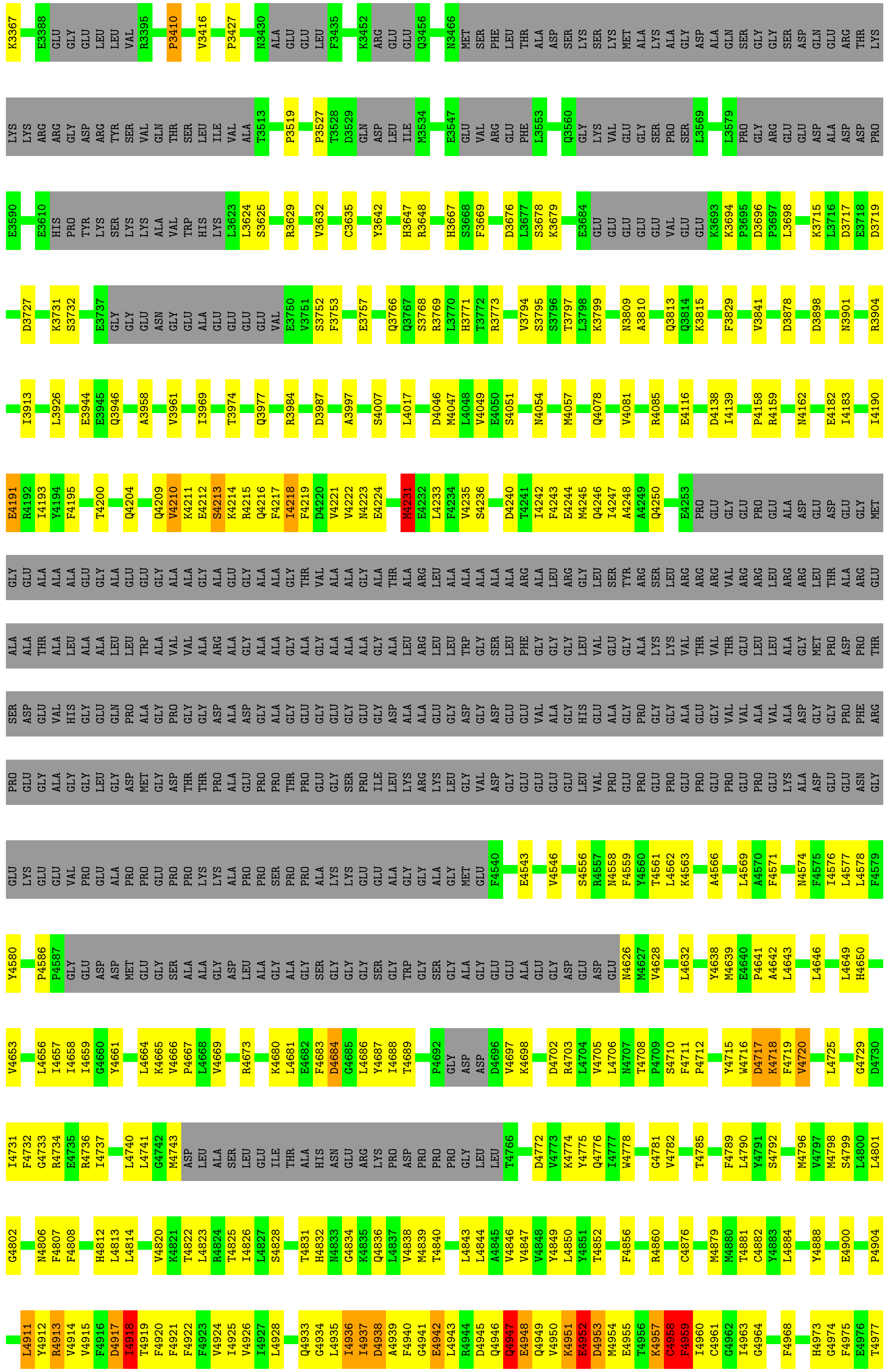


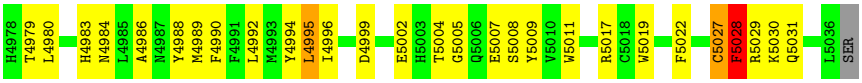
• Molecule 1: Ryanodine receptor 1

Chain D:

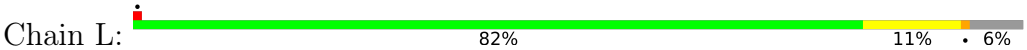


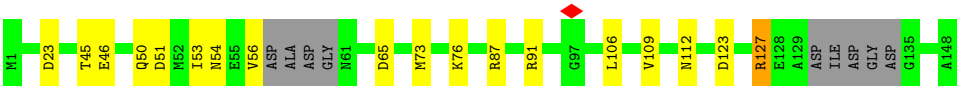




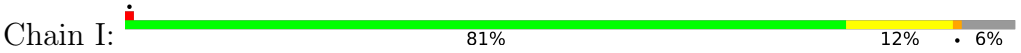


• Molecule 2: Calmodulin-1

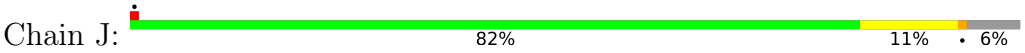


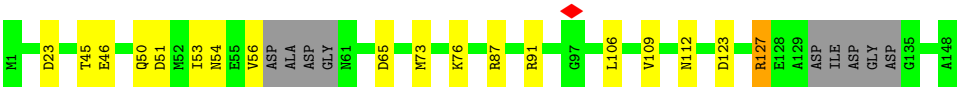


• Molecule 2: Calmodulin-1

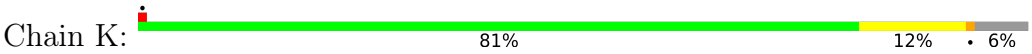


• Molecule 2: Calmodulin-1

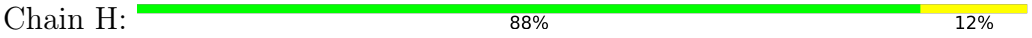




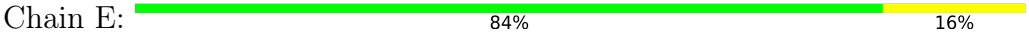
• Molecule 2: Calmodulin-1



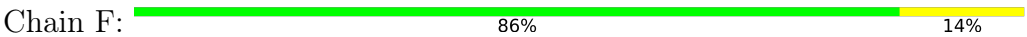
• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

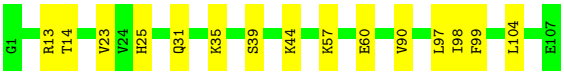


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.484	Depositor
Minimum map value	-0.814	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	613.2, 613.2, 613.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2775, 1.2775, 1.2775	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.40	1/28349 (0.0%)	0.58	33/38619 (0.1%)
1	B	0.40	1/28349 (0.0%)	0.58	32/38619 (0.1%)
1	C	0.40	1/28349 (0.0%)	0.58	33/38619 (0.1%)
1	D	0.40	1/28349 (0.0%)	0.58	33/38619 (0.1%)
2	I	0.28	0/1052	0.50	0/1416
2	J	0.28	0/1052	0.50	0/1416
2	K	0.28	0/1052	0.50	0/1416
2	L	0.28	0/1052	0.50	0/1416
3	E	0.31	0/820	0.55	0/1105
3	F	0.31	0/820	0.55	0/1105
3	G	0.31	0/820	0.55	0/1105
3	H	0.31	0/820	0.55	0/1105
All	All	0.39	4/120884 (0.0%)	0.58	131/164560 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4200	THR	C-N	5.19	1.46	1.34
1	B	4200	THR	C-N	5.19	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4200	THR	C-N	5.19	1.46	1.34
1	D	4200	THR	C-N	5.19	1.46	1.34

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	836	GLY	C-N-CD	-13.39	91.14	120.60
1	A	836	GLY	C-N-CD	-13.37	91.18	120.60
1	C	836	GLY	C-N-CD	-13.37	91.18	120.60
1	B	836	GLY	C-N-CD	-13.36	91.21	120.60
1	A	4200	THR	O-C-N	-10.40	106.05	122.70
1	B	4200	THR	O-C-N	-10.40	106.05	122.70
1	C	4200	THR	O-C-N	-10.40	106.05	122.70
1	D	4200	THR	O-C-N	-10.40	106.05	122.70
1	A	4200	THR	CA-C-N	7.93	134.65	117.20
1	B	4200	THR	CA-C-N	7.91	134.60	117.20
1	C	4200	THR	CA-C-N	7.91	134.60	117.20
1	D	4200	THR	CA-C-N	7.91	134.60	117.20
1	A	5028	PHE	N-CA-CB	6.79	122.83	110.60
1	B	3282	PRO	N-CA-CB	6.62	111.25	103.30
1	C	3282	PRO	N-CA-CB	6.61	111.23	103.30
1	A	3282	PRO	N-CA-CB	6.58	111.20	103.30
1	D	3282	PRO	N-CA-CB	6.58	111.20	103.30
1	A	3302	PRO	N-CA-CB	6.48	111.07	103.30
1	C	3302	PRO	N-CA-CB	6.48	111.07	103.30
1	D	3302	PRO	N-CA-CB	6.48	111.07	103.30
1	B	3302	PRO	N-CA-CB	6.47	111.06	103.30
1	A	4200	THR	C-N-CA	6.47	137.87	121.70
1	D	4200	THR	C-N-CA	6.47	137.87	121.70
1	B	4200	THR	C-N-CA	6.45	137.83	121.70
1	C	4200	THR	C-N-CA	6.45	137.83	121.70
1	A	3297	PRO	N-CA-CB	6.29	110.85	103.30
1	D	3297	PRO	N-CA-CB	6.29	110.85	103.30
1	C	3303	PRO	N-CA-CB	6.27	110.83	103.30
1	D	3303	PRO	N-CA-CB	6.27	110.83	103.30
1	C	3297	PRO	N-CA-CB	6.27	110.82	103.30
1	A	3303	PRO	N-CA-CB	6.26	110.81	103.30
1	B	3303	PRO	N-CA-CB	6.25	110.81	103.30
1	A	3301	PRO	N-CA-CB	6.25	110.80	103.30
1	B	3301	PRO	N-CA-CB	6.25	110.80	103.30
1	C	3301	PRO	N-CA-CB	6.25	110.80	103.30
1	D	3301	PRO	N-CA-CB	6.25	110.80	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3208	PRO	N-CA-CB	6.25	110.80	103.30
1	B	3208	PRO	N-CA-CB	6.24	110.79	103.30
1	C	3208	PRO	N-CA-CB	6.24	110.79	103.30
1	A	3208	PRO	N-CA-CB	6.24	110.79	103.30
1	B	3297	PRO	N-CA-CB	6.24	110.78	103.30
1	D	3519	PRO	N-CA-CB	6.23	110.77	103.30
1	C	3519	PRO	N-CA-CB	6.21	110.75	103.30
1	A	3519	PRO	N-CA-CB	6.20	110.74	103.30
1	A	4715	TYR	N-CA-C	-6.20	94.28	111.00
1	C	4715	TYR	N-CA-C	-6.20	94.28	111.00
1	D	4715	TYR	N-CA-C	-6.20	94.27	111.00
1	B	4715	TYR	N-CA-C	-6.18	94.31	111.00
1	B	3519	PRO	N-CA-CB	6.18	110.72	103.30
1	B	2640	PRO	N-CA-CB	6.17	110.70	103.30
1	C	2640	PRO	N-CA-CB	6.17	110.70	103.30
1	B	3275	PRO	N-CA-CB	6.16	110.70	103.30
1	D	3275	PRO	N-CA-CB	6.16	110.70	103.30
1	A	2640	PRO	N-CA-CB	6.16	110.69	103.30
1	A	3427	PRO	N-CA-CB	6.16	110.69	103.30
1	B	3427	PRO	N-CA-CB	6.16	110.69	103.30
1	C	3427	PRO	N-CA-CB	6.16	110.69	103.30
1	D	3427	PRO	N-CA-CB	6.16	110.69	103.30
1	A	3275	PRO	N-CA-CB	6.15	110.67	103.30
1	C	3275	PRO	N-CA-CB	6.14	110.67	103.30
1	D	2640	PRO	N-CA-CB	6.13	110.66	103.30
1	B	3224	PRO	N-CA-CB	6.12	110.64	103.30
1	A	3344	PRO	N-CA-CB	6.09	110.60	103.30
1	B	3344	PRO	N-CA-CB	6.09	110.60	103.30
1	C	3344	PRO	N-CA-CB	6.08	110.60	103.30
1	A	3224	PRO	N-CA-CB	6.08	110.60	103.30
1	D	3224	PRO	N-CA-CB	6.08	110.60	103.30
1	C	3224	PRO	N-CA-CB	6.07	110.59	103.30
1	D	3351	PRO	N-CA-CB	6.07	110.59	103.30
1	B	3351	PRO	N-CA-CB	6.07	110.59	103.30
1	A	3351	PRO	N-CA-CB	6.06	110.57	103.30
1	D	3344	PRO	N-CA-CB	6.06	110.57	103.30
1	D	3188	PRO	N-CA-CB	6.05	110.56	103.30
1	C	3351	PRO	N-CA-CB	6.04	110.55	103.30
1	B	3527	PRO	N-CA-CB	6.02	110.52	103.30
1	A	3188	PRO	N-CA-CB	6.01	110.52	103.30
1	C	3293	PRO	N-CA-CB	6.01	110.51	103.30
1	B	3188	PRO	N-CA-CB	6.00	110.50	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3188	PRO	N-CA-CB	6.00	110.50	103.30
1	C	5028	PHE	N-CA-CB	5.99	121.39	110.60
1	A	3527	PRO	N-CA-CB	5.99	110.49	103.30
1	D	3527	PRO	N-CA-CB	5.99	110.49	103.30
1	B	4995	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	C	4995	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	A	4995	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	A	3293	PRO	N-CA-CB	5.97	110.47	103.30
1	B	3293	PRO	N-CA-CB	5.97	110.47	103.30
1	C	3062	PRO	N-CA-CB	5.97	110.47	103.30
1	C	3202	PRO	N-CA-CB	5.97	110.46	103.30
1	D	4995	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	C	3527	PRO	N-CA-CB	5.96	110.45	103.30
1	D	3202	PRO	N-CA-CB	5.96	110.45	103.30
1	A	3062	PRO	N-CA-CB	5.96	110.45	103.30
1	B	3062	PRO	N-CA-CB	5.96	110.45	103.30
1	A	3202	PRO	N-CA-CB	5.95	110.44	103.30
1	D	3293	PRO	N-CA-CB	5.94	110.43	103.30
1	C	3294	PRO	N-CA-CB	5.93	110.42	103.30
1	D	3294	PRO	N-CA-CB	5.93	110.42	103.30
1	B	3202	PRO	N-CA-CB	5.93	110.42	103.30
1	D	3062	PRO	N-CA-CB	5.93	110.42	103.30
1	D	5028	PHE	N-CA-CB	5.93	121.27	110.60
1	A	3294	PRO	N-CA-CB	5.92	110.40	103.30
1	B	3294	PRO	N-CA-CB	5.90	110.38	103.30
1	B	3004	PRO	N-CA-CB	5.86	110.34	103.30
1	A	3004	PRO	N-CA-CB	5.86	110.33	103.30
1	C	3004	PRO	N-CA-CB	5.86	110.33	103.30
1	D	3004	PRO	N-CA-CB	5.86	110.33	103.30
1	B	3410	PRO	N-CA-CB	5.84	110.31	103.30
1	D	3410	PRO	N-CA-CB	5.81	110.27	103.30
1	A	3410	PRO	N-CA-CB	5.80	110.26	103.30
1	C	3410	PRO	N-CA-CB	5.80	110.26	103.30
1	A	4911	LEU	CA-CB-CG	-5.76	102.04	115.30
1	B	4911	LEU	CA-CB-CG	-5.76	102.04	115.30
1	C	4911	LEU	CA-CB-CG	-5.76	102.04	115.30
1	D	4911	LEU	CA-CB-CG	-5.76	102.06	115.30
1	B	4958	CYS	CA-CB-SG	-5.74	103.68	114.00
1	A	3360	PRO	N-CA-CB	5.73	110.17	103.30
1	B	3360	PRO	N-CA-CB	5.73	110.17	103.30
1	C	3360	PRO	N-CA-CB	5.72	110.17	103.30
1	C	4958	CYS	CA-CB-SG	-5.72	103.70	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4958	CYS	CA-CB-SG	-5.71	103.72	114.00
1	A	4958	CYS	CA-CB-SG	-5.71	103.73	114.00
1	D	3360	PRO	N-CA-CB	5.70	110.14	103.30
1	B	180	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	180	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	180	LEU	CA-CB-CG	5.66	128.31	115.30
1	C	180	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	4942	GLU	O-C-N	-5.24	114.32	122.70
1	B	4942	GLU	O-C-N	-5.23	114.34	122.70
1	A	4942	GLU	O-C-N	-5.22	114.34	122.70
1	C	4942	GLU	O-C-N	-5.22	114.34	122.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4231	MET	Peptide
1	A	4957	LYS	Peptide
1	A	4959	PHE	Peptide
1	B	4231	MET	Peptide
1	B	4957	LYS	Peptide
1	B	4959	PHE	Peptide
1	C	4231	MET	Peptide
1	C	4957	LYS	Peptide
1	C	4959	PHE	Peptide
1	D	4231	MET	Peptide
1	D	4957	LYS	Peptide
1	D	4959	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27821	0	24966	494	0
1	B	27821	0	24966	499	0
1	C	27821	0	24966	506	0
1	D	27821	0	24966	495	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1042	0	972	12	0
2	J	1042	0	972	11	0
2	K	1042	0	972	12	0
2	L	1042	0	972	12	0
3	E	804	0	812	9	0
3	F	804	0	812	8	0
3	G	804	0	812	7	0
3	H	804	0	812	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	12	12	1	0
6	B	31	12	12	1	0
6	C	31	12	12	1	0
6	D	31	12	12	1	0
7	A	14	10	10	1	0
7	B	14	10	10	1	0
7	C	14	10	10	1	0
7	D	14	10	10	1	0
All	All	118856	88	107088	2037	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4586:PRO:HG3	1:B:4628:VAL:HG11	1.39	1.04
1:A:4586:PRO:HG3	1:A:4628:VAL:HG11	1.39	1.03
1:C:4586:PRO:HG3	1:C:4628:VAL:HG11	1.39	1.00
1:D:4586:PRO:HG3	1:D:4628:VAL:HG11	1.39	1.00
1:B:4569:LEU:HD21	1:B:4649:LEU:HD23	1.47	0.97
1:B:4957:LYS:HA	1:B:4964:GLY:HA2	1.48	0.95
1:A:4569:LEU:HD21	1:A:4649:LEU:HD23	1.47	0.95
1:C:4569:LEU:HD21	1:C:4649:LEU:HD23	1.47	0.95
1:A:4957:LYS:HA	1:A:4964:GLY:HA2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4569:LEU:HD21	1:D:4649:LEU:HD23	1.47	0.94
1:D:4957:LYS:HA	1:D:4964:GLY:HA2	1.48	0.94
1:C:4957:LYS:HA	1:C:4964:GLY:HA2	1.48	0.92
1:B:4182:GLU:OE2	1:B:5028:PHE:N	2.06	0.89
1:D:4904:PRO:HG3	1:D:4913:ARG:HD2	1.57	0.87
1:A:4904:PRO:HG3	1:A:4913:ARG:HD2	1.57	0.86
1:B:4904:PRO:HG3	1:B:4913:ARG:HD2	1.57	0.86
1:C:4904:PRO:HG3	1:C:4913:ARG:HD2	1.57	0.85
1:B:4716:TRP:O	1:B:4717:ASP:HB2	1.76	0.85
1:C:4716:TRP:O	1:C:4717:ASP:HB2	1.76	0.85
1:A:4716:TRP:O	1:A:4717:ASP:HB2	1.76	0.85
1:D:4716:TRP:O	1:D:4717:ASP:HB2	1.76	0.85
1:D:4183:ILE:HD13	1:D:4193:ILE:HD11	1.62	0.82
1:C:4183:ILE:HD13	1:C:4193:ILE:HD11	1.62	0.81
1:C:4832:HIS:HE1	1:C:4939:ALA:HB1	1.46	0.81
1:D:4980:LEU:HA	1:D:4984:ASN:HD22	1.46	0.81
1:A:4980:LEU:HA	1:A:4984:ASN:HD22	1.46	0.81
1:B:4832:HIS:HE1	1:B:4939:ALA:HB1	1.46	0.80
1:A:4832:HIS:HE1	1:A:4939:ALA:HB1	1.46	0.80
1:D:4832:HIS:HE1	1:D:4939:ALA:HB1	1.46	0.80
1:A:4183:ILE:HD13	1:A:4193:ILE:HD11	1.63	0.80
1:B:4980:LEU:HA	1:B:4984:ASN:HD22	1.46	0.80
1:C:4980:LEU:HA	1:C:4984:ASN:HD22	1.46	0.79
1:B:4183:ILE:HD13	1:B:4193:ILE:HD11	1.64	0.79
1:C:4731:ILE:HG23	1:C:4732:PHE:HD1	1.49	0.78
1:A:4222:VAL:HG11	1:A:4950:VAL:HG22	1.66	0.78
1:B:4958:CYS:SG	1:B:4959:PHE:N	2.57	0.78
1:B:4731:ILE:HG23	1:B:4732:PHE:HD1	1.49	0.78
1:B:4222:VAL:HG11	1:B:4950:VAL:HG22	1.66	0.77
1:D:4222:VAL:HG11	1:D:4950:VAL:HG22	1.66	0.77
1:C:4563:LYS:HA	1:C:4657:ILE:HD11	1.67	0.76
1:C:4958:CYS:SG	1:C:4959:PHE:N	2.57	0.76
1:B:4563:LYS:HA	1:B:4657:ILE:HD11	1.67	0.76
1:A:4731:ILE:HG23	1:A:4732:PHE:HD1	1.49	0.76
1:C:4222:VAL:HG11	1:C:4950:VAL:HG22	1.66	0.76
1:D:4563:LYS:HA	1:D:4657:ILE:HD11	1.67	0.76
1:D:4731:ILE:HG23	1:D:4732:PHE:HD1	1.49	0.76
1:C:4688:ILE:HD11	1:C:4737:ILE:HG12	1.68	0.76
1:D:4958:CYS:SG	1:D:4959:PHE:N	2.57	0.75
1:B:4688:ILE:HD11	1:B:4737:ILE:HG12	1.68	0.75
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.57	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4680:LYS:HE2	1:C:4686:LEU:HD11	1.70	0.74
1:A:4563:LYS:HA	1:A:4657:ILE:HD11	1.67	0.74
1:B:4680:LYS:HE2	1:B:4686:LEU:HD11	1.70	0.74
1:A:4688:ILE:HD11	1:A:4737:ILE:HG12	1.68	0.74
1:D:4688:ILE:HD11	1:D:4737:ILE:HG12	1.68	0.73
1:A:4680:LYS:HE2	1:A:4686:LEU:HD11	1.70	0.72
1:D:4680:LYS:HE2	1:D:4686:LEU:HD11	1.70	0.72
1:C:4826:ILE:HD13	1:C:4940:PHE:CZ	2.25	0.72
1:C:4562:LEU:HD21	1:C:4656:LEU:HD23	1.72	0.71
1:B:4562:LEU:HD21	1:B:4656:LEU:HD23	1.72	0.71
1:D:4826:ILE:HD13	1:D:4940:PHE:CZ	2.25	0.71
1:A:4826:ILE:HD13	1:A:4940:PHE:CZ	2.25	0.71
1:B:4826:ILE:HD13	1:B:4940:PHE:CZ	2.25	0.71
1:D:4190:ILE:HG22	1:D:4191:GLU:H	1.55	0.71
1:A:4562:LEU:HD21	1:A:4656:LEU:HD23	1.72	0.71
1:A:4687:TYR:HE2	1:A:4703:ARG:HG2	1.56	0.71
1:D:4687:TYR:HE2	1:D:4703:ARG:HG2	1.56	0.71
1:D:4562:LEU:HD21	1:D:4656:LEU:HD23	1.72	0.70
1:C:5028:PHE:H	1:C:5028:PHE:HD2	1.39	0.70
1:B:4684:ASP:OD1	1:B:4684:ASP:N	2.25	0.70
1:C:4684:ASP:N	1:C:4684:ASP:OD1	2.25	0.70
1:B:4219:PHE:CD1	1:B:4950:VAL:HG21	2.27	0.70
1:B:5027:CYS:O	1:B:5028:PHE:C	2.27	0.70
1:C:4219:PHE:CD1	1:C:4950:VAL:HG21	2.27	0.70
1:C:4937:ILE:HG13	1:C:4938:ASP:N	2.07	0.70
1:A:4219:PHE:CD1	1:A:4950:VAL:HG21	2.27	0.69
1:A:4937:ILE:HG13	1:A:4938:ASP:N	2.07	0.69
1:B:4219:PHE:O	1:B:4222:VAL:HG12	1.92	0.69
1:A:4219:PHE:O	1:A:4222:VAL:HG12	1.92	0.69
1:B:4687:TYR:HE2	1:B:4703:ARG:HG2	1.56	0.69
1:A:4952:GLU:O	1:A:4954:MET:N	2.26	0.69
1:D:4219:PHE:CD1	1:D:4950:VAL:HG21	2.27	0.69
1:B:4937:ILE:HG13	1:B:4938:ASP:N	2.07	0.69
1:C:4219:PHE:O	1:C:4222:VAL:HG12	1.92	0.69
1:C:4687:TYR:HE2	1:C:4703:ARG:HG2	1.56	0.69
1:D:4231:MET:HG3	1:D:5022:PHE:HD2	1.58	0.69
1:D:4937:ILE:HG13	1:D:4938:ASP:N	2.07	0.69
1:C:4231:MET:HG3	1:C:5022:PHE:HD2	1.58	0.69
1:A:4231:MET:HG3	1:A:5022:PHE:HD2	1.58	0.69
1:C:4952:GLU:O	1:C:4954:MET:N	2.26	0.69
1:D:4952:GLU:O	1:D:4954:MET:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5028:PHE:H	1:D:5028:PHE:HD2	1.41	0.69
1:A:4222:VAL:CG1	1:A:4950:VAL:HG22	2.23	0.69
1:B:4231:MET:HG3	1:B:5022:PHE:HD2	1.58	0.68
1:D:4182:GLU:OE2	1:D:5028:PHE:N	2.27	0.68
1:D:4968:PHE:O	1:D:4974:GLY:HA3	1.94	0.68
1:A:4219:PHE:HD1	1:A:4950:VAL:HG21	1.58	0.68
1:B:4219:PHE:HD1	1:B:4950:VAL:HG21	1.58	0.68
1:D:4684:ASP:OD1	1:D:4684:ASP:N	2.25	0.68
1:D:4920:PHE:O	1:D:4921:PHE:C	2.32	0.68
1:B:4952:GLU:O	1:B:4954:MET:N	2.26	0.68
1:C:4968:PHE:O	1:C:4974:GLY:HA3	1.94	0.68
1:A:4190:ILE:HD11	1:A:5028:PHE:HA	1.75	0.68
1:B:4222:VAL:CG1	1:B:4950:VAL:HG22	2.23	0.68
1:B:4920:PHE:O	1:B:4921:PHE:C	2.32	0.68
1:D:4958:CYS:O	6:D:5103:ATP:N6	2.27	0.68
1:D:4219:PHE:O	1:D:4222:VAL:HG12	1.92	0.68
1:D:4219:PHE:HD1	1:D:4950:VAL:HG21	1.58	0.68
1:A:4958:CYS:O	6:A:5103:ATP:N6	2.27	0.68
1:D:5027:CYS:H	1:D:5030:LYS:CB	2.07	0.68
1:C:4958:CYS:O	6:C:5103:ATP:N6	2.27	0.67
1:D:4222:VAL:CG1	1:D:4950:VAL:HG22	2.23	0.67
1:B:4958:CYS:O	6:B:5103:ATP:N6	2.27	0.67
1:C:4222:VAL:CG1	1:C:4950:VAL:HG22	2.23	0.67
1:A:4920:PHE:O	1:A:4921:PHE:C	2.32	0.67
1:B:4968:PHE:O	1:B:4974:GLY:HA3	1.94	0.67
1:A:4975:PHE:O	1:A:4979:THR:HG22	1.95	0.67
1:C:4219:PHE:HD1	1:C:4950:VAL:HG21	1.58	0.67
1:C:4975:PHE:O	1:C:4979:THR:HG22	1.95	0.67
1:D:4661:TYR:HE2	1:D:4789:PHE:HB2	1.60	0.67
1:C:4182:GLU:OE2	1:C:5028:PHE:N	2.27	0.67
1:C:4661:TYR:HE2	1:C:4789:PHE:HB2	1.60	0.67
1:A:4968:PHE:O	1:A:4974:GLY:HA3	1.94	0.67
1:D:4975:PHE:O	1:D:4979:THR:HG22	1.95	0.67
1:C:5027:CYS:H	1:C:5030:LYS:CB	2.08	0.67
1:B:4661:TYR:HE2	1:B:4789:PHE:HB2	1.60	0.67
1:B:4569:LEU:HD21	1:B:4649:LEU:CD2	2.24	0.66
1:A:4999:ASP:HB3	1:A:5002:GLU:OE2	1.95	0.66
1:C:4904:PRO:CG	1:C:4913:ARG:HD2	2.26	0.66
1:D:4904:PRO:CG	1:D:4913:ARG:HD2	2.26	0.66
1:D:4999:ASP:HB3	1:D:5002:GLU:OE2	1.95	0.66
1:A:4569:LEU:HD21	1:A:4649:LEU:CD2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4661:TYR:HE2	1:A:4789:PHE:HB2	1.60	0.66
1:A:4684:ASP:OD1	1:A:4684:ASP:N	2.25	0.66
1:B:4182:GLU:OE2	1:B:4190:ILE:HD11	1.96	0.66
1:A:4904:PRO:CG	1:A:4913:ARG:HD2	2.26	0.66
1:B:4952:GLU:O	1:B:4955:GLU:N	2.29	0.66
1:B:4975:PHE:O	1:B:4979:THR:HG22	1.95	0.66
1:B:4999:ASP:HB3	1:B:5002:GLU:OE2	1.95	0.66
1:A:4952:GLU:O	1:A:4955:GLU:N	2.29	0.66
1:A:4562:LEU:HD21	1:A:4656:LEU:HB3	1.77	0.66
1:B:4562:LEU:HD21	1:B:4656:LEU:HB3	1.77	0.66
1:C:4999:ASP:HB3	1:C:5002:GLU:OE2	1.95	0.65
1:C:4920:PHE:O	1:C:4921:PHE:C	2.32	0.65
1:C:4952:GLU:O	1:C:4955:GLU:N	2.29	0.65
1:D:4569:LEU:HD21	1:D:4649:LEU:CD2	2.24	0.65
1:D:289:ARG:HE	1:D:303:ASP:HA	1.61	0.65
1:B:4904:PRO:CG	1:B:4913:ARG:HD2	2.26	0.65
1:D:4562:LEU:HD21	1:D:4656:LEU:HB3	1.77	0.65
1:A:289:ARG:HE	1:A:303:ASP:HA	1.61	0.65
1:A:393:CYS:SG	1:A:394:GLN:N	2.70	0.65
1:C:4586:PRO:HA	1:C:4628:VAL:HG21	1.79	0.65
1:D:4796:MET:O	1:D:4799:SER:N	2.30	0.65
1:C:4562:LEU:HD21	1:C:4656:LEU:HB3	1.77	0.65
1:C:4796:MET:O	1:C:4799:SER:N	2.30	0.64
1:D:4586:PRO:HA	1:D:4628:VAL:HG21	1.79	0.64
1:A:4796:MET:O	1:A:4799:SER:N	2.30	0.64
1:A:4586:PRO:HA	1:A:4628:VAL:HG21	1.79	0.64
1:B:4586:PRO:HA	1:B:4628:VAL:HG21	1.79	0.64
1:D:393:CYS:SG	1:D:394:GLN:N	2.70	0.64
1:B:289:ARG:HE	1:B:303:ASP:HA	1.61	0.64
1:B:4796:MET:O	1:B:4799:SER:N	2.30	0.64
1:D:4952:GLU:O	1:D:4955:GLU:N	2.29	0.64
1:C:3678:SER:HB2	1:C:3698:LEU:HD12	1.80	0.64
1:B:393:CYS:SG	1:B:394:GLN:N	2.70	0.64
1:C:393:CYS:SG	1:C:394:GLN:N	2.70	0.63
1:B:3678:SER:HB2	1:B:3698:LEU:HD12	1.80	0.63
1:C:4840:THR:O	1:C:4843:LEU:N	2.27	0.63
1:D:4247:ILE:HA	1:D:4250:GLN:HG2	1.81	0.63
1:A:711:LEU:O	1:A:1470:ARG:NH2	2.31	0.63
1:D:3678:SER:HB2	1:D:3698:LEU:HD12	1.80	0.63
1:A:4705:VAL:HG13	1:A:4706:LEU:HD12	1.81	0.63
1:C:289:ARG:HE	1:C:303:ASP:HA	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4705:VAL:HG13	1:B:4706:LEU:HD12	1.81	0.62
1:C:4247:ILE:HA	1:C:4250:GLN:HG2	1.81	0.62
1:C:4569:LEU:HD21	1:C:4649:LEU:CD2	2.24	0.62
1:A:3678:SER:HB2	1:A:3698:LEU:HD12	1.80	0.62
1:D:711:LEU:O	1:D:1470:ARG:NH2	2.31	0.62
1:A:4247:ILE:HA	1:A:4250:GLN:HG2	1.81	0.62
1:B:711:LEU:O	1:B:1470:ARG:NH2	2.32	0.62
1:C:711:LEU:O	1:C:1470:ARG:NH2	2.32	0.62
1:C:731:THR:O	1:C:765:GLN:NE2	2.33	0.62
1:C:4844:LEU:HB2	1:C:4928:LEU:HD23	1.82	0.62
1:A:1473:THR:HA	1:A:1488:LYS:HA	1.82	0.62
1:D:4556:SER:OG	1:D:4664:LEU:HB2	1.99	0.62
1:A:4844:LEU:HB2	1:A:4928:LEU:HD23	1.82	0.62
1:B:4844:LEU:HB2	1:B:4928:LEU:HD23	1.82	0.62
1:D:731:THR:O	1:D:765:GLN:NE2	2.33	0.62
1:D:1473:THR:HA	1:D:1488:LYS:HA	1.82	0.62
1:B:731:THR:O	1:B:765:GLN:NE2	2.33	0.62
1:B:1473:THR:HA	1:B:1488:LYS:HA	1.82	0.62
1:C:4556:SER:OG	1:C:4664:LEU:HB2	1.99	0.62
1:D:4563:LYS:O	1:D:4566:ALA:N	2.32	0.62
1:B:1452:TRP:HE1	1:B:1518:CYS:HG	1.44	0.62
1:C:4235:VAL:HG11	1:C:5019:TRP:CH2	2.36	0.61
1:C:1473:THR:HA	1:C:1488:LYS:HA	1.82	0.61
1:D:4844:LEU:HB2	1:D:4928:LEU:HD23	1.82	0.61
1:B:4247:ILE:HA	1:B:4250:GLN:HG2	1.81	0.61
1:D:4705:VAL:HG13	1:D:4706:LEU:HD12	1.81	0.61
1:B:4556:SER:OG	1:B:4664:LEU:HB2	1.99	0.61
1:C:4888:TYR:CD1	1:D:4914:VAL:HG23	2.35	0.61
1:C:4957:LYS:HD2	1:C:4964:GLY:HA3	1.83	0.61
1:A:731:THR:O	1:A:765:GLN:NE2	2.33	0.61
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.82	0.61
1:C:4242:ILE:HD11	7:C:5104:CFF:H142	1.83	0.61
1:D:4840:THR:O	1:D:4843:LEU:N	2.27	0.61
1:A:4556:SER:OG	1:A:4664:LEU:HB2	1.99	0.61
1:B:2233:CYS:HG	1:B:2270:SER:HG	1.48	0.61
1:C:1452:TRP:NE1	1:C:1518:CYS:SG	2.73	0.61
1:C:4705:VAL:HG13	1:C:4706:LEU:HD12	1.81	0.61
1:A:102:LEU:H	1:A:105:HIS:HD2	1.49	0.61
1:A:4235:VAL:HG11	1:A:5019:TRP:CH2	2.36	0.60
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.81	0.60
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.81	0.60
1:A:4957:LYS:HD2	1:A:4964:GLY:HA3	1.83	0.60
1:B:102:LEU:H	1:B:105:HIS:HD2	1.49	0.60
1:B:5008:SER:O	1:B:5011:TRP:N	2.34	0.60
1:D:5028:PHE:O	1:D:5030:LYS:N	2.34	0.60
1:B:4242:ILE:HD11	7:B:5104:CFF:H142	1.83	0.60
1:B:4957:LYS:HD2	1:B:4964:GLY:HA3	1.83	0.60
1:D:102:LEU:H	1:D:105:HIS:HD2	1.49	0.60
1:A:4836:GLN:O	1:A:4840:THR:HG23	2.02	0.60
1:A:4946:GLN:O	1:A:4948:GLU:N	2.35	0.60
3:H:13:ARG:HG3	3:H:14:THR:HG23	1.83	0.60
1:B:1927:LEU:O	1:B:2104:ARG:NH2	2.35	0.60
1:B:4778:TRP:O	1:B:4781:GLY:N	2.32	0.60
1:D:4235:VAL:HG11	1:D:5019:TRP:CH2	2.36	0.60
1:C:1927:LEU:O	1:C:2104:ARG:NH2	2.35	0.60
1:D:4957:LYS:HD2	1:D:4964:GLY:HA3	1.83	0.60
1:A:2117:VAL:HA	1:A:2120:MET:HB3	1.83	0.60
1:B:4235:VAL:HG11	1:B:5019:TRP:CH2	2.35	0.60
1:A:5008:SER:O	1:A:5011:TRP:N	2.34	0.60
1:B:4836:GLN:O	1:B:4840:THR:HG23	2.02	0.60
1:C:4836:GLN:O	1:C:4840:THR:HG23	2.02	0.60
1:D:4242:ILE:HD11	7:D:5104:CFF:H142	1.83	0.60
1:B:415:ILE:O	1:B:493:ARG:NH2	2.35	0.60
1:B:4946:GLN:O	1:B:4948:GLU:N	2.35	0.60
1:C:102:LEU:H	1:C:105:HIS:HD2	1.49	0.60
1:C:1100:MET:H	1:C:1126:GLY:HA3	1.67	0.60
1:D:1100:MET:H	1:D:1126:GLY:HA3	1.67	0.60
1:D:2117:VAL:HA	1:D:2120:MET:HB3	1.83	0.60
1:A:4839:MET:HG2	1:D:4820:VAL:HG21	1.82	0.60
3:F:13:ARG:HG3	3:F:14:THR:HG23	1.82	0.60
1:A:1452:TRP:NE1	1:A:1518:CYS:SG	2.73	0.60
1:B:1023:PRO:HG2	1:B:1026:LEU:HD13	1.84	0.60
1:C:1023:PRO:HG2	1:C:1026:LEU:HD13	1.84	0.60
1:C:4957:LYS:HD2	1:C:4964:GLY:CA	2.32	0.59
1:D:1023:PRO:HG2	1:D:1026:LEU:HD13	1.84	0.59
1:D:4957:LYS:HD2	1:D:4964:GLY:CA	2.32	0.59
1:A:4247:ILE:HA	1:A:4250:GLN:CG	2.32	0.59
1:B:4247:ILE:HA	1:B:4250:GLN:CG	2.32	0.59
1:C:5008:SER:O	1:C:5011:TRP:N	2.34	0.59
3:G:13:ARG:HG3	3:G:14:THR:HG23	1.82	0.59
1:A:1023:PRO:HG2	1:A:1026:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4888:TYR:CD1	1:C:4914:VAL:HG23	2.36	0.59
1:C:2117:VAL:HA	1:C:2120:MET:HB3	1.83	0.59
1:A:1927:LEU:O	1:A:2104:ARG:NH2	2.35	0.59
1:B:1100:MET:H	1:B:1126:GLY:HA3	1.67	0.59
1:B:4957:LYS:HD2	1:B:4964:GLY:CA	2.32	0.59
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.85	0.59
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.85	0.59
1:D:4946:GLN:O	1:D:4948:GLU:N	2.35	0.59
1:D:5008:SER:O	1:D:5011:TRP:N	2.34	0.59
1:A:1100:MET:H	1:A:1126:GLY:HA3	1.67	0.59
1:A:4778:TRP:O	1:A:4781:GLY:N	2.32	0.59
1:C:4946:GLN:O	1:C:4948:GLU:N	2.35	0.59
1:D:415:ILE:O	1:D:493:ARG:NH2	2.35	0.59
1:D:4778:TRP:O	1:D:4781:GLY:N	2.32	0.59
1:A:4934:GLY:O	1:A:4935:LEU:C	2.41	0.59
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.85	0.59
1:A:4242:ILE:HD11	7:A:5104:CFF:H142	1.83	0.59
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.85	0.59
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.36	0.59
1:D:4836:GLN:O	1:D:4840:THR:HG23	2.02	0.59
1:C:4934:GLY:O	1:C:4935:LEU:C	2.41	0.59
1:B:2117:VAL:HA	1:B:2120:MET:HB3	1.83	0.59
1:C:4980:LEU:HA	1:C:4984:ASN:ND2	2.18	0.59
3:E:13:ARG:HG3	3:E:14:THR:HG23	1.82	0.59
1:C:415:ILE:O	1:C:493:ARG:NH2	2.35	0.59
1:D:2233:CYS:HG	1:D:2270:SER:HG	1.50	0.59
1:A:415:ILE:O	1:A:493:ARG:NH2	2.35	0.58
1:B:4798:MET:O	1:B:4801:LEU:N	2.36	0.58
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.85	0.58
1:C:5028:PHE:O	1:C:5030:LYS:N	2.35	0.58
1:D:3752:SER:OG	1:D:3753:PHE:N	2.36	0.58
1:D:4247:ILE:HA	1:D:4250:GLN:CG	2.32	0.58
1:A:4960:ILE:HD13	1:A:4988:TYR:CE2	2.38	0.58
2:L:123:ASP:O	2:L:127:ARG:NH1	2.35	0.58
1:B:3696:ASP:N	1:B:3696:ASP:OD1	2.36	0.58
1:C:2474:LEU:HD21	1:C:2494:PHE:HB3	1.85	0.58
1:C:3987:ASP:N	1:C:3987:ASP:OD1	2.36	0.58
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.36	0.58
1:D:4822:THR:O	1:D:4826:ILE:HG12	2.04	0.58
1:D:4831:THR:O	1:D:4834:GLY:N	2.36	0.58
1:D:4960:ILE:HD13	1:D:4988:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4798:MET:O	1:A:4801:LEU:N	2.36	0.58
1:B:1721:GLU:OE1	1:B:1725:ARG:NH1	2.37	0.58
1:B:4980:LEU:HA	1:B:4984:ASN:ND2	2.18	0.58
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.77	0.58
1:D:4798:MET:O	1:D:4801:LEU:N	2.36	0.58
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.36	0.58
1:B:4563:LYS:O	1:B:4566:ALA:N	2.32	0.58
1:D:2474:LEU:HD21	1:D:2494:PHE:HB3	1.85	0.58
1:A:194:SER:OG	1:A:195:PHE:N	2.37	0.58
1:A:2474:LEU:HD21	1:A:2494:PHE:HB3	1.85	0.58
1:A:4822:THR:O	1:A:4826:ILE:HG12	2.04	0.58
1:A:4957:LYS:HD2	1:A:4964:GLY:CA	2.32	0.58
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.85	0.58
1:C:1721:GLU:OE1	1:C:1725:ARG:NH1	2.37	0.58
1:C:4247:ILE:HA	1:C:4250:GLN:CG	2.32	0.58
1:C:4822:THR:O	1:C:4826:ILE:HG12	2.03	0.58
1:D:1927:LEU:O	1:D:2104:ARG:NH2	2.35	0.58
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.36	0.58
1:A:2233:CYS:HG	1:A:2270:SER:HG	1.49	0.58
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.77	0.58
1:C:120:CYS:SG	1:C:121:LEU:N	2.77	0.58
1:D:120:CYS:SG	1:D:121:LEU:N	2.77	0.58
1:D:1721:GLU:OE1	1:D:1725:ARG:NH1	2.37	0.58
1:B:2474:LEU:HD21	1:B:2494:PHE:HB3	1.85	0.58
1:B:4683:PHE:HE2	1:B:5017:ARG:HD2	1.69	0.58
1:C:4683:PHE:HE2	1:C:5017:ARG:HD2	1.69	0.58
1:D:2254:LEU:HA	1:D:2257:LEU:HB2	1.85	0.58
1:D:5028:PHE:C	1:D:5030:LYS:H	2.06	0.58
1:A:615:ARG:HH12	1:A:1678:ASN:HA	1.69	0.58
1:B:4960:ILE:HD13	1:B:4988:TYR:CE2	2.38	0.58
1:C:194:SER:OG	1:C:195:PHE:N	2.37	0.58
1:D:615:ARG:HH12	1:D:1678:ASN:HA	1.69	0.58
1:A:569:ILE:HD13	1:A:605:SER:HB2	1.86	0.58
1:D:4946:GLN:O	1:D:4947:GLN:C	2.41	0.58
1:A:4820:VAL:HG21	1:B:4839:MET:HG2	1.84	0.58
1:A:4888:TYR:CD1	1:B:4914:VAL:HG23	2.38	0.58
1:B:569:ILE:HD13	1:B:605:SER:HB2	1.86	0.58
1:C:3752:SER:OG	1:C:3753:PHE:N	2.36	0.58
1:A:1721:GLU:OE1	1:A:1725:ARG:NH1	2.37	0.57
1:B:4986:ALA:O	1:B:4989:MET:HE2	2.04	0.57
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3987:ASP:OD1	1:B:3987:ASP:N	2.36	0.57
1:C:2254:LEU:HA	1:C:2257:LEU:HB2	1.85	0.57
1:C:4986:ALA:O	1:C:4989:MET:HE2	2.04	0.57
1:B:4820:VAL:HG21	1:C:4839:MET:HG2	1.86	0.57
1:C:4798:MET:O	1:C:4801:LEU:N	2.36	0.57
1:C:4990:PHE:O	1:C:4994:TYR:N	2.37	0.57
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.37	0.57
1:D:4558:ASN:O	1:D:4561:THR:HG22	2.05	0.57
1:B:120:CYS:SG	1:B:121:LEU:N	2.77	0.57
1:B:4822:THR:O	1:B:4826:ILE:HG12	2.04	0.57
1:C:569:ILE:HD13	1:C:605:SER:HB2	1.86	0.57
1:D:569:ILE:HD13	1:D:605:SER:HB2	1.86	0.57
1:D:4986:ALA:O	1:D:4989:MET:HE2	2.04	0.57
1:A:1452:TRP:HE1	1:A:1518:CYS:HG	1.46	0.57
1:A:4990:PHE:O	1:A:4994:TYR:N	2.37	0.57
1:B:2254:LEU:HA	1:B:2257:LEU:HB2	1.85	0.57
1:B:4737:ILE:O	1:B:4740:LEU:N	2.38	0.57
1:C:4960:ILE:HD13	1:C:4988:TYR:CE2	2.38	0.57
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.77	0.57
1:A:4558:ASN:O	1:A:4561:THR:HG22	2.05	0.57
1:B:4577:LEU:HD21	1:B:4807:PHE:CD1	2.40	0.57
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.37	0.57
1:C:4638:TYR:C	1:C:4641:PRO:HD2	2.24	0.57
1:A:2254:LEU:HA	1:A:2257:LEU:HB2	1.85	0.57
1:A:4638:TYR:C	1:A:4641:PRO:HD2	2.24	0.57
1:B:1232:ARG:NH1	1:B:1828:ASP:O	2.37	0.57
1:B:4946:GLN:O	1:B:4947:GLN:C	2.41	0.57
1:C:4737:ILE:O	1:C:4740:LEU:N	2.38	0.57
1:C:4820:VAL:HG21	1:D:4839:MET:HG2	1.87	0.57
1:D:1781:CYS:SG	1:D:1782:PHE:N	2.78	0.57
1:D:4959:PHE:O	1:D:4960:ILE:HG13	2.05	0.57
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.37	0.57
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.77	0.57
1:A:4942:GLU:O	1:A:4943:LEU:C	2.42	0.57
1:B:1101:ARG:HB2	1:B:1193:SER:HB3	1.87	0.57
1:C:4778:TRP:O	1:C:4781:GLY:N	2.32	0.57
1:C:5028:PHE:C	1:C:5030:LYS:H	2.08	0.57
1:D:4577:LEU:HD21	1:D:4807:PHE:CD1	2.40	0.57
2:K:123:ASP:O	2:K:127:ARG:NH1	2.35	0.57
1:A:2282:ASP:OD1	1:A:2342:ASN:ND2	2.38	0.57
1:A:4577:LEU:HD21	1:A:4807:PHE:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4737:ILE:O	1:A:4740:LEU:N	2.38	0.57
1:B:194:SER:OG	1:B:195:PHE:N	2.37	0.57
1:C:4558:ASN:O	1:C:4561:THR:HG22	2.05	0.57
2:J:123:ASP:O	2:J:127:ARG:NH1	2.35	0.57
1:D:4138:ASP:OD1	1:D:4138:ASP:N	2.38	0.57
1:A:1101:ARG:HB2	1:A:1193:SER:HB3	1.87	0.57
1:A:4244:GLU:HA	1:A:4247:ILE:HG12	1.87	0.57
1:A:4980:LEU:HA	1:A:4984:ASN:ND2	2.18	0.57
1:B:4638:TYR:C	1:B:4641:PRO:HD2	2.24	0.57
1:C:1781:CYS:SG	1:C:1782:PHE:N	2.78	0.57
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.57
1:C:4577:LEU:HD21	1:C:4807:PHE:CD1	2.40	0.57
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.85	0.57
1:D:1232:ARG:NH1	1:D:1828:ASP:O	2.37	0.57
1:D:4688:ILE:HD11	1:D:4737:ILE:CG1	2.35	0.57
1:A:120:CYS:SG	1:A:121:LEU:N	2.77	0.56
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.85	0.56
1:A:4683:PHE:HE2	1:A:5017:ARG:HD2	1.69	0.56
1:C:2336:ARG:HG2	1:C:2435:ARG:HD2	1.87	0.56
1:A:4688:ILE:HD11	1:A:4737:ILE:CG1	2.35	0.56
1:A:4986:ALA:O	1:A:4989:MET:HE2	2.04	0.56
1:B:615:ARG:HH12	1:B:1678:ASN:HA	1.69	0.56
1:B:4990:PHE:O	1:B:4994:TYR:N	2.37	0.56
1:C:3732:SER:O	1:C:3766:GLN:NE2	2.38	0.56
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.38	0.56
1:A:5028:PHE:O	1:A:5030:LYS:N	2.36	0.56
1:B:2516:ASP:N	1:B:2516:ASP:OD1	2.39	0.56
1:B:4772:ASP:O	1:B:4776:GLN:HG2	2.05	0.56
1:B:4826:ILE:HD13	1:B:4940:PHE:CE1	2.40	0.56
2:I:123:ASP:O	2:I:127:ARG:NH1	2.35	0.56
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.38	0.56
1:D:194:SER:OG	1:D:195:PHE:N	2.37	0.56
1:D:2282:ASP:OD1	1:D:2342:ASN:ND2	2.38	0.56
1:D:4638:TYR:C	1:D:4641:PRO:HD2	2.24	0.56
1:D:4737:ILE:O	1:D:4740:LEU:N	2.38	0.56
1:D:4832:HIS:CE1	1:D:4939:ALA:HB1	2.36	0.56
1:A:1008:SER:HB3	1:A:1017:ARG:HE	1.70	0.56
1:A:1781:CYS:SG	1:A:1782:PHE:N	2.78	0.56
1:A:4577:LEU:HD21	1:A:4807:PHE:CE1	2.41	0.56
1:A:4959:PHE:O	1:A:4960:ILE:HG13	2.05	0.56
1:B:1008:SER:HB3	1:B:1017:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2282:ASP:OD1	1:B:2342:ASN:ND2	2.38	0.56
1:B:2515:GLN:HA	1:B:2568:LEU:HD21	1.88	0.56
1:B:4558:ASN:O	1:B:4561:THR:HG22	2.05	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:D:4683:PHE:HE2	1:D:5017:ARG:HD2	1.69	0.56
1:B:1192:CYS:SG	1:B:1193:SER:N	2.79	0.56
1:C:1101:ARG:HB2	1:C:1193:SER:HB3	1.87	0.56
1:A:320:LYS:HG3	1:A:356:TRP:HE1	1.71	0.56
1:A:2336:ARG:HG2	1:A:2435:ARG:HD2	1.87	0.56
1:A:3732:SER:O	1:A:3766:GLN:NE2	2.38	0.56
1:A:5008:SER:OG	1:A:5009:TYR:N	2.39	0.56
1:B:1781:CYS:SG	1:B:1782:PHE:N	2.78	0.56
1:B:4650:HIS:O	1:B:4653:VAL:N	2.39	0.56
1:B:4959:PHE:O	1:B:4960:ILE:HG13	2.05	0.56
1:C:2458:ARG:HH21	1:C:2510:TYR:HA	1.71	0.56
1:C:4772:ASP:O	1:C:4776:GLN:HG2	2.05	0.56
1:C:4831:THR:O	1:C:4834:GLY:N	2.36	0.56
1:D:3732:SER:O	1:D:3766:GLN:NE2	2.38	0.56
1:D:4650:HIS:O	1:D:4653:VAL:N	2.39	0.56
1:D:4934:GLY:O	1:D:4935:LEU:C	2.41	0.56
1:A:4826:ILE:HD13	1:A:4940:PHE:CE1	2.41	0.56
1:B:2302:LEU:HD23	1:B:2363:CYS:HB3	1.88	0.56
1:B:3732:SER:O	1:B:3766:GLN:NE2	2.38	0.56
1:C:615:ARG:HH12	1:C:1678:ASN:HA	1.69	0.56
1:C:4825:THR:HA	1:C:4828:SER:OG	2.06	0.56
1:C:4826:ILE:HD13	1:C:4940:PHE:CE1	2.41	0.56
1:D:320:LYS:HG3	1:D:356:TRP:HE1	1.71	0.56
1:D:1192:CYS:SG	1:D:1193:SER:N	2.79	0.56
1:A:4563:LYS:O	1:A:4566:ALA:N	2.32	0.56
1:A:4650:HIS:O	1:A:4653:VAL:N	2.39	0.56
1:A:4840:THR:O	1:A:4843:LEU:N	2.27	0.56
1:A:4986:ALA:HA	1:A:4989:MET:HE1	1.88	0.56
1:B:2336:ARG:HG2	1:B:2435:ARG:HD2	1.87	0.56
1:C:2302:LEU:HD23	1:C:2363:CYS:HB3	1.88	0.56
1:D:2634:ASN:O	1:D:2638:LYS:N	2.39	0.56
1:A:1192:CYS:SG	1:A:1193:SER:N	2.79	0.56
1:A:1856:ASP:N	1:A:1856:ASP:OD1	2.39	0.56
1:A:3987:ASP:OD1	1:A:3987:ASP:N	2.36	0.56
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.36	0.56
1:C:4138:ASP:N	1:C:4138:ASP:OD1	2.38	0.56
1:A:2634:ASN:O	1:A:2638:LYS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.56
1:A:4831:THR:O	1:A:4834:GLY:N	2.36	0.56
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.56
1:B:4825:THR:HA	1:B:4828:SER:OG	2.06	0.56
1:B:4934:GLY:O	1:B:4935:LEU:C	2.41	0.56
1:C:4986:ALA:HA	1:C:4989:MET:HE1	1.88	0.56
1:D:1101:ARG:HB2	1:D:1193:SER:HB3	1.87	0.56
1:D:1271:ARG:NH2	1:D:1560:ASN:OD1	2.39	0.56
1:D:4577:LEU:HD21	1:D:4807:PHE:CE1	2.41	0.56
1:D:5008:SER:OG	1:D:5009:TYR:N	2.39	0.56
1:B:4190:ILE:HG23	1:B:5031:GLN:HE22	1.70	0.55
1:C:2515:GLN:HA	1:C:2568:LEU:HD21	1.88	0.55
1:C:4959:PHE:O	1:C:4960:ILE:HG13	2.05	0.55
1:D:3987:ASP:OD1	1:D:3987:ASP:N	2.36	0.55
1:A:1607:ARG:NH2	1:A:1610:ASN:OD1	2.40	0.55
1:A:4850:LEU:HD11	1:D:4814:LEU:HD21	1.88	0.55
1:A:4914:VAL:HG23	1:D:4888:TYR:CD1	2.42	0.55
1:B:2458:ARG:HH21	1:B:2510:TYR:HA	1.71	0.55
1:B:3752:SER:OG	1:B:3753:PHE:N	2.36	0.55
1:B:4831:THR:O	1:B:4834:GLY:N	2.36	0.55
1:C:1271:ARG:NH2	1:C:1560:ASN:OD1	2.39	0.55
1:D:2336:ARG:HG2	1:D:2435:ARG:HD2	1.87	0.55
1:A:4832:HIS:CE1	1:A:4939:ALA:HB1	2.36	0.55
1:B:4244:GLU:HA	1:B:4247:ILE:HG12	1.87	0.55
1:C:1008:SER:HB3	1:C:1017:ARG:HE	1.70	0.55
1:C:2282:ASP:OD1	1:C:2342:ASN:ND2	2.38	0.55
1:C:4946:GLN:O	1:C:4947:GLN:C	2.41	0.55
1:D:1607:ARG:NH2	1:D:1610:ASN:OD1	2.40	0.55
1:D:4772:ASP:O	1:D:4776:GLN:HG2	2.05	0.55
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.40	0.55
1:C:2634:ASN:O	1:C:2638:LYS:N	2.39	0.55
1:C:4244:GLU:HA	1:C:4247:ILE:HG12	1.87	0.55
1:A:2515:GLN:HA	1:A:2568:LEU:HD21	1.88	0.55
1:A:4772:ASP:O	1:A:4776:GLN:HG2	2.05	0.55
1:A:4881:THR:O	1:A:4884:LEU:N	2.40	0.55
1:A:5028:PHE:C	1:A:5030:LYS:H	2.09	0.55
1:B:2634:ASN:O	1:B:2638:LYS:N	2.39	0.55
1:B:4138:ASP:OD1	1:B:4138:ASP:N	2.38	0.55
1:B:4942:GLU:O	1:B:4943:LEU:C	2.42	0.55
1:C:1192:CYS:SG	1:C:1193:SER:N	2.79	0.55
1:C:4577:LEU:HD21	1:C:4807:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4666:VAL:HG23	1:D:4667:PRO:HD3	1.89	0.55
1:D:4826:ILE:HD13	1:D:4940:PHE:CE1	2.41	0.55
1:A:4825:THR:HA	1:A:4828:SER:OG	2.06	0.55
1:B:134:ASP:N	1:B:134:ASP:OD1	2.39	0.55
1:B:320:LYS:HG3	1:B:356:TRP:HE1	1.71	0.55
1:B:4577:LEU:HD21	1:B:4807:PHE:CE1	2.41	0.55
1:B:4666:VAL:HG23	1:B:4667:PRO:HD3	1.89	0.55
1:C:4650:HIS:O	1:C:4653:VAL:N	2.39	0.55
1:D:1974:ARG:NH2	1:D:3642:TYR:O	2.40	0.55
1:A:134:ASP:OD1	1:A:134:ASP:N	2.39	0.55
1:A:2530:MET:SD	1:A:2531:ARG:NH1	2.79	0.55
1:A:4666:VAL:HG23	1:A:4667:PRO:HD3	1.89	0.55
3:H:23:VAL:HG22	3:H:104:LEU:HD13	1.89	0.55
1:C:320:LYS:HG3	1:C:356:TRP:HE1	1.71	0.55
1:C:4814:LEU:HD21	1:D:4850:LEU:HD11	1.88	0.55
1:D:4825:THR:HA	1:D:4828:SER:OG	2.06	0.55
1:D:4920:PHE:O	1:D:4922:PHE:N	2.40	0.55
1:A:4195:PHE:HD2	1:A:4994:TYR:CD2	2.25	0.55
1:B:1856:ASP:OD1	1:B:1856:ASP:N	2.39	0.55
1:C:1607:ARG:NH2	1:C:1610:ASN:OD1	2.40	0.55
1:D:4195:PHE:HD2	1:D:4994:TYR:CD2	2.25	0.55
1:A:24:CYS:SG	1:A:25:SER:N	2.80	0.55
1:B:4920:PHE:O	1:B:4922:PHE:N	2.40	0.55
1:C:4920:PHE:O	1:C:4922:PHE:N	2.40	0.55
1:D:1008:SER:HB3	1:D:1017:ARG:HE	1.70	0.55
1:D:4244:GLU:HA	1:D:4247:ILE:HG12	1.87	0.55
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.39	0.55
1:A:4920:PHE:O	1:A:4922:PHE:N	2.40	0.55
1:B:4240:ASP:O	1:B:4243:PHE:N	2.35	0.55
1:C:2333:ASP:OD1	1:C:2333:ASP:N	2.40	0.55
1:C:4563:LYS:O	1:C:4566:ALA:N	2.32	0.55
1:C:4881:THR:O	1:C:4884:LEU:N	2.40	0.55
1:A:1271:ARG:NH2	1:A:1560:ASN:OD1	2.39	0.54
1:A:1974:ARG:NH2	1:A:3642:TYR:O	2.40	0.54
1:A:2302:LEU:HD23	1:A:2363:CYS:HB3	1.88	0.54
1:B:1607:ARG:NH2	1:B:1610:ASN:OD1	2.40	0.54
1:B:1974:ARG:NH2	1:B:3642:TYR:O	2.40	0.54
1:C:4231:MET:HG3	1:C:5022:PHE:CD2	2.40	0.54
1:C:4244:GLU:CA	1:C:4247:ILE:HG12	2.37	0.54
1:C:4900:GLU:OE1	1:C:4900:GLU:N	2.41	0.54
1:D:2232:CYS:SG	1:D:2233:CYS:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2458:ARG:HH21	1:D:2510:TYR:HA	1.71	0.54
1:D:4571:PHE:HE1	1:D:4813:LEU:HD11	1.72	0.54
1:D:4990:PHE:O	1:D:4994:TYR:N	2.37	0.54
1:A:4244:GLU:CA	1:A:4247:ILE:HG12	2.37	0.54
3:E:23:VAL:HG22	3:E:104:LEU:HD13	1.89	0.54
1:D:3878:ASP:N	1:D:3878:ASP:OD1	2.41	0.54
1:D:5004:THR:OG1	1:D:5005:GLY:N	2.38	0.54
1:B:756:SER:HB2	1:B:767:VAL:HG12	1.89	0.54
1:B:3809:ASN:O	1:B:3813:GLN:NE2	2.41	0.54
1:C:1422:ASP:N	1:C:1570:LYS:O	2.41	0.54
1:C:2531:ARG:NH2	1:C:2581:SER:OG	2.41	0.54
1:C:4195:PHE:HD2	1:C:4994:TYR:CD2	2.25	0.54
1:D:24:CYS:SG	1:D:25:SER:N	2.80	0.54
1:D:134:ASP:N	1:D:134:ASP:OD1	2.39	0.54
1:D:2516:ASP:OD1	1:D:2516:ASP:N	2.39	0.54
1:D:4231:MET:HG3	1:D:5022:PHE:CD2	2.40	0.54
1:A:2324:ASN:OD1	1:A:2327:GLY:N	2.41	0.54
1:A:3809:ASN:O	1:A:3813:GLN:NE2	2.41	0.54
1:A:4900:GLU:OE1	1:A:4900:GLU:N	2.41	0.54
1:B:2030:ASP:OD1	1:B:2030:ASP:N	2.39	0.54
1:C:1974:ARG:NH2	1:C:3642:TYR:O	2.40	0.54
1:C:2232:CYS:SG	1:C:2233:CYS:N	2.80	0.54
1:D:2030:ASP:N	1:D:2030:ASP:OD1	2.39	0.54
1:D:2333:ASP:N	1:D:2333:ASP:OD1	2.40	0.54
1:D:3809:ASN:O	1:D:3813:GLN:NE2	2.41	0.54
1:D:4725:LEU:O	1:D:4734:ARG:NH1	2.41	0.54
1:A:221:ARG:NH1	1:A:253:CYS:O	2.41	0.54
1:A:2458:ARG:HH21	1:A:2510:TYR:HA	1.71	0.54
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.40	0.54
1:B:4195:PHE:HD2	1:B:4994:TYR:CD2	2.25	0.54
1:B:4688:ILE:HD11	1:B:4737:ILE:CG1	2.35	0.54
1:B:4832:HIS:CE1	1:B:4939:ALA:HB1	2.36	0.54
1:B:4881:THR:O	1:B:4884:LEU:N	2.40	0.54
1:B:4900:GLU:OE1	1:B:4900:GLU:N	2.41	0.54
1:B:5008:SER:OG	1:B:5009:TYR:N	2.39	0.54
1:C:24:CYS:SG	1:C:25:SER:N	2.80	0.54
1:C:3878:ASP:N	1:C:3878:ASP:OD1	2.41	0.54
1:D:756:SER:HB2	1:D:767:VAL:HG12	1.89	0.54
1:D:2302:LEU:HD23	1:D:2363:CYS:HB3	1.88	0.54
1:D:2515:GLN:HA	1:D:2568:LEU:HD21	1.88	0.54
1:D:2531:ARG:NH2	1:D:2581:SER:OG	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2232:CYS:SG	1:A:2233:CYS:N	2.80	0.54
1:A:2333:ASP:N	1:A:2333:ASP:OD1	2.40	0.54
1:B:221:ARG:NH1	1:B:253:CYS:O	2.41	0.54
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.40	0.54
1:C:1232:ARG:NH1	1:C:1828:ASP:O	2.37	0.54
1:C:2030:ASP:N	1:C:2030:ASP:OD1	2.39	0.54
1:D:4900:GLU:OE1	1:D:4900:GLU:N	2.41	0.54
1:A:756:SER:HB2	1:A:767:VAL:HG12	1.89	0.54
1:A:2030:ASP:N	1:A:2030:ASP:OD1	2.39	0.54
1:B:2324:ASN:OD1	1:B:2327:GLY:N	2.41	0.54
1:C:1106:ARG:NH2	1:C:1183:GLU:O	2.40	0.54
1:C:3809:ASN:O	1:C:3813:GLN:NE2	2.41	0.54
1:C:4666:VAL:HG23	1:C:4667:PRO:HD3	1.89	0.54
1:D:4992:LEU:O	1:D:4996:ILE:HG12	2.08	0.54
1:A:1652:GLU:OE1	1:A:1656:ARG:NH1	2.41	0.54
1:B:1290:ARG:NH1	1:B:1291:LEU:O	2.41	0.54
1:B:1422:ASP:N	1:B:1570:LYS:O	2.41	0.54
1:B:2232:CYS:SG	1:B:2233:CYS:N	2.80	0.54
1:B:3717:ASP:OD1	1:B:3717:ASP:N	2.41	0.54
1:B:4725:LEU:O	1:B:4734:ARG:NH1	2.41	0.54
1:C:1856:ASP:N	1:C:1856:ASP:OD1	2.39	0.54
1:C:4571:PHE:HE1	1:C:4813:LEU:HD11	1.72	0.54
1:C:4942:GLU:O	1:C:4943:LEU:C	2.42	0.54
1:D:1290:ARG:NH1	1:D:1291:LEU:O	2.41	0.54
1:D:4940:PHE:O	1:D:4941:GLY:C	2.46	0.54
1:D:4980:LEU:HA	1:D:4984:ASN:ND2	2.18	0.54
1:A:3752:SER:OG	1:A:3753:PHE:N	2.36	0.54
1:A:4571:PHE:HE1	1:A:4813:LEU:HD11	1.72	0.54
1:A:4950:VAL:O	1:A:4951:LYS:C	2.45	0.54
1:A:4992:LEU:O	1:A:4996:ILE:HG12	2.08	0.54
1:B:4571:PHE:HE1	1:B:4813:LEU:HD11	1.72	0.54
1:B:4666:VAL:CG2	1:B:4667:PRO:HD3	2.38	0.54
1:C:113:HIS:O	1:C:399:GLN:NE2	2.41	0.54
1:C:4725:LEU:O	1:C:4734:ARG:NH1	2.41	0.54
1:A:1290:ARG:NH1	1:A:1291:LEU:O	2.41	0.54
1:A:4946:GLN:O	1:A:4947:GLN:C	2.41	0.54
1:B:2531:ARG:NH2	1:B:2581:SER:OG	2.41	0.54
1:B:3794:VAL:HA	1:B:3797:THR:HG22	1.90	0.54
1:B:4244:GLU:CA	1:B:4247:ILE:HG12	2.37	0.54
1:C:1652:GLU:OE1	1:C:1656:ARG:NH1	2.41	0.54
1:D:4881:THR:O	1:D:4884:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:23:VAL:HG22	3:G:104:LEU:HD13	1.89	0.54
1:A:1422:ASP:N	1:A:1570:LYS:O	2.41	0.53
1:A:3794:VAL:HA	1:A:3797:THR:HG22	1.90	0.53
1:B:24:CYS:SG	1:B:25:SER:N	2.80	0.53
1:B:1106:ARG:NH2	1:B:1183:GLU:O	2.41	0.53
1:B:1271:ARG:NH2	1:B:1560:ASN:OD1	2.39	0.53
1:C:1290:ARG:NH1	1:C:1291:LEU:O	2.41	0.53
2:J:87:ARG:O	2:J:91:ARG:NH1	2.42	0.53
1:D:1422:ASP:N	1:D:1570:LYS:O	2.41	0.53
1:D:1652:GLU:OE1	1:D:1656:ARG:NH1	2.41	0.53
1:D:4244:GLU:CA	1:D:4247:ILE:HG12	2.37	0.53
1:A:4725:LEU:O	1:A:4734:ARG:NH1	2.41	0.53
1:B:4814:LEU:HD21	1:C:4850:LEU:HD11	1.89	0.53
1:C:134:ASP:OD1	1:C:134:ASP:N	2.39	0.53
1:C:4992:LEU:O	1:C:4996:ILE:HG12	2.08	0.53
1:D:4217:PHE:CE1	1:D:4221:VAL:HG11	2.43	0.53
1:A:113:HIS:O	1:A:399:GLN:NE2	2.41	0.53
1:A:4940:PHE:O	1:A:4941:GLY:C	2.46	0.53
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.38	0.53
1:C:756:SER:HB2	1:C:767:VAL:HG12	1.89	0.53
1:C:784:SER:OG	1:C:785:ALA:N	2.41	0.53
1:C:4688:ILE:HD11	1:C:4737:ILE:CG1	2.35	0.53
1:C:5008:SER:OG	1:C:5009:TYR:N	2.39	0.53
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.40	0.53
2:K:87:ARG:O	2:K:91:ARG:NH1	2.42	0.53
1:A:831:ARG:HB3	1:A:838:HIS:HB2	1.91	0.53
1:A:4217:PHE:CE1	1:A:4221:VAL:HG11	2.44	0.53
1:A:4814:LEU:HD21	1:B:4850:LEU:CD1	2.38	0.53
1:C:4217:PHE:CE1	1:C:4221:VAL:HG11	2.43	0.53
1:C:4814:LEU:HD21	1:D:4850:LEU:CD1	2.39	0.53
1:D:391:THR:OG1	1:D:392:ARG:N	2.42	0.53
1:A:4231:MET:HG3	1:A:5022:PHE:CD2	2.40	0.53
1:B:831:ARG:HB3	1:B:838:HIS:HB2	1.91	0.53
1:B:1024:TYR:HA	1:B:1027:LEU:HD12	1.90	0.53
1:B:3901:ASN:HD22	1:B:3904:ARG:HH12	1.56	0.53
1:B:4195:PHE:HB2	1:B:4994:TYR:CE2	2.44	0.53
1:B:4231:MET:HG3	1:B:5022:PHE:CD2	2.40	0.53
1:C:831:ARG:HB3	1:C:838:HIS:HB2	1.91	0.53
1:C:4666:VAL:CG2	1:C:4667:PRO:HD3	2.39	0.53
3:F:23:VAL:HG22	3:F:104:LEU:HD13	1.89	0.53
1:D:221:ARG:NH1	1:D:253:CYS:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4195:PHE:HB2	1:D:4994:TYR:CE2	2.44	0.53
1:A:391:THR:OG1	1:A:392:ARG:N	2.42	0.53
1:A:784:SER:OG	1:A:785:ALA:N	2.41	0.53
1:A:3878:ASP:N	1:A:3878:ASP:OD1	2.41	0.53
1:B:1477:GLY:HA3	1:B:1483:VAL:HA	1.91	0.53
1:C:4950:VAL:O	1:C:4951:LYS:C	2.45	0.53
1:D:784:SER:OG	1:D:785:ALA:N	2.41	0.53
1:D:2530:MET:SD	1:D:2531:ARG:NH1	2.79	0.53
1:D:4849:TYR:O	1:D:4852:THR:N	2.42	0.53
1:A:1477:GLY:HA3	1:A:1483:VAL:HA	1.91	0.53
1:C:4658:ILE:HD11	1:C:4792:SER:O	2.09	0.53
1:D:831:ARG:HB3	1:D:838:HIS:HB2	1.91	0.53
1:D:1024:TYR:HA	1:D:1027:LEU:HD12	1.90	0.53
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.40	0.53
1:D:2381:GLU:HA	1:D:2384:ILE:HD12	1.91	0.53
1:D:4950:VAL:O	1:D:4951:LYS:C	2.45	0.53
1:A:2531:ARG:NH2	1:A:2581:SER:OG	2.41	0.53
1:B:391:THR:OG1	1:B:392:ARG:N	2.42	0.53
1:B:1452:TRP:NE1	1:B:1518:CYS:SG	2.73	0.53
1:C:221:ARG:NH1	1:C:253:CYS:O	2.41	0.53
1:D:1856:ASP:OD1	1:D:1856:ASP:N	2.39	0.53
1:D:3794:VAL:HA	1:D:3797:THR:HG22	1.90	0.53
1:D:4666:VAL:CG2	1:D:4667:PRO:HD3	2.38	0.53
1:B:4643:LEU:O	1:B:4643:LEU:HD23	2.09	0.53
1:C:4195:PHE:HB2	1:C:4994:TYR:CE2	2.44	0.53
1:D:1477:GLY:HA3	1:D:1483:VAL:HA	1.91	0.53
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.42	0.53
1:A:4666:VAL:CG2	1:A:4667:PRO:HD3	2.39	0.53
1:B:1652:GLU:OE1	1:B:1656:ARG:NH1	2.41	0.53
1:C:1171:SER:HG	1:C:1175:SER:HG	1.57	0.53
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.42	0.53
1:C:3901:ASN:HD22	1:C:3904:ARG:HH12	1.56	0.53
1:A:4658:ILE:HD11	1:A:4792:SER:O	2.09	0.52
1:A:4814:LEU:HD21	1:B:4850:LEU:HD11	1.90	0.52
3:E:25:HIS:HB2	3:E:104:LEU:HD11	1.91	0.52
1:C:229:GLU:N	1:C:248:GLU:O	2.42	0.52
1:C:4711:PHE:HB3	1:C:4712:PRO:HD3	1.91	0.52
1:D:4834:GLY:O	1:D:4838:VAL:HG12	2.09	0.52
1:A:3676:ASP:HA	1:A:3679:LYS:HG2	1.91	0.52
1:A:3717:ASP:OD1	1:A:3717:ASP:N	2.41	0.52
1:A:3901:ASN:HD22	1:A:3904:ARG:HH12	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4643:LEU:HD23	1:A:4643:LEU:O	2.09	0.52
1:B:4217:PHE:CE1	1:B:4221:VAL:HG11	2.43	0.52
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.42	0.52
1:B:4658:ILE:HD11	1:B:4792:SER:O	2.09	0.52
1:B:4950:VAL:O	1:B:4951:LYS:C	2.45	0.52
1:C:391:THR:OG1	1:C:392:ARG:N	2.42	0.52
1:C:1477:GLY:HA3	1:C:1483:VAL:HA	1.91	0.52
1:D:4210:VAL:O	1:D:4211:LYS:C	2.48	0.52
1:D:4711:PHE:HB3	1:D:4712:PRO:HD3	1.91	0.52
1:A:4571:PHE:CE1	1:A:4813:LEU:HD11	2.45	0.52
1:B:229:GLU:N	1:B:248:GLU:O	2.42	0.52
1:C:3794:VAL:HA	1:C:3797:THR:HG22	1.90	0.52
1:C:4643:LEU:HD23	1:C:4643:LEU:O	2.09	0.52
1:D:2189:LYS:O	1:D:2193:GLN:NE2	2.42	0.52
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.42	0.52
1:A:1024:TYR:HA	1:A:1027:LEU:HD12	1.90	0.52
1:A:1106:ARG:NH2	1:A:1183:GLU:O	2.40	0.52
1:A:4850:LEU:CD1	1:D:4814:LEU:HD21	2.39	0.52
1:B:2195:PRO:O	1:B:2199:ARG:NH1	2.42	0.52
1:B:2381:GLU:HA	1:B:2384:ILE:HD12	1.91	0.52
1:B:4639:MET:O	1:B:4642:ALA:N	2.43	0.52
1:B:4814:LEU:HD21	1:C:4850:LEU:CD1	2.40	0.52
1:B:4834:GLY:O	1:B:4838:VAL:HG12	2.09	0.52
1:B:4846:VAL:O	1:B:4849:TYR:N	2.43	0.52
1:C:771:PHE:HB3	1:C:1472:VAL:HG22	1.92	0.52
1:C:2195:PRO:O	1:C:2199:ARG:NH1	2.42	0.52
1:C:2530:MET:SD	1:C:2531:ARG:NH1	2.79	0.52
1:C:4940:PHE:O	1:C:4941:GLY:C	2.46	0.52
1:D:1716:ILE:HG22	1:D:1720:LEU:HD12	1.92	0.52
1:D:2195:PRO:O	1:D:2199:ARG:NH1	2.42	0.52
1:D:2324:ASN:OD1	1:D:2327:GLY:N	2.41	0.52
1:D:3901:ASN:HD22	1:D:3904:ARG:HH12	1.56	0.52
1:D:4217:PHE:CE2	1:D:4959:PHE:HZ	2.28	0.52
1:D:4961:CYS:HB3	1:D:4983:HIS:CE1	2.45	0.52
1:A:2189:LYS:O	1:A:2193:GLN:NE2	2.42	0.52
1:A:4195:PHE:HB2	1:A:4994:TYR:CE2	2.44	0.52
1:A:4217:PHE:CE2	1:A:4959:PHE:HZ	2.28	0.52
1:A:4834:GLY:O	1:A:4838:VAL:HG12	2.09	0.52
3:H:25:HIS:HB2	3:H:104:LEU:HD11	1.92	0.52
1:B:113:HIS:O	1:B:399:GLN:NE2	2.41	0.52
1:C:1024:TYR:HA	1:C:1027:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4195:PHE:CD2	1:C:4994:TYR:CD2	2.98	0.52
1:C:4849:TYR:O	1:C:4852:THR:N	2.42	0.52
1:D:4571:PHE:CE1	1:D:4813:LEU:HD11	2.45	0.52
1:B:350:HIS:O	1:B:354:GLY:N	2.42	0.52
1:B:4158:PRO:O	1:B:4162:ASN:ND2	2.43	0.52
1:C:2381:GLU:HA	1:C:2384:ILE:HD12	1.91	0.52
1:C:4639:MET:O	1:C:4642:ALA:N	2.43	0.52
1:C:4961:CYS:HB3	1:C:4983:HIS:CE1	2.45	0.52
1:D:113:HIS:O	1:D:399:GLN:NE2	2.41	0.52
1:D:4643:LEU:O	1:D:4643:LEU:HD23	2.09	0.52
1:A:543:ASN:OD1	1:A:543:ASN:N	2.43	0.52
1:A:4656:LEU:O	1:A:4659:ILE:N	2.43	0.52
1:A:4849:TYR:O	1:A:4852:THR:N	2.42	0.52
1:B:784:SER:OG	1:B:785:ALA:N	2.41	0.52
1:B:3676:ASP:HA	1:B:3679:LYS:HG2	1.91	0.52
1:B:4195:PHE:CD2	1:B:4994:TYR:CD2	2.98	0.52
1:B:4849:TYR:O	1:B:4852:THR:N	2.42	0.52
1:B:4992:LEU:O	1:B:4996:ILE:HG12	2.08	0.52
1:C:4936:ILE:O	1:C:4937:ILE:C	2.47	0.52
1:D:4673:ARG:HE	1:D:4782:VAL:HG21	1.75	0.52
1:A:2195:PRO:O	1:A:2199:ARG:NH1	2.42	0.52
1:A:4846:VAL:O	1:A:4849:TYR:N	2.43	0.52
1:C:1716:ILE:HG22	1:C:1720:LEU:HD12	1.92	0.52
1:C:3676:ASP:HA	1:C:3679:LYS:HG2	1.91	0.52
1:D:4183:ILE:CD1	1:D:4193:ILE:HD11	2.38	0.52
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.40	0.52
1:A:3696:ASP:OD1	1:A:3696:ASP:N	2.36	0.52
1:A:4235:VAL:HG11	1:A:5019:TRP:CZ3	2.45	0.52
1:B:2333:ASP:OD1	1:B:2333:ASP:N	2.40	0.52
1:B:4571:PHE:CE1	1:B:4813:LEU:HD11	2.45	0.52
1:B:4965:SER:O	1:B:4965:SER:OG	2.28	0.52
1:C:552:ASP:N	1:C:552:ASP:OD1	2.42	0.52
1:C:4656:LEU:O	1:C:4659:ILE:N	2.43	0.52
1:C:4740:LEU:HD23	1:C:4741:LEU:HD23	1.91	0.52
1:D:4195:PHE:CD2	1:D:4994:TYR:CD2	2.98	0.52
1:A:1232:ARG:NH1	1:A:1828:ASP:O	2.37	0.51
1:A:4158:PRO:O	1:A:4162:ASN:ND2	2.43	0.51
1:A:4195:PHE:CD2	1:A:4994:TYR:CD2	2.98	0.51
1:B:543:ASN:OD1	1:B:543:ASN:N	2.43	0.51
1:B:4217:PHE:CE2	1:B:4959:PHE:HZ	2.28	0.51
1:B:4235:VAL:HG11	1:B:5019:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4936:ILE:O	1:B:4937:ILE:C	2.47	0.51
1:C:645:ARG:NE	1:C:824:GLU:OE2	2.41	0.51
1:D:3696:ASP:OD1	1:D:3696:ASP:N	2.36	0.51
1:D:4658:ILE:HD11	1:D:4792:SER:O	2.09	0.51
1:D:4942:GLU:O	1:D:4943:LEU:C	2.42	0.51
1:B:4961:CYS:HB3	1:B:4983:HIS:CE1	2.45	0.51
2:I:87:ARG:O	2:I:91:ARG:NH1	2.42	0.51
1:C:2324:ASN:OD1	1:C:2327:GLY:N	2.41	0.51
1:C:4210:VAL:O	1:C:4211:LYS:C	2.48	0.51
1:C:4834:GLY:O	1:C:4838:VAL:HG12	2.09	0.51
1:C:4933:GLN:HG2	1:D:4926:VAL:HG13	1.92	0.51
1:D:4158:PRO:O	1:D:4162:ASN:ND2	2.43	0.51
1:D:4802:GLY:O	1:D:4806:ASN:N	2.44	0.51
1:A:681:HIS:H	1:A:784:SER:HB3	1.76	0.51
1:A:2381:GLU:HA	1:A:2384:ILE:HD12	1.91	0.51
1:A:4639:MET:O	1:A:4642:ALA:N	2.43	0.51
1:B:771:PHE:HB3	1:B:1472:VAL:HG22	1.92	0.51
1:C:350:HIS:O	1:C:354:GLY:N	2.42	0.51
3:F:25:HIS:HB2	3:F:104:LEU:HD11	1.92	0.51
1:A:229:GLU:N	1:A:248:GLU:O	2.43	0.51
1:A:4740:LEU:HD23	1:A:4741:LEU:HD23	1.91	0.51
1:B:1243:PRO:HB3	1:B:1602:PRO:HA	1.92	0.51
1:C:579:GLN:H	1:C:582:HIS:HD2	1.59	0.51
1:D:579:GLN:H	1:D:582:HIS:HD2	1.59	0.51
1:D:4740:LEU:HD23	1:D:4741:LEU:HD23	1.91	0.51
2:K:51:ASP:N	2:K:51:ASP:OD1	2.44	0.51
1:A:4961:CYS:HB3	1:A:4983:HIS:CE1	2.45	0.51
1:B:4656:LEU:O	1:B:4659:ILE:N	2.43	0.51
1:C:681:HIS:H	1:C:784:SER:HB3	1.76	0.51
1:C:1029:GLU:HA	1:C:1032:LYS:HB2	1.92	0.51
1:C:1438:ARG:HD2	1:C:1563:GLN:HE21	1.76	0.51
1:C:4673:ARG:HE	1:C:4782:VAL:HG21	1.75	0.51
1:C:4733:GLY:O	1:C:4736:ARG:N	2.44	0.51
1:D:229:GLU:N	1:D:248:GLU:O	2.42	0.51
1:D:3676:ASP:HA	1:D:3679:LYS:HG2	1.91	0.51
1:D:4656:LEU:O	1:D:4659:ILE:N	2.43	0.51
1:A:579:GLN:H	1:A:582:HIS:HD2	1.59	0.51
1:A:771:PHE:HB3	1:A:1472:VAL:HG22	1.92	0.51
1:A:1095:VAL:HG23	1:A:1200:GLY:HA2	1.93	0.51
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	1.91	0.51
1:B:217:GLY:O	1:B:261:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:GLN:H	1:B:582:HIS:HD2	1.59	0.51
1:B:4711:PHE:HB3	1:B:4712:PRO:HD3	1.91	0.51
1:B:4840:THR:O	1:B:4843:LEU:N	2.27	0.51
2:I:51:ASP:OD1	2:I:51:ASP:N	2.44	0.51
1:C:217:GLY:O	1:C:261:ARG:NH1	2.44	0.51
1:C:4217:PHE:CE2	1:C:4959:PHE:HZ	2.28	0.51
1:C:4235:VAL:HG11	1:C:5019:TRP:CZ3	2.45	0.51
1:C:4571:PHE:CE1	1:C:4813:LEU:HD11	2.45	0.51
1:D:681:HIS:H	1:D:784:SER:HB3	1.76	0.51
1:D:4235:VAL:HG11	1:D:5019:TRP:CZ3	2.45	0.51
1:A:1029:GLU:HA	1:A:1032:LYS:HB2	1.92	0.51
1:A:1992:ALA:O	1:A:1996:ARG:NH1	2.44	0.51
1:A:4138:ASP:OD1	1:A:4138:ASP:N	2.38	0.51
1:B:4210:VAL:O	1:B:4211:LYS:C	2.48	0.51
1:B:4214:LYS:O	1:B:4215:ARG:C	2.49	0.51
1:B:4740:LEU:HD23	1:B:4741:LEU:HD23	1.91	0.51
1:C:4158:PRO:O	1:C:4162:ASN:ND2	2.43	0.51
1:D:2554:LEU:HA	1:D:2558:VAL:HG22	1.92	0.51
1:A:1716:ILE:HG22	1:A:1720:LEU:HD12	1.92	0.51
1:B:2554:LEU:HA	1:B:2558:VAL:HG22	1.92	0.51
1:B:4917:ASP:O	1:B:4920:PHE:N	2.37	0.51
1:C:2189:LYS:O	1:C:2193:GLN:NE2	2.42	0.51
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.40	0.51
3:G:25:HIS:HB2	3:G:104:LEU:HD11	1.91	0.51
1:A:1438:ARG:HD2	1:A:1563:GLN:HE21	1.76	0.51
1:B:645:ARG:NE	1:B:824:GLU:OE2	2.41	0.51
1:B:4986:ALA:HA	1:B:4989:MET:HE1	1.93	0.51
1:C:1095:VAL:HG23	1:C:1200:GLY:HA2	1.93	0.51
1:C:4183:ILE:CD1	1:C:4193:ILE:HD11	2.38	0.51
1:A:1243:PRO:HB3	1:A:1602:PRO:HA	1.92	0.51
1:A:4578:LEU:HD12	1:B:4879:MET:HG2	1.93	0.51
1:A:4673:ARG:HE	1:A:4782:VAL:HG21	1.75	0.51
1:B:552:ASP:OD1	1:B:552:ASP:N	2.43	0.51
1:B:1716:ILE:HG22	1:B:1720:LEU:HD12	1.92	0.51
1:B:2189:LYS:O	1:B:2193:GLN:NE2	2.42	0.51
1:B:4733:GLY:O	1:B:4736:ARG:N	2.44	0.51
1:C:232:THR:OG1	1:C:233:ILE:N	2.44	0.51
1:C:543:ASN:OD1	1:C:543:ASN:N	2.43	0.51
1:D:1095:VAL:HG23	1:D:1200:GLY:HA2	1.93	0.51
1:D:1438:ARG:HD2	1:D:1563:GLN:HE21	1.76	0.51
1:D:3717:ASP:OD1	1:D:3717:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4626:ASN:O	1:D:4628:VAL:HG13	2.11	0.51
1:D:4639:MET:O	1:D:4642:ALA:N	2.43	0.51
1:D:4689:THR:HG22	1:D:4732:PHE:CZ	2.46	0.51
1:A:2554:LEU:HA	1:A:2558:VAL:HG22	1.92	0.50
1:A:2572:THR:OG1	1:A:2615:ARG:NH1	2.44	0.50
1:B:681:HIS:H	1:B:784:SER:HB3	1.76	0.50
1:B:1438:ARG:HD2	1:B:1563:GLN:HE21	1.76	0.50
1:C:1144:GLN:HE21	1:C:1147:ASP:HB3	1.75	0.50
1:C:2554:LEU:HA	1:C:2558:VAL:HG22	1.92	0.50
1:D:217:GLY:O	1:D:261:ARG:NH1	2.44	0.50
1:D:771:PHE:HB3	1:D:1472:VAL:HG22	1.92	0.50
1:D:1144:GLN:HE21	1:D:1147:ASP:HB3	1.75	0.50
1:A:217:GLY:O	1:A:261:ARG:NH1	2.44	0.50
1:A:350:HIS:O	1:A:354:GLY:N	2.42	0.50
1:A:1204:LEU:HD21	1:A:1226:PHE:HD2	1.77	0.50
1:A:4210:VAL:O	1:A:4211:LYS:C	2.48	0.50
1:A:4689:THR:HG22	1:A:4732:PHE:CZ	2.46	0.50
2:L:87:ARG:O	2:L:91:ARG:NH1	2.42	0.50
1:C:2516:ASP:OD1	1:C:2516:ASP:N	2.39	0.50
1:C:4790:LEU:O	1:C:4790:LEU:HD23	2.12	0.50
1:D:989:ALA:HA	1:D:1039:LEU:HD13	1.93	0.50
1:A:989:ALA:HA	1:A:1039:LEU:HD13	1.93	0.50
1:A:4733:GLY:O	1:A:4736:ARG:N	2.44	0.50
1:B:2530:MET:SD	1:B:2531:ARG:NH1	2.79	0.50
1:B:4626:ASN:O	1:B:4628:VAL:HG13	2.11	0.50
1:C:4214:LYS:O	1:C:4215:ARG:C	2.49	0.50
1:D:1186:ASP:OD1	1:D:1186:ASP:N	2.43	0.50
1:A:4626:ASN:O	1:A:4628:VAL:HG13	2.11	0.50
1:B:4673:ARG:HE	1:B:4782:VAL:HG21	1.75	0.50
1:C:710:ASP:OD1	1:C:710:ASP:N	2.44	0.50
1:C:1204:LEU:HD21	1:C:1226:PHE:HD2	1.77	0.50
1:D:1204:LEU:HD21	1:D:1226:PHE:HD2	1.77	0.50
1:D:4733:GLY:O	1:D:4736:ARG:N	2.44	0.50
1:D:4986:ALA:HA	1:D:4989:MET:HE1	1.92	0.50
1:B:4823:LEU:HA	1:B:4826:ILE:CG1	2.42	0.50
1:C:1243:PRO:HB3	1:C:1602:PRO:HA	1.92	0.50
1:C:1992:ALA:O	1:C:1996:ARG:NH1	2.44	0.50
1:C:4802:GLY:O	1:C:4806:ASN:N	2.44	0.50
1:C:4846:VAL:O	1:C:4849:TYR:N	2.43	0.50
1:D:552:ASP:OD1	1:D:552:ASP:N	2.43	0.50
1:D:1029:GLU:HA	1:D:1032:LYS:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.85	0.50
1:D:2199:ARG:NH1	1:D:2246:ASN:OD1	2.45	0.50
1:D:4823:LEU:HA	1:D:4826:ILE:CG1	2.42	0.50
1:D:4917:ASP:O	1:D:4920:PHE:N	2.37	0.50
1:A:4210:VAL:HG12	1:A:4211:LYS:N	2.26	0.50
1:B:1029:GLU:HA	1:B:1032:LYS:HB2	1.92	0.50
1:B:1095:VAL:HG23	1:B:1200:GLY:HA2	1.93	0.50
1:B:1144:GLN:HE21	1:B:1147:ASP:HB3	1.76	0.50
1:C:4689:THR:HG22	1:C:4732:PHE:CZ	2.46	0.50
1:C:4933:GLN:O	1:C:4937:ILE:HG23	2.12	0.50
1:D:919:ASN:HA	1:D:922:LEU:HB2	1.93	0.50
1:D:1992:ALA:O	1:D:1996:ARG:NH1	2.44	0.50
1:D:4790:LEU:HD23	1:D:4790:LEU:O	2.12	0.50
2:K:23:ASP:N	2:K:23:ASP:OD1	2.45	0.50
1:B:989:ALA:HA	1:B:1039:LEU:HD13	1.93	0.50
1:D:232:THR:OG1	1:D:233:ILE:N	2.44	0.50
1:D:4244:GLU:O	1:D:4248:ALA:N	2.44	0.50
1:D:4717:ASP:O	1:D:4718:LYS:CB	2.60	0.50
1:A:232:THR:OG1	1:A:233:ILE:N	2.44	0.50
1:B:2617:SER:OG	1:B:2618:MET:SD	2.67	0.50
1:B:3810:ALA:HA	1:B:3813:GLN:HE21	1.77	0.50
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.85	0.50
1:D:4846:VAL:O	1:D:4849:TYR:N	2.43	0.50
1:A:35:LEU:HB3	1:A:49:LEU:HD21	1.94	0.50
1:A:4823:LEU:HA	1:A:4826:ILE:CG1	2.42	0.50
1:A:4917:ASP:O	1:A:4919:THR:N	2.45	0.50
1:A:4936:ILE:O	1:A:4937:ILE:C	2.47	0.50
1:B:251:ALA:O	1:B:255:HIS:ND1	2.37	0.50
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.85	0.50
1:B:3878:ASP:OD1	1:B:3878:ASP:N	2.41	0.50
1:B:4936:ILE:HG22	1:B:4937:ILE:N	2.26	0.50
1:D:4933:GLN:O	1:D:4937:ILE:HG23	2.12	0.50
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.45	0.49
1:B:4689:THR:HG22	1:B:4732:PHE:CZ	2.46	0.49
1:D:4719:PHE:O	1:D:4720:VAL:C	2.50	0.49
1:A:4217:PHE:O	1:A:4221:VAL:HG22	2.12	0.49
1:B:232:THR:OG1	1:B:233:ILE:N	2.44	0.49
1:B:4244:GLU:O	1:B:4247:ILE:HG12	2.12	0.49
1:B:4940:PHE:O	1:B:4941:GLY:C	2.46	0.49
1:C:4717:ASP:O	1:C:4718:LYS:CB	2.60	0.49
1:D:4214:LYS:O	1:D:4215:ARG:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2199:ARG:NH1	1:A:2246:ASN:OD1	2.45	0.49
1:A:4790:LEU:HD23	1:A:4790:LEU:O	2.12	0.49
1:B:1771:LEU:HD23	1:B:2153:MET:HG3	1.95	0.49
1:B:1992:ALA:O	1:B:1996:ARG:NH1	2.44	0.49
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.40	0.49
1:B:4802:GLY:O	1:B:4806:ASN:N	2.44	0.49
1:B:4823:LEU:HA	1:B:4826:ILE:HG12	1.94	0.49
1:C:2199:ARG:NH1	1:C:2246:ASN:OD1	2.45	0.49
1:C:3810:ALA:HA	1:C:3813:GLN:HE21	1.77	0.49
1:D:35:LEU:HB3	1:D:49:LEU:HD21	1.94	0.49
1:D:143:GLY:HA3	1:D:147:TRP:HE1	1.78	0.49
1:D:516:LYS:NZ	1:D:520:ASN:OD1	2.46	0.49
1:D:543:ASN:OD1	1:D:543:ASN:N	2.43	0.49
1:D:4936:ILE:O	1:D:4937:ILE:C	2.47	0.49
1:A:1771:LEU:HD23	1:A:2153:MET:HG3	1.94	0.49
1:A:4823:LEU:HA	1:A:4826:ILE:HG12	1.94	0.49
1:A:4933:GLN:O	1:A:4937:ILE:HG23	2.12	0.49
1:B:718:GLY:HA3	1:B:737:LEU:HA	1.95	0.49
1:B:919:ASN:HA	1:B:922:LEU:HB2	1.93	0.49
1:C:35:LEU:HB3	1:C:49:LEU:HD21	1.94	0.49
1:C:919:ASN:HA	1:C:922:LEU:HB2	1.93	0.49
1:C:1008:SER:OG	1:C:1010:VAL:O	2.31	0.49
1:C:1771:LEU:HD23	1:C:2153:MET:HG3	1.94	0.49
1:C:4210:VAL:HG12	1:C:4211:LYS:N	2.26	0.49
1:C:4626:ASN:O	1:C:4628:VAL:HG13	2.11	0.49
1:D:1769:THR:OG1	1:D:1956:GLU:OE1	2.28	0.49
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.45	0.49
1:A:1144:GLN:HE21	1:A:1147:ASP:HB3	1.76	0.49
1:B:4933:GLN:O	1:B:4937:ILE:HG23	2.12	0.49
1:C:1769:THR:OG1	1:C:1956:GLU:OE1	2.28	0.49
1:C:4823:LEU:HA	1:C:4826:ILE:CG1	2.42	0.49
1:C:4917:ASP:O	1:C:4919:THR:N	2.45	0.49
1:D:1771:LEU:HD23	1:D:2153:MET:HG3	1.95	0.49
1:D:4936:ILE:HG22	1:D:4937:ILE:N	2.26	0.49
1:A:143:GLY:HA3	1:A:147:TRP:HE1	1.78	0.49
1:A:718:GLY:HA3	1:A:737:LEU:HA	1.95	0.49
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.85	0.49
1:A:3810:ALA:HA	1:A:3813:GLN:HE21	1.77	0.49
1:A:4244:GLU:O	1:A:4247:ILE:HG12	2.12	0.49
1:B:1204:LEU:HD21	1:B:1226:PHE:HD2	1.77	0.49
1:C:143:GLY:HA3	1:C:147:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:ASP:OD1	1:C:1147:ASP:N	2.46	0.49
1:C:4673:ARG:NH1	1:C:4702:ASP:OD2	2.46	0.49
1:D:350:HIS:O	1:D:354:GLY:N	2.42	0.49
1:D:1243:PRO:HB3	1:D:1602:PRO:HA	1.92	0.49
1:D:3810:ALA:HA	1:D:3813:GLN:HE21	1.77	0.49
1:A:4673:ARG:NH1	1:A:4702:ASP:OD2	2.46	0.49
2:L:51:ASP:OD1	2:L:51:ASP:N	2.44	0.49
1:B:1856:ASP:O	1:B:1860:LYS:NZ	2.45	0.49
1:B:2199:ARG:NH1	1:B:2246:ASN:OD1	2.45	0.49
1:B:4933:GLN:HG2	1:C:4926:VAL:HG13	1.93	0.49
1:C:989:ALA:HA	1:C:1039:LEU:HD13	1.93	0.49
1:C:4244:GLU:O	1:C:4247:ILE:HG12	2.12	0.49
1:D:718:GLY:HA3	1:D:737:LEU:HA	1.95	0.49
1:D:4673:ARG:NH1	1:D:4702:ASP:OD2	2.46	0.49
1:D:4957:LYS:CA	1:D:4964:GLY:HA2	2.32	0.49
1:A:516:LYS:NZ	1:A:520:ASN:OD1	2.46	0.49
1:A:4802:GLY:O	1:A:4806:ASN:N	2.44	0.49
1:B:1008:SER:OG	1:B:1010:VAL:O	2.31	0.49
1:B:4673:ARG:NH1	1:B:4702:ASP:OD2	2.46	0.49
1:B:4790:LEU:O	1:B:4790:LEU:HD23	2.12	0.49
1:C:158:SER:OG	1:C:159:GLU:N	2.46	0.49
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.46	0.49
1:C:1279:SER:OG	1:C:1280:GLN:N	2.46	0.49
1:C:4223:ASN:HB3	1:C:4224:GLU:OE1	2.13	0.49
1:C:4832:HIS:CE1	1:C:4939:ALA:HB1	2.36	0.49
1:C:4917:ASP:O	1:C:4920:PHE:N	2.37	0.49
1:C:4963:ILE:HD12	1:C:4964:GLY:H	1.78	0.49
1:D:158:SER:OG	1:D:159:GLU:N	2.46	0.49
1:D:4244:GLU:O	1:D:4247:ILE:HG12	2.12	0.49
1:B:4049:VAL:HG11	1:B:4159:ARG:HD2	1.95	0.49
1:B:4986:ALA:HA	1:B:4989:MET:CE	2.43	0.49
2:I:23:ASP:N	2:I:23:ASP:OD1	2.45	0.49
1:C:2886:TRP:O	1:C:2890:LYS:N	2.46	0.49
1:C:4217:PHE:O	1:C:4221:VAL:HG22	2.12	0.49
1:C:4244:GLU:O	1:C:4248:ALA:N	2.44	0.49
1:D:2617:SER:OG	1:D:2618:MET:SD	2.66	0.49
1:D:4210:VAL:HG12	1:D:4211:LYS:N	2.26	0.49
1:D:5028:PHE:N	1:D:5028:PHE:CD2	2.77	0.49
1:A:158:SER:OG	1:A:159:GLU:N	2.46	0.49
1:A:4820:VAL:HG23	1:A:4823:LEU:HG	1.95	0.49
1:A:4933:GLN:HG2	1:B:4926:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4936:ILE:HG22	1:A:4937:ILE:N	2.26	0.49
1:B:710:ASP:OD1	1:B:710:ASP:N	2.44	0.49
1:B:4820:VAL:HG23	1:B:4823:LEU:HG	1.95	0.49
1:D:1008:SER:OG	1:D:1010:VAL:O	2.31	0.49
1:D:1972:ASN:O	1:D:1976:ARG:NH1	2.46	0.49
1:D:4217:PHE:O	1:D:4221:VAL:HG22	2.12	0.49
1:D:4917:ASP:O	1:D:4919:THR:N	2.45	0.49
1:A:1966:VAL:O	1:A:1970:GLN:N	2.45	0.48
1:A:2883:HIS:O	1:A:2887:GLY:N	2.42	0.48
1:A:4801:LEU:HB3	1:A:4808:PHE:CD2	2.48	0.48
2:L:23:ASP:N	2:L:23:ASP:OD1	2.45	0.48
1:B:35:LEU:HB3	1:B:49:LEU:HD21	1.94	0.48
1:B:143:GLY:HA3	1:B:147:TRP:HE1	1.78	0.48
1:B:4210:VAL:HG12	1:B:4211:LYS:N	2.26	0.48
1:C:492:ASP:OD1	1:C:492:ASP:N	2.46	0.48
1:C:4986:ALA:HA	1:C:4989:MET:CE	2.43	0.48
1:D:831:ARG:O	1:D:838:HIS:N	2.46	0.48
1:D:1147:ASP:OD1	1:D:1147:ASP:N	2.46	0.48
1:D:1279:SER:OG	1:D:1280:GLN:N	2.46	0.48
1:A:1444:GLU:HG3	1:A:1446:SER:H	1.78	0.48
1:B:831:ARG:O	1:B:838:HIS:N	2.46	0.48
1:C:718:GLY:HA3	1:C:737:LEU:HA	1.95	0.48
1:C:4801:LEU:HB3	1:C:4808:PHE:CD2	2.48	0.48
1:C:4936:ILE:HG22	1:C:4937:ILE:N	2.26	0.48
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.46	0.48
1:D:4190:ILE:H	1:D:5031:GLN:HE22	1.58	0.48
1:D:4973:HIS:O	1:D:4977:THR:HG23	2.14	0.48
1:A:919:ASN:HA	1:A:922:LEU:HB2	1.93	0.48
1:B:492:ASP:N	1:B:492:ASP:OD1	2.45	0.48
1:B:1279:SER:OG	1:B:1280:GLN:N	2.46	0.48
1:B:4217:PHE:O	1:B:4221:VAL:HG22	2.12	0.48
1:C:831:ARG:O	1:C:838:HIS:N	2.46	0.48
1:D:645:ARG:NE	1:D:824:GLU:OE2	2.41	0.48
1:D:2886:TRP:O	1:D:2890:LYS:N	2.46	0.48
1:A:4049:VAL:HG11	1:A:4159:ARG:HD2	1.95	0.48
1:A:4963:ILE:HD12	1:A:4964:GLY:H	1.78	0.48
1:A:4986:ALA:HA	1:A:4989:MET:CE	2.43	0.48
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	1.96	0.48
1:B:1966:VAL:O	1:B:1970:GLN:N	2.45	0.48
1:B:4223:ASN:HB3	1:B:4224:GLU:OE1	2.13	0.48
1:B:4801:LEU:HB3	1:B:4808:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:65:ASP:OD1	2:I:65:ASP:N	2.46	0.48
1:C:4049:VAL:HG11	1:C:4159:ARG:HD2	1.95	0.48
1:D:4801:LEU:HB3	1:D:4808:PHE:CD2	2.48	0.48
1:A:552:ASP:OD1	1:A:552:ASP:N	2.43	0.48
1:B:2572:THR:OG1	1:B:2615:ARG:NH1	2.44	0.48
1:B:4233:LEU:O	1:B:4236:SER:OG	2.25	0.48
1:B:4963:ILE:HD12	1:B:4964:GLY:H	1.78	0.48
1:C:4190:ILE:HD11	1:C:5028:PHE:HA	1.95	0.48
1:C:4820:VAL:HG23	1:C:4823:LEU:HG	1.95	0.48
1:D:4823:LEU:HA	1:D:4826:ILE:HG12	1.93	0.48
1:D:4937:ILE:HG13	1:D:4938:ASP:H	1.79	0.48
1:D:4986:ALA:HA	1:D:4989:MET:CE	2.43	0.48
1:A:710:ASP:N	1:A:710:ASP:OD1	2.44	0.48
1:A:1279:SER:OG	1:A:1280:GLN:N	2.46	0.48
1:A:2579:VAL:HA	1:A:2582:MET:HB2	1.96	0.48
1:A:4719:PHE:O	1:A:4720:VAL:C	2.50	0.48
1:B:158:SER:OG	1:B:159:GLU:N	2.46	0.48
1:B:1490:SER:OG	1:B:1491:ASN:N	2.47	0.48
1:C:4823:LEU:HA	1:C:4826:ILE:HG12	1.94	0.48
1:D:1490:SER:OG	1:D:1491:ASN:N	2.47	0.48
1:D:4223:ASN:HB3	1:D:4224:GLU:OE1	2.13	0.48
1:D:4681:LEU:HD23	1:D:4681:LEU:O	2.14	0.48
1:A:2617:SER:OG	1:A:2618:MET:SD	2.67	0.48
1:A:4183:ILE:CD1	1:A:4193:ILE:HD11	2.39	0.48
1:A:4973:HIS:O	1:A:4977:THR:HG23	2.14	0.48
1:B:516:LYS:NZ	1:B:520:ASN:OD1	2.46	0.48
1:B:4717:ASP:O	1:B:4718:LYS:CB	2.60	0.48
1:A:492:ASP:OD1	1:A:492:ASP:N	2.46	0.48
1:A:1008:SER:OG	1:A:1010:VAL:O	2.31	0.48
1:A:4244:GLU:O	1:A:4248:ALA:N	2.44	0.48
1:B:2886:TRP:O	1:B:2890:LYS:N	2.46	0.48
1:B:4719:PHE:O	1:B:4720:VAL:C	2.50	0.48
1:C:1972:ASN:O	1:C:1976:ARG:NH1	2.46	0.48
2:J:23:ASP:OD1	2:J:23:ASP:N	2.45	0.48
1:D:1106:ARG:NH2	1:D:1183:GLU:O	2.40	0.48
1:D:3795:SER:O	1:D:3799:LYS:NZ	2.45	0.48
1:D:4574:ASN:ND2	1:D:4813:LEU:HD22	2.29	0.48
1:D:4950:VAL:O	1:D:4952:GLU:N	2.46	0.48
1:A:4046:ASP:HA	1:A:4049:VAL:HG22	1.96	0.48
1:A:4214:LYS:O	1:A:4215:ARG:C	2.49	0.48
1:A:4574:ASN:ND2	1:A:4813:LEU:HD22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4950:VAL:O	1:B:4952:GLU:N	2.46	0.48
1:C:516:LYS:NZ	1:C:520:ASN:OD1	2.46	0.48
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.47	0.48
1:C:1966:VAL:O	1:C:1970:GLN:N	2.45	0.48
1:C:2518:LEU:HD13	1:C:2568:LEU:HD22	1.96	0.48
1:C:2572:THR:OG1	1:C:2615:ARG:NH1	2.44	0.48
2:J:51:ASP:N	2:J:51:ASP:OD1	2.44	0.48
2:J:106:LEU:HA	2:J:109:VAL:HG12	1.96	0.48
1:D:2579:VAL:HA	1:D:2582:MET:HB2	1.96	0.48
1:A:4950:VAL:O	1:A:4952:GLU:N	2.46	0.48
1:B:498:THR:H	1:B:503:PHE:HD2	1.62	0.48
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.47	0.48
1:B:1972:ASN:O	1:B:1976:ARG:NH1	2.46	0.48
1:B:2023:LEU:O	1:B:2028:ARG:NH2	2.45	0.48
1:C:1610:ASN:O	1:C:1611:HIS:ND1	2.47	0.48
1:C:2883:HIS:O	1:C:2887:GLY:N	2.42	0.48
1:C:4973:HIS:O	1:C:4977:THR:HG23	2.14	0.48
1:D:2276:ALA:O	1:D:2279:SER:OG	2.30	0.48
1:A:645:ARG:NE	1:A:824:GLU:OE2	2.41	0.47
1:A:831:ARG:O	1:A:838:HIS:N	2.46	0.47
1:A:4681:LEU:O	1:A:4681:LEU:HD23	2.14	0.47
1:A:4917:ASP:O	1:A:4920:PHE:N	2.37	0.47
1:A:4995:LEU:HA	1:A:4995:LEU:HD23	1.42	0.47
1:C:596:ASN:HB3	1:C:599:VAL:HG22	1.96	0.47
1:D:4049:VAL:HG11	1:D:4159:ARG:HD2	1.94	0.47
1:D:4215:ARG:O	1:D:4216:GLN:C	2.52	0.47
1:D:4240:ASP:O	1:D:4243:PHE:N	2.35	0.47
1:A:1972:ASN:O	1:A:1976:ARG:NH1	2.46	0.47
1:B:1610:ASN:O	1:B:1611:HIS:ND1	2.47	0.47
1:B:4681:LEU:HD23	1:B:4681:LEU:O	2.14	0.47
1:C:1644:GLU:OE2	1:C:1646:ARG:NE	2.48	0.47
1:C:3717:ASP:N	1:C:3717:ASP:OD1	2.41	0.47
1:D:915:GLU:O	1:D:919:ASN:ND2	2.46	0.47
1:D:1610:ASN:O	1:D:1611:HIS:ND1	2.47	0.47
1:D:2518:LEU:HD13	1:D:2568:LEU:HD22	1.96	0.47
1:D:4799:SER:HB2	1:D:4812:HIS:CE1	2.49	0.47
1:A:251:ALA:O	1:A:255:HIS:ND1	2.37	0.47
1:A:1610:ASN:O	1:A:1611:HIS:ND1	2.47	0.47
1:A:1644:GLU:OE2	1:A:1646:ARG:NE	2.48	0.47
1:A:4223:ASN:HB3	1:A:4224:GLU:OE1	2.13	0.47
1:B:2518:LEU:HD13	1:B:2568:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4576:ILE:HD12	1:C:4639:MET:SD	2.55	0.47
1:D:4925:ILE:HG22	1:D:4925:ILE:O	2.14	0.47
1:A:4665:LYS:HA	1:A:4665:LYS:HD2	1.68	0.47
1:B:1444:GLU:HG3	1:B:1446:SER:H	1.78	0.47
1:B:4576:ILE:HD12	1:B:4639:MET:SD	2.55	0.47
1:B:4666:VAL:HA	1:B:4669:VAL:HG12	1.97	0.47
1:B:4799:SER:HB2	1:B:4812:HIS:CE1	2.49	0.47
1:C:4574:ASN:ND2	1:C:4813:LEU:HD22	2.29	0.47
1:C:4950:VAL:O	1:C:4952:GLU:N	2.46	0.47
2:J:65:ASP:OD1	2:J:65:ASP:N	2.46	0.47
1:D:596:ASN:HB3	1:D:599:VAL:HG22	1.96	0.47
1:D:1644:GLU:OE2	1:D:1646:ARG:NE	2.48	0.47
1:D:3757:GLU:OE2	1:D:4719:PHE:HE2	1.98	0.47
1:D:4820:VAL:HG23	1:D:4823:LEU:HG	1.95	0.47
1:D:4963:ILE:HD12	1:D:4964:GLY:H	1.78	0.47
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.47	0.47
1:A:1632:ASP:OD1	1:A:1632:ASP:N	2.44	0.47
1:B:2579:VAL:HA	1:B:2582:MET:HB2	1.96	0.47
1:B:4574:ASN:ND2	1:B:4813:LEU:HD22	2.29	0.47
1:B:4917:ASP:O	1:B:4919:THR:N	2.45	0.47
2:I:106:LEU:HA	2:I:109:VAL:HG12	1.96	0.47
1:C:2617:SER:OG	1:C:2618:MET:SD	2.67	0.47
1:C:4681:LEU:O	1:C:4681:LEU:HD23	2.14	0.47
1:C:5027:CYS:O	1:C:5028:PHE:C	2.49	0.47
2:K:65:ASP:OD1	2:K:65:ASP:N	2.46	0.47
2:K:106:LEU:HA	2:K:109:VAL:HG12	1.96	0.47
1:A:14:LEU:HB3	1:A:101:LEU:HD21	1.97	0.47
1:A:4937:ILE:HG13	1:A:4938:ASP:H	1.79	0.47
1:B:4046:ASP:HA	1:B:4049:VAL:HG22	1.96	0.47
1:C:613:ALA:HB2	1:C:1676:LEU:HD12	1.95	0.47
1:C:1490:SER:OG	1:C:1491:ASN:N	2.47	0.47
1:C:4666:VAL:HA	1:C:4669:VAL:HG12	1.96	0.47
1:D:710:ASP:N	1:D:710:ASP:OD1	2.44	0.47
1:A:1490:SER:OG	1:A:1491:ASN:N	2.47	0.47
1:A:4666:VAL:HA	1:A:4669:VAL:HG12	1.97	0.47
1:A:4926:VAL:HG13	1:D:4933:GLN:HG2	1.96	0.47
1:B:1769:THR:OG1	1:B:1956:GLU:OE1	2.28	0.47
1:B:4563:LYS:CA	1:B:4657:ILE:HD11	2.43	0.47
1:B:4925:ILE:HG22	1:B:4925:ILE:O	2.14	0.47
1:B:4973:HIS:O	1:B:4977:THR:HG23	2.14	0.47
1:C:1735:ILE:HG22	1:C:2142:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3757:GLU:OE2	1:C:4719:PHE:HE2	1.98	0.47
1:C:3795:SER:O	1:C:3799:LYS:NZ	2.45	0.47
1:C:4719:PHE:O	1:C:4720:VAL:C	2.51	0.47
1:D:14:LEU:HB3	1:D:101:LEU:HD21	1.97	0.47
1:D:492:ASP:OD1	1:D:492:ASP:N	2.46	0.47
1:D:498:THR:H	1:D:503:PHE:HD2	1.62	0.47
1:D:613:ALA:HB2	1:D:1676:LEU:HD12	1.95	0.47
1:D:1444:GLU:HG3	1:D:1446:SER:H	1.78	0.47
1:D:2572:THR:OG1	1:D:2615:ARG:NH1	2.44	0.47
1:D:4046:ASP:HA	1:D:4049:VAL:HG22	1.96	0.47
1:A:498:THR:H	1:A:503:PHE:HD2	1.62	0.47
1:A:745:SER:OG	1:A:758:ARG:O	2.29	0.47
1:A:4576:ILE:HD12	1:A:4639:MET:SD	2.55	0.47
2:L:106:LEU:HA	2:L:109:VAL:HG12	1.96	0.47
1:B:1028:ASP:OD1	1:B:1028:ASP:N	2.43	0.47
1:B:2873:ALA:O	1:B:2877:GLN:N	2.46	0.47
1:B:3795:SER:O	1:B:3799:LYS:NZ	2.45	0.47
1:B:4190:ILE:HG23	1:B:5031:GLN:NE2	2.30	0.47
1:B:4543:GLU:HA	1:B:4546:VAL:HG22	1.96	0.47
1:B:4646:LEU:HD12	1:B:4646:LEU:HA	1.73	0.47
1:C:4543:GLU:HA	1:C:4546:VAL:HG22	1.96	0.47
1:D:1241:SER:HA	1:D:1603:VAL:HG12	1.97	0.47
1:D:4576:ILE:HD12	1:D:4639:MET:SD	2.55	0.47
1:D:4665:LYS:HA	1:D:4665:LYS:HD2	1.68	0.47
1:D:4666:VAL:HA	1:D:4669:VAL:HG12	1.97	0.47
1:A:596:ASN:HB3	1:A:599:VAL:HG22	1.96	0.47
1:A:2518:LEU:HD13	1:A:2568:LEU:HD22	1.96	0.47
1:A:2873:ALA:O	1:A:2877:GLN:N	2.46	0.47
1:A:3969:ILE:HD11	1:A:3977:GLN:HA	1.97	0.47
1:A:4543:GLU:HA	1:A:4546:VAL:HG22	1.96	0.47
1:B:3757:GLU:OE2	1:B:4719:PHE:HE2	1.98	0.47
1:C:498:THR:H	1:C:503:PHE:HD2	1.62	0.47
1:C:915:GLU:O	1:C:919:ASN:ND2	2.46	0.47
1:C:2579:VAL:HA	1:C:2582:MET:HB2	1.96	0.47
1:C:4233:LEU:O	1:C:4236:SER:OG	2.25	0.47
1:D:1966:VAL:O	1:D:1970:GLN:N	2.45	0.47
1:A:2886:TRP:O	1:A:2890:LYS:N	2.46	0.47
1:A:4233:LEU:O	1:A:4236:SER:OG	2.25	0.47
1:B:4183:ILE:CD1	1:B:4193:ILE:HD11	2.40	0.47
1:D:3969:ILE:HD11	1:D:3977:GLN:HA	1.97	0.47
1:D:4543:GLU:HA	1:D:4546:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4799:SER:HB2	1:A:4812:HIS:CE1	2.49	0.46
2:L:65:ASP:OD1	2:L:65:ASP:N	2.46	0.46
1:B:1735:ILE:HG22	1:B:2142:TYR:HB3	1.97	0.46
1:C:4182:GLU:OE2	1:C:4190:ILE:HD13	2.15	0.46
1:C:4813:LEU:HD12	1:C:4813:LEU:HA	1.66	0.46
1:D:2536:LEU:HD13	1:D:2544:THR:HG21	1.97	0.46
1:A:916:PRO:HA	1:A:919:ASN:HB2	1.98	0.46
1:A:2536:LEU:HD13	1:A:2544:THR:HG21	1.97	0.46
1:A:4054:ASN:OD1	1:A:4054:ASN:N	2.47	0.46
1:A:4717:ASP:O	1:A:4718:LYS:CB	2.60	0.46
1:B:1241:SER:HA	1:B:1603:VAL:HG12	1.97	0.46
1:B:3969:ILE:HD11	1:B:3977:GLN:HA	1.97	0.46
1:B:4832:HIS:CE1	1:B:4943:LEU:HD21	2.51	0.46
1:B:4957:LYS:CA	1:B:4964:GLY:HA2	2.32	0.46
1:C:1444:GLU:HG3	1:C:1446:SER:H	1.78	0.46
1:D:2883:HIS:O	1:D:2887:GLY:N	2.42	0.46
1:A:1735:ILE:HG22	1:A:2142:TYR:HB3	1.96	0.46
1:B:229:GLU:N	1:B:249:GLY:O	2.49	0.46
1:B:1644:GLU:OE2	1:B:1646:ARG:NE	2.48	0.46
1:B:2536:LEU:HD13	1:B:2544:THR:HG21	1.97	0.46
1:B:3944:GLU:OE1	1:B:3946:GLN:N	2.47	0.46
1:B:4244:GLU:O	1:B:4248:ALA:N	2.44	0.46
1:B:4957:LYS:HA	1:B:4964:GLY:CA	2.33	0.46
1:C:4578:LEU:HD12	1:D:4879:MET:HG2	1.97	0.46
1:C:4646:LEU:HD12	1:C:4646:LEU:HA	1.73	0.46
1:C:4799:SER:HB2	1:C:4812:HIS:CE1	2.49	0.46
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	1.95	0.46
1:B:596:ASN:HB3	1:B:599:VAL:HG22	1.96	0.46
1:B:916:PRO:HA	1:B:919:ASN:HB2	1.98	0.46
1:C:916:PRO:HA	1:C:919:ASN:HB2	1.98	0.46
1:C:3969:ILE:HD11	1:C:3977:GLN:HA	1.97	0.46
1:C:4937:ILE:HG13	1:C:4938:ASP:H	1.79	0.46
1:D:4708:THR:HG23	1:D:4710:SER:H	1.81	0.46
1:A:340:LYS:O	1:A:344:SER:OG	2.34	0.46
1:A:1147:ASP:OD1	1:A:1147:ASP:N	2.46	0.46
1:A:4218:ILE:HD13	1:A:4218:ILE:HA	1.62	0.46
1:B:786:GLY:N	1:B:1630:CYS:SG	2.89	0.46
1:C:1297:PHE:HD1	1:C:1522:LEU:HA	1.81	0.46
1:C:4046:ASP:HA	1:C:4049:VAL:HG22	1.96	0.46
1:C:4243:PHE:O	1:C:4246:GLN:HB3	2.16	0.46
1:C:4563:LYS:CA	1:C:4657:ILE:HD11	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4957:LYS:HA	1:C:4964:GLY:CA	2.33	0.46
1:D:1011:GLN:NE2	1:D:1017:ARG:O	2.49	0.46
1:A:786:GLY:N	1:A:1630:CYS:SG	2.89	0.46
1:A:1297:PHE:HD1	1:A:1522:LEU:HA	1.81	0.46
1:A:2024:PRO:HG2	1:A:2027:ILE:HG12	1.98	0.46
1:B:501:ALA:HA	1:B:504:ALA:HB3	1.98	0.46
1:B:1297:PHE:HD1	1:B:1522:LEU:HA	1.81	0.46
1:C:4708:THR:HG23	1:C:4710:SER:H	1.81	0.46
1:D:229:GLU:N	1:D:249:GLY:O	2.49	0.46
1:D:786:GLY:N	1:D:1630:CYS:SG	2.89	0.46
1:D:4832:HIS:CE1	1:D:4943:LEU:HD21	2.51	0.46
1:A:3372:VAL:O	1:A:3376:GLU:N	2.48	0.46
1:A:3757:GLU:OE2	1:A:4719:PHE:HE2	1.98	0.46
1:A:4243:PHE:O	1:A:4246:GLN:HB3	2.16	0.46
1:A:4813:LEU:HD12	1:A:4813:LEU:HA	1.66	0.46
1:A:4925:ILE:O	1:A:4925:ILE:HG22	2.14	0.46
1:B:720:HIS:HD2	1:B:729:PRO:HA	1.80	0.46
1:B:3372:VAL:O	1:B:3376:GLU:N	2.48	0.46
1:C:229:GLU:N	1:C:249:GLY:O	2.49	0.46
1:C:501:ALA:HA	1:C:504:ALA:HB3	1.98	0.46
1:C:1005:TRP:HE3	1:C:1021:LEU:HD11	1.81	0.46
1:C:1241:SER:HA	1:C:1603:VAL:HG12	1.97	0.46
1:C:2171:GLY:N	1:C:2174:GLU:OE2	2.49	0.46
1:C:4832:HIS:CE1	1:C:4943:LEU:HD21	2.50	0.46
1:D:501:ALA:HA	1:D:504:ALA:HB3	1.98	0.46
1:D:916:PRO:HA	1:D:919:ASN:HB2	1.98	0.46
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.47	0.46
1:D:1735:ILE:HG22	1:D:2142:TYR:HB3	1.96	0.46
1:A:3944:GLU:OE1	1:A:3946:GLN:N	2.47	0.46
1:A:4212:GLU:O	1:A:4213:SER:C	2.54	0.46
1:A:4708:THR:HG23	1:A:4710:SER:H	1.81	0.46
1:B:4708:THR:HG23	1:B:4710:SER:H	1.81	0.46
1:C:485:SER:O	1:C:489:ASN:N	2.45	0.46
1:C:4925:ILE:O	1:C:4925:ILE:HG22	2.14	0.46
1:D:1099:GLU:H	1:D:1198:GLN:HG3	1.80	0.46
1:D:4658:ILE:HD13	1:D:4658:ILE:HA	1.76	0.46
1:D:4952:GLU:HB3	1:D:4953:ASP:H	1.65	0.46
1:A:1241:SER:HA	1:A:1603:VAL:HG12	1.97	0.46
1:A:2171:GLY:N	1:A:2174:GLU:OE2	2.49	0.46
1:A:4215:ARG:O	1:A:4216:GLN:C	2.52	0.46
1:A:4807:PHE:CE1	1:B:4879:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4832:HIS:CE1	1:A:4943:LEU:HD21	2.50	0.46
1:A:4879:MET:HE2	1:A:4879:MET:HB2	1.77	0.46
1:B:485:SER:O	1:B:489:ASN:N	2.46	0.46
1:B:2305:CYS:HB2	1:B:2324:ASN:HB3	1.98	0.46
2:I:112:ASN:N	2:I:112:ASN:OD1	2.49	0.46
1:C:2536:LEU:HD13	1:C:2544:THR:HG21	1.97	0.46
1:C:4017:LEU:HD12	1:C:4139:ILE:HG21	1.98	0.46
1:D:340:LYS:O	1:D:344:SER:OG	2.34	0.46
1:D:4017:LEU:HD12	1:D:4139:ILE:HG21	1.98	0.46
1:D:4247:ILE:O	1:D:4250:GLN:HB2	2.16	0.46
1:A:1856:ASP:O	1:A:1860:LYS:NZ	2.45	0.46
1:A:4247:ILE:O	1:A:4250:GLN:HB2	2.16	0.46
1:A:5027:CYS:H	1:A:5030:LYS:CB	2.28	0.46
1:B:412:ASN:O	1:B:416:LYS:NZ	2.47	0.46
1:B:985:VAL:HA	1:B:988:LEU:HB2	1.98	0.46
2:J:73:MET:HA	2:J:76:LYS:HB2	1.98	0.46
1:D:2024:PRO:HG2	1:D:2027:ILE:HG12	1.98	0.46
1:D:4243:PHE:O	1:D:4246:GLN:HB3	2.16	0.46
1:A:229:GLU:N	1:A:249:GLY:O	2.49	0.45
1:A:501:ALA:HA	1:A:504:ALA:HB3	1.98	0.45
1:A:915:GLU:O	1:A:919:ASN:ND2	2.46	0.45
1:A:985:VAL:HA	1:A:988:LEU:HB2	1.98	0.45
1:A:1005:TRP:HE3	1:A:1021:LEU:HD11	1.81	0.45
1:A:1769:THR:OG1	1:A:1956:GLU:OE1	2.28	0.45
1:C:2023:LEU:O	1:C:2028:ARG:NH2	2.45	0.45
1:C:2121:PHE:HD1	1:C:2124:LEU:HD21	1.81	0.45
1:C:5028:PHE:N	1:C:5028:PHE:CD2	2.77	0.45
1:D:2171:GLY:N	1:D:2174:GLU:OE2	2.49	0.45
2:K:73:MET:HA	2:K:76:LYS:HB2	1.98	0.45
2:L:53:ILE:HD12	2:L:53:ILE:HA	1.87	0.45
1:B:2024:PRO:HG2	1:B:2027:ILE:HG12	1.98	0.45
1:B:2151:ASP:O	1:B:2154:SER:OG	2.34	0.45
1:B:2276:ALA:O	1:B:2279:SER:OG	2.30	0.45
1:C:652:ARG:HE	1:C:773:LEU:HD22	1.81	0.45
1:C:4244:GLU:OE1	1:C:4244:GLU:N	2.46	0.45
1:D:1856:ASP:O	1:D:1860:LYS:NZ	2.45	0.45
1:A:1739:THR:HG23	1:A:1742:THR:H	1.82	0.45
1:A:4244:GLU:OE1	1:A:4244:GLU:N	2.46	0.45
1:B:14:LEU:HB3	1:B:101:LEU:HD21	1.97	0.45
1:B:1096:THR:OG1	1:B:1198:GLN:OE1	2.35	0.45
1:B:2171:GLY:N	1:B:2174:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4243:PHE:O	1:B:4246:GLN:HB3	2.16	0.45
1:C:14:LEU:HB3	1:C:101:LEU:HD21	1.97	0.45
1:C:786:GLY:N	1:C:1630:CYS:SG	2.89	0.45
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.81	0.45
1:D:4731:ILE:HG23	1:D:4732:PHE:CD1	2.40	0.45
1:A:720:HIS:HD2	1:A:729:PRO:HA	1.80	0.45
1:A:1011:GLN:NE2	1:A:1017:ARG:O	2.49	0.45
1:A:2121:PHE:HD1	1:A:2124:LEU:HD21	1.81	0.45
1:A:4957:LYS:HA	1:A:4964:GLY:CA	2.33	0.45
1:B:1782:PHE:HE1	3:E:90:VAL:HG21	1.82	0.45
1:B:2503:VAL:HG21	1:B:2558:VAL:HG12	1.99	0.45
1:C:340:LYS:O	1:C:344:SER:OG	2.34	0.45
1:C:1782:PHE:HE1	3:F:90:VAL:HG21	1.82	0.45
1:A:1171:SER:HG	1:A:1175:SER:HG	1.57	0.45
1:A:4879:MET:HE1	1:D:4807:PHE:CE1	2.51	0.45
1:B:4017:LEU:HD12	1:B:4139:ILE:HG21	1.98	0.45
1:B:4813:LEU:HA	1:B:4813:LEU:HD12	1.66	0.45
1:C:720:HIS:HD2	1:C:729:PRO:HA	1.80	0.45
1:C:3944:GLU:OE1	1:C:3946:GLN:N	2.47	0.45
1:C:4665:LYS:HD2	1:C:4665:LYS:HA	1.68	0.45
1:C:4741:LEU:HB2	1:C:4743:MET:HE2	1.98	0.45
1:D:1739:THR:HG23	1:D:1742:THR:H	1.82	0.45
1:A:652:ARG:HE	1:A:773:LEU:HD22	1.81	0.45
1:A:1099:GLU:H	1:A:1198:GLN:HG3	1.81	0.45
1:A:2305:CYS:HB2	1:A:2324:ASN:HB3	1.98	0.45
1:A:2433:LEU:HD12	1:A:2457:LEU:HD13	1.99	0.45
1:A:4017:LEU:HD12	1:A:4139:ILE:HG21	1.98	0.45
1:B:4247:ILE:O	1:B:4250:GLN:HB2	2.16	0.45
1:C:1011:GLN:NE2	1:C:1017:ARG:O	2.49	0.45
1:C:1095:VAL:HB	1:C:1199:VAL:HG13	1.98	0.45
1:C:2151:ASP:O	1:C:2154:SER:OG	2.34	0.45
2:J:50:GLN:O	2:J:54:ASN:N	2.44	0.45
1:D:652:ARG:HE	1:D:773:LEU:HD22	1.81	0.45
1:D:665:GLU:HG2	1:D:745:SER:HB3	1.99	0.45
1:D:720:HIS:HD2	1:D:729:PRO:HA	1.80	0.45
1:D:985:VAL:HA	1:D:988:LEU:HB2	1.98	0.45
1:D:1005:TRP:HE3	1:D:1021:LEU:HD11	1.81	0.45
1:A:4731:ILE:HG23	1:A:4732:PHE:CD1	2.40	0.45
1:B:340:LYS:O	1:B:344:SER:OG	2.34	0.45
1:B:1011:GLN:NE2	1:B:1017:ARG:O	2.49	0.45
1:B:2121:PHE:HD1	1:B:2124:LEU:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2301:TYR:HB3	1:B:2331:TYR:CZ	2.52	0.45
1:B:4731:ILE:HG23	1:B:4732:PHE:CD1	2.40	0.45
2:I:73:MET:HA	2:I:76:LYS:HB2	1.98	0.45
1:C:1099:GLU:H	1:C:1198:GLN:HG3	1.81	0.45
1:A:2301:TYR:HB3	1:A:2331:TYR:CZ	2.52	0.45
1:A:2592:GLY:H	1:A:2600:ARG:HH21	1.65	0.45
1:C:665:GLU:HG2	1:C:745:SER:HB3	1.99	0.45
1:C:2024:PRO:HG2	1:C:2027:ILE:HG12	1.98	0.45
1:C:4247:ILE:O	1:C:4250:GLN:HB2	2.16	0.45
1:D:2575:ARG:HD2	1:D:2575:ARG:HA	1.79	0.45
1:D:2592:GLY:H	1:D:2600:ARG:HH21	1.65	0.45
1:A:1782:PHE:HE1	3:H:90:VAL:HG21	1.82	0.45
1:A:4957:LYS:CA	1:A:4964:GLY:HA2	2.32	0.45
1:B:652:ARG:HE	1:B:773:LEU:HD22	1.81	0.45
1:B:665:GLU:HG2	1:B:745:SER:HB3	1.99	0.45
1:B:915:GLU:O	1:B:919:ASN:ND2	2.46	0.45
1:B:1005:TRP:HE3	1:B:1021:LEU:HD11	1.81	0.45
1:C:2301:TYR:HB3	1:C:2331:TYR:CZ	2.52	0.45
1:C:2305:CYS:HB2	1:C:2324:ASN:HB3	1.98	0.45
1:C:4215:ARG:O	1:C:4216:GLN:C	2.52	0.45
1:D:412:ASN:O	1:D:416:LYS:NZ	2.47	0.45
1:D:3727:ASP:O	1:D:3731:LYS:N	2.45	0.45
1:D:4688:ILE:HD11	1:D:4737:ILE:CD1	2.47	0.45
1:A:1095:VAL:HB	1:A:1199:VAL:HG13	1.98	0.45
1:A:4741:LEU:HB2	1:A:4743:MET:HE2	1.98	0.45
1:B:1739:THR:HG23	1:B:1742:THR:H	1.82	0.45
1:B:4688:ILE:HD11	1:B:4737:ILE:CD1	2.47	0.45
1:B:5027:CYS:H	1:B:5030:LYS:CB	2.29	0.45
1:C:1739:THR:HG23	1:C:1742:THR:H	1.82	0.45
1:C:2191:PHE:HD1	1:C:2198:MET:HG3	1.82	0.45
1:D:1782:PHE:HE1	3:G:90:VAL:HG21	1.82	0.45
1:D:2301:TYR:HB3	1:D:2331:TYR:CZ	2.52	0.45
1:D:4212:GLU:O	1:D:4213:SER:C	2.54	0.45
1:A:665:GLU:HG2	1:A:745:SER:HB3	1.99	0.44
1:A:3997:ALA:HB1	1:A:4057:MET:HB2	1.99	0.44
1:A:4688:ILE:HD11	1:A:4737:ILE:CD1	2.47	0.44
1:B:1099:GLU:H	1:B:1198:GLN:HG3	1.81	0.44
1:C:1096:THR:OG1	1:C:1198:GLN:OE1	2.35	0.44
1:C:1856:ASP:O	1:C:1860:LYS:NZ	2.45	0.44
1:C:3804:ILE:HD12	1:C:3804:ILE:HA	1.84	0.44
1:D:1018:ASN:HB3	1:D:1021:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1095:VAL:HB	1:D:1199:VAL:HG13	1.98	0.44
1:D:2151:ASP:O	1:D:2154:SER:OG	2.34	0.44
1:D:2305:CYS:HB2	1:D:2324:ASN:HB3	1.98	0.44
1:D:2873:ALA:O	1:D:2877:GLN:N	2.46	0.44
2:L:73:MET:HA	2:L:76:LYS:HB2	1.98	0.44
1:C:3997:ALA:HB1	1:C:4057:MET:HB2	1.99	0.44
1:D:2575:ARG:HH22	1:D:2577:ILE:HG22	1.82	0.44
1:D:4813:LEU:HD12	1:D:4813:LEU:HA	1.66	0.44
1:A:1018:ASN:HB3	1:A:1021:LEU:HG	1.99	0.44
1:A:3795:SER:O	1:A:3799:LYS:NZ	2.45	0.44
1:B:2191:PHE:HD1	1:B:2198:MET:HG3	1.82	0.44
1:B:4213:SER:O	1:B:4214:LYS:C	2.55	0.44
1:B:4825:THR:HG22	1:B:4940:PHE:CE1	2.53	0.44
1:C:2519:LEU:HA	1:C:2522:LEU:HB3	1.99	0.44
1:C:2592:GLY:H	1:C:2600:ARG:HH21	1.65	0.44
1:C:4212:GLU:O	1:C:4213:SER:C	2.54	0.44
1:D:875:ALA:O	1:D:921:ASN:ND2	2.50	0.44
1:D:4233:LEU:O	1:D:4236:SER:OG	2.25	0.44
1:D:4741:LEU:HB2	1:D:4743:MET:HE2	1.98	0.44
1:A:2191:PHE:HD1	1:A:2198:MET:HG3	1.82	0.44
1:A:5027:CYS:O	1:A:5028:PHE:C	2.46	0.44
1:B:2592:GLY:H	1:B:2600:ARG:HH21	1.65	0.44
1:B:4578:LEU:HD12	1:C:4879:MET:HG2	1.98	0.44
1:B:4665:LYS:HA	1:B:4665:LYS:HD2	1.68	0.44
1:C:2233:CYS:SG	1:C:2270:SER:OG	2.64	0.44
1:C:2503:VAL:HG21	1:C:2558:VAL:HG12	1.99	0.44
1:C:3974:THR:HA	1:C:3977:GLN:HB2	1.99	0.44
1:C:4562:LEU:HD21	1:C:4656:LEU:CD2	2.45	0.44
1:C:4825:THR:HG22	1:C:4940:PHE:CE1	2.53	0.44
1:C:4957:LYS:CA	1:C:4964:GLY:HA2	2.32	0.44
1:D:2433:LEU:HD12	1:D:2457:LEU:HD13	1.99	0.44
1:D:3997:ALA:HB1	1:D:4057:MET:HB2	1.99	0.44
1:A:1096:THR:OG1	1:A:1198:GLN:OE1	2.35	0.44
1:A:1961:PHE:HD1	1:A:1964:ARG:HH21	1.66	0.44
1:A:2575:ARG:HH22	1:A:2577:ILE:HG22	1.83	0.44
1:A:4774:LYS:HG3	1:A:4775:TYR:N	2.33	0.44
1:C:1018:ASN:HB3	1:C:1021:LEU:HG	1.99	0.44
1:C:2575:ARG:HH22	1:C:2577:ILE:HG22	1.83	0.44
1:D:2121:PHE:HD1	1:D:2124:LEU:HD21	1.81	0.44
1:B:1095:VAL:HB	1:B:1199:VAL:HG13	1.98	0.44
1:B:2433:LEU:HD12	1:B:2457:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2519:LEU:HA	1:B:2522:LEU:HB3	1.99	0.44
1:B:3997:ALA:HB1	1:B:4057:MET:HB2	1.99	0.44
1:B:4212:GLU:O	1:B:4213:SER:C	2.54	0.44
1:C:875:ALA:O	1:C:921:ASN:ND2	2.50	0.44
1:C:2873:ALA:O	1:C:2877:GLN:N	2.46	0.44
1:C:4240:ASP:O	1:C:4243:PHE:N	2.35	0.44
1:C:4562:LEU:CD2	1:C:4656:LEU:HD23	2.45	0.44
1:C:4774:LYS:HG3	1:C:4775:TYR:N	2.33	0.44
1:C:4995:LEU:HA	1:C:4995:LEU:HD23	1.42	0.44
2:J:112:ASN:OD1	2:J:112:ASN:N	2.49	0.44
1:D:251:ALA:O	1:D:255:HIS:ND1	2.37	0.44
1:D:2104:ARG:HA	1:D:2107:GLN:HB3	2.00	0.44
1:A:4190:ILE:H	1:A:5031:GLN:HE22	1.64	0.44
1:B:37:LEU:HD21	1:B:191:VAL:HG11	2.00	0.44
2:I:53:ILE:HD12	2:I:56:VAL:HG23	1.99	0.44
1:C:3761:GLN:O	1:C:3765:TYR:N	2.48	0.44
1:D:1961:PHE:HD1	1:D:1964:ARG:HH21	1.66	0.44
1:D:4825:THR:HG22	1:D:4940:PHE:CE1	2.53	0.44
3:G:39:SER:OG	3:G:44:LYS:O	2.36	0.44
1:A:3898:ASP:OD1	1:A:3898:ASP:N	2.51	0.44
2:L:53:ILE:HD12	2:L:56:VAL:HG23	1.99	0.44
1:B:608:VAL:HG12	1:B:613:ALA:HA	2.00	0.44
1:B:1961:PHE:HD1	1:B:1964:ARG:HH21	1.66	0.44
1:B:2575:ARG:HH22	1:B:2577:ILE:HG22	1.82	0.44
1:B:4774:LYS:HG3	1:B:4775:TYR:N	2.33	0.44
1:B:4937:ILE:CG1	1:B:4938:ASP:N	2.80	0.44
1:C:985:VAL:HA	1:C:988:LEU:HB2	1.98	0.44
1:D:1745:ILE:HD12	1:D:1745:ILE:HA	1.86	0.44
1:D:2023:LEU:O	1:D:2028:ARG:NH2	2.45	0.44
1:D:2191:PHE:HD1	1:D:2198:MET:HG3	1.82	0.44
2:K:53:ILE:HD12	2:K:56:VAL:HG23	1.99	0.44
1:A:37:LEU:HD21	1:A:191:VAL:HG11	2.00	0.44
1:A:2023:LEU:O	1:A:2028:ARG:NH2	2.45	0.44
1:A:4825:THR:HG22	1:A:4940:PHE:CE1	2.53	0.44
1:A:4839:MET:HG3	1:D:4823:LEU:HD11	1.99	0.44
1:A:4914:VAL:O	1:A:4918:ILE:HG13	2.18	0.44
1:B:4059:LEU:HD23	1:B:4059:LEU:HA	1.86	0.44
1:B:4215:ARG:O	1:B:4216:GLN:C	2.52	0.44
1:B:4729:GLY:O	1:B:4734:ARG:HG3	2.18	0.44
1:C:477:LEU:HD23	1:C:477:LEU:HA	1.88	0.44
1:C:840:VAL:HG23	1:C:1199:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2104:ARG:HA	1:C:2107:GLN:HB3	2.00	0.44
1:C:4688:ILE:HD11	1:C:4737:ILE:CD1	2.47	0.44
1:C:4729:GLY:O	1:C:4734:ARG:HG3	2.18	0.44
1:D:1432:THR:HG23	1:D:1572:ILE:HG22	2.00	0.44
1:D:3898:ASP:OD1	1:D:3898:ASP:N	2.51	0.44
2:K:112:ASN:OD1	2:K:112:ASN:N	2.49	0.44
1:A:3841:VAL:HG12	1:A:3926:LEU:HD22	2.00	0.43
1:B:123:THR:OG1	1:B:124:SER:N	2.51	0.43
1:B:4924:VAL:HG22	1:B:4924:VAL:O	2.18	0.43
1:C:4785:THR:O	1:C:4785:THR:HG22	2.19	0.43
1:C:4937:ILE:CG1	1:C:4938:ASP:N	2.80	0.43
2:J:45:THR:OG1	2:J:46:GLU:N	2.51	0.43
3:F:39:SER:OG	3:F:44:LYS:O	2.36	0.43
1:D:1087:ARG:HH21	1:D:1222:GLY:HA3	1.83	0.43
1:D:2503:VAL:HG21	1:D:2558:VAL:HG12	1.99	0.43
1:D:3944:GLU:OE1	1:D:3946:GLN:N	2.47	0.43
1:D:4054:ASN:OD1	1:D:4054:ASN:N	2.47	0.43
1:A:875:ALA:O	1:A:921:ASN:ND2	2.50	0.43
1:A:2519:LEU:HA	1:A:2522:LEU:HB3	1.99	0.43
1:A:4562:LEU:HD21	1:A:4656:LEU:CD2	2.45	0.43
2:L:112:ASN:N	2:L:112:ASN:OD1	2.49	0.43
1:B:2883:HIS:O	1:B:2887:GLY:N	2.42	0.43
1:C:412:ASN:O	1:C:416:LYS:NZ	2.47	0.43
1:C:608:VAL:HG12	1:C:613:ALA:HA	2.00	0.43
1:C:1685:LEU:HA	1:C:1688:HIS:HD2	1.84	0.43
1:C:4914:VAL:O	1:C:4918:ILE:HG13	2.18	0.43
1:C:4924:VAL:O	1:C:4924:VAL:HG22	2.18	0.43
1:D:37:LEU:HD21	1:D:191:VAL:HG11	2.00	0.43
1:D:123:THR:OG1	1:D:124:SER:N	2.51	0.43
1:D:716:PHE:HE1	1:D:730:VAL:HG11	1.83	0.43
1:D:1452:TRP:NE1	1:D:1518:CYS:SG	2.73	0.43
1:D:2519:LEU:HA	1:D:2522:LEU:HB3	1.99	0.43
1:D:4209:GLN:O	1:D:4209:GLN:HG2	2.19	0.43
1:D:4914:VAL:O	1:D:4918:ILE:HG13	2.18	0.43
1:D:4924:VAL:HG22	1:D:4924:VAL:O	2.18	0.43
1:D:5028:PHE:C	1:D:5030:LYS:N	2.71	0.43
1:A:2618:MET:SD	1:A:2618:MET:N	2.91	0.43
1:A:4562:LEU:CD2	1:A:4656:LEU:HD23	2.45	0.43
1:A:4920:PHE:HB3	1:A:4921:PHE:H	1.54	0.43
1:B:1177:THR:OG1	1:B:1179:PHE:O	2.34	0.43
1:B:4937:ILE:HG13	1:B:4938:ASP:H	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:GLU:O	1:D:466:SER:OG	2.35	0.43
1:D:840:VAL:HG23	1:D:1199:VAL:HB	2.00	0.43
1:D:3974:THR:HA	1:D:3977:GLN:HB2	1.99	0.43
1:D:4785:THR:HG22	1:D:4785:THR:O	2.19	0.43
1:A:412:ASN:O	1:A:416:LYS:NZ	2.47	0.43
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.89	0.43
1:A:4240:ASP:O	1:A:4243:PHE:N	2.35	0.43
2:L:45:THR:OG1	2:L:46:GLU:N	2.51	0.43
1:B:3761:GLN:O	1:B:3765:TYR:N	2.48	0.43
1:C:916:PRO:O	1:C:920:TYR:N	2.50	0.43
1:C:3898:ASP:N	1:C:3898:ASP:OD1	2.51	0.43
1:D:309:THR:O	1:D:313:SER:OG	2.31	0.43
1:D:745:SER:OG	1:D:758:ARG:O	2.29	0.43
1:D:916:PRO:O	1:D:920:TYR:N	2.50	0.43
1:D:1096:THR:OG1	1:D:1198:GLN:OE1	2.35	0.43
1:D:2529:ASP:O	1:D:2533:ALA:N	2.47	0.43
1:A:256:ALA:HB2	1:A:477:LEU:HD22	2.00	0.43
1:A:581:ASN:N	1:A:581:ASN:OD1	2.52	0.43
1:A:1177:THR:OG1	1:A:1179:PHE:O	2.34	0.43
1:A:1242:LEU:HD12	1:A:1242:LEU:HA	1.90	0.43
1:A:1283:LEU:HD23	1:A:1283:LEU:HA	1.88	0.43
1:A:2616:PRO:HB3	1:A:2619:LEU:HD22	2.01	0.43
1:A:3974:THR:HA	1:A:3977:GLN:HB2	1.99	0.43
1:A:4729:GLY:O	1:A:4734:ARG:HG3	2.18	0.43
1:B:1432:THR:HG23	1:B:1572:ILE:HG22	2.00	0.43
1:B:4943:LEU:HD13	1:B:4943:LEU:HA	1.89	0.43
1:C:37:LEU:HD21	1:C:191:VAL:HG11	2.00	0.43
1:C:636:ASN:HB3	1:C:702:TRP:HZ2	1.84	0.43
1:C:2433:LEU:HD12	1:C:2457:LEU:HD13	1.99	0.43
1:C:4213:SER:O	1:C:4214:LYS:C	2.55	0.43
1:C:4705:VAL:O	1:C:4708:THR:HG22	2.19	0.43
2:J:53:ILE:HD12	2:J:56:VAL:HG23	1.99	0.43
1:D:256:ALA:HB2	1:D:477:LEU:HD22	2.00	0.43
1:D:581:ASN:N	1:D:581:ASN:OD1	2.52	0.43
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.88	0.43
1:D:2233:CYS:SG	1:D:2270:SER:OG	2.64	0.43
1:D:2616:PRO:HB3	1:D:2619:LEU:HD22	2.01	0.43
1:D:4957:LYS:HA	1:D:4964:GLY:CA	2.33	0.43
1:A:2503:VAL:HG21	1:A:2558:VAL:HG12	1.99	0.43
1:A:4204:GLN:HG3	1:A:4245:MET:HE3	2.01	0.43
1:A:4856:PHE:O	1:A:4860:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:ALA:O	1:B:921:ASN:ND2	2.51	0.43
1:B:1087:ARG:HH21	1:B:1222:GLY:HA3	1.83	0.43
1:B:3841:VAL:HG12	1:B:3926:LEU:HD22	2.00	0.43
1:B:4559:PHE:O	1:B:4562:LEU:N	2.52	0.43
1:B:4785:THR:O	1:B:4785:THR:HG22	2.19	0.43
1:C:251:ALA:O	1:C:255:HIS:ND1	2.37	0.43
1:C:1961:PHE:HD1	1:C:1964:ARG:HH21	1.66	0.43
1:C:4820:VAL:CG2	1:C:4823:LEU:HG	2.49	0.43
1:D:608:VAL:HG12	1:D:613:ALA:HA	2.00	0.43
1:D:636:ASN:HB3	1:D:702:TRP:HZ2	1.84	0.43
1:D:3632:VAL:HA	1:D:3635:CYS:HB2	2.01	0.43
1:D:4085:ARG:H	1:D:4085:ARG:HG2	1.65	0.43
1:A:479:GLN:HA	1:A:484:LEU:HD23	2.01	0.43
1:A:608:VAL:HG12	1:A:613:ALA:HA	2.00	0.43
1:A:716:PHE:HE1	1:A:730:VAL:HG11	1.83	0.43
1:A:1432:THR:HG23	1:A:1572:ILE:HG22	2.00	0.43
1:A:2244:ARG:NH2	1:A:2283:ASN:OD1	2.52	0.43
1:A:3632:VAL:HA	1:A:3635:CYS:HB2	2.01	0.43
1:A:4785:THR:HG22	1:A:4785:THR:O	2.19	0.43
1:B:916:PRO:O	1:B:920:TYR:N	2.50	0.43
1:B:1018:ASN:HB3	1:B:1021:LEU:HG	1.99	0.43
1:B:2618:MET:SD	1:B:2618:MET:N	2.92	0.43
1:B:4697:VAL:HG13	1:B:4698:LYS:HD3	2.00	0.43
1:C:581:ASN:OD1	1:C:581:ASN:N	2.52	0.43
1:C:4059:LEU:HD23	1:C:4059:LEU:HA	1.86	0.43
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.52	0.43
1:D:4190:ILE:HG22	1:D:4191:GLU:N	2.28	0.43
1:D:4244:GLU:OE1	1:D:4244:GLU:N	2.46	0.43
1:D:4705:VAL:O	1:D:4708:THR:HG22	2.19	0.43
1:D:5028:PHE:HD2	1:D:5028:PHE:N	2.13	0.43
1:A:4847:VAL:O	1:A:4847:VAL:HG22	2.19	0.43
1:B:1283:LEU:HD23	1:B:1283:LEU:HA	1.88	0.43
1:B:4218:ILE:HD13	1:B:4218:ILE:HA	1.62	0.43
3:E:39:SER:OG	3:E:44:LYS:O	2.36	0.43
1:C:1186:ASP:N	1:C:1186:ASP:OD1	2.43	0.43
1:C:3841:VAL:HG12	1:C:3926:LEU:HD22	2.00	0.43
1:C:5028:PHE:C	1:C:5030:LYS:N	2.72	0.43
1:D:275:ARG:NH1	1:D:278:GLN:OE1	2.52	0.43
1:D:479:GLN:HA	1:D:484:LEU:HD23	2.01	0.43
1:D:1242:LEU:HD12	1:D:1242:LEU:HA	1.90	0.43
1:D:4559:PHE:O	1:D:4562:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4562:LEU:CD2	1:D:4656:LEU:HD23	2.45	0.43
2:K:45:THR:OG1	2:K:46:GLU:N	2.51	0.43
1:A:916:PRO:O	1:A:920:TYR:N	2.50	0.43
1:A:2104:ARG:HA	1:A:2107:GLN:HB3	2.00	0.43
1:B:691:GLY:HA3	1:B:712:TYR:CZ	2.54	0.43
1:B:2616:PRO:HB3	1:B:2619:LEU:HD22	2.01	0.43
1:B:4705:VAL:O	1:B:4708:THR:HG22	2.19	0.43
2:I:45:THR:OG1	2:I:46:GLU:N	2.51	0.43
1:C:2618:MET:SD	1:C:2618:MET:N	2.91	0.43
1:C:4085:ARG:H	1:C:4085:ARG:HG2	1.65	0.43
1:C:4218:ILE:HD13	1:C:4218:ILE:HA	1.62	0.43
1:D:2244:ARG:NH2	1:D:2283:ASN:OD1	2.52	0.43
1:D:4213:SER:O	1:D:4214:LYS:C	2.55	0.43
1:D:4729:GLY:O	1:D:4734:ARG:HG3	2.18	0.43
1:D:4820:VAL:CG2	1:D:4823:LEU:HG	2.49	0.43
1:D:5027:CYS:O	1:D:5028:PHE:C	2.50	0.43
1:A:3625:SER:O	1:A:3629:ARG:NH1	2.52	0.43
1:B:275:ARG:NH1	1:B:278:GLN:OE1	2.52	0.43
1:B:479:GLN:HA	1:B:484:LEU:HD23	2.01	0.43
1:B:3974:THR:HA	1:B:3977:GLN:HB2	1.99	0.43
1:C:1125:ASN:HB2	1:C:1130:GLN:H	1.84	0.43
1:C:4559:PHE:O	1:C:4562:LEU:N	2.52	0.43
1:C:4697:VAL:HG13	1:C:4698:LYS:HD3	2.00	0.43
1:D:2815:ALA:O	1:D:2819:TRP:N	2.52	0.43
1:D:4774:LYS:HG3	1:D:4775:TYR:N	2.33	0.43
1:A:162:LYS:HG3	1:D:3984:ARG:HH12	1.84	0.42
1:A:758:ARG:HG2	1:A:763:PRO:HA	2.01	0.42
1:A:1087:ARG:HH21	1:A:1222:GLY:HA3	1.83	0.42
1:A:3958:ALA:HA	1:A:3961:VAL:HG12	2.01	0.42
1:A:4705:VAL:O	1:A:4708:THR:HG22	2.19	0.42
1:B:840:VAL:HG23	1:B:1199:VAL:HB	2.00	0.42
1:B:2104:ARG:HA	1:B:2107:GLN:HB3	2.00	0.42
1:B:4844:LEU:HD12	1:B:4928:LEU:HB3	2.01	0.42
2:I:50:GLN:O	2:I:54:ASN:N	2.44	0.42
1:C:123:THR:OG1	1:C:124:SER:N	2.51	0.42
1:C:256:ALA:HB2	1:C:477:LEU:HD22	2.00	0.42
1:C:1432:THR:HG23	1:C:1572:ILE:HG22	2.00	0.42
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.52	0.42
1:C:2815:ALA:O	1:C:2819:TRP:N	2.52	0.42
1:C:4856:PHE:O	1:C:4860:ARG:HD3	2.19	0.42
1:C:4945:ASP:O	1:C:4948:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:SER:O	1:D:489:ASN:N	2.46	0.42
1:D:1125:ASN:HB2	1:D:1130:GLN:H	1.84	0.42
1:D:4562:LEU:HD21	1:D:4656:LEU:CD2	2.45	0.42
1:D:4697:VAL:HG13	1:D:4698:LYS:HD3	2.00	0.42
1:D:4716:TRP:CD1	1:D:4716:TRP:N	2.87	0.42
1:A:691:GLY:HA3	1:A:712:TYR:CZ	2.54	0.42
1:A:2529:ASP:O	1:A:2533:ALA:N	2.47	0.42
1:B:716:PHE:HE1	1:B:730:VAL:HG11	1.83	0.42
1:B:1125:ASN:HB2	1:B:1130:GLN:H	1.84	0.42
1:B:3625:SER:O	1:B:3629:ARG:NH1	2.52	0.42
1:B:4820:VAL:CG2	1:B:4823:LEU:HG	2.49	0.42
1:B:4847:VAL:HG22	1:B:4847:VAL:O	2.19	0.42
1:B:5004:THR:HG22	1:B:5007:GLU:HB2	2.01	0.42
1:C:716:PHE:HE1	1:C:730:VAL:HG11	1.83	0.42
1:C:1259:ARG:HH12	1:C:1593:PRO:HA	1.84	0.42
1:C:4847:VAL:O	1:C:4847:VAL:HG22	2.19	0.42
1:D:676:THR:OG1	1:D:677:ALA:N	2.53	0.42
1:D:3841:VAL:HG12	1:D:3926:LEU:HD22	2.00	0.42
1:A:1568:LYS:HB2	1:A:1568:LYS:HE3	1.82	0.42
1:A:4213:SER:O	1:A:4214:LYS:C	2.55	0.42
1:B:357:LEU:HA	1:B:378:LEU:HA	2.02	0.42
1:B:636:ASN:HB3	1:B:702:TRP:HZ2	1.84	0.42
1:B:671:VAL:HG23	1:B:787:VAL:HG22	2.02	0.42
1:B:1186:ASP:OD1	1:B:1186:ASP:N	2.43	0.42
1:B:2815:ALA:O	1:B:2819:TRP:N	2.52	0.42
1:B:3632:VAL:HA	1:B:3635:CYS:HB2	2.01	0.42
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.51	0.42
1:B:4085:ARG:H	1:B:4085:ARG:HG2	1.65	0.42
1:B:4209:GLN:O	1:B:4209:GLN:HG2	2.19	0.42
1:B:4244:GLU:OE1	1:B:4244:GLU:N	2.46	0.42
1:B:4698:LYS:H	1:B:4698:LYS:HG2	1.62	0.42
1:C:479:GLN:HA	1:C:484:LEU:HD23	2.01	0.42
1:C:4731:ILE:HG23	1:C:4732:PHE:CD1	2.40	0.42
1:D:1259:ARG:HH12	1:D:1593:PRO:HA	1.84	0.42
1:D:2618:MET:SD	1:D:2618:MET:N	2.92	0.42
1:D:3676:ASP:OD1	1:D:3676:ASP:N	2.52	0.42
1:D:4218:ILE:HD13	1:D:4218:ILE:HA	1.62	0.42
1:D:4979:THR:O	1:D:4984:ASN:ND2	2.53	0.42
1:A:671:VAL:HG23	1:A:787:VAL:HG22	2.02	0.42
1:A:2151:ASP:O	1:A:2154:SER:OG	2.34	0.42
1:A:4924:VAL:O	1:A:4924:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3958:ALA:HA	1:B:3961:VAL:HG12	2.02	0.42
1:B:4204:GLN:HG3	1:B:4245:MET:HE3	2.01	0.42
1:B:4914:VAL:O	1:B:4918:ILE:HG13	2.18	0.42
1:B:4995:LEU:HA	1:B:4995:LEU:HD23	1.42	0.42
1:C:3632:VAL:HA	1:C:3635:CYS:HB2	2.01	0.42
1:C:4007:SER:OG	1:C:4116:GLU:OE2	2.37	0.42
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.38	0.42
1:D:1685:LEU:HA	1:D:1688:HIS:HD2	1.84	0.42
1:D:5017:ARG:HG2	1:D:5019:TRP:CZ2	2.55	0.42
1:A:1685:LEU:HA	1:A:1688:HIS:HD2	1.84	0.42
1:A:3629:ARG:HA	1:A:3632:VAL:HG22	2.02	0.42
1:A:4697:VAL:HG13	1:A:4698:LYS:HD3	2.00	0.42
1:B:256:ALA:HB2	1:B:477:LEU:HD22	2.00	0.42
1:B:2623:LEU:HD12	1:B:2626:LEU:HD22	2.01	0.42
1:C:357:LEU:HA	1:C:378:LEU:HA	2.02	0.42
1:C:1087:ARG:HH21	1:C:1222:GLY:HA3	1.83	0.42
1:C:2810:LYS:O	1:C:2814:LYS:N	2.50	0.42
1:C:3958:ALA:HA	1:C:3961:VAL:HG12	2.01	0.42
1:C:4844:LEU:HD12	1:C:4928:LEU:HB3	2.01	0.42
1:C:4879:MET:HE2	1:C:4879:MET:HB2	1.74	0.42
1:D:544:LEU:HD23	1:D:544:LEU:HA	1.89	0.42
1:D:3625:SER:O	1:D:3629:ARG:NH1	2.52	0.42
1:D:4856:PHE:O	1:D:4860:ARG:HD3	2.19	0.42
1:D:5004:THR:HG22	1:D:5007:GLU:HB2	2.01	0.42
1:A:485:SER:O	1:A:489:ASN:N	2.45	0.42
1:A:636:ASN:HB3	1:A:702:TRP:HZ2	1.84	0.42
1:A:840:VAL:HG23	1:A:1199:VAL:HB	2.00	0.42
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.38	0.42
1:B:758:ARG:HG2	1:B:763:PRO:HA	2.01	0.42
1:B:2244:ARG:NH2	1:B:2283:ASN:OD1	2.52	0.42
1:B:4562:LEU:HD21	1:B:4656:LEU:CD2	2.45	0.42
1:B:4856:PHE:O	1:B:4860:ARG:HD3	2.19	0.42
1:D:599:VAL:HA	1:D:602:VAL:HG12	2.02	0.42
1:A:123:THR:OG1	1:A:124:SER:N	2.51	0.42
1:A:1125:ASN:HB2	1:A:1130:GLN:H	1.84	0.42
1:B:599:VAL:HA	1:B:602:VAL:HG12	2.02	0.42
1:B:2810:LYS:O	1:B:2814:LYS:N	2.50	0.42
1:B:3624:LEU:HD23	1:B:3624:LEU:HA	1.87	0.42
1:C:671:VAL:HG23	1:C:787:VAL:HG22	2.02	0.42
1:C:2575:ARG:HH12	1:C:2577:ILE:HG22	1.85	0.42
1:C:2623:LEU:HD12	1:C:2626:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4965:SER:O	1:C:4965:SER:OG	2.28	0.42
1:D:671:VAL:HG23	1:D:787:VAL:HG22	2.02	0.42
1:D:758:ARG:HG2	1:D:763:PRO:HA	2.01	0.42
1:D:3629:ARG:HA	1:D:3632:VAL:HG22	2.02	0.42
1:A:689:THR:HA	1:A:778:PHE:HE2	1.85	0.42
1:A:1203:ASN:ND2	1:A:1210:SER:OG	2.51	0.42
1:A:1746:THR:OG1	1:A:1747:LEU:N	2.53	0.42
1:A:2815:ALA:O	1:A:2819:TRP:N	2.52	0.42
1:A:4820:VAL:CG2	1:A:4823:LEU:HG	2.49	0.42
1:A:4945:ASP:O	1:A:4948:GLU:HB3	2.19	0.42
2:L:50:GLN:O	2:L:54:ASN:N	2.44	0.42
1:B:2360:LYS:HD2	1:B:2360:LYS:HA	1.82	0.42
1:C:275:ARG:NH1	1:C:278:GLN:OE1	2.52	0.42
1:C:599:VAL:HA	1:C:602:VAL:HG12	2.02	0.42
1:C:676:THR:OG1	1:C:677:ALA:N	2.52	0.42
1:C:4658:ILE:HD13	1:C:4658:ILE:HA	1.76	0.42
1:D:4995:LEU:HA	1:D:4995:LEU:HD23	1.42	0.42
1:A:275:ARG:NH1	1:A:278:GLN:OE1	2.52	0.42
1:A:599:VAL:HA	1:A:602:VAL:HG12	2.02	0.42
1:A:4559:PHE:O	1:A:4562:LEU:N	2.52	0.42
1:A:4562:LEU:HD21	1:A:4656:LEU:CB	2.47	0.42
3:H:39:SER:OG	3:H:44:LYS:O	2.36	0.42
1:B:1963:GLU:HA	1:B:1966:VAL:HG22	2.02	0.42
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.52	0.42
1:B:2575:ARG:HH12	1:B:2577:ILE:HG22	1.85	0.42
1:B:4007:SER:OG	1:B:4116:GLU:OE2	2.37	0.42
1:B:4945:ASP:O	1:B:4948:GLU:HB3	2.19	0.42
1:C:2244:ARG:NH2	1:C:2283:ASN:OD1	2.52	0.42
1:C:2616:PRO:HB3	1:C:2619:LEU:HD22	2.01	0.42
1:C:3946:GLN:O	1:C:3950:ASN:ND2	2.44	0.42
1:D:691:GLY:HA3	1:D:712:TYR:CZ	2.54	0.42
1:D:2760:GLU:O	1:D:2764:GLU:N	2.53	0.42
1:D:3958:ALA:HA	1:D:3961:VAL:HG12	2.01	0.42
1:A:4937:ILE:CG1	1:A:4938:ASP:N	2.80	0.42
1:A:5017:ARG:HG2	1:A:5019:TRP:CZ2	2.55	0.42
1:B:2116:LEU:O	1:B:2120:MET:N	2.53	0.42
1:B:3698:LEU:HD23	1:B:3698:LEU:HA	1.91	0.42
1:B:4979:THR:O	1:B:4984:ASN:ND2	2.53	0.42
1:C:392:ARG:HA	1:C:392:ARG:HD2	1.87	0.42
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.31	0.42
1:C:1466:LEU:HD23	1:C:1466:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1568:LYS:HB2	1:C:1568:LYS:HE3	1.82	0.42
1:C:2578:MET:O	1:C:2582:MET:N	2.50	0.42
1:C:5017:ARG:HG2	1:C:5019:TRP:CZ2	2.55	0.42
1:D:1963:GLU:HA	1:D:1966:VAL:HG22	2.02	0.42
1:D:4204:GLN:HG3	1:D:4245:MET:HE3	2.01	0.42
1:D:4847:VAL:O	1:D:4847:VAL:HG22	2.19	0.42
1:D:4912:TYR:O	1:D:4915:VAL:HG12	2.20	0.42
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.87	0.41
1:A:836:GLY:HA2	1:A:837:PRO:HD2	1.50	0.41
3:H:31:GLN:HA	3:H:98:ILE:HD13	2.02	0.41
1:B:3676:ASP:N	1:B:3676:ASP:OD1	2.52	0.41
1:B:3829:PHE:HB3	1:B:3913:ILE:HG13	2.02	0.41
1:B:4914:VAL:O	1:B:4914:VAL:HG22	2.20	0.41
1:C:4875:LYS:HA	1:C:4875:LYS:HD3	1.81	0.41
1:C:4876:CYS:CB	1:C:4882:CYS:HB2	2.50	0.41
3:F:31:GLN:HA	3:F:98:ILE:HD13	2.02	0.41
3:F:97:LEU:HB3	3:F:99:PHE:HE1	1.85	0.41
1:D:689:THR:HA	1:D:778:PHE:HE2	1.85	0.41
1:D:2575:ARG:HH12	1:D:2577:ILE:HG22	1.85	0.41
1:A:2575:ARG:HH12	1:A:2577:ILE:HG22	1.85	0.41
1:A:4876:CYS:CB	1:A:4882:CYS:HB2	2.50	0.41
1:B:689:THR:HA	1:B:778:PHE:HE2	1.85	0.41
1:B:2575:ARG:HA	1:B:2575:ARG:HD2	1.80	0.41
1:C:691:GLY:HA3	1:C:712:TYR:CZ	2.54	0.41
1:C:3279:SER:O	1:C:3283:ARG:N	2.52	0.41
1:C:4204:GLN:HG3	1:C:4245:MET:HE3	2.01	0.41
1:C:4840:THR:OG1	1:C:4841:VAL:N	2.53	0.41
1:C:4914:VAL:O	1:C:4914:VAL:HG22	2.20	0.41
1:D:2360:LYS:HA	1:D:2360:LYS:HD2	1.82	0.41
1:D:4562:LEU:HD21	1:D:4656:LEU:CB	2.47	0.41
1:A:2760:GLU:O	1:A:2764:GLU:N	2.53	0.41
1:A:4875:LYS:HA	1:A:4875:LYS:HD3	1.81	0.41
1:B:1685:LEU:HA	1:B:1688:HIS:HD2	1.84	0.41
1:B:3647:HIS:CE1	1:B:3648:ARG:HG3	2.56	0.41
1:B:4054:ASN:OD1	1:B:4054:ASN:N	2.47	0.41
1:B:4562:LEU:CD2	1:B:4656:LEU:HD23	2.45	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.87	0.41
1:C:651:GLY:O	1:C:658:GLN:NE2	2.53	0.41
1:C:2021:CYS:HA	1:C:2022:PRO:HD3	1.90	0.41
1:C:3629:ARG:HA	1:C:3632:VAL:HG22	2.01	0.41
1:C:3647:HIS:CE1	1:C:3648:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3829:PHE:HB3	1:C:3913:ILE:HG13	2.02	0.41
1:C:4920:PHE:HB3	1:C:4921:PHE:H	1.54	0.41
1:C:4946:GLN:C	1:C:4948:GLU:N	2.74	0.41
1:D:4054:ASN:HA	1:D:4057:MET:HG3	2.02	0.41
1:D:4876:CYS:CB	1:D:4882:CYS:HB2	2.50	0.41
1:D:4945:ASP:O	1:D:4948:GLU:HB3	2.19	0.41
3:G:31:GLN:HA	3:G:98:ILE:HD13	2.02	0.41
1:A:255:HIS:HD2	1:A:480:GLU:HG2	1.86	0.41
1:A:357:LEU:HA	1:A:378:LEU:HA	2.02	0.41
1:A:4979:THR:O	1:A:4984:ASN:ND2	2.53	0.41
1:B:569:ILE:HD12	1:B:569:ILE:HA	1.90	0.41
1:C:255:HIS:HD2	1:C:480:GLU:HG2	1.86	0.41
1:C:1963:GLU:HA	1:C:1966:VAL:HG22	2.02	0.41
1:C:2760:GLU:O	1:C:2764:GLU:N	2.53	0.41
1:C:3917:ILE:HD13	1:C:3917:ILE:HA	1.95	0.41
1:C:4209:GLN:O	1:C:4209:GLN:HG2	2.18	0.41
1:C:4943:LEU:HD13	1:C:4943:LEU:HA	1.89	0.41
1:D:1457:TYR:CE1	1:D:1459:GLN:HB2	2.56	0.41
1:D:4946:GLN:C	1:D:4948:GLU:N	2.74	0.41
1:A:309:THR:O	1:A:313:SER:OG	2.31	0.41
1:A:551:LEU:HD12	1:A:589:LEU:HD22	2.02	0.41
1:A:1963:GLU:HA	1:A:1966:VAL:HG22	2.02	0.41
1:A:3829:PHE:HB3	1:A:3913:ILE:HG13	2.02	0.41
1:A:5004:THR:HG22	1:A:5007:GLU:HB2	2.01	0.41
1:B:644:ILE:HD11	1:B:1628:VAL:HG11	2.03	0.41
1:B:3984:ARG:HH12	1:C:162:LYS:HG3	1.86	0.41
3:E:31:GLN:HA	3:E:98:ILE:HD13	2.02	0.41
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.38	0.41
1:C:1749:PRO:HA	1:C:1750:PRO:HD3	1.88	0.41
1:C:3625:SER:O	1:C:3629:ARG:NH1	2.52	0.41
1:C:4979:THR:O	1:C:4984:ASN:ND2	2.53	0.41
1:D:2623:LEU:HD12	1:D:2626:LEU:HD22	2.01	0.41
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.52	0.41
1:A:4209:GLN:O	1:A:4209:GLN:HG2	2.19	0.41
1:A:4563:LYS:CA	1:A:4657:ILE:HD11	2.43	0.41
1:A:4912:TYR:O	1:A:4915:VAL:HG12	2.20	0.41
1:A:4914:VAL:O	1:A:4914:VAL:HG22	2.20	0.41
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.38	0.41
1:B:1203:ASN:ND2	1:B:1210:SER:OG	2.51	0.41
1:B:2623:LEU:HD12	1:B:2623:LEU:HA	1.94	0.41
1:B:4840:THR:OG1	1:B:4841:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4876:CYS:CB	1:B:4882:CYS:HB2	2.50	0.41
1:B:5017:ARG:HG2	1:B:5019:TRP:CZ2	2.55	0.41
1:C:644:ILE:HD11	1:C:1628:VAL:HG11	2.03	0.41
1:C:1969:LEU:HD11	1:C:2023:LEU:HD11	2.03	0.41
1:D:4844:LEU:HD12	1:D:4928:LEU:HB3	2.01	0.41
1:A:644:ILE:HD11	1:A:1628:VAL:HG11	2.03	0.41
1:A:1457:TYR:CE1	1:A:1459:GLN:HB2	2.56	0.41
1:A:2113:SER:HA	1:A:2114:PRO:HD3	1.93	0.41
1:A:4937:ILE:HG23	1:A:4937:ILE:H	1.63	0.41
1:B:255:HIS:HD2	1:B:480:GLU:HG2	1.86	0.41
1:B:683:ARG:NH1	1:B:707:VAL:O	2.49	0.41
1:B:1259:ARG:HH12	1:B:1593:PRO:HA	1.84	0.41
1:B:1746:THR:OG1	1:B:1747:LEU:N	2.53	0.41
1:C:569:ILE:HD12	1:C:569:ILE:HA	1.90	0.41
1:C:758:ARG:HG2	1:C:763:PRO:HA	2.01	0.41
1:C:3372:VAL:O	1:C:3376:GLU:N	2.48	0.41
1:C:3676:ASP:N	1:C:3676:ASP:OD1	2.52	0.41
1:D:2474:LEU:HD23	1:D:2474:LEU:HA	1.92	0.41
2:K:3:ASP:OD1	2:K:3:ASP:N	2.45	0.41
1:A:2623:LEU:HD12	1:A:2626:LEU:HD22	2.01	0.41
1:A:4646:LEU:HD12	1:A:4646:LEU:HA	1.73	0.41
1:A:4716:TRP:CD1	1:A:4716:TRP:N	2.87	0.41
1:B:581:ASN:OD1	1:B:581:ASN:N	2.52	0.41
1:B:1568:LYS:HB2	1:B:1568:LYS:HE3	1.82	0.41
1:B:1804:LEU:HD23	1:B:1804:LEU:HA	1.91	0.41
1:B:2118:ARG:NH2	1:B:3719:ASP:OD1	2.48	0.41
1:B:3629:ARG:HA	1:B:3632:VAL:HG22	2.02	0.41
3:E:97:LEU:HB3	3:E:99:PHE:HE1	1.85	0.41
1:C:4573:ILE:HG21	1:C:4573:ILE:HD13	1.81	0.41
1:D:551:LEU:HD12	1:D:589:LEU:HD22	2.02	0.41
1:D:4007:SER:OG	1:D:4116:GLU:OE2	2.37	0.41
3:G:97:LEU:HB3	3:G:99:PHE:HE1	1.85	0.41
1:A:852:VAL:HA	1:A:853:PRO:HD3	1.94	0.41
1:A:1475:THR:HA	1:A:1486:SER:HA	2.03	0.41
1:A:1863:LEU:HA	1:A:1866:ILE:HG22	2.03	0.41
1:A:3647:HIS:CE1	1:A:3648:ARG:HG3	2.56	0.41
1:A:4658:ILE:HD13	1:A:4658:ILE:HA	1.76	0.41
1:A:4879:MET:HG2	1:D:4578:LEU:HD12	2.01	0.41
1:A:4917:ASP:C	1:A:4919:THR:H	2.23	0.41
1:A:4925:ILE:HD13	1:A:4925:ILE:HG21	1.71	0.41
1:A:5028:PHE:C	1:A:5030:LYS:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LEU:HB3	1:B:1688:HIS:CE1	2.56	0.41
1:B:1595:LEU:HD12	1:B:1595:LEU:HA	1.92	0.41
1:B:1778:SER:HA	1:B:1779:PRO:HD3	1.94	0.41
1:B:3804:ILE:HD12	1:B:3804:ILE:HA	1.84	0.41
1:B:3917:ILE:HD13	1:B:3917:ILE:HA	1.95	0.41
1:B:4911:LEU:O	1:B:4911:LEU:HG	2.20	0.41
1:C:626:LEU:HB3	1:C:1688:HIS:CE1	2.56	0.41
1:C:689:THR:HA	1:C:778:PHE:HE2	1.85	0.41
1:C:1177:THR:OG1	1:C:1179:PHE:O	2.34	0.41
1:C:4917:ASP:C	1:C:4919:THR:H	2.23	0.41
1:D:852:VAL:HA	1:D:853:PRO:HD3	1.94	0.41
1:D:3279:SER:O	1:D:3283:ARG:N	2.52	0.41
1:D:3624:LEU:HD23	1:D:3624:LEU:HA	1.87	0.41
1:D:3667:HIS:NE2	1:D:3669:PHE:HB3	2.36	0.41
1:D:3829:PHE:HB3	1:D:3913:ILE:HG13	2.02	0.41
1:D:4914:VAL:O	1:D:4914:VAL:HG22	2.20	0.41
1:D:4917:ASP:C	1:D:4919:THR:H	2.23	0.41
1:A:2531:ARG:HH12	1:A:2582:MET:HA	1.86	0.41
1:A:4078:GLN:HA	1:A:4081:VAL:HG12	2.02	0.41
1:B:392:ARG:HA	1:B:392:ARG:HD2	1.87	0.41
1:B:1863:LEU:HA	1:B:1866:ILE:HG22	2.03	0.41
1:B:2187:ASN:HB2	2:I:14:LYS:HE2	2.03	0.41
1:B:4157:ASP:HA	1:B:4158:PRO:HD3	1.95	0.41
1:B:4875:LYS:HD3	1:B:4875:LYS:HA	1.81	0.41
3:E:26:TYR:OH	3:E:37:ASP:OD2	2.32	0.41
1:C:4952:GLU:O	1:C:4953:ASP:C	2.60	0.41
3:F:57:LYS:HA	3:F:60:GLU:HB3	2.03	0.41
1:D:357:LEU:HA	1:D:378:LEU:HA	2.02	0.41
1:D:3647:HIS:CE1	1:D:3648:ARG:HG3	2.56	0.41
1:D:3768:SER:HA	1:D:3771:HIS:CE1	2.56	0.41
1:D:4646:LEU:HD12	1:D:4646:LEU:HA	1.73	0.41
1:A:3768:SER:HA	1:A:3771:HIS:CE1	2.56	0.40
1:A:3984:ARG:HH12	1:B:162:LYS:HG3	1.86	0.40
1:A:4844:LEU:HD12	1:A:4928:LEU:HB3	2.01	0.40
1:B:1969:LEU:HD11	1:B:2023:LEU:HD11	2.03	0.40
1:B:2529:ASP:O	1:B:2533:ALA:N	2.47	0.40
1:B:2531:ARG:HH12	1:B:2582:MET:HA	1.86	0.40
1:B:4912:TYR:O	1:B:4915:VAL:HG12	2.20	0.40
1:C:1457:TYR:CE1	1:C:1459:GLN:HB2	2.56	0.40
1:C:1475:THR:HA	1:C:1486:SER:HA	2.03	0.40
1:C:2474:LEU:HD23	1:C:2474:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2575:ARG:HD2	1:C:2575:ARG:HA	1.80	0.40
1:C:3667:HIS:NE2	1:C:3669:PHE:HB3	2.36	0.40
1:C:3768:SER:HA	1:C:3771:HIS:CE1	2.57	0.40
1:D:2021:CYS:HA	1:D:2022:PRO:HD3	1.90	0.40
1:D:2531:ARG:HH12	1:D:2582:MET:HA	1.86	0.40
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.43	0.40
1:A:1259:ARG:HH12	1:A:1593:PRO:HA	1.84	0.40
1:A:4054:ASN:HA	1:A:4057:MET:HG3	2.02	0.40
1:A:4190:ILE:HD12	1:A:4191:GLU:N	2.36	0.40
1:B:1242:LEU:HD12	1:B:1242:LEU:HA	1.90	0.40
1:B:4054:ASN:HA	1:B:4057:MET:HG3	2.02	0.40
1:B:4655:PHE:O	1:B:4659:ILE:HG12	2.22	0.40
1:B:4920:PHE:HB3	1:B:4921:PHE:H	1.54	0.40
3:E:57:LYS:HA	3:E:60:GLU:HB3	2.03	0.40
1:C:4054:ASN:OD1	1:C:4054:ASN:N	2.47	0.40
1:C:4078:GLN:HA	1:C:4081:VAL:HG12	2.02	0.40
1:C:4912:TYR:O	1:C:4915:VAL:HG12	2.20	0.40
1:D:644:ILE:HD11	1:D:1628:VAL:HG11	2.03	0.40
1:D:4911:LEU:O	1:D:4914:VAL:HG12	2.21	0.40
1:D:4937:ILE:CG1	1:D:4938:ASP:N	2.81	0.40
2:K:50:GLN:O	2:K:54:ASN:N	2.44	0.40
1:A:392:ARG:HA	1:A:392:ARG:HD2	1.87	0.40
1:A:2575:ARG:HA	1:A:2575:ARG:HD2	1.80	0.40
1:A:2586:VAL:HA	1:A:2589:LEU:HB2	2.03	0.40
3:H:97:LEU:HB3	3:H:99:PHE:HE1	1.85	0.40
1:B:676:THR:OG1	1:B:677:ALA:N	2.52	0.40
1:B:1457:TYR:CE1	1:B:1459:GLN:HB2	2.56	0.40
1:B:4946:GLN:C	1:B:4948:GLU:N	2.74	0.40
1:C:1595:LEU:HD12	1:C:1595:LEU:HA	1.92	0.40
1:C:1863:LEU:HA	1:C:1866:ILE:HG22	2.03	0.40
1:C:4211:LYS:O	1:C:4212:GLU:C	2.59	0.40
1:C:4655:PHE:O	1:C:4659:ILE:HG12	2.22	0.40
1:C:4669:VAL:HG22	1:C:4669:VAL:O	2.22	0.40
1:D:626:LEU:HB3	1:D:1688:HIS:CE1	2.56	0.40
1:D:1259:ARG:HH22	1:D:1593:PRO:HA	1.87	0.40
1:D:2118:ARG:NH2	1:D:3719:ASP:OD1	2.48	0.40
1:D:4047:MET:O	1:D:4051:SER:OG	2.35	0.40
1:D:4632:LEU:HA	1:D:4632:LEU:HD12	1.89	0.40
1:A:257:ARG:H	1:A:257:ARG:HG2	1.70	0.40
1:A:2360:LYS:HD2	1:A:2360:LYS:HA	1.82	0.40
1:B:551:LEU:HD12	1:B:589:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4911:LEU:O	1:B:4914:VAL:HG12	2.21	0.40
1:B:5002:GLU:OE1	1:B:5002:GLU:N	2.55	0.40
1:C:1242:LEU:HD12	1:C:1242:LEU:HA	1.90	0.40
1:C:3892:CYS:HB3	1:C:3900:GLN:HE21	1.87	0.40
1:C:5004:THR:HG22	1:C:5007:GLU:HB2	2.01	0.40
1:D:4911:LEU:O	1:D:4911:LEU:HG	2.20	0.40
1:A:676:THR:OG1	1:A:677:ALA:N	2.52	0.40
1:A:3676:ASP:N	1:A:3676:ASP:OD1	2.52	0.40
1:A:4655:PHE:O	1:A:4659:ILE:HG12	2.22	0.40
1:B:3892:CYS:HB3	1:B:3900:GLN:HE21	1.87	0.40
1:B:4952:GLU:O	1:B:4953:ASP:C	2.59	0.40
1:C:670:GLU:HB3	1:C:788:LYS:HB3	2.03	0.40
1:C:2559:LEU:HD23	1:C:2559:LEU:HA	1.91	0.40
1:C:4054:ASN:HA	1:C:4057:MET:HG3	2.02	0.40
1:C:4673:ARG:HE	1:C:4782:VAL:CG2	2.34	0.40
1:C:4911:LEU:O	1:C:4914:VAL:HG12	2.21	0.40
1:D:2586:VAL:HA	1:D:2589:LEU:HB2	2.03	0.40
1:D:4078:GLN:HA	1:D:4081:VAL:HG12	2.02	0.40
1:D:4669:VAL:O	1:D:4669:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3800/5037 (75%)	3436 (90%)	337 (9%)	27 (1%)	19 53
1	B	3800/5037 (75%)	3439 (90%)	335 (9%)	26 (1%)	19 53
1	C	3800/5037 (75%)	3437 (90%)	336 (9%)	27 (1%)	19 53
1	D	3800/5037 (75%)	3436 (90%)	337 (9%)	27 (1%)	19 53
2	I	133/148 (90%)	124 (93%)	9 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	133/148 (90%)	124 (93%)	9 (7%)	0	100	100
2	K	133/148 (90%)	124 (93%)	9 (7%)	0	100	100
2	L	133/148 (90%)	124 (93%)	9 (7%)	0	100	100
3	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	16152/21168 (76%)	14636 (91%)	1409 (9%)	107 (1%)	21	53

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	837	PRO
1	A	3003	LEU
1	A	3004	PRO
1	A	3061	ALA
1	A	3350	ARG
1	A	4717	ASP
1	A	4718	LYS
1	A	4918	ILE
1	A	4953	ASP
1	A	4959	PHE
1	B	837	PRO
1	B	3003	LEU
1	B	3004	PRO
1	B	3061	ALA
1	B	3350	ARG
1	B	4717	ASP
1	B	4718	LYS
1	B	4918	ILE
1	B	4953	ASP
1	B	4959	PHE
1	C	837	PRO
1	C	3003	LEU
1	C	3004	PRO
1	C	3061	ALA
1	C	3350	ARG
1	C	4717	ASP
1	C	4718	LYS
1	C	4918	ILE

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Mol	Chain	Res	Type
1	C	4953	ASP
1	C	4959	PHE
1	D	837	PRO
1	D	3003	LEU
1	D	3004	PRO
1	D	3061	ALA
1	D	3350	ARG
1	D	4717	ASP
1	D	4718	LYS
1	D	4918	ILE
1	D	4953	ASP
1	D	4959	PHE
1	A	4958	CYS
1	B	4958	CYS
1	C	4958	CYS
1	D	4958	CYS
1	A	3041	SER
1	A	3306	ALA
1	A	3317	GLY
1	A	4951	LYS
1	B	3041	SER
1	B	3306	ALA
1	B	3317	GLY
1	B	4951	LYS
1	C	3041	SER
1	C	3306	ALA
1	C	3317	GLY
1	C	4951	LYS
1	C	5029	ARG
1	D	3041	SER
1	D	3306	ALA
1	D	3317	GLY
1	D	4951	LYS
1	D	5029	ARG
1	A	3050	VAL
1	A	4947	GLN
1	A	4952	GLU
1	A	5029	ARG
1	B	3050	VAL
1	B	4947	GLN
1	B	4952	GLU
1	C	3050	VAL

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Mol	Chain	Res	Type
1	C	4947	GLN
1	C	4952	GLU
1	D	3050	VAL
1	D	4947	GLN
1	D	4952	GLU
1	A	3187	ARG
1	A	3294	PRO
1	A	3367	LYS
1	B	3187	ARG
1	B	3294	PRO
1	B	3367	LYS
1	C	3187	ARG
1	C	3294	PRO
1	C	3367	LYS
1	D	3187	ARG
1	D	3294	PRO
1	D	3367	LYS
1	A	3416	VAL
1	B	3416	VAL
1	C	3416	VAL
1	D	3416	VAL
1	A	834	PRO
1	A	3410	PRO
1	A	4936	ILE
1	B	834	PRO
1	B	3410	PRO
1	B	4936	ILE
1	C	834	PRO
1	C	3410	PRO
1	C	4936	ILE
1	D	834	PRO
1	D	3410	PRO
1	D	4936	ILE
1	A	3207	GLU
1	B	3207	GLU
1	C	3207	GLU
1	D	3207	GLU

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	2448/4276 (57%)	2413 (99%)	35 (1%)	62	79
1	B	2448/4276 (57%)	2414 (99%)	34 (1%)	62	79
1	C	2448/4276 (57%)	2414 (99%)	34 (1%)	62	79
1	D	2448/4276 (57%)	2413 (99%)	35 (1%)	62	79
2	I	104/122 (85%)	103 (99%)	1 (1%)	73	84
2	J	104/122 (85%)	103 (99%)	1 (1%)	73	84
2	K	104/122 (85%)	103 (99%)	1 (1%)	73	84
2	L	104/122 (85%)	103 (99%)	1 (1%)	73	84
3	E	84/88 (96%)	83 (99%)	1 (1%)	67	82
3	F	84/88 (96%)	83 (99%)	1 (1%)	67	82
3	G	84/88 (96%)	83 (99%)	1 (1%)	67	82
3	H	84/88 (96%)	83 (99%)	1 (1%)	67	82
All	All	10544/17944 (59%)	10398 (99%)	146 (1%)	62	79

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	266	ARG
1	A	317	ARG
1	A	830	ARG
1	A	838	HIS
1	A	1025	ARG
1	A	1232	ARG
1	A	1275	ARG
1	A	1573	MET
1	A	1982	ARG
1	A	1996	ARG
1	A	2615	ARG
1	A	2624	ARG
1	A	2625	ARG
1	A	3694	LYS
1	A	3715	LYS
1	A	4191	GLU
1	A	4210	VAL

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Mol	Chain	Res	Type
1	A	4213	SER
1	A	4218	ILE
1	A	4231	MET
1	A	4580	TYR
1	A	4684	ASP
1	A	4720	VAL
1	A	4913	ARG
1	A	4917	ASP
1	A	4918	ILE
1	A	4937	ILE
1	A	4938	ASP
1	A	4947	GLN
1	A	4948	GLU
1	A	4949	GLN
1	A	4952	GLU
1	A	5027	CYS
1	A	5028	PHE
2	L	127	ARG
3	H	35	LYS
1	B	99	ARG
1	B	266	ARG
1	B	317	ARG
1	B	830	ARG
1	B	838	HIS
1	B	1025	ARG
1	B	1232	ARG
1	B	1275	ARG
1	B	1573	MET
1	B	1982	ARG
1	B	1996	ARG
1	B	2615	ARG
1	B	2624	ARG
1	B	2625	ARG
1	B	3694	LYS
1	B	3715	LYS
1	B	4190	ILE
1	B	4210	VAL
1	B	4213	SER
1	B	4218	ILE
1	B	4231	MET
1	B	4580	TYR
1	B	4684	ASP

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Mol	Chain	Res	Type
1	B	4720	VAL
1	B	4913	ARG
1	B	4917	ASP
1	B	4918	ILE
1	B	4937	ILE
1	B	4938	ASP
1	B	4947	GLN
1	B	4948	GLU
1	B	4949	GLN
1	B	4952	GLU
1	B	5027	CYS
2	I	127	ARG
3	E	35	LYS
1	C	99	ARG
1	C	266	ARG
1	C	317	ARG
1	C	830	ARG
1	C	838	HIS
1	C	1025	ARG
1	C	1232	ARG
1	C	1275	ARG
1	C	1573	MET
1	C	1982	ARG
1	C	1996	ARG
1	C	2615	ARG
1	C	2624	ARG
1	C	2625	ARG
1	C	3694	LYS
1	C	3715	LYS
1	C	4210	VAL
1	C	4213	SER
1	C	4218	ILE
1	C	4231	MET
1	C	4580	TYR
1	C	4684	ASP
1	C	4720	VAL
1	C	4913	ARG
1	C	4917	ASP
1	C	4918	ILE
1	C	4937	ILE
1	C	4938	ASP
1	C	4947	GLN

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Mol	Chain	Res	Type
1	C	4948	GLU
1	C	4949	GLN
1	C	4952	GLU
1	C	5027	CYS
1	C	5028	PHE
2	J	127	ARG
3	F	35	LYS
1	D	99	ARG
1	D	266	ARG
1	D	317	ARG
1	D	830	ARG
1	D	838	HIS
1	D	1025	ARG
1	D	1232	ARG
1	D	1275	ARG
1	D	1573	MET
1	D	1982	ARG
1	D	1996	ARG
1	D	2615	ARG
1	D	2624	ARG
1	D	2625	ARG
1	D	3694	LYS
1	D	3715	LYS
1	D	4191	GLU
1	D	4210	VAL
1	D	4213	SER
1	D	4218	ILE
1	D	4231	MET
1	D	4580	TYR
1	D	4684	ASP
1	D	4720	VAL
1	D	4913	ARG
1	D	4917	ASP
1	D	4918	ILE
1	D	4937	ILE
1	D	4938	ASP
1	D	4947	GLN
1	D	4948	GLU
1	D	4949	GLN
1	D	4952	GLU
1	D	5027	CYS
1	D	5028	PHE

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Mol	Chain	Res	Type
2	K	127	ARG
3	G	35	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	113	HIS
1	A	582	HIS
1	A	634	GLN
1	A	720	HIS
1	A	765	GLN
1	A	921	ASN
1	A	1011	GLN
1	A	1144	GLN
1	A	1203	ASN
1	A	1299	GLN
1	A	1460	HIS
1	A	1563	GLN
1	A	1569	GLN
1	A	1688	HIS
1	A	1928	GLN
1	A	1970	GLN
1	A	2127	GLN
1	A	2188	ASN
1	A	2213	ASN
1	A	2260	ASN
1	A	2349	ASN
1	A	2417	HIS
1	A	3766	GLN
1	A	3781	GLN
1	A	3813	GLN
1	A	3895	HIS
1	A	3901	ASN
1	A	4162	ASN
1	A	4204	GLN
1	A	4574	ASN
1	A	4650	HIS
1	A	4803	HIS
1	A	4832	HIS
1	A	4933	GLN
1	A	4984	ASN

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Mol	Chain	Res	Type
2	L	54	ASN
3	H	31	GLN
1	B	105	HIS
1	B	113	HIS
1	B	582	HIS
1	B	634	GLN
1	B	720	HIS
1	B	765	GLN
1	B	921	ASN
1	B	1011	GLN
1	B	1144	GLN
1	B	1203	ASN
1	B	1299	GLN
1	B	1460	HIS
1	B	1563	GLN
1	B	1569	GLN
1	B	1688	HIS
1	B	1928	GLN
1	B	1970	GLN
1	B	2127	GLN
1	B	2188	ASN
1	B	2213	ASN
1	B	2260	ASN
1	B	2349	ASN
1	B	2417	HIS
1	B	3766	GLN
1	B	3781	GLN
1	B	3813	GLN
1	B	3895	HIS
1	B	3901	ASN
1	B	4162	ASN
1	B	4204	GLN
1	B	4574	ASN
1	B	4650	HIS
1	B	4803	HIS
1	B	4933	GLN
1	B	4984	ASN
2	I	54	ASN
3	E	31	GLN
1	C	105	HIS
1	C	113	HIS
1	C	582	HIS

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Mol	Chain	Res	Type
1	C	634	GLN
1	C	720	HIS
1	C	765	GLN
1	C	1011	GLN
1	C	1144	GLN
1	C	1203	ASN
1	C	1299	GLN
1	C	1460	HIS
1	C	1563	GLN
1	C	1569	GLN
1	C	1688	HIS
1	C	1928	GLN
1	C	1970	GLN
1	C	2127	GLN
1	C	2188	ASN
1	C	2213	ASN
1	C	2260	ASN
1	C	2349	ASN
1	C	2417	HIS
1	C	3766	GLN
1	C	3781	GLN
1	C	3813	GLN
1	C	3895	HIS
1	C	3901	ASN
1	C	4162	ASN
1	C	4204	GLN
1	C	4574	ASN
1	C	4650	HIS
1	C	4803	HIS
1	C	4933	GLN
1	C	4984	ASN
2	J	54	ASN
3	F	31	GLN
1	D	105	HIS
1	D	113	HIS
1	D	582	HIS
1	D	634	GLN
1	D	720	HIS
1	D	765	GLN
1	D	1011	GLN
1	D	1144	GLN
1	D	1203	ASN

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Mol	Chain	Res	Type
1	D	1299	GLN
1	D	1460	HIS
1	D	1563	GLN
1	D	1569	GLN
1	D	1688	HIS
1	D	1928	GLN
1	D	1970	GLN
1	D	2127	GLN
1	D	2188	ASN
1	D	2213	ASN
1	D	2260	ASN
1	D	2349	ASN
1	D	2417	HIS
1	D	3766	GLN
1	D	3781	GLN
1	D	3813	GLN
1	D	3895	HIS
1	D	3901	ASN
1	D	4162	ASN
1	D	4204	GLN
1	D	4574	ASN
1	D	4650	HIS
1	D	4803	HIS
1	D	4933	GLN
1	D	4984	ASN
2	K	54	ASN
3	G	31	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	ATP	B	5103	-	26,33,33	3.47	15 (57%)	31,52,52	2.22	11 (35%)
7	CFF	A	5104	-	8,15,15	3.59	5 (62%)	8,23,23	3.29	6 (75%)
6	ATP	C	5103	-	26,33,33	3.47	15 (57%)	31,52,52	2.21	11 (35%)
7	CFF	C	5104	-	8,15,15	3.59	5 (62%)	8,23,23	3.32	6 (75%)
7	CFF	B	5104	-	8,15,15	3.58	5 (62%)	8,23,23	3.31	6 (75%)
7	CFF	D	5104	-	8,15,15	3.58	5 (62%)	8,23,23	3.29	6 (75%)
6	ATP	A	5103	-	26,33,33	3.47	15 (57%)	31,52,52	2.21	11 (35%)
6	ATP	D	5103	-	26,33,33	3.46	15 (57%)	31,52,52	2.22	11 (35%)

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	ATP	B	5103	-	-	4/18/38/38	0/3/3/3
7	CFF	A	5104	-	-	-	0/2/2/2
6	ATP	C	5103	-	-	4/18/38/38	0/3/3/3
7	CFF	C	5104	-	-	-	0/2/2/2
7	CFF	B	5104	-	-	-	0/2/2/2
7	CFF	D	5104	-	-	-	0/2/2/2
6	ATP	A	5103	-	-	4/18/38/38	0/3/3/3
6	ATP	D	5103	-	-	4/18/38/38	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5103	ATP	O4'-C1'	12.33	1.58	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	ATP	O4'-C1'	12.28	1.58	1.41
6	B	5103	ATP	O4'-C1'	12.28	1.58	1.41
6	D	5103	ATP	O4'-C1'	12.25	1.58	1.41
7	C	5104	CFF	O13-C6	6.52	1.40	1.24
7	A	5104	CFF	O13-C6	6.51	1.40	1.24
7	B	5104	CFF	O13-C6	6.51	1.40	1.24
7	D	5104	CFF	O13-C6	6.51	1.40	1.24
7	A	5104	CFF	C5-C6	6.17	1.51	1.41
7	B	5104	CFF	C5-C6	6.17	1.51	1.41
7	C	5104	CFF	C5-C6	6.17	1.51	1.41
7	D	5104	CFF	C5-C6	6.13	1.51	1.41
6	A	5103	ATP	O4'-C4'	5.77	1.57	1.45
6	D	5103	ATP	O4'-C4'	5.77	1.57	1.45
6	B	5103	ATP	O4'-C4'	5.75	1.57	1.45
6	C	5103	ATP	O4'-C4'	5.75	1.57	1.45
6	A	5103	ATP	C2'-C3'	-4.88	1.40	1.53
6	B	5103	ATP	C2'-C3'	-4.88	1.40	1.53
6	D	5103	ATP	C2'-C3'	-4.87	1.40	1.53
6	C	5103	ATP	C2'-C3'	-4.86	1.40	1.53
6	A	5103	ATP	C2'-C1'	-4.85	1.46	1.53
6	B	5103	ATP	C2'-C1'	-4.85	1.46	1.53
6	C	5103	ATP	C2'-C1'	-4.85	1.46	1.53
6	D	5103	ATP	C2'-C1'	-4.85	1.46	1.53
6	A	5103	ATP	C3'-C4'	-3.11	1.45	1.53
6	D	5103	ATP	C3'-C4'	-3.11	1.45	1.53
6	B	5103	ATP	C3'-C4'	-3.10	1.45	1.53
6	C	5103	ATP	C3'-C4'	-3.10	1.45	1.53
6	C	5103	ATP	O2'-C2'	2.58	1.49	1.43
6	B	5103	ATP	O2'-C2'	2.57	1.49	1.43
6	D	5103	ATP	O2'-C2'	2.57	1.49	1.43
6	A	5103	ATP	O2'-C2'	2.57	1.49	1.43
6	B	5103	ATP	C6-N6	2.52	1.43	1.34
6	A	5103	ATP	C6-N6	2.50	1.43	1.34
6	C	5103	ATP	C6-N6	2.50	1.43	1.34
6	D	5103	ATP	C6-N6	2.50	1.43	1.34
6	A	5103	ATP	C4-N3	-2.44	1.32	1.35
6	B	5103	ATP	C4-N3	-2.44	1.32	1.35
6	C	5103	ATP	C4-N3	-2.44	1.32	1.35
6	D	5103	ATP	C4-N3	-2.44	1.32	1.35
6	A	5103	ATP	C2-N1	-2.39	1.29	1.33
6	B	5103	ATP	C2-N1	-2.38	1.29	1.33
6	D	5103	ATP	C2-N1	-2.38	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	ATP	O3'-C3'	2.38	1.48	1.43
6	D	5103	ATP	O3'-C3'	2.38	1.48	1.43
6	C	5103	ATP	O3'-C3'	2.37	1.48	1.43
6	B	5103	ATP	O3'-C3'	2.36	1.48	1.43
6	C	5103	ATP	C2-N1	-2.35	1.29	1.33
7	B	5104	CFF	C5-C4	2.34	1.42	1.39
7	C	5104	CFF	C5-C4	2.34	1.42	1.39
7	D	5104	CFF	C8-N9	2.33	1.38	1.34
7	A	5104	CFF	C8-N9	2.33	1.38	1.34
7	C	5104	CFF	C8-N9	2.33	1.38	1.34
7	B	5104	CFF	C6-N1	2.32	1.41	1.38
7	C	5104	CFF	C6-N1	2.31	1.41	1.38
7	D	5104	CFF	C6-N1	2.31	1.41	1.38
7	A	5104	CFF	C6-N1	2.31	1.41	1.38
7	A	5104	CFF	C5-C4	2.31	1.42	1.39
7	D	5104	CFF	C5-C4	2.30	1.42	1.39
7	B	5104	CFF	C8-N9	2.30	1.38	1.34
6	A	5103	ATP	PG-O3G	-2.23	1.46	1.54
6	B	5103	ATP	PG-O3G	-2.23	1.46	1.54
6	C	5103	ATP	PG-O3G	-2.23	1.46	1.54
6	D	5103	ATP	PG-O3G	-2.23	1.46	1.54
6	A	5103	ATP	PG-O2G	-2.21	1.46	1.54
6	B	5103	ATP	PG-O2G	-2.21	1.46	1.54
6	C	5103	ATP	PG-O2G	-2.21	1.46	1.54
6	D	5103	ATP	PG-O2G	-2.21	1.46	1.54
6	B	5103	ATP	C5-N7	2.06	1.47	1.39
6	D	5103	ATP	C5-N7	2.06	1.47	1.39
6	A	5103	ATP	C5-N7	2.05	1.47	1.39
6	C	5103	ATP	C5-N7	2.05	1.47	1.39
6	C	5103	ATP	PA-O2A	-2.02	1.45	1.55
6	A	5103	ATP	PA-O2A	-2.02	1.45	1.55
6	B	5103	ATP	PA-O2A	-2.02	1.45	1.55
6	D	5103	ATP	PA-O2A	-2.02	1.45	1.55
6	A	5103	ATP	PB-O2B	-2.00	1.45	1.55
6	B	5103	ATP	PB-O2B	-2.00	1.45	1.55
6	C	5103	ATP	PB-O2B	-2.00	1.45	1.55
6	D	5103	ATP	PB-O2B	-2.00	1.45	1.55

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	5104	CFF	C4-C5-C6	-7.42	115.20	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	5104	CFF	C4-C5-C6	-7.42	115.20	119.96
7	A	5104	CFF	C4-C5-C6	-7.35	115.24	119.96
7	D	5104	CFF	C4-C5-C6	-7.32	115.26	119.96
6	B	5103	ATP	C4-C5-N7	-4.88	104.32	109.40
6	D	5103	ATP	C4-C5-N7	-4.88	104.32	109.40
6	A	5103	ATP	C4-C5-N7	-4.87	104.32	109.40
6	C	5103	ATP	C4-C5-N7	-4.86	104.34	109.40
6	B	5103	ATP	N3-C2-N1	-4.42	121.76	128.68
6	D	5103	ATP	N3-C2-N1	-4.42	121.76	128.68
6	C	5103	ATP	N3-C2-N1	-4.41	121.78	128.68
6	A	5103	ATP	N3-C2-N1	-4.39	121.81	128.68
6	D	5103	ATP	C3'-C2'-C1'	4.35	107.52	100.98
6	A	5103	ATP	C3'-C2'-C1'	4.33	107.50	100.98
6	B	5103	ATP	C3'-C2'-C1'	4.33	107.50	100.98
6	C	5103	ATP	C3'-C2'-C1'	4.31	107.47	100.98
6	C	5103	ATP	PA-O3A-PB	-4.05	118.94	132.83
6	B	5103	ATP	PA-O3A-PB	-4.04	118.95	132.83
6	A	5103	ATP	PA-O3A-PB	-4.04	118.95	132.83
6	D	5103	ATP	PA-O3A-PB	-4.04	118.95	132.83
6	A	5103	ATP	PB-O3B-PG	-4.02	119.05	132.83
6	B	5103	ATP	PB-O3B-PG	-4.01	119.06	132.83
6	C	5103	ATP	PB-O3B-PG	-4.01	119.06	132.83
6	D	5103	ATP	PB-O3B-PG	-4.00	119.09	132.83
6	C	5103	ATP	C1'-N9-C4	-3.24	120.94	126.64
6	A	5103	ATP	C1'-N9-C4	-3.23	120.97	126.64
6	D	5103	ATP	C1'-N9-C4	-3.22	120.98	126.64
6	B	5103	ATP	C1'-N9-C4	-3.20	121.02	126.64
7	C	5104	CFF	C12-N3-C4	-2.79	114.30	118.25
7	A	5104	CFF	C12-N3-C4	-2.76	114.34	118.25
7	B	5104	CFF	C12-N3-C4	-2.76	114.34	118.25
7	D	5104	CFF	C12-N3-C4	-2.76	114.34	118.25
6	B	5103	ATP	O2G-PG-O3B	2.76	113.88	104.64
6	C	5103	ATP	O2G-PG-O3B	2.76	113.88	104.64
7	A	5104	CFF	C14-N7-C8	-2.75	112.19	125.43
7	D	5104	CFF	C14-N7-C8	-2.75	112.19	125.43
6	A	5103	ATP	O2G-PG-O3B	2.75	113.85	104.64
7	B	5104	CFF	C14-N7-C8	-2.74	112.22	125.43
7	C	5104	CFF	C14-N7-C8	-2.74	112.23	125.43
6	D	5103	ATP	O2G-PG-O3B	2.73	113.80	104.64
6	D	5103	ATP	C2-N1-C6	2.63	123.25	118.75
6	B	5103	ATP	C2-N1-C6	2.62	123.23	118.75
6	A	5103	ATP	C2-N1-C6	2.60	123.20	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	5103	ATP	C2-N1-C6	2.60	123.20	118.75
7	B	5104	CFF	C12-N3-C2	2.54	125.91	119.61
7	D	5104	CFF	C12-N3-C2	2.54	125.91	119.61
7	C	5104	CFF	C12-N3-C2	2.53	125.88	119.61
7	A	5104	CFF	C12-N3-C2	2.52	125.85	119.61
6	A	5103	ATP	O3G-PG-O3B	2.50	113.00	104.64
6	D	5103	ATP	O3G-PG-O3B	2.50	113.00	104.64
6	B	5103	ATP	O3G-PG-O3B	2.49	112.99	104.64
6	C	5103	ATP	O3G-PG-O3B	2.49	112.99	104.64
7	C	5104	CFF	C5-C6-N1	2.31	120.67	118.20
7	D	5104	CFF	C5-C6-N1	2.29	120.64	118.20
7	B	5104	CFF	C5-C6-N1	2.28	120.63	118.20
7	A	5104	CFF	C5-C6-N1	2.27	120.62	118.20
7	C	5104	CFF	C5-C4-N9	-2.15	106.44	110.87
7	B	5104	CFF	C5-C4-N9	-2.15	106.44	110.87
6	C	5103	ATP	O2A-PA-O1A	-2.15	101.59	112.24
6	D	5103	ATP	O2A-PA-O1A	-2.15	101.61	112.24
6	A	5103	ATP	O2A-PA-O1A	-2.15	101.63	112.24
6	B	5103	ATP	O2A-PA-O1A	-2.15	101.63	112.24
7	D	5104	CFF	C5-C4-N9	-2.14	106.48	110.87
7	A	5104	CFF	C5-C4-N9	-2.13	106.49	110.87
6	D	5103	ATP	O2B-PB-O1B	-2.06	102.06	112.24
6	A	5103	ATP	O2B-PB-O1B	-2.06	102.08	112.24
6	B	5103	ATP	O2B-PB-O1B	-2.06	102.08	112.24
6	C	5103	ATP	O2B-PB-O1B	-2.06	102.08	112.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C4'-C5'-O5'-PA
6	B	5103	ATP	C4'-C5'-O5'-PA
6	C	5103	ATP	C4'-C5'-O5'-PA
6	D	5103	ATP	C4'-C5'-O5'-PA
6	A	5103	ATP	PB-O3A-PA-O5'
6	B	5103	ATP	PB-O3A-PA-O5'
6	C	5103	ATP	PB-O3A-PA-O5'
6	D	5103	ATP	PB-O3A-PA-O5'
6	A	5103	ATP	O4'-C4'-C5'-O5'
6	B	5103	ATP	O4'-C4'-C5'-O5'
6	C	5103	ATP	O4'-C4'-C5'-O5'
6	D	5103	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C5'-O5'-PA-O1A
6	B	5103	ATP	C5'-O5'-PA-O1A
6	C	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	C5'-O5'-PA-O1A

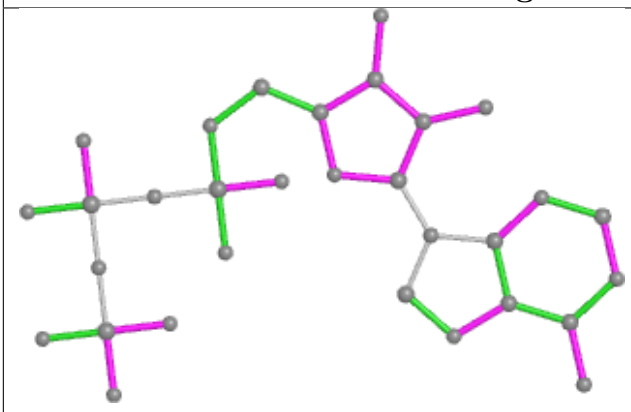
There are no ring outliers.

8 monomers are involved in 8 short contacts:

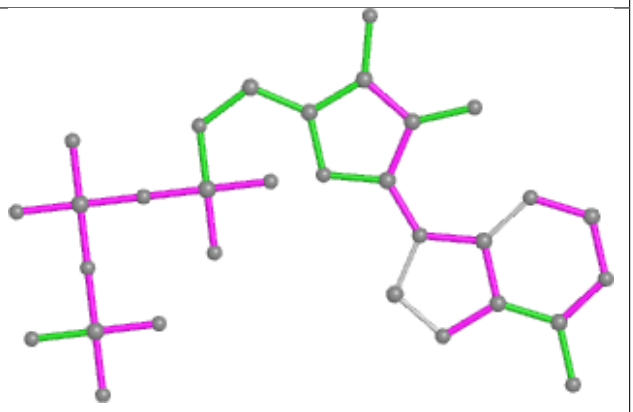
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5103	ATP	1	0
7	A	5104	CFF	1	0
6	C	5103	ATP	1	0
7	C	5104	CFF	1	0
7	B	5104	CFF	1	0
7	D	5104	CFF	1	0
6	A	5103	ATP	1	0
6	D	5103	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

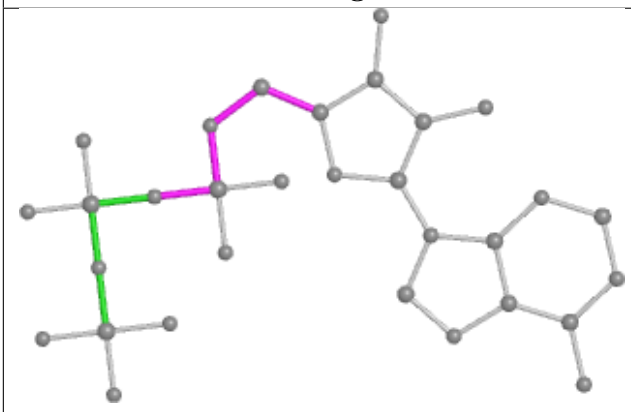
Ligand ATP B 5103



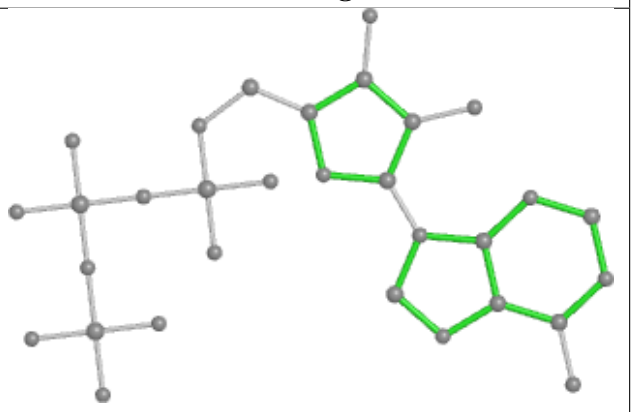
Bond lengths



Bond angles

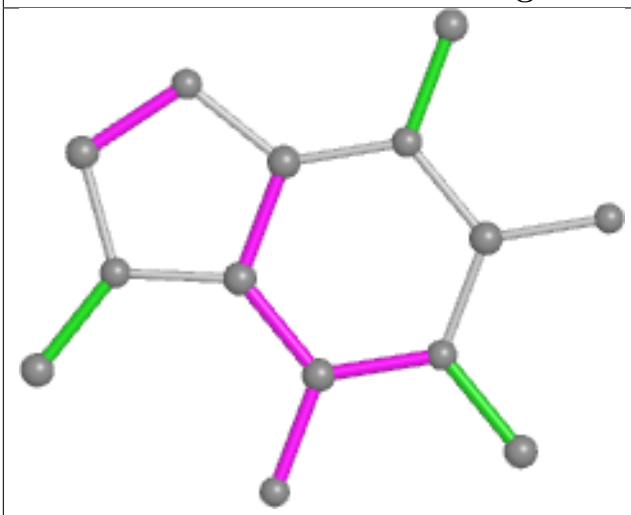


Torsions



Rings

Ligand CFF A 5104



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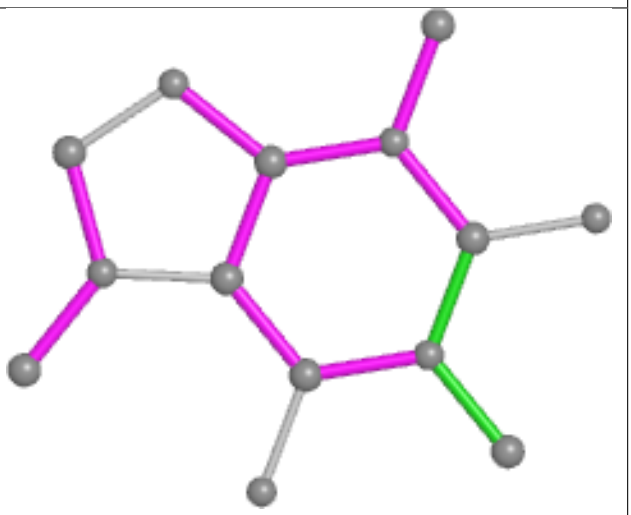
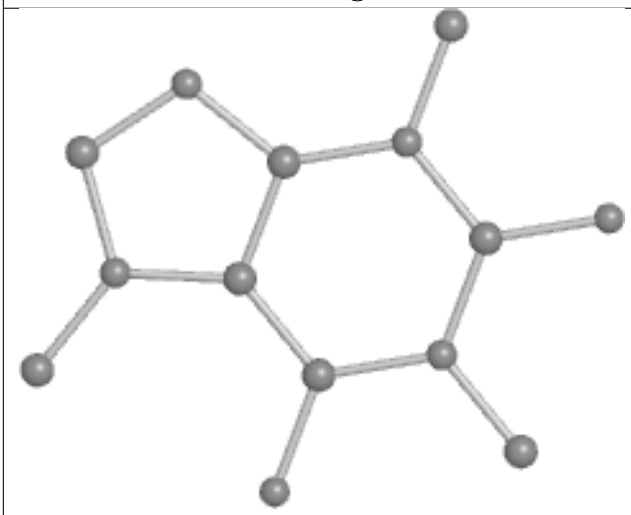


Bond angles



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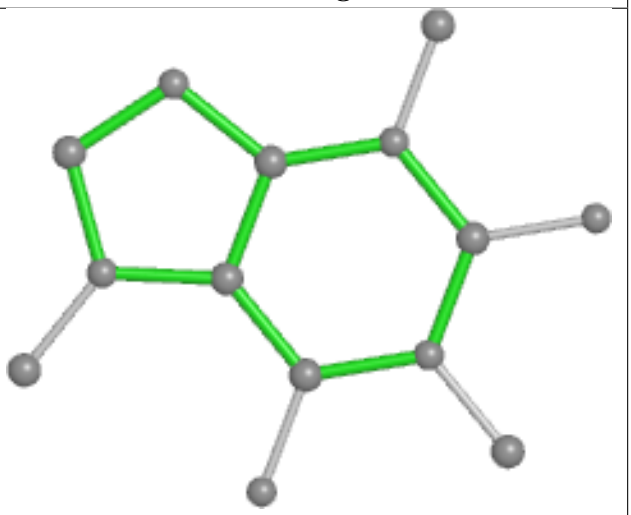
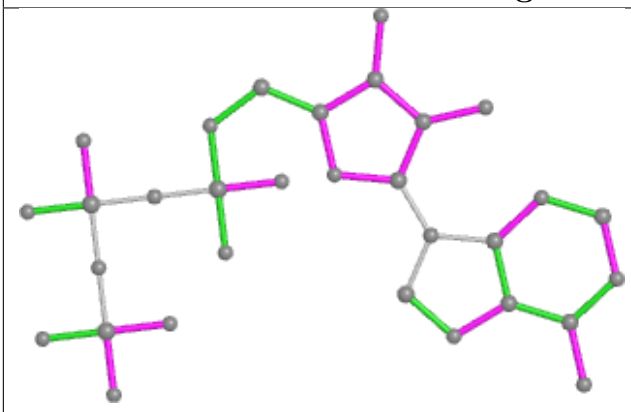


Rings

Ligand ATP C 5103



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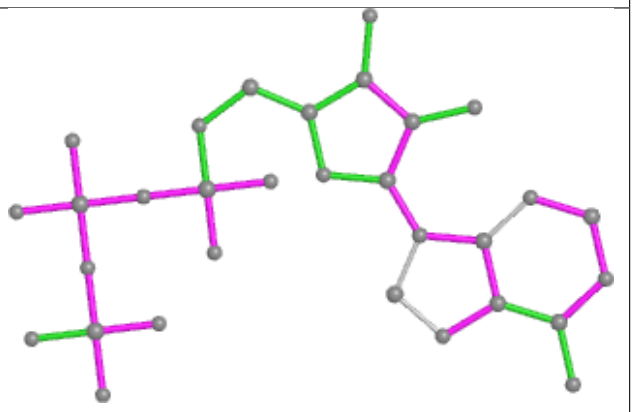
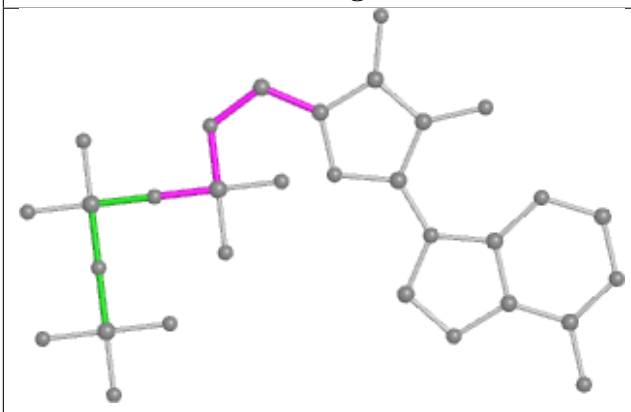


Bond angles



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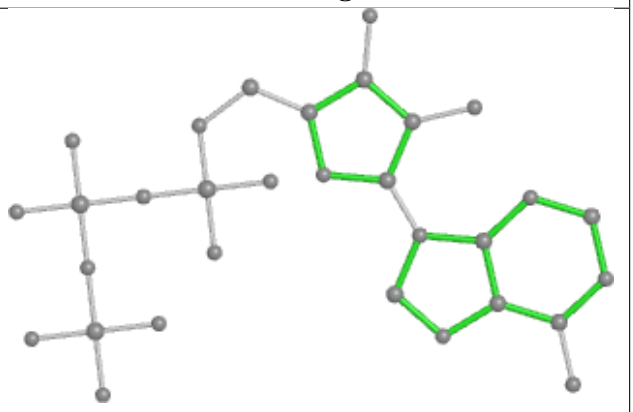
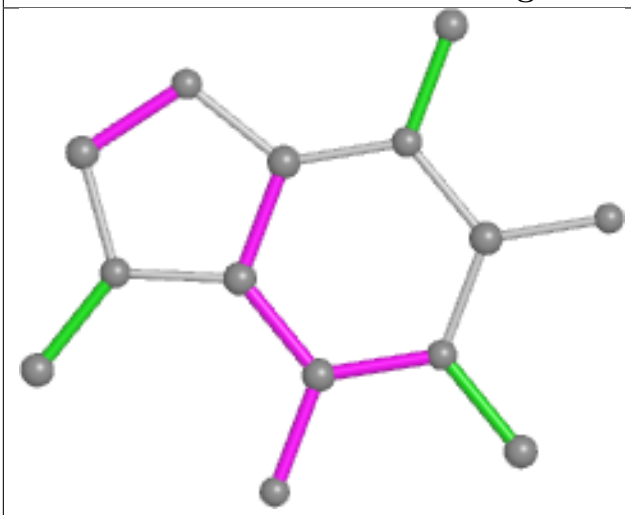


Rings

Ligand CFF C 5104



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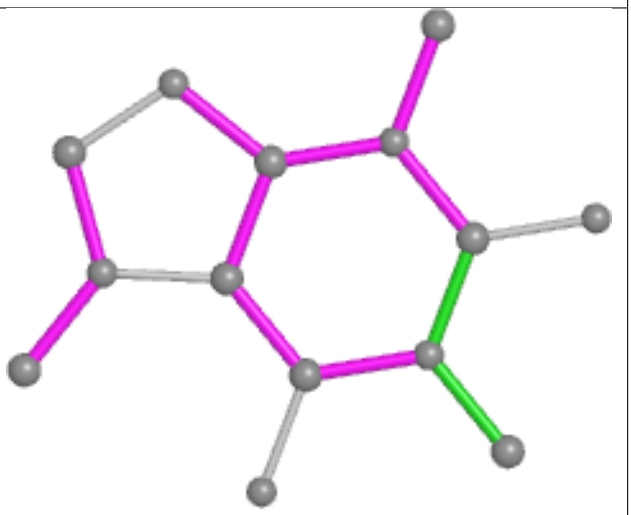
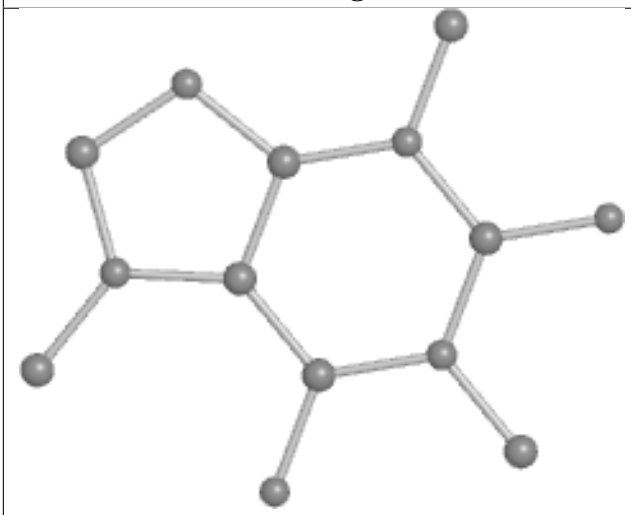


Bond angles



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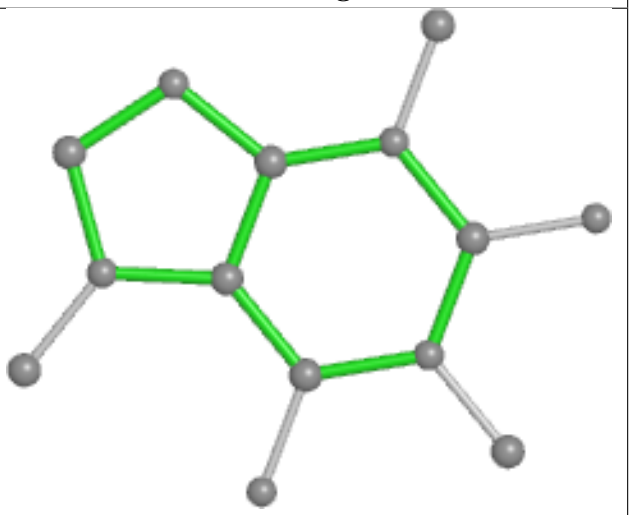
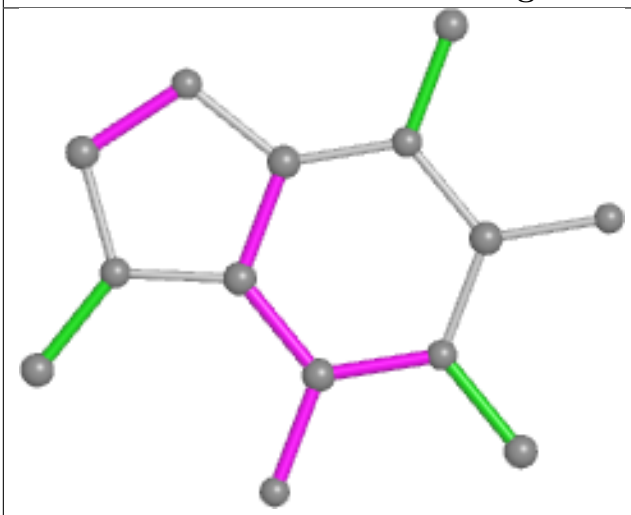
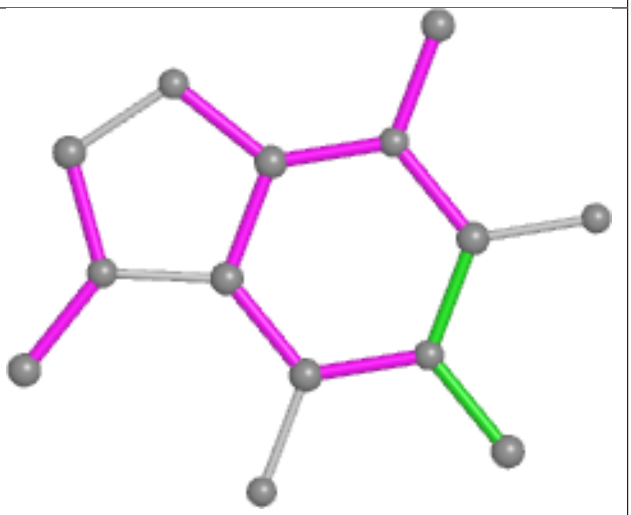


Rings

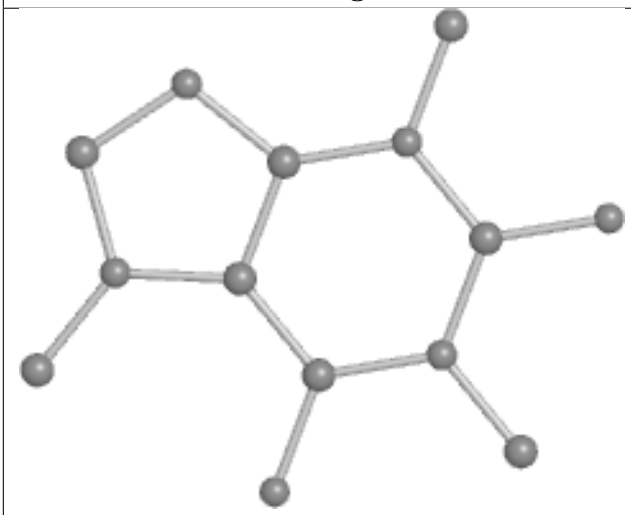
Ligand CFF B 5104



Bond lengths



Bond angles



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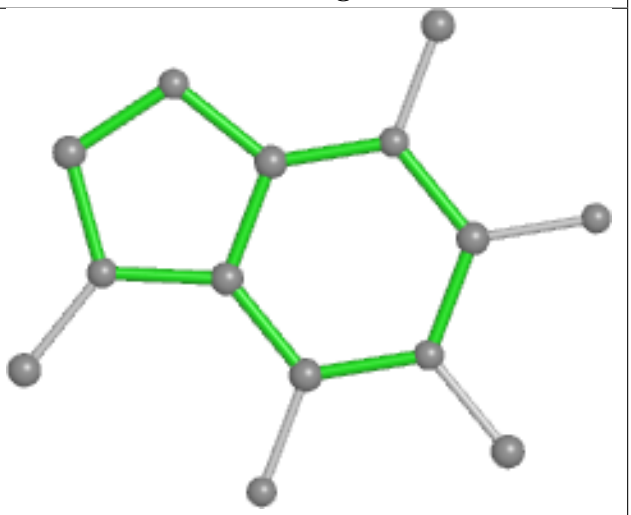
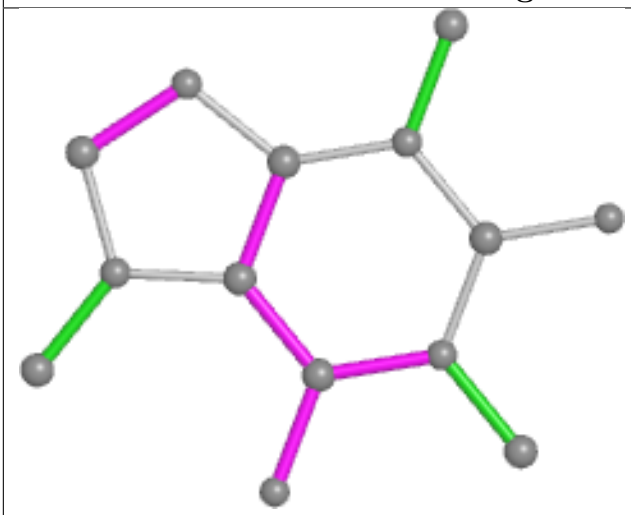
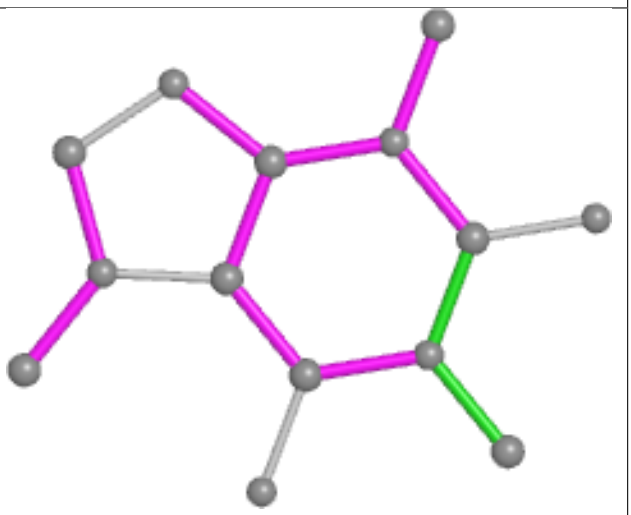


Rings

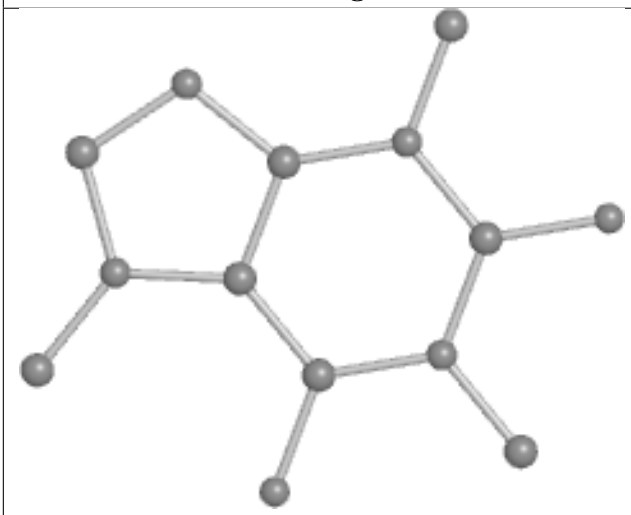
Ligand CFF D 5104



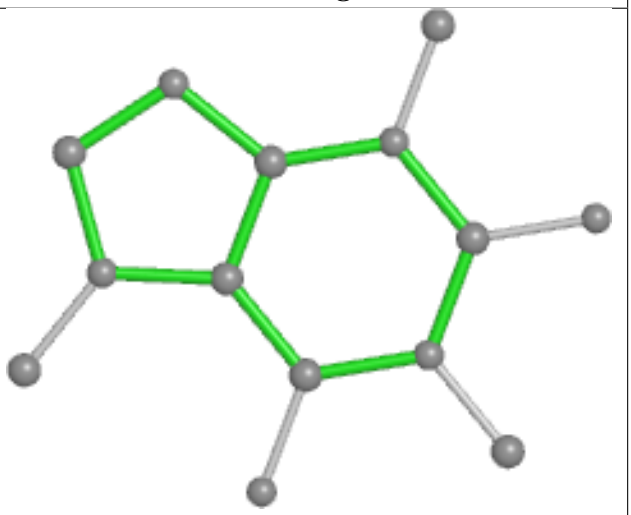
Bond lengths



Bond angles

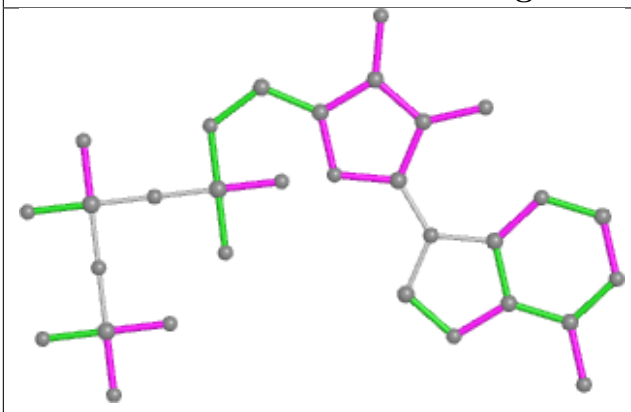


Torsions

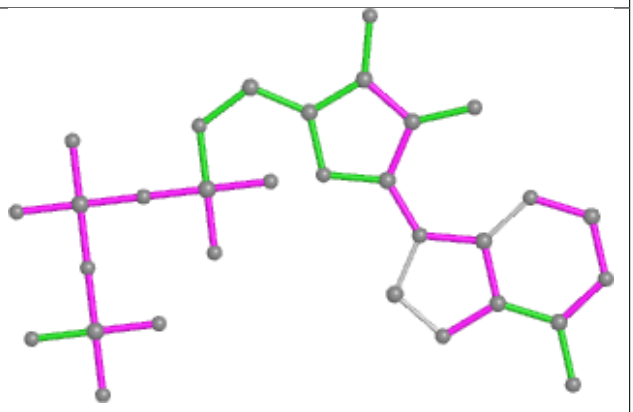


Rings

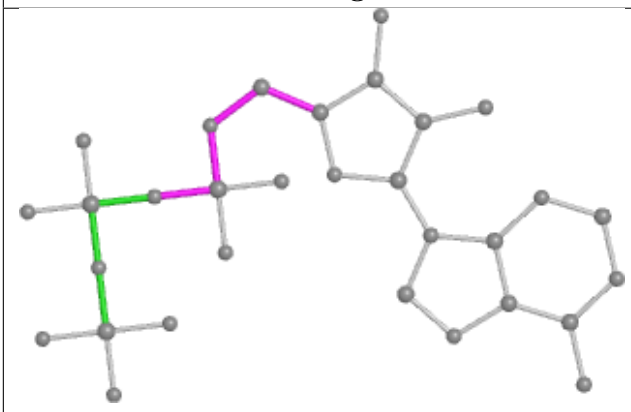
Ligand ATP A 5103



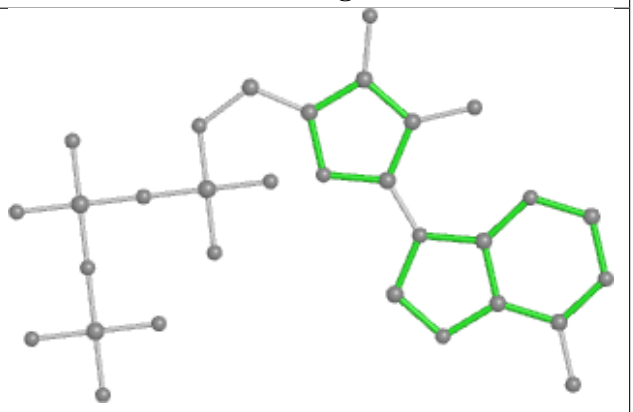
Bond lengths



Bond angles

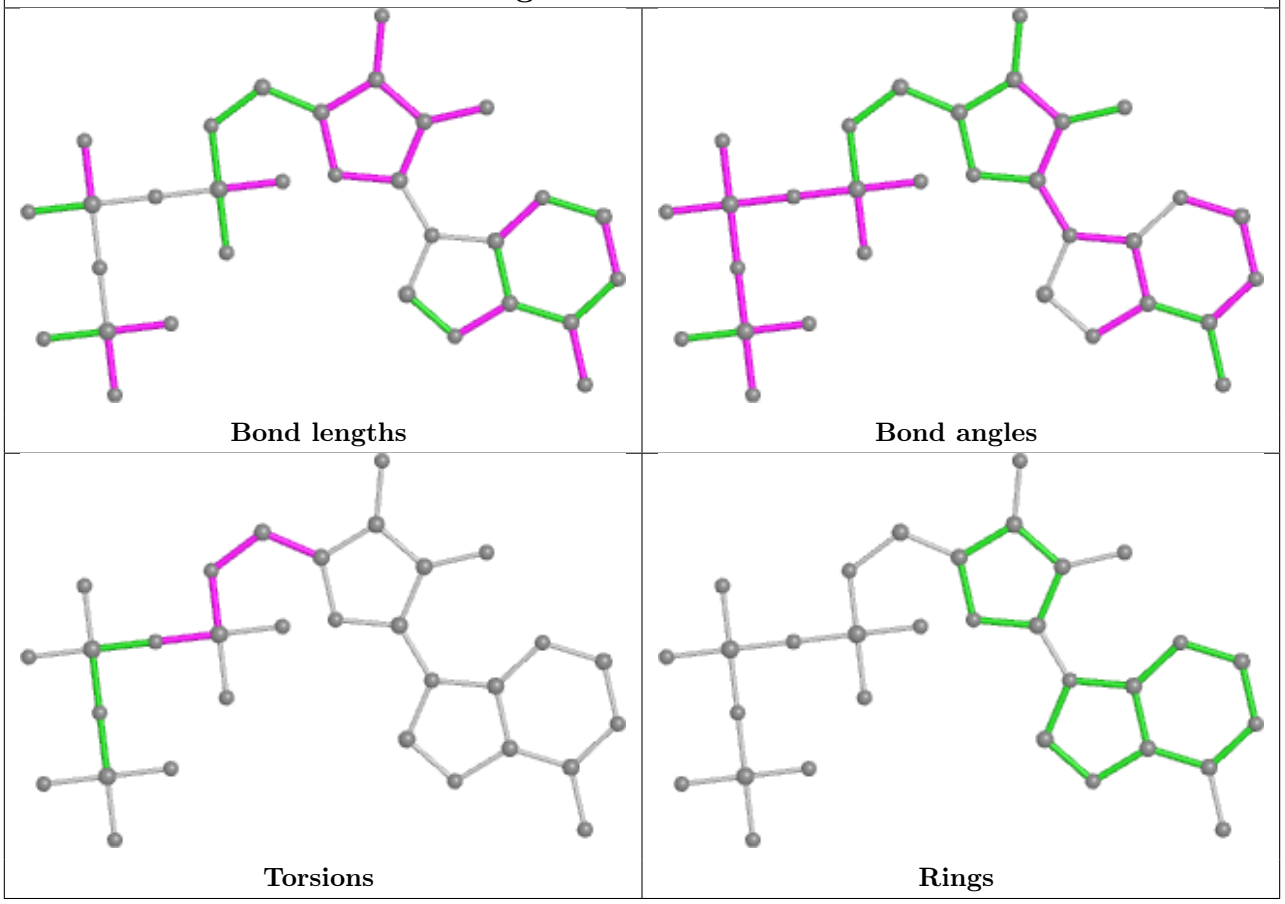


Torsions



Rings

Ligand ATP D 5103



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.

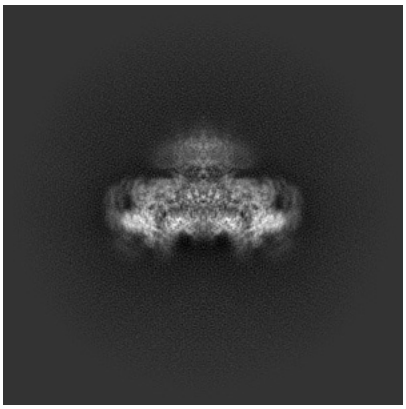
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38447. These allow visual inspection of the internal detail of the map and identification of artifacts.

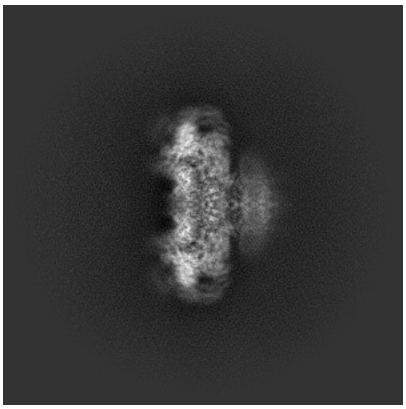
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

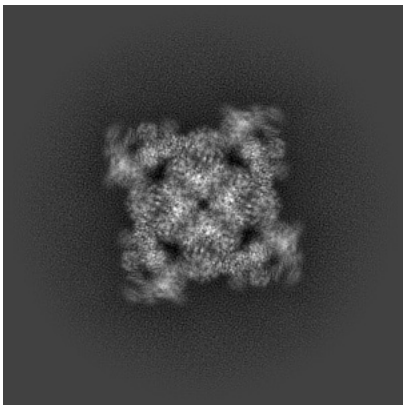
6.1.1 Primary map



X

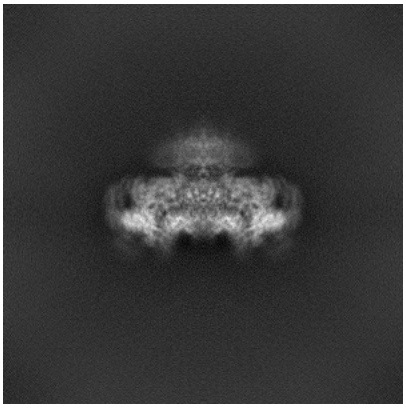


Y

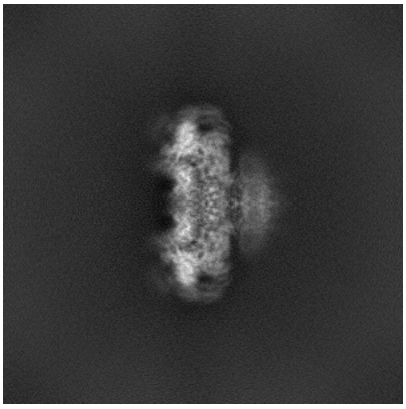


Z

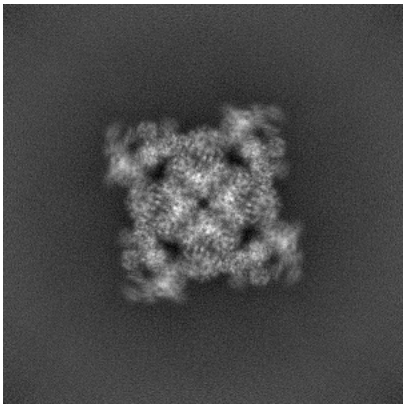
6.1.2 Raw map



X



Y

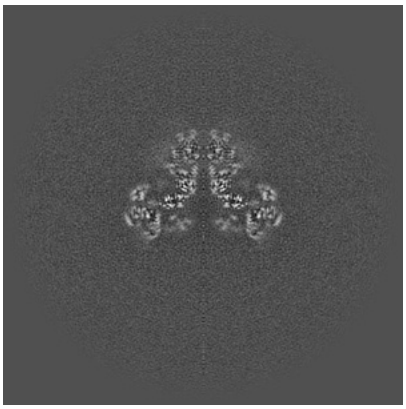


Z

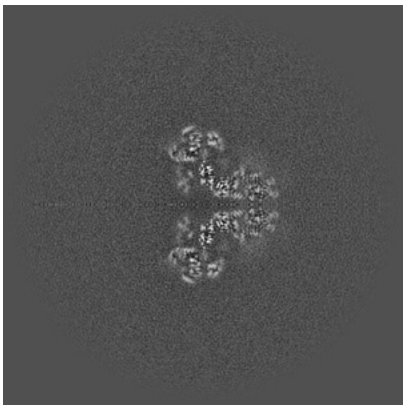
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

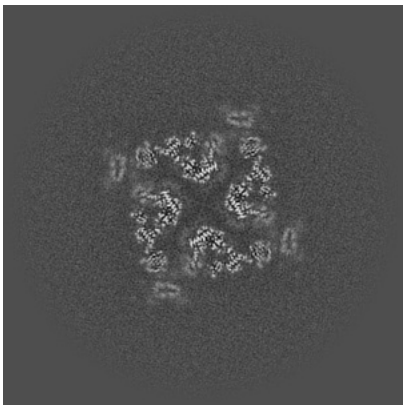
6.2.1 Primary map



X Index: 240

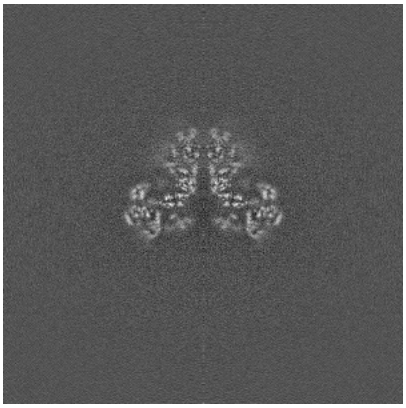


Y Index: 240

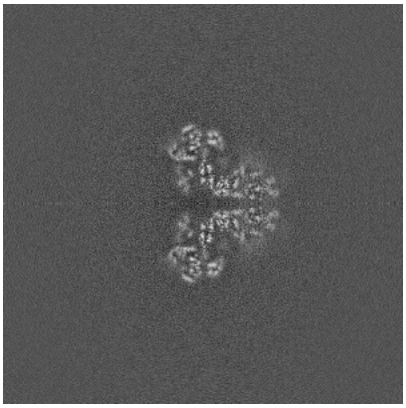


Z Index: 240

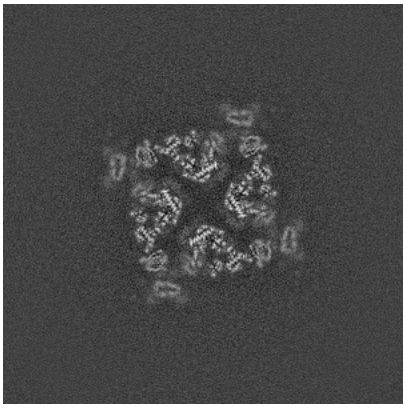
6.2.2 Raw map



X Index: 240



Y Index: 240

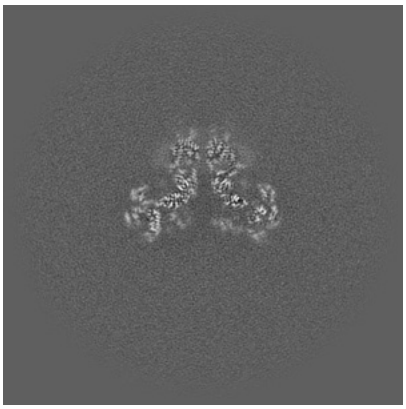


Z Index: 240

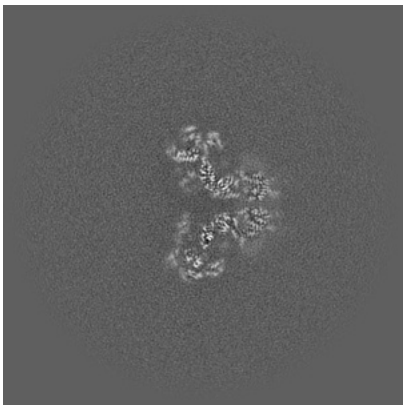
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

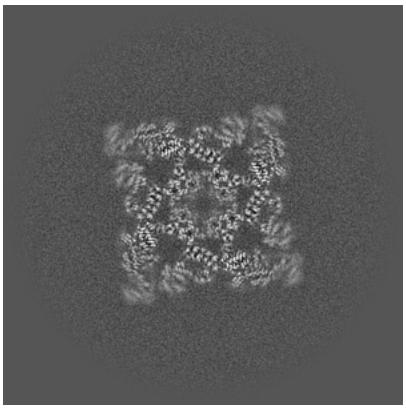
6.3.1 Primary map



X Index: 238

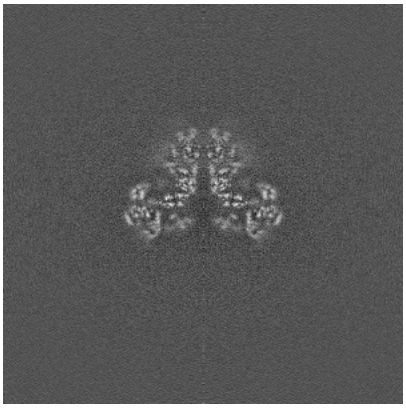


Y Index: 238

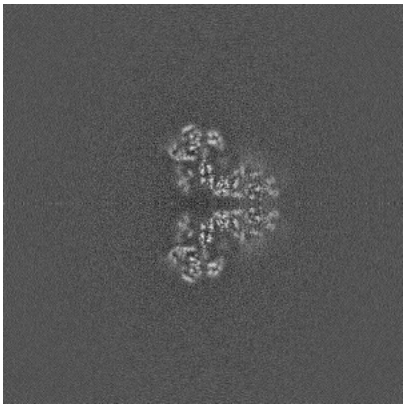


Z Index: 223

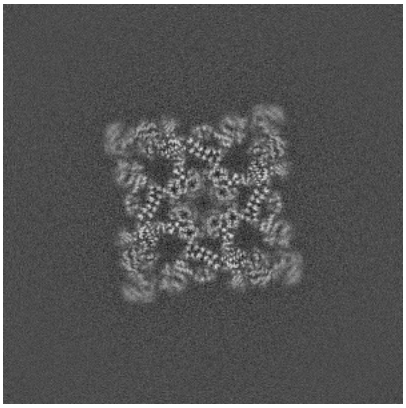
6.3.2 Raw map



X Index: 240



Y Index: 240

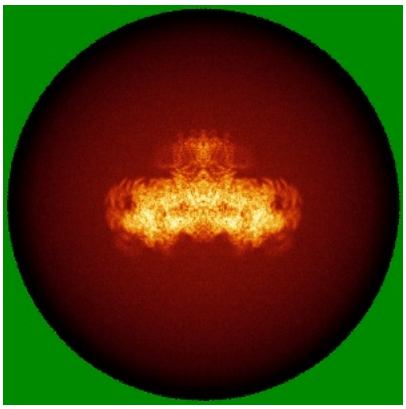


Z Index: 222

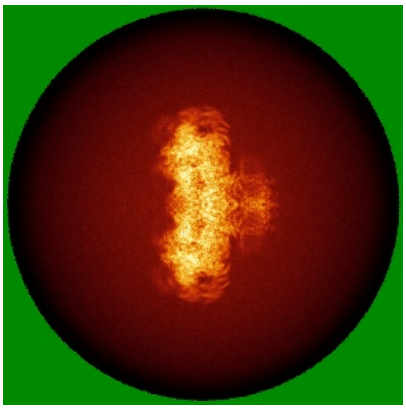
The images above show the largest variance slices of the map in three orthogonal directions.

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

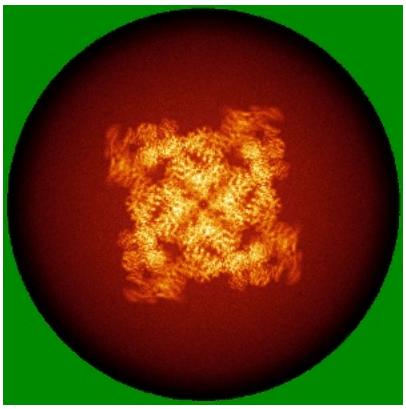
6.4.1 Primary map



X

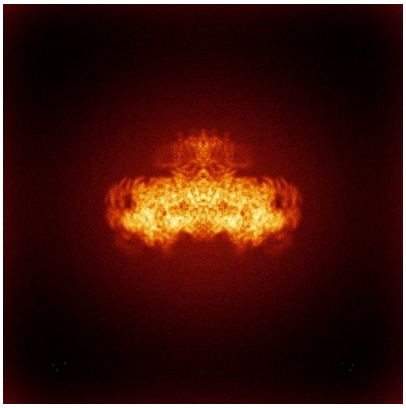


Y

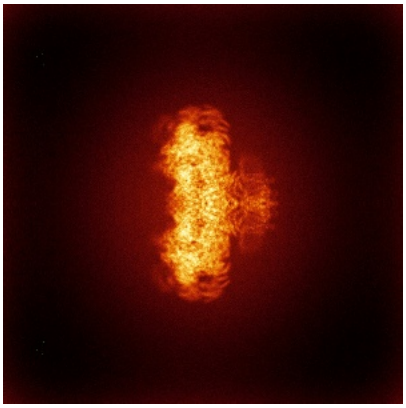


Z

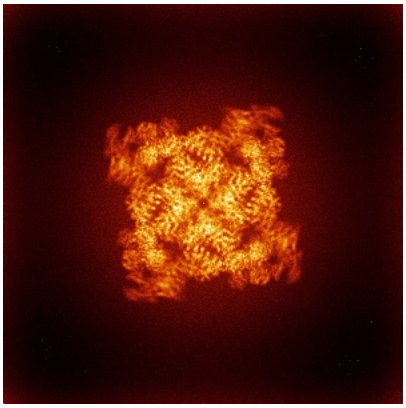
6.4.2 Raw map



X



Y

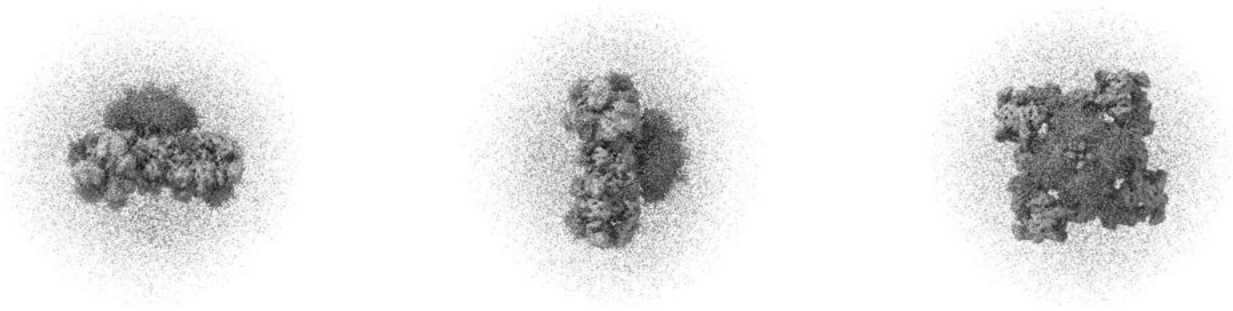


Z

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

6.5 Orthogonal surface views (i)

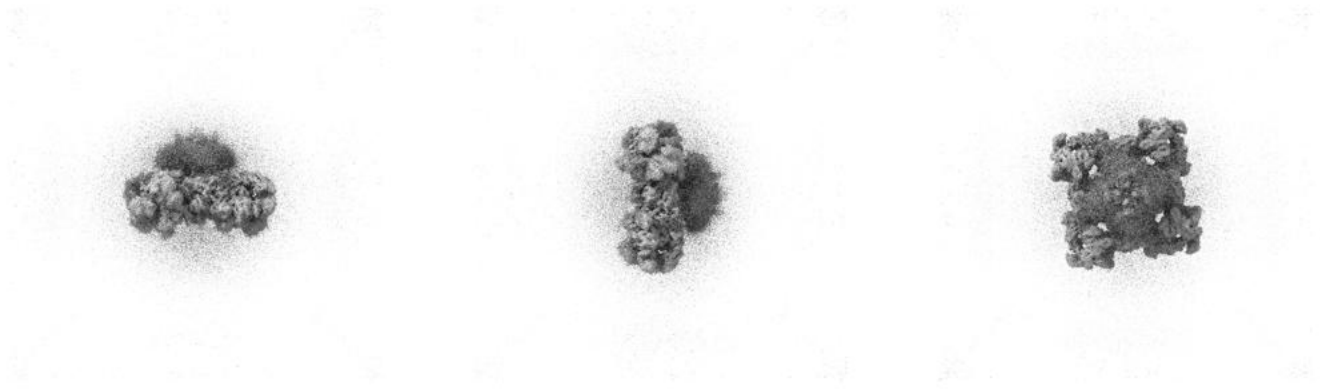
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

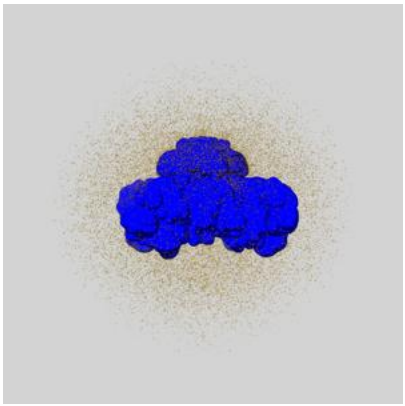
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

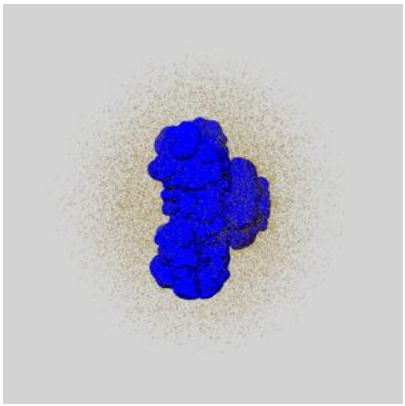
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

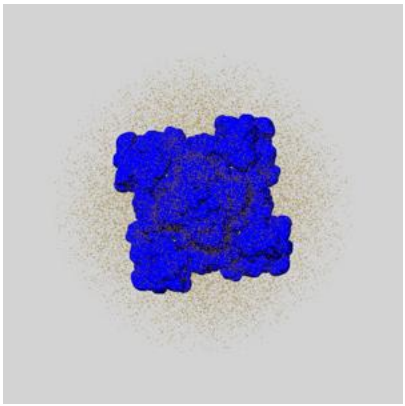
6.6.1 emd_38447_msk_1.map (i)



X



Y

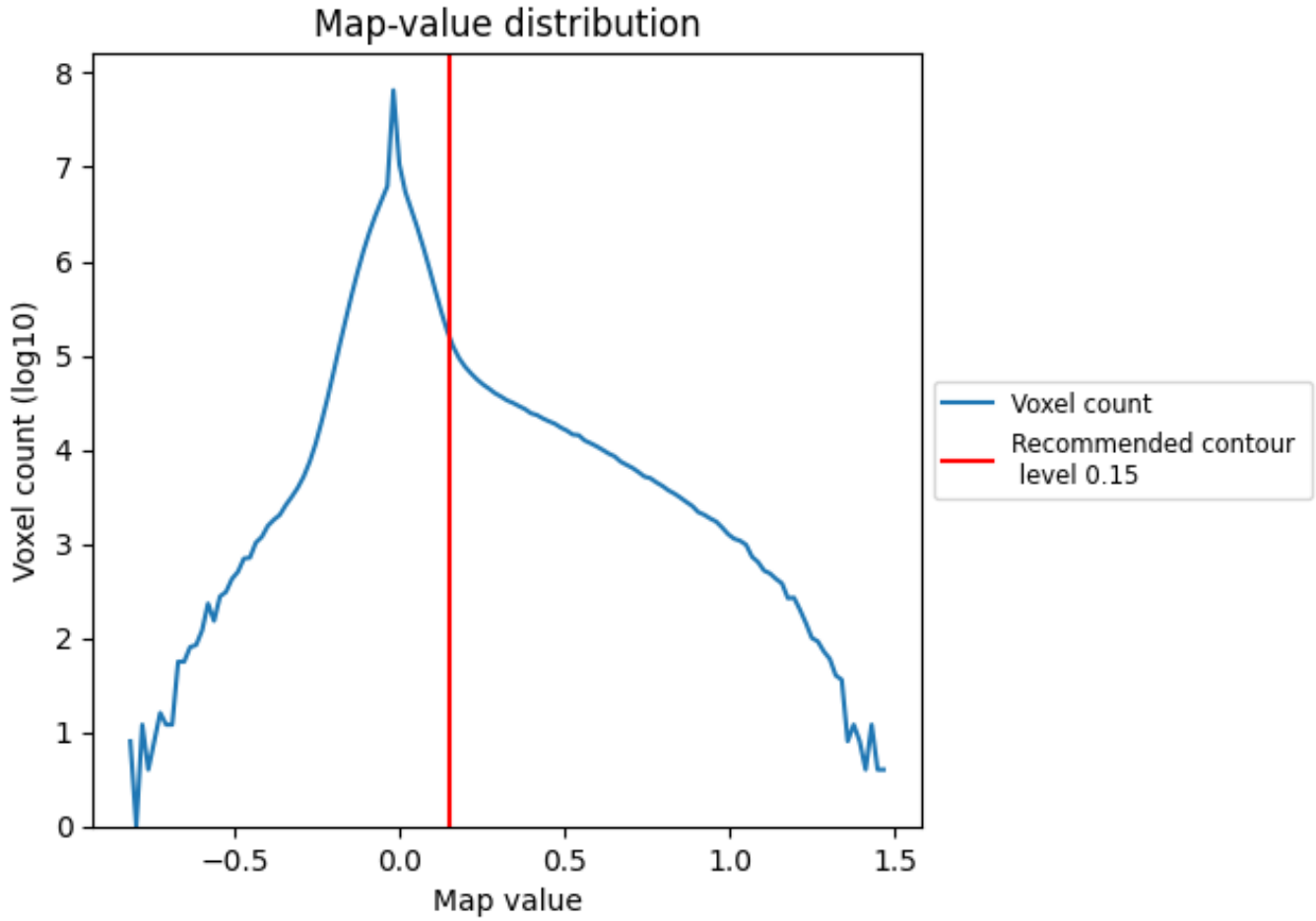


Z

7 Map analysis

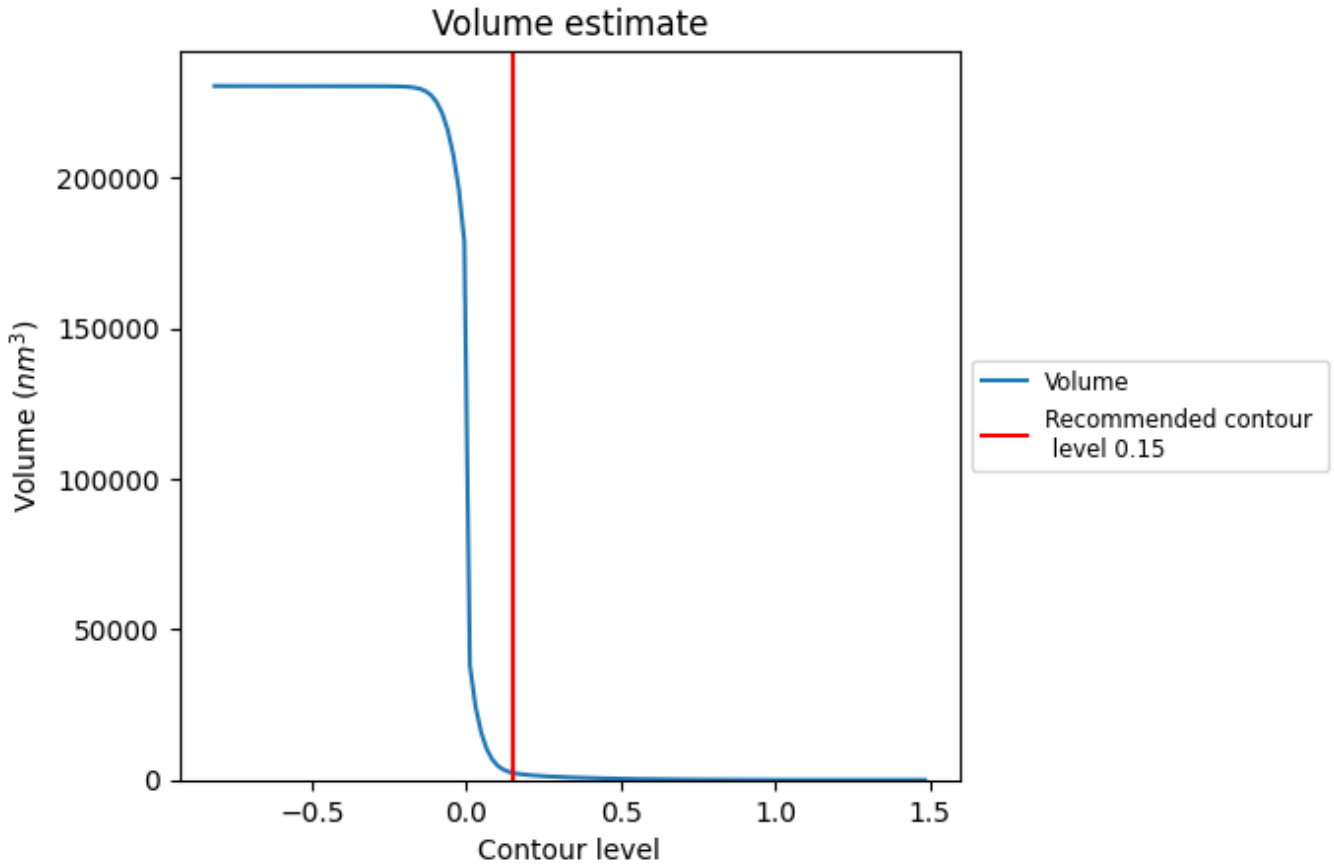
This section contains the results of statistical analysis of the map.

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.

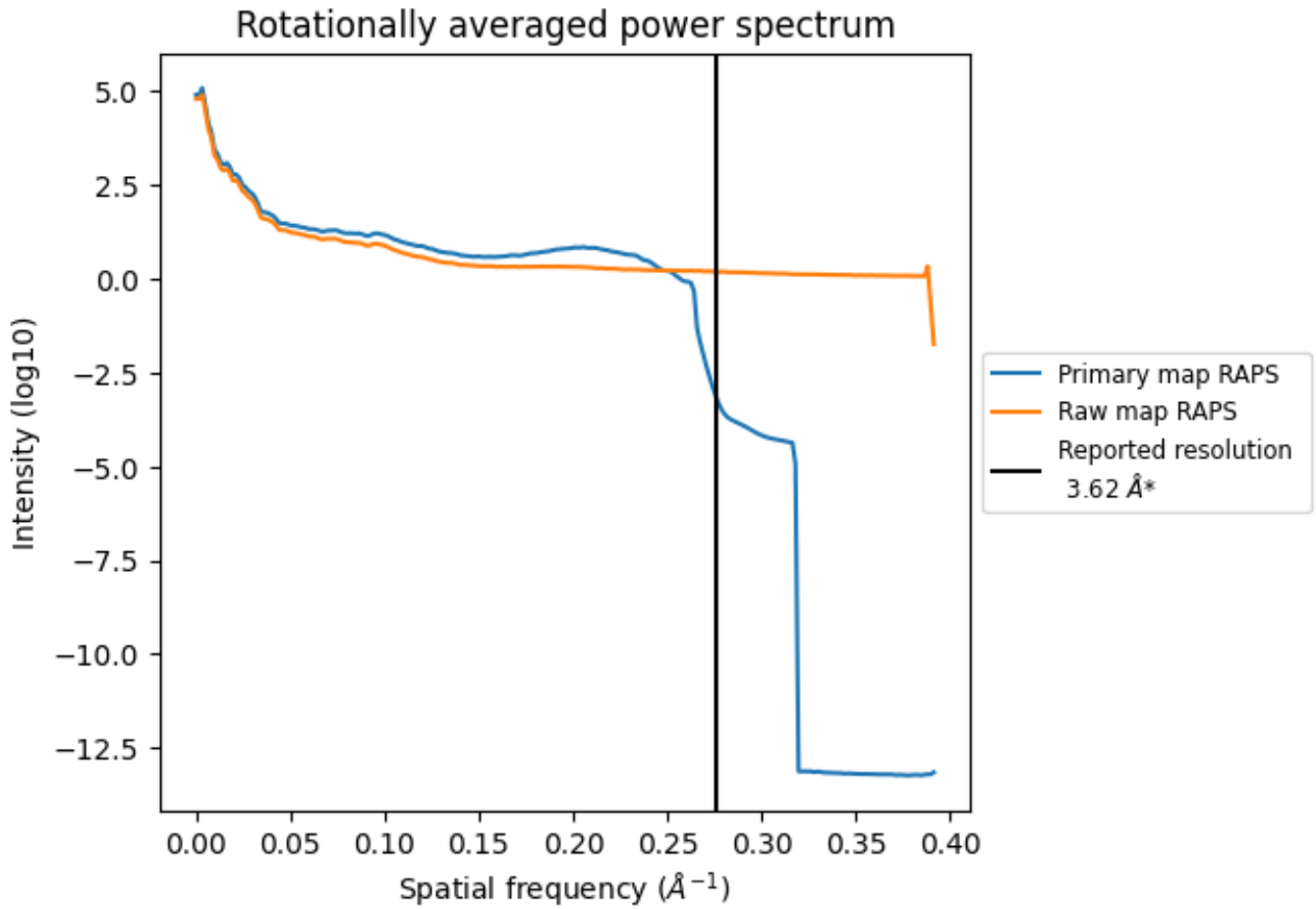
7.2 Volume estimate



The volume at the recommended contour level is 2397 nm^3; this corresponds to an approximate mass of 2166 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)

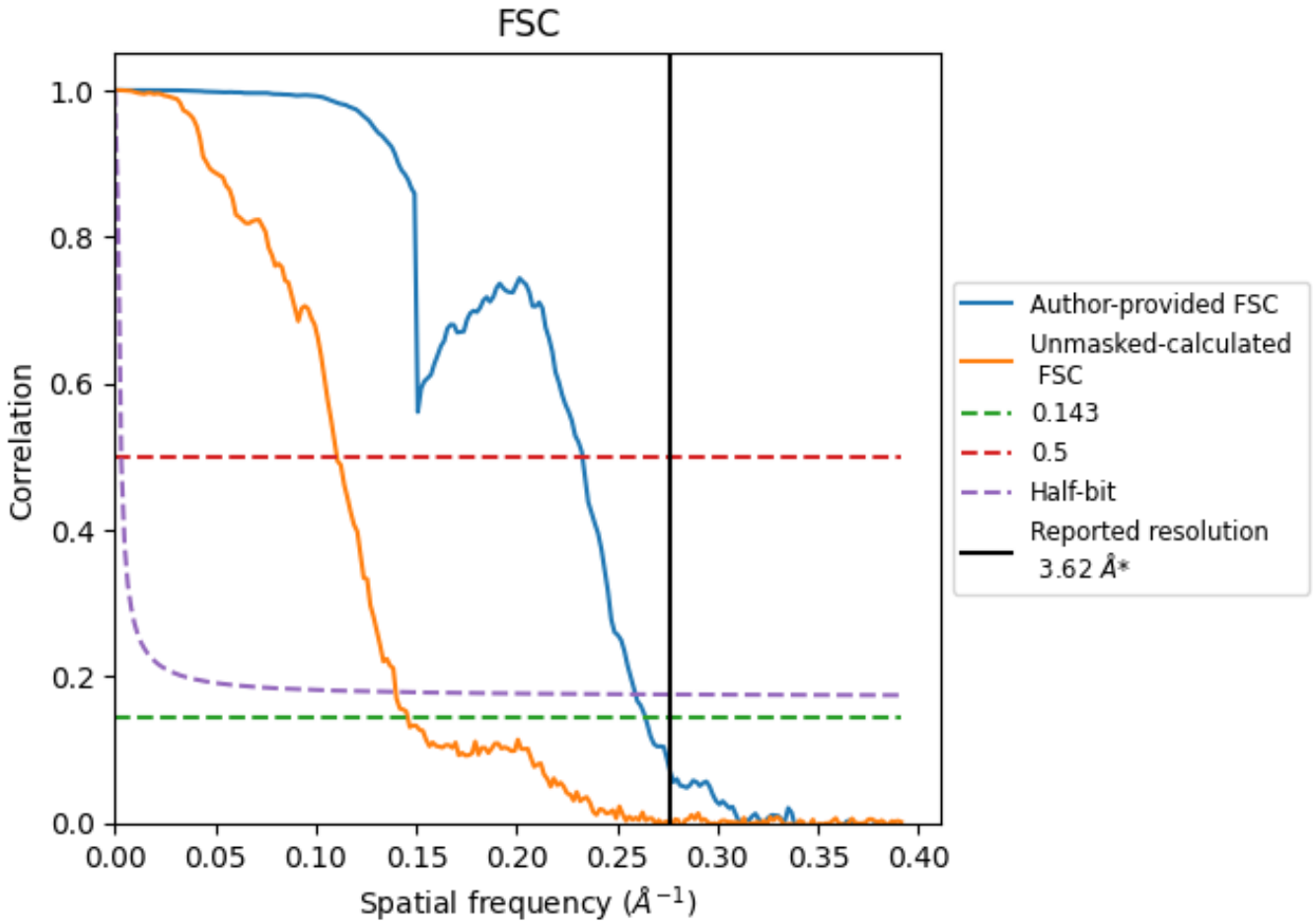


*Reported resolution corresponds to spatial frequency of 0.276 $Å^{-1}$

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 0.276 Å^{-1}

8.2 Resolution estimates (i)

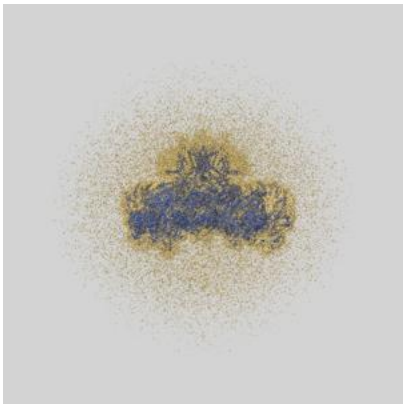
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.79	4.30	3.86
Unmasked-calculated*	6.86	9.05	7.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 3.62 by more than 10 %

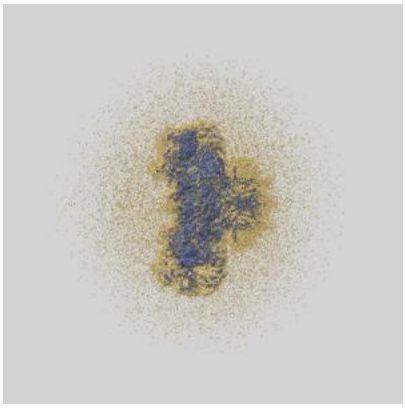
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38447 and PDB model 8XLF. Per-residue inclusion information can be found in section 3 on page 8.

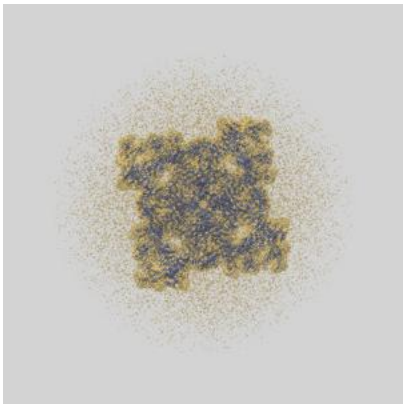
9.1 Map-model overlay



X



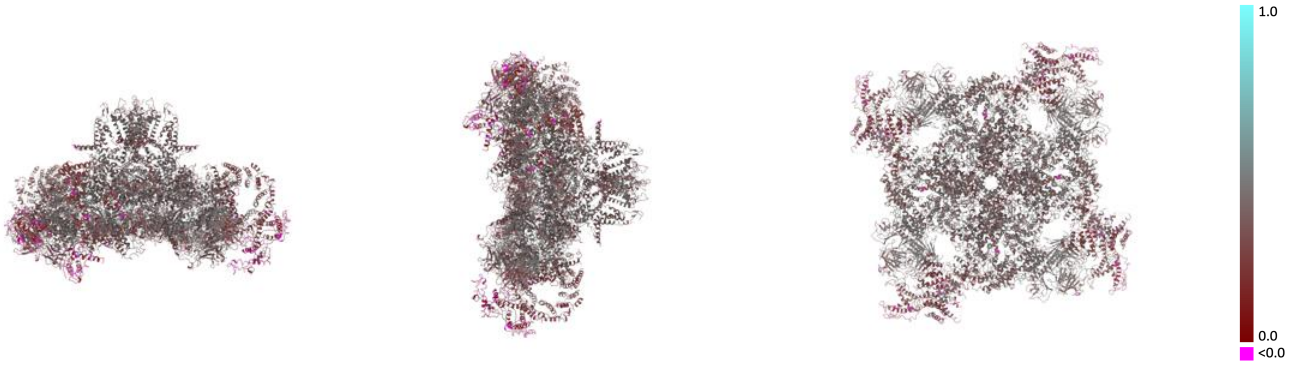
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

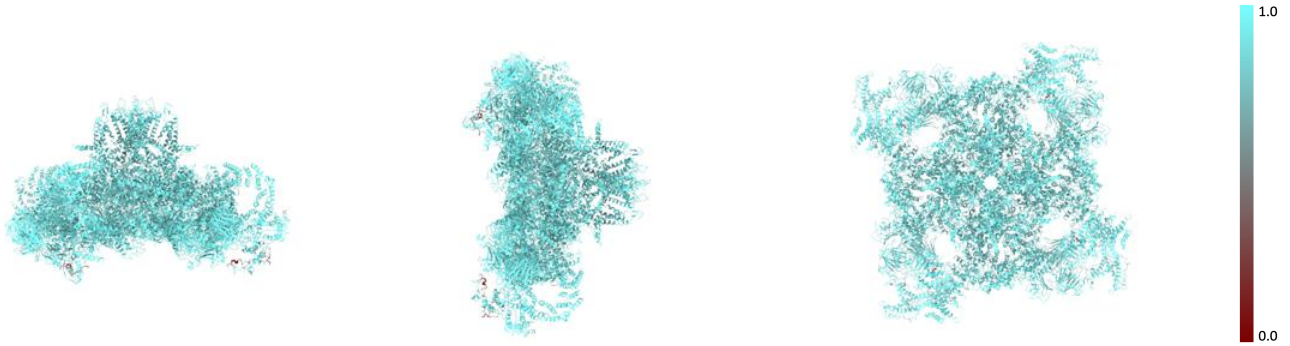
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

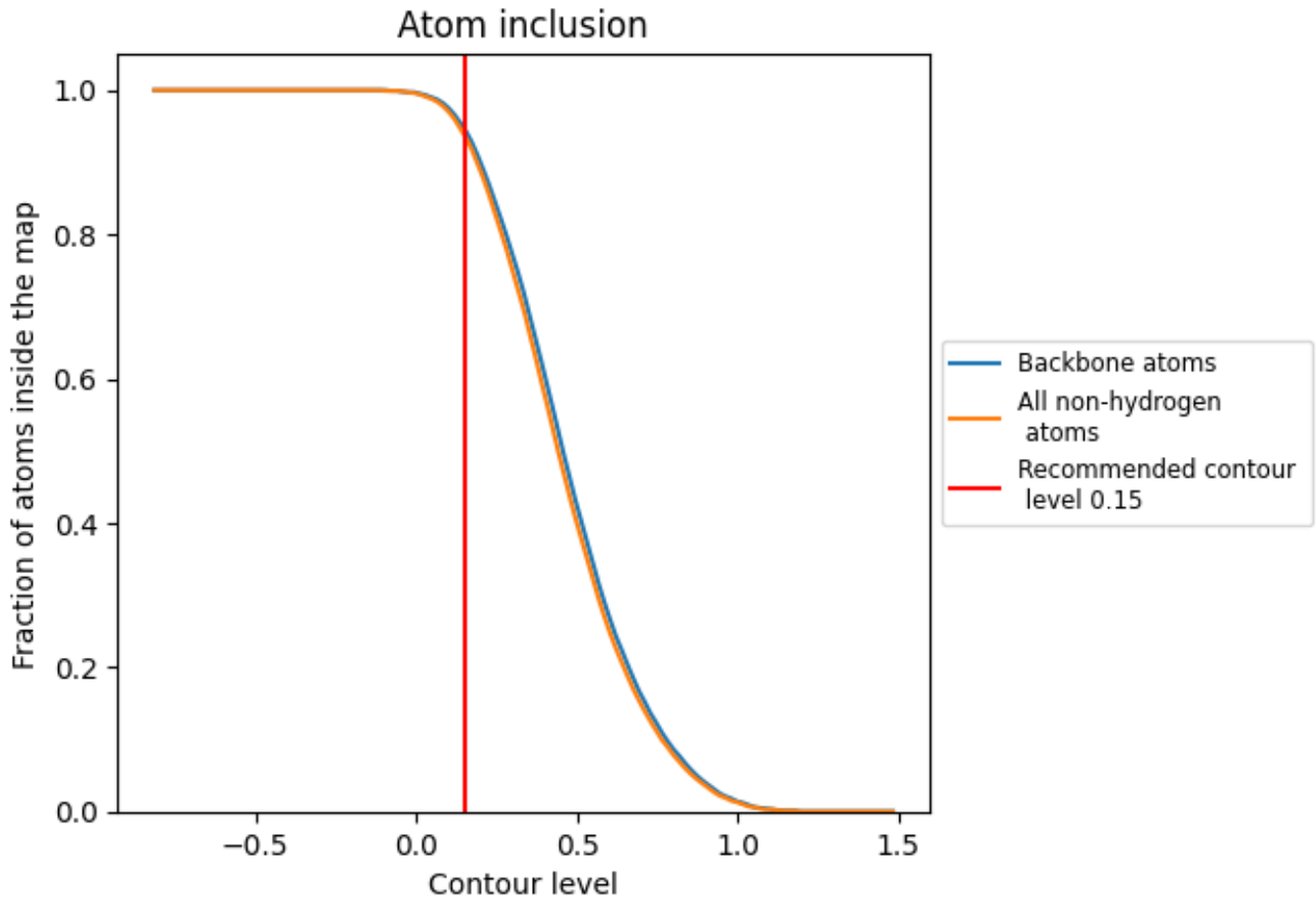
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.3750
A	0.9410	0.3780
B	0.9410	0.3780
C	0.9410	0.3780
D	0.9410	0.3790
E	0.9510	0.3920
F	0.9510	0.3890
G	0.9530	0.3890
H	0.9510	0.3910
I	0.8990	0.2850
J	0.9000	0.2880
K	0.8990	0.2870
L	0.9010	0.2840