



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:11 PM UTC

PDB ID : 8XLF / pdb_00008xlf
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

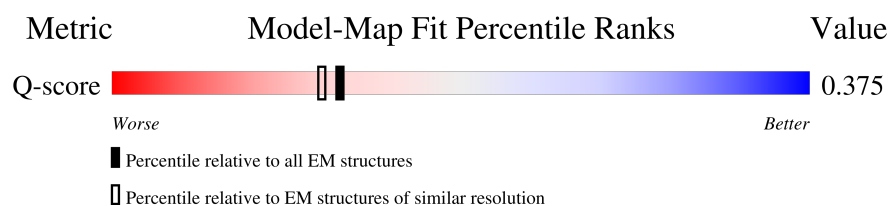
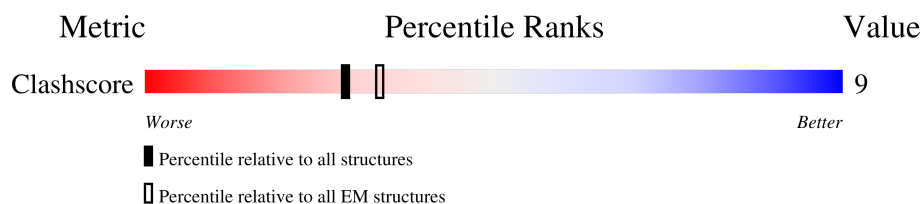
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

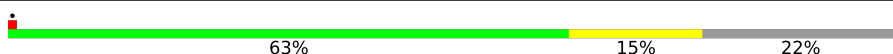
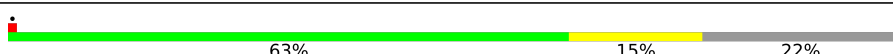
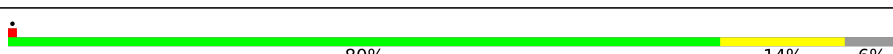
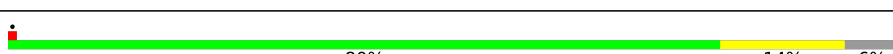
The reported resolution of this entry is 3.62 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11773 (3.12 - 4.12)

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	I	148	
2	J	148	

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Mol	Chain	Length	Quality of chain
2	K	148	
2	L	148	
3	E	107	
3	F	107	
3	G	107	
3	H	107	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	A	5104	-	X	-	-
7	CFF	B	5104	-	X	-	-
7	CFF	C	5104	-	X	-	-
7	CFF	D	5104	-	X	-	-

2 Entry composition

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		

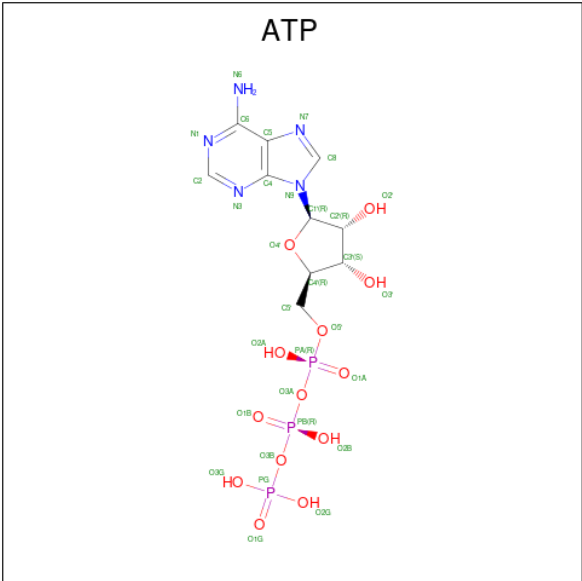
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



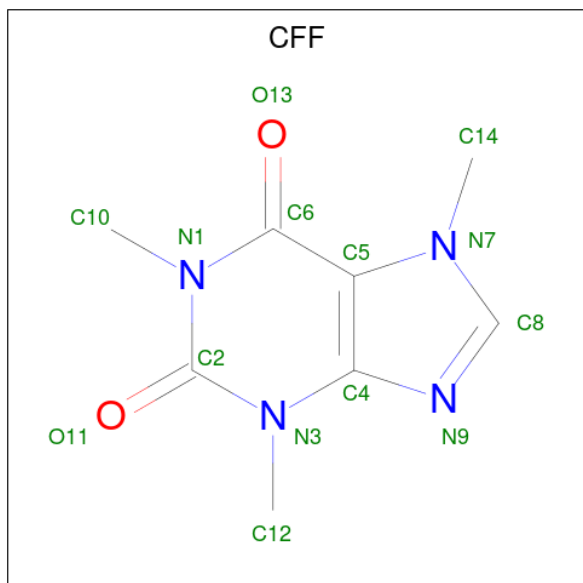
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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

- Molecule 7 is CAFFEINE (CCD ID: 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	
			24	8	10	4	2	0
7	B	1	Total	C	H	N	O	
			24	8	10	4	2	0
7	C	1	Total	C	H	N	O	
			24	8	10	4	2	0
7	D	1	Total	C	H	N	O	
			24	8	10	4	2	0





M4796	V4797	M4798	S4799	L4800	L4801	G4802	N4806	F4807	F4808	H4812	L4813	L4814	V4820	K4821	T4822	L4823	R4824	T4825	L4826	L4827	S4828	T4831	H4832	G4834	K4835	K4836	L4837	V4838	M4839	T4840	L4843	L4844	V4845	V4846	V4847	V4848	L4849	L4850	T4851	F4852	F4856	R4860	K4875	C4876	M4879	V4880	T4881	C4882	Y4883				
L4884	Y4888	E4900	I4901	E4902	D4903	P4904	Y4912	R4913	V4914	V4915	F4916	D4917	I4918	T4919	F4920	F4921	F4922	F4923	V4924	I4925	V4926	I4927	L4928	Q4933	G4934	L4935	I4936	I4937	D4938	M4939	F4940	G4941	E4942	R4943	R4944	V4945	Q4946	Q4947	E4948	Q4949	K4950	E4951	D4952	M4954	E4955	T4956	K4957	C4958	F4959	I4960	C4961	G4962	G4964
S4965	F4968	G4973	G4974	F4975	E4976	T4977	H4978	T4979	L4980	H4983	N4984	L4985	A4986	N4987	Y4988	M4989	F4991	L4992	N4993	Y4994	L4995	L4996	D4999	E5002	H5003	T5004	G5005	Q5006	E5007	S5008	Y5009	V5010	N5011	V5012	N5013	E5016	R5017	C5018	N5019	F5022	C5027	F5028	R5029	K5030	Q5031	L5036	SER						

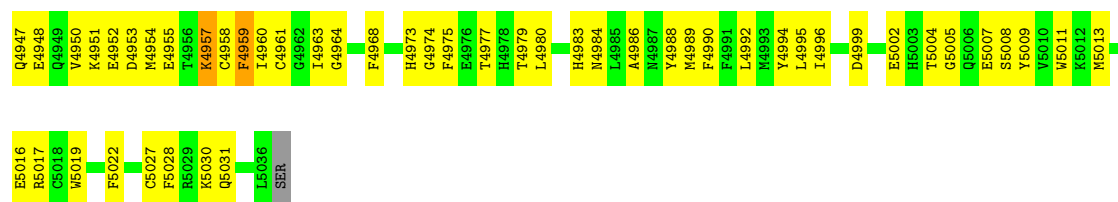
● Molecule 1: Ryanodine receptor 1

Chain B:  63% 15% 22%

R1438	Q1443	Q1444	E1444	P1445	S1446	W1452	Y1457	H1458	Q1459	R1470	A1471	V1472	T1473	G1477	V1483	K1488	C1489	S1490	N1491	V1501	SER	PRO	GLY	GLN	GLN	GLY	ARG	T1509	C1518	L1522	L1555	N1560	Q1563	K1568	Q1569	K1570	N1571	L1572	L1575	M1579	P1593	R1594						
GLY	VAL	GLU	ALA	GLN	PRO	ARG	ALA	ASN	GLY	GLU	GLY	ASN	GLN	LYS	ARG	GLY	PHE	LEU	PHE	LYS	ALA	LYS	ASN	LYS	ALA	GLY	GLN	GLN	GLY	THR	GLN	TRP	GLY	LYS	GLU	GLY	VAL	GLY	GLY	GLY	GLY	GLY	THR					
Q1144	A989	P763	A613	G427	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299	GLY	L299	G143	GLY	L299				
D1147	W1005	V764	V614	SER	GLY	L299	GLY	GLY	L299	GLY	L299	GLY	GLY	L299	GLY	L299	GLY	GLY	L299	GLY	L299	GLY	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299	GLY	L299		
D1154	Y1007	G766	R615	PRO	ALA	L477	PRO	PRO	D303	PRO	D303	PRO	PRO	D303	PRO	D303	PRO	PRO	D303	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	D303	PRO	PRO	
L1155	S1008	V767	Q618	ALA	GLY	L477	ALA	ALA	D303	ALA	D303	ALA	ALA	D303	ALA	D303	ALA	ALA	D303	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	D303	ALA	ALA	
T1156	A1009	F771	D619	GLY	GLY	L477	GLY	GLY	D303	GLY	D303	GLY	GLY	D303	GLY	D303	GLY	GLY	D303	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	D303	GLY	GLY	
M1170	Q1011	L773	T622	P434	K320	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	
A1177	R1017	F778	L626	L477	L323	ASP	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	ASP	L323	V191	
T1178	N1018	S784	N636	Q479	THR	THR	S194	THR	THR	THR	S194	THR	THR	THR	THR	S194	THR	THR	THR	THR	THR	S194	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
F1179	V1021	A785	V636	E480	ALA	ALA	F195	ALA	ALA	ALA	F195	ALA	ALA	ALA	ALA	F195	ALA	ALA	ALA	ALA	ALA	F195	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
E1183	P1022	G786	I644	L484	LYS	LYS	C217	PRO	PRO	PRO	C217	PRO	PRO	PRO	PRO	C217	PRO	PRO	PRO	PRO	PRO	C217	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
D1186	Y1024	V787	R645	S485	ARG	ARG	R221	ASP	ASP	ASP	R221	ASP	ASP	ASP	ASP	R221	ASP	ASP	ASP	ASP	ASP	R221	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
G1192	R1025	R818	R652	M489	VAL	VAL	H224	GLY	GLY	GLY	H224	GLY	GLY	GLY	GLY	H224	GLY	GLY	GLY	GLY	GLY	H224	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
S1193	L1026	E524	E665	D492	G333	G333	GLY	HIS	HIS	HIS	GLY	HIS	HIS	HIS	HIS	GLY	HIS	HIS	HIS	HIS	HIS	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	
Q1198	E1029	R831	V671	T498	K340	K340	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	
V1199	D1028	E831	T676	A501	S344	S344	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
G1200	K1032	G836	A677	A501	S344	S344	E229	ASP	ASP	ASP	E229	ASP	ASP	ASP	ASP	E229	ASP	ASP	ASP	ASP	ASP	E229	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
N1203	L1039	H838	T689	N520	A360	A360	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
L1204	P1055	V940	H681	A504	G354	G354	S234	ALA	ALA	ALA	S234	ALA	ALA	ALA	ALA	S234	ALA	ALA	ALA	ALA	ALA	S234	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		
S1210	PRO	P855	T689	K516	V356	V356	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		
G1222	ASN	VAL	E690	N520	L357	L357	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
F1226	PRO	THR	E690	N520	L357	L357	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	
R1232	GLN	GLN	T661	N543	PRO	PRO	Q241	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
S1241	VAL	I861	S1241	L551	PRO	PRO	Q241	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	GLU	Q241	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
L1242	ASN	A875	L1242	D552	PRO	PRO	E248	GLU	GLU	GLU	E248	GLU	GLU	GLU	GLU	E248	GLU	GLU	GLU	GLU	GLU	E248	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
P1243	GLN	GLN	P1243	I569	LYS	LYS	G249	GLY	GLY	GLY	G249	GLY	GLY	GLY	GLY	G249	GLY	GLY	GLY	GLY	GLY	G249	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
H1252	ALA	E915	H1252	P572	ARG	ARG	A251	LEU	LEU	LEU	A251	LEU	LEU	LEU	LEU	A251	LEU	LEU	LEU	LEU	LEU	A251	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU		
R1259	TRP	D1070	R1259	L575	GLY	GLY	C253	GLY	GLY	GLY	C253	GLY	GLY	GLY	GLY	C253	GLY	GLY	GLY	GLY	GLY	C253	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
R1271	R1087	N921	R1271	Q579	GLY	GLY	H255	GLY	GLY	GLY	H255	GLY	GLY	GLY	GLY	H255	GLY	GLY	GLY	GLY	GLY	H255	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
R1275	V1095	L922	R1275	L719	VAL	VAL	A256	VAL	VAL	VAL	A256	VAL	VAL	VAL	VAL	A256	VAL	VAL	VAL	VAL	VAL	A256	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL		
S1279	T1096	D943	S1279	E580	THR	THR	R261	THR	THR	THR	R261	THR	THR	THR	THR	R261	THR	THR	THR	THR	THR	R261	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
Q1280	E1099	L950	Q1280	N589	LYS	LYS	R275	LYS	LYS	LYS	R275	LYS	LYS	LYS	LYS	R275	LYS	LYS	LYS	LYS	LYS	R275	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS		
L1283	R1101	K951	L1283	N596	GLY	GLY	Q278	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
R1290	R1106	K952	R1290	V599	PRO	PRO	R289	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	
L1291	L1096	D943	L1291	N589	GLY	GLY	Q278	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	GLY	Q278	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
F1297	M1125	R976	F1297	V599	PRO	PRO	R289	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	PRO	R289	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
C1303	Q1130	V985	C1303	T958	GLN	GLN	D134	GLN	GLN	GLN	D134	GLN	GLN	GLN	GLN	D134	GLN	GLN	GLN	GLN	GLN	D134	GLN	GLN	GLN	GL																						

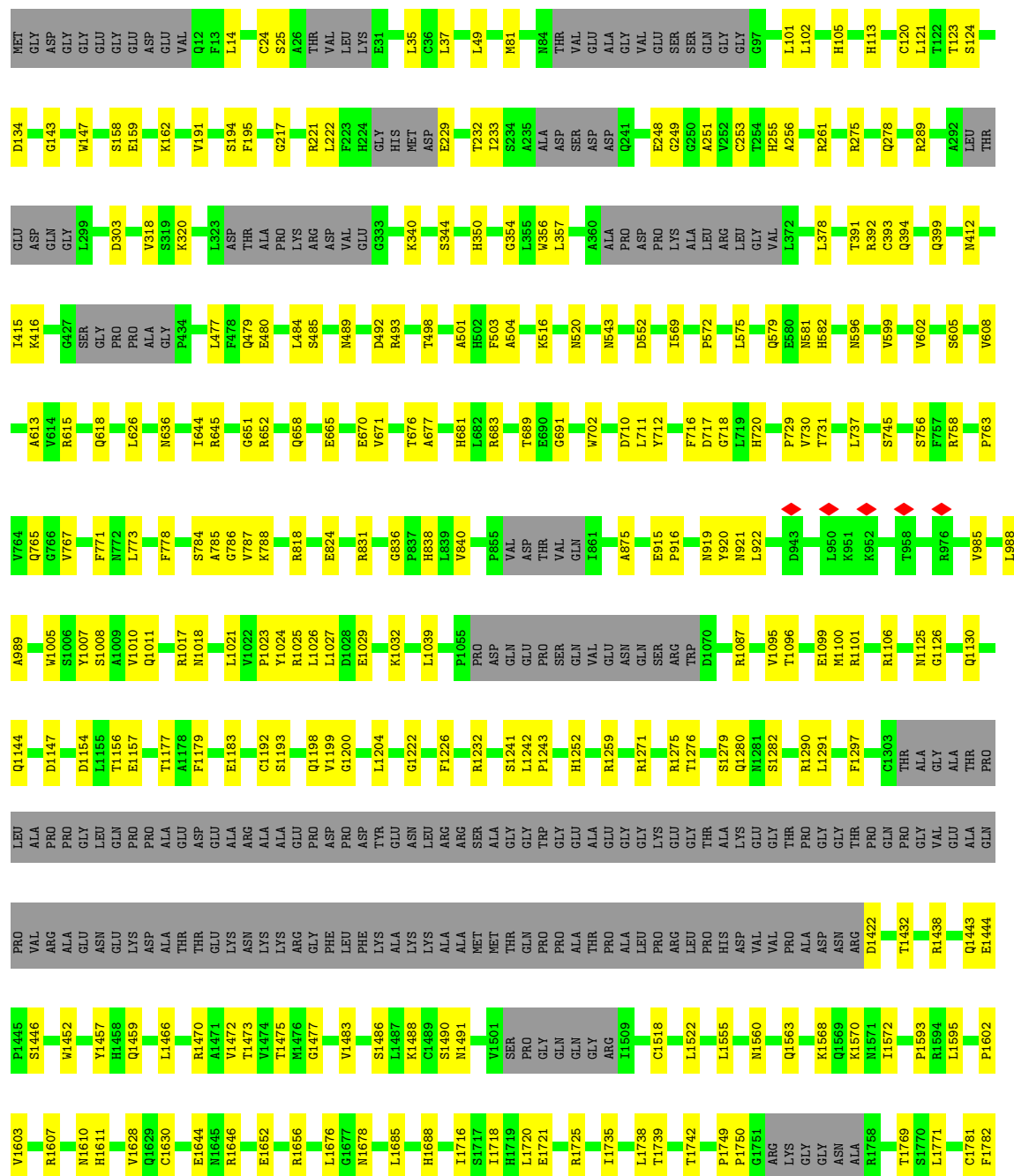


Y4849	K4774	B4703	G4656	V4245	I4058	V3841	P3697	L3579	GLN	P3344
L4850	Y4775	L4704	R4557	Q4246	L4059	D3877	L3698	PRO	SER	GLY
T4852	Q4776	V4705	N4558	T4247	R4085	D3878	D3717	GLY	GLY	P3351
F4856	Y4778	L4706	F4559	A4248	Q4249	C3892	E3718	GLU	SER	H3356
G4781	T4708	T4707	Y4561	Q4250	E4116	C3892	D3719	GLU	ASP	SER
Y4782	P4709	P4709	F4560	F4283	D4138	D3898	S3732	ASP	GLN	HIS
T4785	S4710	F4711	L4562	PRO	I4139	F3899	E3737	ALA	GLU	PHE
F4789	P4712	P4712	K4563	GLY	D4157	Q3900	GLY	ASP	ARG	P3359
L4790	Y4715	Y4715	A4566	GLU	P4158	N3901	GLY	ASP	THR	P3360
Y4791	D4717	D4717	F4571	PRO	R4159	R3904	GLU	E3590	LYS	V3372
S4792	K4718	K4718	N4574	GLU	M4162	T3913	ASN	E3610	LYS	V3372
F4796	F4719	F4719	F4575	ALA	N4162	T3913	GLY	HIS	ARG	E3376
M4798	V4720	V4720	L4577	ASP	E4182	T3917	GLY	PRO	ARG	E3388
S4799	L4725	L4725	L4578	GLU	I4183	L3926	GLU	TYR	GLY	GLY
L4800	G4729	G4729	P4586	GLY	I4190	E3944	GLU	SER	LEU	LEU
L4801	L4730	L4730	P4587	MET	I4193	E3945	GLU	LYS	VAL	VAL
G4802	I4731	I4731	F4587	ALA	Y4194	Q3946	VAL	ALA	GLN	THR
N4806	F4732	F4732	GLY	ALA	F4195	Q3946	E3750	TRP	THR	R3395
F4807	G4733	G4733	ASP	ALA	ALA	A3958	S3752	HIS	SER	P3410
F4808	R4734	R4734	ASP	ALA	T4200	A3958	F3753	LYS	ILE	P3410
H4812	E4735	E4735	PRO	GLU	W4205	V3961	E3757	L3623	VAL	P3427
L4813	L4737	L4737	MET	GLU	E4206	T3969	GLY	L3624	ALA	T3513
L4814	L4740	L4740	GLY	ALA	M4207	T3969	Q3761	S3625	ALA	P3427
Y4820	L4741	L4741	GLY	ALA	P4208	T3974	Y3765	R3629	ALA	ALA
K4821	Q4742	Q4742	ALA	GLY	Q4209	Q3977	Q3766	V3632	GLU	GLU
L4823	L4668	L4668	GLY	VAL	K4211	R3984	R3769	C3635	LEU	F3435
L4824	V4669	V4669	ASP	ALA	K4213	D3987	H3771	M3638	GLN	K3482
T4825	R4673	R4673	LEU	ALA	K4214	D3987	T3772	Y3642	ASP	ARG
I4826	E4676	E4676	GLY	GLY	R4215	K3997	R3773	H3647	GLU	GLU
S4828	K4680	K4680	ALA	ALA	F4217	H3998	M3793	R3648	ILE	M3534
T4831	L4681	L4681	PRO	ALA	I4218	M3999	V3794	H3647	GLU	E3547
H4832	F4682	F4682	PRO	ALA	D4219	M3999	S3795	D3676	SER	MET
N4833	G4683	G4683	GLY	LYS	W4221	L4003	S3796	L3677	VAL	PHE
G4834	D4684	D4684	SER	LYS	V4222	S4007	T3797	S3678	ARG	THR
Q4835	L4686	L4686	GLY	GLU	N4223	D4046	L3798	K3679	GLU	LEU
Q4836	Y4687	Y4687	GLY	ALA	E4224	M4047	K3799	L3563	PHE	THR
L4837	I4688	I4688	SER	ALA	M4231	L4048	I3604	E3684	ALA	ALA
V4838	T4689	T4689	GLY	LEU	M4231	V4049	S3604	GLU	ASP	ASP
M4839	P4692	P4692	ALA	ARG	E4232	Q4043	N3809	GLU	SER	SER
T4840	GLY	GLY	ALA	LEU	L4233	Q4043	A3810	GLU	LYS	LYS
V4841	GLY	GLY	MET	GLY	F4234	D4046	Q3813	GLU	VAL	VAL
G4842	ASP	ASP	GLU	TRP	V4235	M4047	Q3814	VAL	GLY	GLY
L4843	GLY	GLY	GLU	GLY	S4236	L4048	Q3815	GLU	ALA	ALA
L4844	ASP	ASP	ALA	ALA	D4240	V4049	K3815	GLU	SER	LYS
A4845	D4696	D4696	GLY	ALA	T4241	M4054	F3829	GLU	ALA	ALA
V4846	V4697	V4697	GLY	ARG	I4242	M4054	F3829	F3693	GLY	GLY
V4847	K4698	K4698	ASP	ALA	F4243	M4054	F3829	K3693	SER	ASP
V4848	D4702	D4702	ASP	GLY	E4244	M4057	S3840	D3696	ALA	ALA



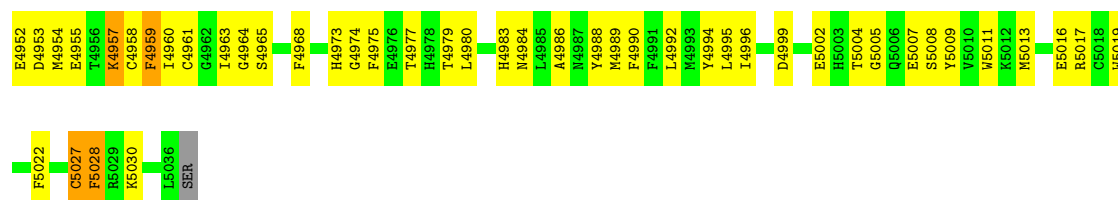
• Molecule 1: Ryanodine receptor 1

Chain C: 63% 15% 22%

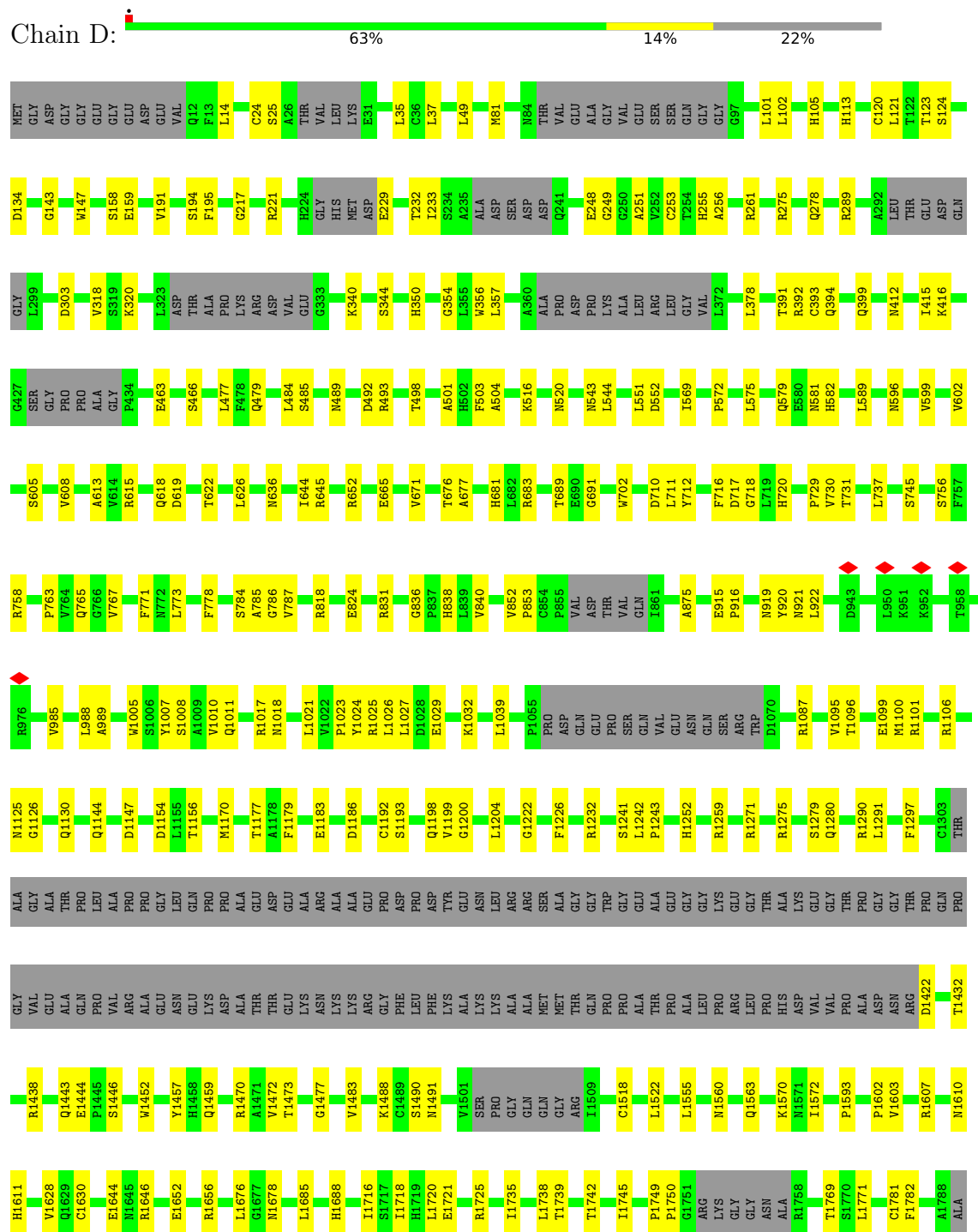








• Molecule 1: Ryanodine receptor 1

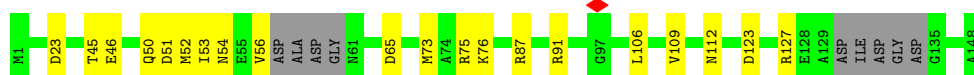
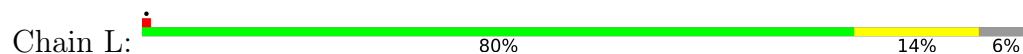




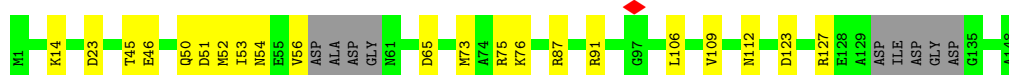
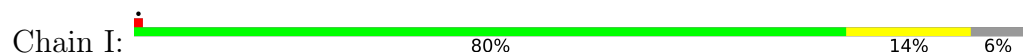




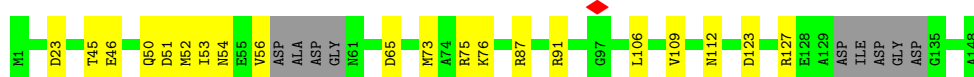
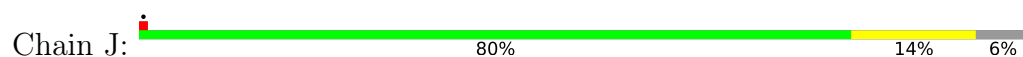
• Molecule 2: Calmodulin-1



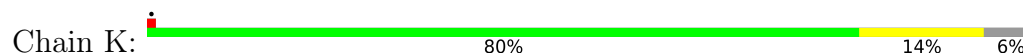
• Molecule 2: Calmodulin-1



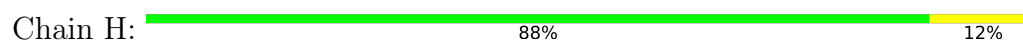
• Molecule 2: Calmodulin-1



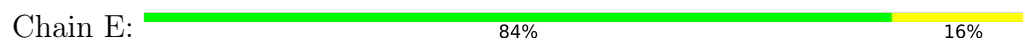
• Molecule 2: Calmodulin-1



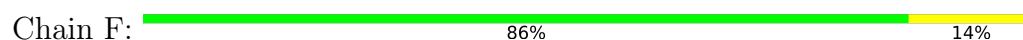
• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

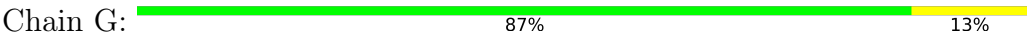


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B





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



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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, ATP, CA

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	0.39	6/28349 (0.0%)	0.67	49/38619 (0.1%)
1	B	0.39	6/28349 (0.0%)	0.66	43/38619 (0.1%)
1	C	0.39	6/28349 (0.0%)	0.67	48/38619 (0.1%)
1	D	0.39	7/28349 (0.0%)	0.67	48/38619 (0.1%)
2	I	0.20	0/1052	0.44	0/1416
2	J	0.20	0/1052	0.44	0/1416
2	K	0.20	0/1052	0.44	0/1416
2	L	0.20	0/1052	0.44	0/1416
3	E	0.23	0/820	0.52	0/1105
3	F	0.23	0/820	0.52	0/1105
3	G	0.23	0/820	0.51	0/1105
3	H	0.23	0/820	0.52	0/1105
All	All	0.38	25/120884 (0.0%)	0.66	188/164560 (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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4200	THR	C-N	8.97	1.46	1.34
1	B	4200	THR	C-N	8.97	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4200	THR	C-N	8.97	1.46	1.34
1	D	4200	THR	C-N	8.97	1.46	1.34
1	A	4943	LEU	C-O	6.56	1.31	1.24
1	B	4943	LEU	C-O	6.56	1.31	1.24
1	C	4943	LEU	C-O	6.56	1.31	1.24
1	D	4943	LEU	C-O	6.56	1.31	1.24
1	A	4717	ASP	CA-C	-6.26	1.44	1.52
1	B	4717	ASP	CA-C	-6.26	1.44	1.52
1	C	4717	ASP	CA-C	-6.26	1.44	1.52
1	D	4717	ASP	CA-C	-6.26	1.44	1.52
1	A	4716	TRP	CA-C	-6.07	1.44	1.52
1	B	4716	TRP	CA-C	-6.07	1.44	1.52
1	C	4716	TRP	CA-C	-6.07	1.44	1.52
1	D	4716	TRP	CA-C	-6.06	1.44	1.52
1	A	4920	PHE	CA-C	-5.87	1.45	1.52
1	B	4920	PHE	CA-C	-5.87	1.45	1.52
1	C	4920	PHE	CA-C	-5.87	1.45	1.52
1	D	4920	PHE	CA-C	-5.87	1.45	1.52
1	A	4917	ASP	CA-C	-5.66	1.47	1.53
1	B	4917	ASP	CA-C	-5.66	1.47	1.53
1	C	4917	ASP	CA-C	-5.66	1.47	1.53
1	D	4917	ASP	CA-C	-5.66	1.47	1.53
1	D	5027	CYS	CA-C	-5.08	1.46	1.52

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	GLY	CA-C-N	15.87	139.68	119.84
1	A	836	GLY	C-N-CA	15.87	139.68	119.84
1	B	836	GLY	CA-C-N	15.87	139.68	119.84
1	B	836	GLY	C-N-CA	15.87	139.68	119.84
1	C	836	GLY	CA-C-N	15.87	139.68	119.84
1	C	836	GLY	C-N-CA	15.87	139.68	119.84
1	D	836	GLY	CA-C-N	15.85	139.65	119.84
1	D	836	GLY	C-N-CA	15.85	139.65	119.84
1	C	4919	THR	N-CA-C	-13.14	97.88	114.56
1	A	4919	THR	N-CA-C	-13.13	97.88	114.56
1	B	4919	THR	N-CA-C	-13.13	97.88	114.56
1	D	4919	THR	N-CA-C	-13.13	97.88	114.56
1	A	4200	THR	CA-C-N	12.21	137.87	120.28
1	A	4200	THR	C-N-CA	12.21	137.87	120.28
1	D	4200	THR	CA-C-N	12.21	137.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4200	THR	C-N-CA	12.21	137.87	120.28
1	B	4200	THR	CA-C-N	12.19	137.83	120.28
1	B	4200	THR	C-N-CA	12.19	137.83	120.28
1	C	4200	THR	CA-C-N	12.19	137.83	120.28
1	C	4200	THR	C-N-CA	12.19	137.83	120.28
1	A	4200	THR	O-C-N	-11.48	106.05	122.36
1	B	4200	THR	O-C-N	-11.48	106.05	122.36
1	C	4200	THR	O-C-N	-11.48	106.05	122.36
1	D	4200	THR	O-C-N	-11.48	106.05	122.36
1	D	3188	PRO	N-CA-CB	11.04	110.56	102.28
1	A	3188	PRO	N-CA-CB	10.98	110.52	102.28
1	B	3188	PRO	N-CA-CB	10.96	110.50	102.28
1	C	3188	PRO	N-CA-CB	10.96	110.50	102.28
1	D	5028	PHE	N-CA-C	-9.47	100.96	111.28
1	A	4933	GLN	N-CA-C	-9.04	101.37	111.14
1	C	4933	GLN	N-CA-C	-9.04	101.37	111.14
1	C	5028	PHE	N-CA-C	-9.04	101.42	111.28
1	D	4933	GLN	N-CA-C	-9.04	101.37	111.14
1	B	4933	GLN	N-CA-C	-9.04	101.38	111.14
1	A	5028	PHE	N-CA-CB	8.64	122.83	110.12
1	D	4715	TYR	N-CA-C	-8.57	94.27	108.32
1	A	4715	TYR	N-CA-C	-8.56	94.28	108.32
1	C	4715	TYR	N-CA-C	-8.56	94.28	108.32
1	B	4715	TYR	N-CA-C	-8.55	94.31	108.32
1	D	836	GLY	C-N-CD	-8.26	91.14	125.00
1	A	836	GLY	C-N-CD	-8.25	91.18	125.00
1	C	836	GLY	C-N-CD	-8.25	91.18	125.00
1	B	836	GLY	C-N-CD	-8.24	91.21	125.00
1	A	3302	PRO	N-CA-CB	8.24	111.07	103.08
1	C	3302	PRO	N-CA-CB	8.24	111.07	103.08
1	D	3302	PRO	N-CA-CB	8.24	111.07	103.08
1	B	3302	PRO	N-CA-CB	8.23	111.06	103.08
1	A	5028	PHE	N-CA-C	-8.17	102.37	111.28
1	A	3301	PRO	N-CA-CB	7.96	110.80	103.08
1	B	3301	PRO	N-CA-CB	7.96	110.80	103.08
1	C	3301	PRO	N-CA-CB	7.96	110.80	103.08
1	D	3301	PRO	N-CA-CB	7.96	110.80	103.08
1	B	3527	PRO	N-CA-CB	7.96	110.52	102.17
1	A	3527	PRO	N-CA-CB	7.92	110.49	102.17
1	D	3527	PRO	N-CA-CB	7.92	110.49	102.17
1	C	3527	PRO	N-CA-CB	7.89	110.45	102.17
1	B	2640	PRO	N-CA-CB	7.79	110.70	103.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2640	PRO	N-CA-CB	7.79	110.70	103.46
1	A	2640	PRO	N-CA-CB	7.78	110.69	103.46
1	D	2640	PRO	N-CA-CB	7.74	110.66	103.46
1	A	3344	PRO	N-CA-CB	7.68	110.60	103.46
1	B	3344	PRO	N-CA-CB	7.68	110.60	103.46
1	C	3344	PRO	N-CA-CB	7.68	110.60	103.46
1	B	3351	PRO	N-CA-CB	7.66	110.59	103.46
1	C	5028	PHE	N-CA-CB	7.66	121.39	110.12
1	D	3351	PRO	N-CA-CB	7.66	110.59	103.46
1	A	3351	PRO	N-CA-CB	7.65	110.57	103.46
1	D	3344	PRO	N-CA-CB	7.64	110.57	103.46
1	D	4676	GLU	N-CA-C	-7.64	104.86	114.56
1	C	3351	PRO	N-CA-CB	7.63	110.55	103.46
1	B	4676	GLU	N-CA-C	-7.62	104.89	114.56
1	A	4676	GLU	N-CA-C	-7.62	104.89	114.56
1	C	4676	GLU	N-CA-C	-7.62	104.89	114.56
1	D	5028	PHE	N-CA-CB	7.58	121.27	110.12
1	B	3282	PRO	N-CA-CB	7.29	111.25	103.52
1	C	3282	PRO	N-CA-CB	7.28	111.23	103.52
1	A	3282	PRO	N-CA-CB	7.25	111.20	103.52
1	D	3282	PRO	N-CA-CB	7.25	111.20	103.52
1	C	3303	PRO	N-CA-CB	7.22	110.83	103.25
1	D	3303	PRO	N-CA-CB	7.22	110.83	103.25
1	A	3303	PRO	N-CA-CB	7.20	110.81	103.25
1	B	3303	PRO	N-CA-CB	7.20	110.81	103.25
1	D	3208	PRO	N-CA-CB	7.19	110.80	103.25
1	B	3208	PRO	N-CA-CB	7.18	110.79	103.25
1	C	3208	PRO	N-CA-CB	7.18	110.79	103.25
1	A	3208	PRO	N-CA-CB	7.18	110.79	103.25
1	B	3275	PRO	N-CA-CB	7.09	110.70	102.76
1	D	3275	PRO	N-CA-CB	7.09	110.70	102.76
1	A	3427	PRO	N-CA-CB	7.08	110.69	103.25
1	B	3427	PRO	N-CA-CB	7.08	110.69	103.25
1	C	3427	PRO	N-CA-CB	7.08	110.69	103.25
1	D	3427	PRO	N-CA-CB	7.08	110.69	103.25
1	A	3275	PRO	N-CA-CB	7.07	110.67	102.76
1	C	3275	PRO	N-CA-CB	7.06	110.67	102.76
1	A	3297	PRO	N-CA-CB	6.91	110.85	103.52
1	D	3297	PRO	N-CA-CB	6.91	110.85	103.52
1	C	3297	PRO	N-CA-CB	6.89	110.82	103.52
1	C	3202	PRO	N-CA-CB	6.87	110.46	103.25
1	D	3202	PRO	N-CA-CB	6.86	110.45	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3297	PRO	N-CA-CB	6.85	110.78	103.52
1	A	3202	PRO	N-CA-CB	6.85	110.44	103.25
1	D	3519	PRO	N-CA-CB	6.84	110.77	103.52
1	C	3294	PRO	N-CA-CB	6.83	110.42	103.25
1	D	3294	PRO	N-CA-CB	6.83	110.42	103.25
1	C	3293	PRO	N-CA-CB	6.83	110.51	103.00
1	B	3202	PRO	N-CA-CB	6.83	110.42	103.25
1	C	3519	PRO	N-CA-CB	6.83	110.75	103.52
1	A	3519	PRO	N-CA-CB	6.81	110.74	103.52
1	A	3294	PRO	N-CA-CB	6.81	110.40	103.25
1	B	3519	PRO	N-CA-CB	6.79	110.72	103.52
1	A	3293	PRO	N-CA-CB	6.79	110.47	103.00
1	B	3293	PRO	N-CA-CB	6.79	110.47	103.00
1	C	3062	PRO	N-CA-CB	6.79	110.47	103.00
1	B	3294	PRO	N-CA-CB	6.79	110.38	103.25
1	A	5027	CYS	N-CA-C	-6.78	98.70	108.60
1	A	3062	PRO	N-CA-CB	6.77	110.45	103.00
1	B	3062	PRO	N-CA-CB	6.77	110.45	103.00
1	D	3293	PRO	N-CA-CB	6.75	110.43	103.00
1	B	3004	PRO	N-CA-CB	6.75	110.34	103.25
1	A	3004	PRO	N-CA-CB	6.74	110.33	103.25
1	C	3004	PRO	N-CA-CB	6.74	110.33	103.25
1	D	3004	PRO	N-CA-CB	6.74	110.33	103.25
1	D	3062	PRO	N-CA-CB	6.74	110.42	103.00
1	B	3410	PRO	N-CA-CB	6.72	110.31	103.25
1	B	3224	PRO	N-CA-CB	6.72	110.64	103.52
1	A	5027	CYS	CA-C-N	-6.70	111.30	120.28
1	A	5027	CYS	C-N-CA	-6.70	111.30	120.28
1	A	3360	PRO	N-CA-CB	6.69	110.17	102.88
1	B	3360	PRO	N-CA-CB	6.69	110.17	102.88
1	C	5016	GLU	N-CA-C	-6.69	104.26	114.16
1	C	3360	PRO	N-CA-CB	6.69	110.17	102.88
1	D	3410	PRO	N-CA-CB	6.69	110.27	103.25
1	A	3224	PRO	N-CA-CB	6.68	110.60	103.52
1	D	3224	PRO	N-CA-CB	6.68	110.60	103.52
1	D	5016	GLU	N-CA-C	-6.68	104.28	114.16
1	A	3410	PRO	N-CA-CB	6.68	110.26	103.25
1	C	3410	PRO	N-CA-CB	6.68	110.26	103.25
1	B	5016	GLU	N-CA-C	-6.67	104.28	114.16
1	A	5016	GLU	N-CA-C	-6.67	104.29	114.16
1	C	3224	PRO	N-CA-CB	6.67	110.59	103.52
1	D	3360	PRO	N-CA-CB	6.66	110.14	102.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4942	GLU	O-C-N	-6.46	114.32	122.27
1	B	4942	GLU	O-C-N	-6.45	114.34	122.27
1	A	4942	GLU	O-C-N	-6.44	114.34	122.27
1	C	4942	GLU	O-C-N	-6.44	114.34	122.27
1	D	4920	PHE	N-CA-C	-6.18	97.62	110.80
1	B	4920	PHE	N-CA-C	-6.18	97.64	110.80
1	A	4920	PHE	N-CA-C	-6.17	97.66	110.80
1	C	4920	PHE	N-CA-C	-6.17	97.66	110.80
1	D	5027	CYS	CA-C-N	-6.14	112.06	120.28
1	D	5027	CYS	C-N-CA	-6.14	112.06	120.28
1	D	4851	TYR	N-CA-C	-6.13	104.68	111.36
1	B	4851	TYR	N-CA-C	-6.11	104.70	111.36
1	A	4851	TYR	N-CA-C	-6.11	104.70	111.36
1	C	4851	TYR	N-CA-C	-6.09	104.73	111.36
1	C	4717	ASP	N-CA-C	-6.07	97.88	110.80
1	C	5027	CYS	CA-C-N	-6.06	112.16	120.28
1	C	5027	CYS	C-N-CA	-6.06	112.16	120.28
1	A	4717	ASP	N-CA-C	-6.06	97.90	110.80
1	B	4717	ASP	N-CA-C	-6.05	97.92	110.80
1	D	4717	ASP	N-CA-C	-6.05	97.92	110.80
1	B	1718	ILE	N-CA-C	-5.92	108.08	113.71
1	C	1718	ILE	N-CA-C	-5.91	108.10	113.71
1	A	1718	ILE	N-CA-C	-5.90	108.11	113.71
1	D	1718	ILE	N-CA-C	-5.90	108.11	113.71
1	A	4902	GLU	CA-C-N	-5.88	110.05	123.15
1	A	4902	GLU	C-N-CA	-5.88	110.05	123.15
1	B	4902	GLU	CA-C-N	-5.88	110.05	123.15
1	B	4902	GLU	C-N-CA	-5.88	110.05	123.15
1	D	4902	GLU	CA-C-N	-5.88	110.05	123.15
1	D	4902	GLU	C-N-CA	-5.88	110.05	123.15
1	C	4902	GLU	CA-C-N	-5.86	110.07	123.15
1	C	4902	GLU	C-N-CA	-5.86	110.07	123.15
1	D	5027	CYS	N-CA-C	-5.80	100.32	108.96
1	C	5027	CYS	N-CA-C	-5.42	100.88	108.96
1	C	4943	LEU	CA-C-O	5.42	126.48	120.63
1	A	4943	LEU	CA-C-O	5.39	126.45	120.63
1	B	4943	LEU	CA-C-O	5.39	126.45	120.63
1	D	4943	LEU	CA-C-O	5.39	126.45	120.63
1	A	4191	GLU	N-CA-C	5.34	115.58	108.38
1	C	318	VAL	N-CA-C	-5.31	108.33	113.53
1	B	318	VAL	N-CA-C	-5.30	108.34	113.53
1	A	318	VAL	N-CA-C	-5.28	108.35	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	VAL	N-CA-C	-5.28	108.35	113.53
1	C	4791	TYR	N-CA-C	-5.27	104.97	111.40
1	A	4791	TYR	N-CA-C	-5.24	105.00	111.40
1	D	4791	TYR	N-CA-C	-5.23	105.02	111.40
1	B	4791	TYR	N-CA-C	-5.21	105.04	111.40

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	519	0
1	B	27821	0	24966	522	0
1	C	27821	0	24966	524	0
1	D	27821	0	24966	516	0
2	I	1042	0	972	13	0
2	J	1042	0	972	12	0
2	K	1042	0	972	13	0
2	L	1042	0	972	13	0
3	E	804	0	812	10	0
3	F	804	0	812	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	804	0	812	8	0
3	H	804	0	812	8	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	2134	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 (2134) 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
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:4986:ALA:HA	1:B:4989:MET:HE1	1.55	0.89
1:C:4986:ALA:HA	1:C:4989:MET:HE1	1.55	0.89
1:B:4182:GLU:OE2	1:B:5028:PHE:N	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4986:ALA:HA	1:D:4989:MET:HE1	1.55	0.88
1:A:4986:ALA:HA	1:A:4989:MET:HE1	1.55	0.88
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:A:4741:LEU:HB2	1:A:4743:MET:HE3	1.64	0.78
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:D:4741:LEU:HB2	1:D:4743:MET:HE3	1.64	0.78
1:B:4958:CYS:SG	1:B:4959:PHE:N	2.57	0.78
1:C:4741:LEU:HB2	1:C:4743:MET:HE3	1.64	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:B:4741:LEU:HB2	1:B:4743:MET:HE3	1.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.57	0.75
1:B:5027:CYS:O	1:B:5028:PHE:C	2.27	0.74
1:C:4680:LYS:HE2	1:C:4686:LEU:HD11	1.70	0.74
1:C:4958:CYS:SG	1:C:4959:PHE:N	2.57	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:D:4920:PHE:O	1:D:4921:PHE:C	2.32	0.73
1:B:4920:PHE:O	1:B:4921:PHE:C	2.32	0.72
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:A:4920:PHE:O	1:A:4921:PHE:C	2.32	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:C:4920:PHE:O	1:C:4921:PHE:C	2.32	0.70
1:B:4219:PHE:CD1	1:B:4950:VAL:HG21	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:B:4631:PHE:HE2	1:B:4639:MET:HE3	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4631:PHE:HE2	1:C:4639:MET:HE3	1.58	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:C:4231:MET:HG3	1:C:5022:PHE:HD2	1.58	0.69
1:D:4937:ILE:HG13	1:D:4938:ASP:N	2.07	0.69
1:A:4231:MET:HG3	1:A:5022:PHE:HD2	1.58	0.69
1:A:4631:PHE:HE2	1:A:4639:MET:HE3	1.58	0.69
1:C:4952:GLU:O	1:C:4954:MET:N	2.26	0.69
1:D:4631:PHE:HE2	1:D:4639:MET:HE3	1.58	0.69
1:D:4952:GLU:O	1:D:4954:MET:N	2.26	0.69
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:4934:GLY:O	1:A:4935:LEU:C	2.41	0.64
1:B:393:CYS:SG	1:B:394:GLN:N	2.70	0.64
1:C:4934:GLY:O	1:C:4935:LEU:C	2.41	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:393:CYS:SG	1:C:394:GLN:N	2.70	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
1:D:5028:PHE:C	1:D:5030:LYS:H	2.06	0.63
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:D:4946:GLN:O	1:D:4947:GLN:C	2.41	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:B:2233:CYS:HG	1:B:2270:SER:HG	1.48	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:A:4638:TYR:C	1:A:4641:PRO:HD2	2.24	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:C:4638:TYR:C	1:C:4641:PRO:HD2	2.24	0.62
1:D:4563:LYS:O	1:D:4566:ALA:N	2.32	0.62
1:B:4716:TRP:CD1	1:B:4716:TRP:H	2.18	0.62
1:A:4741:LEU:CB	1:A:4743:MET:HE3	2.30	0.61
1:C:5028:PHE:C	1:C:5030:LYS:H	2.08	0.61
1:C:4235:VAL:HG11	1:C:5019:TRP:CH2	2.36	0.61
1:C:4716:TRP:H	1:C:4716:TRP:CD1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4638:TYR:C	1:B:4641:PRO:HD2	2.24	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:B:4741:LEU:CB	1:B:4743:MET:HE3	2.30	0.61
1:C:4741:LEU:CB	1:C:4743:MET:HE3	2.30	0.61
1:D:4638:TYR:C	1:D:4641:PRO:HD2	2.24	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: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:D:4934:GLY:O	1:D:4935:LEU:C	2.41	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
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:4716:TRP:CD1	1:A:4716:TRP:H	2.18	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:B:4934:GLY:O	1:B:4935:LEU:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:4946:GLN:O	1:C:4947:GLN:C	2.41	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
1:A:5028:PHE:C	1:A:5030:LYS:H	2.09	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:D:4716:TRP:CD1	1:D:4716:TRP:H	2.18	0.60
1:B:4942:GLU:O	1:B:4943:LEU:C	2.42	0.59
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
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:2233:CYS:HG	1:A:2270:SER:HG	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1452:TRP:NE1	1:B:1518:CYS:SG	2.73	0.59
1:D:4741:LEU:CB	1:D:4743:MET:HE3	2.30	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
1:B:4946:GLN:O	1:B:4947:GLN:C	2.41	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:A:415:ILE:O	1:A:493:ARG:NH2	2.35	0.58
1:A:4942:GLU:O	1:A:4943:LEU:C	2.42	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:D:4940:PHE:O	1:D:4941:GLY:C	2.46	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:OD1	1:C:3987:ASP:N	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
1:A:4798:MET:O	1:A:4801:LEU:N	2.36	0.58
1:A:4950:VAL:O	1:A:4951:LYS:C	2.45	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:A:4946:GLN:O	1:A:4947:GLN:C	2.41	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:C:4631:PHE:CE2	1:C:4639:MET:HE3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1929:MET:HE3	1:D:1931:LEU:HD21	1.85	0.58
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.36	0.58
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.77	0.58
1:B:4631:PHE:CE2	1:B:4639:MET:HE3	2.39	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:D:4631:PHE:CE2	1:D:4639:MET:HE3	2.39	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:1452:TRP:NE1	1:D:1518:CYS:SG	2.73	0.58
1:D:2254:LEU:HA	1:D:2257:LEU:HB2	1.85	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:A:4631:PHE:CE2	1:A:4639:MET:HE3	2.39	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:4950:VAL:O	1:C:4951:LYS:C	2.45	0.58
1:A:1721:GLU:OE1	1:A:1725:ARG:NH1	2.37	0.57
1:A:4940:PHE:O	1:A:4941:GLY:C	2.46	0.57
1:D:4950:VAL:O	1:D:4951:LYS:C	2.45	0.57
1:A:1929:MET:HE3	1:A:1931:LEU:HD21	1.85	0.57
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.37	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1929:MET:HE3	1:C:1931:LEU:HD21	1.85	0.57
1:D:569:ILE:HD13	1:D:605:SER:HB2	1.86	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:A:2254:LEU:HA	1:A:2257:LEU:HB2	1.85	0.57
1:B:1232:ARG:NH1	1:B:1828:ASP:O	2.37	0.57
1:B:4950:VAL:O	1:B:4951:LYS:C	2.45	0.57
1:C:120:CYS:SG	1:C:121:LEU:N	2.77	0.57
1:C:3752:SER:OG	1:C:3753:PHE:N	2.36	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:4210:VAL:O	1:D:4211:LYS:C	2.48	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: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: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
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
1:C:4940:PHE:O	1:C:4941:GLY:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:4942:GLU:O	1:C:4943:LEU:C	2.42	0.56
1:A:4688:ILE:HD11	1:A:4737:ILE:CG1	2.35	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: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
1:B:1929:MET:HE3	1:B:1931:LEU:HD21	1.85	0.56
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:C:4210:VAL:O	1:C:4211:LYS:C	2.48	0.56
1:A:320:LYS:HG3	1:A:356:TRP:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:4942:GLU:O	1:D:4943:LEU:C	2.42	0.56
1:A:1192:CYS:SG	1:A:1193:SER:N	2.79	0.56
1:A:1856:ASP:OD1	1:A:1856:ASP:N	2.39	0.56
1:A:3987:ASP:OD1	1:A:3987:ASP:N	2.36	0.56
1:B:4214:LYS:O	1:B:4215:ARG:C	2.49	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
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:4210:VAL:O	1:B:4211:LYS:C	2.48	0.56
1:B:4825:THR:HA	1:B:4828:SER:OG	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:4210:VAL:O	1:A:4211:LYS:C	2.48	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: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: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
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: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:4214:LYS:O	1:C:4215:ARG:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4920:PHE:O	1:A:4922:PHE:N	2.40	0.55
1:B:134:ASP:N	1:B:134:ASP:OD1	2.39	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
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
1:A:4936:ILE:O	1:A:4937:ILE:C	2.47	0.54
3:E:23:VAL:HG22	3:E:104:LEU:HD13	1.89	0.54
1:D:3878:ASP:OD1	1:D:3878:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4719:PHE:O	1:D:4720:VAL:C	2.50	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:B:4940:PHE:O	1:B:4941:GLY:C	2.46	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:3809:ASN:O	1:D:3813:GLN:NE2	2.41	0.54
1:D:4214:LYS:O	1:D:4215:ARG:C	2.49	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:OD1	1:C:3878:ASP:N	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
1:D:4936:ILE:O	1:D:4937:ILE:C	2.47	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1290:ARG:NH1	1:D:1291:LEU:O	2.41	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: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: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
2:I:52:MET:HE1	2:I:75:ARG:HH21	1.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:52:MET:HE1	2:K:75:ARG:HH21	1.73	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
2:L:52:MET:HE1	2:L:75:ARG:HH21	1.73	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
1:D:4195:PHE:HB2	1:D:4994:TYR:CE2	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2531:ARG:NH2	1:A:2581:SER:OG	2.41	0.53
1:A:4719:PHE:O	1:A:4720:VAL:C	2.50	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:B:4719:PHE:O	1:B:4720:VAL:C	2.50	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:4214:LYS:O	1:A:4215:ARG:C	2.49	0.52
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
2:J:52:MET:HE1	2:J:75:ARG:HH21	1.73	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
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:C:1477:GLY:HA3	1:C:1483:VAL:HA	1.91	0.52
1:D:4215:ARG:O	1:D:4216:GLN:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:4936:ILE:O	1:C:4937:ILE:C	2.47	0.52
1:C:4961:CYS:HB3	1:C:4983:HIS:CE1	2.45	0.52
1:C:5027:CYS:O	1:C:5028:PHE:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:2333:ASP:N	1:D:2333:ASP:OD1	2.40	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:C:4719:PHE:O	1:C:4720:VAL:C	2.51	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:C:552:ASP:OD1	1:C:552:ASP:N	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:2516:ASP:OD1	1:A:2516:ASP:N	2.39	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4205:TRP:CH2	1:A:4989:MET:HE3	2.46	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
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
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:4205:TRP:CH2	1:D:4989:MET:HE3	2.46	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:4740:LEU:HD23	1:B:4741:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4158:PRO:O	1:C:4162:ASN:ND2	2.43	0.51
1:D:745:SER:OG	1:D:758:ARG:O	2.29	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:4205:TRP:CH2	1:B:4989:MET:HE3	2.46	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: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: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:A:4212:GLU:O	1:A:4213:SER:C	2.54	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:B:4936:ILE:O	1:B:4937:ILE:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:LEU:HD21	1:A:1226:PHE:HD2	1.77	0.50
1:A:4215:ARG:O	1:A:4216:GLN:C	2.52	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: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:1769:THR:OG1	1:D:1956:GLU:OE1	2.28	0.50
1:D:4733:GLY:O	1:D:4736:ARG:N	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3795:SER:O	1:A:3799:LYS:NZ	2.45	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
2:I:51:ASP:OD1	2:I:51:ASP:N	2.44	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:B:251:ALA:O	1:B:255:HIS:ND1	2.37	0.50
1:B:391:THR:OG1	1:B:392:ARG:N	2.42	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:C:4205:TRP:CH2	1:C:4989:MET:HE3	2.46	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: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:C:4717:ASP:O	1:C:4718:LYS:CB	2.60	0.49
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:C:4215:ARG:O	1:C:4216:GLN:C	2.52	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:A:1771:LEU:HD23	1:A:2153:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4212:GLU:O	1:D:4213:SER:C	2.54	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:745:SER:OG	1:B:758:ARG:O	2.29	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
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:2199:ARG:NH1	1:B:2246:ASN:OD1	2.45	0.49
1:B:4213:SER:O	1:B:4214:LYS:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:5027:CYS:O	1:A:5028:PHE:C	2.46	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
2:I:23:ASP:OD1	2:I:23:ASP:N	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: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
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:C:3999:MET:HE3	1:C:4003:LEU:HD11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4210:VAL:HG12	1:D:4211:LYS:N	2.26	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:4215:ARG:O	1:B:4216:GLN:C	2.52	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:4989:MET:HB2	1:A:4989:MET:HE2	1.33	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
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:3795:SER:O	1:D:3799:LYS:NZ	2.45	0.48
1:D:4801:LEU:HB3	1:D:4808:PHE:CD2	2.48	0.48
1:D:4989:MET:HB2	1:D:4989:MET:HE2	1.33	0.48
1:A:391:THR:OG1	1:A:392:ARG:N	2.42	0.48
1:A:552:ASP:OD1	1:A:552:ASP:N	2.43	0.48
2:L:23:ASP:OD1	2:L:23:ASP:N	2.45	0.48
1:B:2572:THR:OG1	1:B:2615:ARG:NH1	2.44	0.48
1:B:4963:ILE:HD12	1:B:4964:GLY:H	1.78	0.48
1:C:3795:SER:O	1:C:3799:LYS:NZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4937:ILE:HG13	1:D:4938:ASP:H	1.79	0.48
1:A:710:ASP:N	1:A:710:ASP:OD1	2.44	0.48
1:A:1769:THR:OG1	1:A:1956:GLU:OE1	2.28	0.48
1:A:2579:VAL:HA	1:A:2582:MET:HB2	1.96	0.48
1:A:3999:MET:HE3	1:A:4003:LEU:HD11	1.95	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: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:C:1972:ASN:O	1:C:1976:ARG:NH1	2.46	0.48
1:C:4212:GLU:O	1:C:4213:SER:C	2.54	0.48
1:C:4213:SER:O	1:C:4214:LYS:C	2.55	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: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:4574:ASN:ND2	1:A:4813:LEU:HD22	2.29	0.48
1:B:4212:GLU:O	1:B:4213:SER:C	2.54	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1452:TRP:NE1	1:B:1518:CYS:HG	2.11	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:D:3999:MET:HE3	1:D:4003:LEU:HD11	1.95	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:1490:SER:OG	1:D:1491:ASN:N	2.47	0.47
1:D:4049:VAL:HG11	1:D:4159:ARG:HD2	1.94	0.47
1:D:4213:SER:O	1:D:4214:LYS:C	2.55	0.47
1:D:4240:ASP:O	1:D:4243:PHE:N	2.35	0.47
1:D:5027:CYS:O	1:D:5028:PHE:C	2.50	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:OD1	1:C:3717:ASP:N	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:D:5028:PHE:C	1:D:5030:LYS:N	2.71	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
1:B:3999:MET:HE3	1:B:4003:LEU:HD11	1.95	0.47
1:C:412:ASN:O	1:C:416:LYS:NZ	2.47	0.47
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:412:ASN:O	1:B:416:LYS:NZ	2.47	0.47
1:B:1444:GLU:HG3	1:B:1446:SER:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:5028:PHE:C	1:C:5030:LYS:N	2.72	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:A:4213:SER:O	1:A:4214:LYS:C	2.55	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
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:B:4233:LEU:O	1:B:4236:SER:OG	2.25	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
1:C:1926:LEU:HA	1:C:1929:MET:HE2	1.96	0.47
1:C:2165:LEU:HD21	1:C:2178:MET:HE2	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: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:D:4047:MET:HE2	1:D:4047:MET:HB2	1.80	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:1926:LEU:HA	1:B:1929:MET:HE2	1.96	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:3717:ASP:OD1	1:D:3717:ASP:N	2.41	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: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:4047:MET:HE2	1:A:4047:MET:HB2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4543:GLU:HA	1:D:4546:VAL:HG22	1.96	0.47
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:784:SER:OG	1:C:785:ALA:N	2.41	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:D:1926:LEU:HA	1:D:1929:MET:HE2	1.96	0.46
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	1.95	0.46
1:A:1926:LEU:HA	1:A:1929:MET:HE2	1.96	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:412:ASN:O	1:D:416:LYS:NZ	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4047:MET:HE2	1:C:4047:MET:HB2	1.80	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
1:C:4946:GLN:C	1:C:4948:GLU:N	2.74	0.46
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:340:LYS:O	1:B:344:SER:OG	2.34	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:B:4917:ASP:C	1:B:4919:THR:H	2.23	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:D:4946:GLN:C	1:D:4948:GLU:N	2.74	0.46
1:A:1279:SER:OG	1:A:1280:GLN:N	2.46	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:4708:THR:HG23	1:A:4710:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2165:LEU:HD21	1:A:2178:MET:HE2	1.97	0.46
1:A:2171:GLY:N	1:A:2174:GLU:OE2	2.49	0.46
1:A:4832:HIS:CE1	1:A:4943:LEU:HD21	2.50	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:2107:GLN:O	1:A:3694:LYS:NZ	2.40	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: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:2165:LEU:HD21	1:D:2178:MET:HE2	1.97	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:4917:ASP:C	1:A:4919:THR:H	2.23	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:4917:ASP:C	1:C:4919:THR:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2151:ASP:O	1:B:2154:SER:OG	2.34	0.45
1:B:2165:LEU:HD21	1:B:2178:MET:HE2	1.97	0.45
1:C:652:ARG:HE	1:C:773:LEU:HD22	1.81	0.45
1:C:4205:TRP:CZ3	1:C:4989:MET:HE3	2.51	0.45
1:C:4244:GLU:OE1	1:C:4244:GLU:N	2.46	0.45
1:D:4231:MET:HE3	1:D:4231:MET:HB3	1.82	0.45
1:D:4917:ASP:C	1:D:4919:THR:H	2.23	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
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:C:4952:GLU:O	1:C:4953:ASP:C	2.60	0.45
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.81	0.45
1:D:4205:TRP:CZ3	1:D:4989:MET:HE3	2.51	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:2276:ALA:O	1:B:2279:SER:OG	2.30	0.45
1:B:2503:VAL:HG21	1:B:2558:VAL:HG12	1.99	0.45
1:B:4207:MET:HE2	1:B:4207:MET:HB2	1.89	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: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:1939:MET:HE3	1:C:1939:MET:HB2	1.83	0.45
1:C:2276:ALA:O	1:C:2279:SER:OG	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4946:GLN:C	1:B:4948:GLU:N	2.74	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
1:C:4211:LYS:O	1:C:4212:GLU:C	2.59	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:4205:TRP:CZ3	1:A:4989:MET:HE3	2.51	0.45
1:A:4731:ILE:HG23	1:A:4732:PHE:CD1	2.40	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
1:B:2301:TYR:HB3	1:B:2331:TYR:CZ	2.52	0.45
1:B:4205:TRP:CZ3	1:B:4989:MET:HE3	2.51	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:391:THR:OG1	1:C:392:ARG:N	2.42	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:B:4879:MET:HE2	1:B:4879:MET:HB2	1.68	0.45
1:B:4952:GLU:O	1:B:4953:ASP:C	2.59	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:4207:MET:HE2	1:C:4207:MET:HB2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1170:MET:HE3	1:A:1170:MET:HB3	1.88	0.45
1:A:1177:THR:OG1	1:A:1179:PHE:O	2.34	0.45
1:A:4946:GLN:C	1:A:4948:GLU:N	2.74	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: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:A:4965:SER:O	1:A:4965:SER:OG	2.28	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
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
1:D:4211:LYS:O	1:D:4212:GLU:C	2.59	0.44
1:A:463:GLU:O	1:A:466:SER:OG	2.35	0.44
2:L:73:MET:HA	2:L:76:LYS:HB2	1.98	0.44
1:B:4211:LYS:O	1:B:4212:GLU:C	2.59	0.44
1:C:3997:ALA:HB1	1:C:4057:MET:HB2	1.99	0.44
1:C:4148:THR:O	1:C:4151:SER:OG	2.32	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:4879:MET:HE2	1:A:4879:MET:HB2	1.68	0.44
1:A:4952:GLU:O	1:A:4953:ASP:C	2.59	0.44
1:B:2191:PHE:HD1	1:B:2198:MET:HG3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5009:TYR:CE1	1:D:5013:MET:HE2	2.53	0.44
1:A:2191:PHE:HD1	1:A:2198:MET:HG3	1.82	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:C:5009:TYR:CE1	1:C:5013:MET:HE2	2.53	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:4211:LYS:O	1:A:4212:GLU:C	2.59	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:D:4952:GLU:O	1:D:4953:ASP:C	2.60	0.44
1:A:1171:SER:OG	1:A:1175:SER:OG	2.32	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
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: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:1177:THR:OG1	1:D:1179:PHE:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1851:MET:HE2	1:A:1851:MET:HB2	1.87	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:4729:GLY:O	1:B:4734:ARG:HG3	2.18	0.44
1:B:5009:TYR:CE1	1:B:5013:MET:HE2	2.53	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1856:ASP:O	1:B:1860:LYS:NZ	2.45	0.43
1:B:2883:HIS:O	1:B:2887:GLY:N	2.42	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:2519:LEU:HA	1:D:2522:LEU:HB3	1.99	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: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
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:1156:THR:OG1	1:A:1157:GLU:OE1	2.31	0.43
1:A:4240:ASP:O	1:A:4243:PHE:N	2.35	0.43
1:B:2211:MET:HE3	1:B:2211:MET:HB3	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1749:PRO:HA	1:D:1750:PRO:HD3	1.88	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:4856:PHE:O	1:A:4860:ARG:HD3	2.19	0.43
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:B:4989:MET:HB2	1:B:4989:MET:HE2	1.33	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:4231:MET:HE3	1:C:4231:MET:HB3	1.82	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:A:5009:TYR:CE1	1:A:5013:MET:HE2	2.53	0.43
1:B:916:PRO:O	1:B:920:TYR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:4989:MET:HB2	1:C:4989:MET:HE2	1.33	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:81:MET:HE3	1:C:81:MET:HB3	1.92	0.43
1:C:3841:VAL:HG12	1:C:3926:LEU:HD22	2.00	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
1:D:4562:LEU:CD2	1:D:4656:LEU:HD23	2.45	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:A:4047:MET:O	1:A:4051:SER:OG	2.35	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4047:MET:HB2	1:B:4047:MET:HE2	1.80	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
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
2:L:45:THR:OG1	2:L:46:GLU:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:3958:ALA:HA	1:B:3961:VAL:HG12	2.02	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:B:3840:SER:OG	1:B:3877:ASP:OD1	2.32	0.42
2:I:45:THR:OG1	2:I:46:GLU:N	2.51	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:4216:GLN:O	1:C:4217:PHE:C	2.62	0.42
1:C:4844:LEU:HD12	1:C:4928:LEU:HB3	2.01	0.42
1:D:544:LEU:HD23	1:D:544:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:45:THR:OG1	2:K:46:GLU:N	2.51	0.42
1:A:1125:ASN:HB2	1:A:1130:GLN:H	1.84	0.42
1:A:4039:MET:HE2	1:A:4043:GLN:HE22	1.85	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
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:3898:ASP:OD1	1:A:3898:ASP:N	2.51	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:2211:MET:HE3	1:D:2211:MET:HB3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:29:MET:HE2	3:F:29:MET:HB2	1.94	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:D:4216:GLN:O	1:D:4217:PHE:C	2.62	0.42
1:A:4207:MET:HE2	1:A:4207:MET:HB2	1.89	0.42
1:A:5017:ARG:HG2	1:A:5019:TRP:CZ2	2.55	0.42
3:H:29:MET:HE2	3:H:29:MET:HB2	1.94	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
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:3635:CYS:HA	1:C:3638:MET:HE3	2.01	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:4207:MET:HE2	1:D:4207:MET:HB2	1.89	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: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:B:4945:ASP:O	1:B:4946:GLN:C	2.63	0.41
1:C:4875:LYS:HA	1:C:4875:LYS:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3635:CYS:HA	1:A:3638:MET:HE3	2.01	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:B:4039:MET:HE2	1:B:4043:GLN:HE22	1.85	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: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:619:ASP:O	1:A:622:THR:OG1	2.38	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
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:D:619:ASP:O	1:D:622:THR:OG1	2.38	0.41
1:D:3635:CYS:HA	1:D:3638:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:29:MET:HE2	3:E:29:MET:HB2	1.94	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:1856:ASP:O	1:D:1860:LYS:NZ	2.45	0.41
1:A:551:LEU:HD12	1:A:589:LEU:HD22	2.02	0.41
1:A:692:TYR:O	1:A:827:LYS:NZ	2.47	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:3635:CYS:HA	1:B:3638:MET:HE3	2.01	0.41
1:B:4840:THR:OG1	1:B:4841:VAL:N	2.53	0.41
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:1814:MET:HE3	1:C:1814:MET:HB3	1.89	0.41
1:C:1969:LEU:HD11	1:C:2023:LEU:HD11	2.03	0.41
1:D:4039:MET:HE2	1:D:4043:GLN:HE22	1.85	0.41
1:D:4844:LEU:HD12	1:D:4928:LEU:HB3	2.01	0.41
3:G:15:PHE:O	3:G:17:LYS:NZ	2.49	0.41
1:A:644:ILE:HD11	1:A:1628:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4216:GLN:O	1:B:4217:PHE:C	2.62	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:A:4851:TYR:O	1:A:4852:THR:C	2.62	0.41
1:A:5028:PHE:C	1:A:5030:LYS:N	2.73	0.41
1:B:619:ASP:O	1:B:622:THR:OG1	2.38	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:3858:MET:HE3	1:D:3858:MET:HB3	1.98	0.41
1:D:4007:SER:OG	1:D:4116:GLU:OE2	2.37	0.41
1:D:4879:MET:HE2	1:D:4879:MET:HB2	1.68	0.41
3:G:97:LEU:HB3	3:G:99:PHE:HE1	1.85	0.41
1:A:123:THR:OG1	1:A:124:SER:N	2.51	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:4216:GLN:O	1:A:4217:PHE:C	2.62	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:4925:ILE:HD13	1:A:4925:ILE:HG21	1.71	0.41
1:B:581:ASN:OD1	1:B:581:ASN:N	2.52	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:1170:MET:HE3	1:B:1170:MET:HB3	1.88	0.41
1:B:1575:LEU:HD22	1:B:1579:MET:HE2	2.03	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:3793:MET:HE3	1:B:3793:MET:HB3	1.98	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: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:D:81:MET:HE3	1:D:81:MET:HB3	1.92	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:A:1939:MET:HE3	1:A:1939:MET:HB2	1.83	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
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:1170:MET:HE3	1:D:1170:MET:HB3	1.88	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:1276:THR:O	1:C:1282:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:581:ASN:OD1	1:D:581:ASN:N	2.52	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:3898:ASP:OD1	1:D:3898:ASP:N	2.51	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
1:A:3858:MET:HE3	1:A:3858:MET:HB3	1.98	0.40
1:A:4204:GLN:HG3	1:A:4245:MET:HE3	2.03	0.40
3:H:97:LEU:HB3	3:H:99:PHE:HE1	1.85	0.40
1:B:1457:TYR:CE1	1:B:1459:GLN:HB2	2.56	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: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:3980:LEU:O	1:D:3983:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2608:MET:HE2	1:A:2608:MET:HB2	1.93	0.40
1:B:551:LEU:HD12	1:B:589:LEU:HD22	2.02	0.40
1:B:676:THR:OG1	1:B:677:ALA:N	2.52	0.40
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:4039:MET:HE2	1:C:4043:GLN:HE22	1.85	0.40
1:C:4950:VAL:C	1:C:4952:GLU:N	2.80	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:D:4945:ASP:O	1:D:4946:GLN:C	2.63	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:2608:MET:HE2	1:B:2608:MET:HB2	1.93	0.40
1:B:3892:CYS:HB3	1:B:3900:GLN:HE21	1.87	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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ATP	C	5103	-	32,33,33	3.09	23 (71%)	48,52,52	3.08	20 (41%)
6	ATP	D	5103	-	32,33,33	3.10	22 (68%)	48,52,52	3.08	20 (41%)
6	ATP	B	5103	-	32,33,33	3.10	22 (68%)	48,52,52	3.08	20 (41%)
7	CFF	A	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)
7	CFF	B	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)
6	ATP	A	5103	-	32,33,33	3.10	23 (71%)	48,52,52	3.08	20 (41%)
7	CFF	C	5104	-	15,15,15	4.55	11 (73%)	23,23,23	3.37	12 (52%)
7	CFF	D	5104	-	15,15,15	4.54	11 (73%)	23,23,23	3.36	12 (52%)

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	C	5103	-	-	5/22/38/38	0/3/3/3
6	ATP	D	5103	-	-	5/22/38/38	0/3/3/3
6	ATP	B	5103	-	-	5/22/38/38	0/3/3/3
7	CFF	A	5104	-	-	-	0/2/2/2
7	CFF	B	5104	-	-	-	0/2/2/2
6	ATP	A	5103	-	-	5/22/38/38	0/3/3/3
7	CFF	C	5104	-	-	-	0/2/2/2
7	CFF	D	5104	-	-	-	0/2/2/2

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	5104	CFF	O11-C2	8.99	1.39	1.22
7	A	5104	CFF	O11-C2	8.98	1.39	1.22
7	C	5104	CFF	O11-C2	8.98	1.39	1.22
7	D	5104	CFF	O11-C2	8.98	1.39	1.22
7	C	5104	CFF	O13-C6	8.68	1.40	1.23
7	A	5104	CFF	O13-C6	8.67	1.40	1.23
7	B	5104	CFF	O13-C6	8.67	1.40	1.23
7	D	5104	CFF	O13-C6	8.67	1.40	1.23
7	C	5104	CFF	C4-N9	7.95	1.52	1.36
7	A	5104	CFF	C4-N9	7.94	1.52	1.36
7	B	5104	CFF	C4-N9	7.94	1.52	1.36
7	D	5104	CFF	C4-N9	7.94	1.52	1.36
6	C	5103	ATP	O4'-C1'	7.05	1.58	1.42
6	A	5103	ATP	O4'-C1'	7.02	1.58	1.42
6	B	5103	ATP	O4'-C1'	7.02	1.58	1.42
6	D	5103	ATP	O4'-C1'	7.00	1.58	1.42
6	A	5103	ATP	O4'-C4'	5.81	1.57	1.45
6	D	5103	ATP	O4'-C4'	5.81	1.57	1.45
6	B	5103	ATP	O4'-C4'	5.78	1.57	1.45
6	C	5103	ATP	O4'-C4'	5.78	1.57	1.45
7	A	5104	CFF	C5-N7	-4.94	1.29	1.38
7	B	5104	CFF	C5-N7	-4.94	1.29	1.38
7	C	5104	CFF	C5-N7	-4.94	1.29	1.38
7	D	5104	CFF	C5-N7	-4.94	1.29	1.38
6	A	5103	ATP	C2'-C3'	-4.93	1.40	1.53
6	B	5103	ATP	C2'-C3'	-4.93	1.40	1.53
6	D	5103	ATP	C2'-C3'	-4.93	1.40	1.53
6	C	5103	ATP	C2'-C3'	-4.91	1.40	1.53
6	D	5103	ATP	PB-O3B	4.55	1.64	1.59
6	B	5103	ATP	PB-O3A	4.55	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	ATP	PB-O3B	4.52	1.64	1.59
6	A	5103	ATP	PB-O3A	4.52	1.64	1.59
6	D	5103	ATP	PB-O3A	4.52	1.64	1.59
6	B	5103	ATP	PB-O3B	4.49	1.64	1.59
6	C	5103	ATP	PB-O3B	4.49	1.64	1.59
6	C	5103	ATP	PB-O3A	4.47	1.64	1.59
6	B	5103	ATP	C5-N7	4.44	1.47	1.39
6	D	5103	ATP	C5-N7	4.44	1.47	1.39
6	A	5103	ATP	C5-N7	4.41	1.47	1.39
6	C	5103	ATP	C5-N7	4.41	1.47	1.39
6	A	5103	ATP	PA-O3A	4.07	1.63	1.59
6	B	5103	ATP	PA-O3A	4.07	1.63	1.59
6	C	5103	ATP	PA-O3A	4.07	1.63	1.59
6	D	5103	ATP	PA-O3A	4.07	1.63	1.59
7	B	5104	CFF	C2-N3	3.77	1.46	1.39
7	D	5104	CFF	C2-N3	3.77	1.46	1.39
7	A	5104	CFF	C2-N3	3.76	1.46	1.39
7	C	5104	CFF	C2-N3	3.73	1.46	1.39
6	A	5103	ATP	C8-N9	-3.59	1.31	1.37
6	B	5103	ATP	C8-N9	-3.59	1.31	1.37
6	C	5103	ATP	C8-N9	-3.59	1.31	1.37
6	D	5103	ATP	C8-N9	-3.59	1.31	1.37
6	B	5103	ATP	C6-N6	3.52	1.43	1.34
6	A	5103	ATP	C6-N6	3.49	1.43	1.34
6	C	5103	ATP	C6-N6	3.49	1.43	1.34
6	D	5103	ATP	C6-N6	3.49	1.43	1.34
7	A	5104	CFF	C5-C6	3.25	1.51	1.43
7	B	5104	CFF	C5-C6	3.25	1.51	1.43
7	C	5104	CFF	C5-C6	3.25	1.51	1.43
7	A	5104	CFF	C2-N1	3.23	1.45	1.39
7	C	5104	CFF	C2-N1	3.23	1.45	1.39
7	D	5104	CFF	C2-N1	3.23	1.45	1.39
7	D	5104	CFF	C5-C6	3.22	1.51	1.43
7	B	5104	CFF	C2-N1	3.19	1.45	1.39
6	A	5103	ATP	C3'-C4'	-3.14	1.45	1.53
6	D	5103	ATP	C3'-C4'	-3.14	1.45	1.53
6	B	5103	ATP	C3'-C4'	-3.12	1.45	1.53
6	C	5103	ATP	C3'-C4'	-3.12	1.45	1.53
7	C	5104	CFF	C8-N7	-2.98	1.28	1.35
7	A	5104	CFF	C8-N7	-2.97	1.28	1.35
7	D	5104	CFF	C8-N7	-2.97	1.28	1.35
7	B	5104	CFF	C8-N7	-2.94	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	ATP	C1'-N9	-2.89	1.38	1.46
6	B	5103	ATP	C1'-N9	-2.89	1.38	1.46
6	D	5103	ATP	C1'-N9	-2.89	1.38	1.46
6	C	5103	ATP	C1'-N9	-2.87	1.38	1.46
6	A	5103	ATP	C8-N7	2.59	1.36	1.31
6	B	5103	ATP	C8-N7	2.58	1.36	1.31
6	C	5103	ATP	C8-N7	2.56	1.36	1.31
6	D	5103	ATP	C8-N7	2.56	1.36	1.31
6	A	5103	ATP	C2-N1	-2.53	1.29	1.33
6	B	5103	ATP	C2-N1	-2.51	1.29	1.33
6	D	5103	ATP	C2-N1	-2.51	1.29	1.33
6	C	5103	ATP	C2-N1	-2.49	1.29	1.33
6	C	5103	ATP	O2'-C2'	2.46	1.49	1.43
6	B	5103	ATP	O2'-C2'	2.46	1.49	1.43
6	D	5103	ATP	O2'-C2'	2.46	1.49	1.43
6	A	5103	ATP	O2'-C2'	2.45	1.49	1.43
7	A	5104	CFF	C4-N3	2.42	1.42	1.38
7	B	5104	CFF	C4-N3	2.42	1.42	1.38
7	D	5104	CFF	C4-N3	2.42	1.42	1.38
7	C	5104	CFF	C4-N3	2.41	1.42	1.38
6	A	5103	ATP	PG-O3G	-2.30	1.46	1.54
6	B	5103	ATP	PG-O3G	-2.30	1.46	1.54
6	C	5103	ATP	PG-O3G	-2.30	1.46	1.54
6	D	5103	ATP	PG-O3G	-2.30	1.46	1.54
6	A	5103	ATP	PG-O2G	-2.28	1.46	1.54
6	B	5103	ATP	PG-O2G	-2.28	1.46	1.54
6	C	5103	ATP	PG-O2G	-2.28	1.46	1.54
6	D	5103	ATP	PG-O2G	-2.28	1.46	1.54
6	A	5103	ATP	O3'-C3'	2.27	1.48	1.43
6	D	5103	ATP	O3'-C3'	2.27	1.48	1.43
6	C	5103	ATP	O3'-C3'	2.26	1.48	1.43
6	A	5103	ATP	C2'-C1'	-2.26	1.46	1.53
6	B	5103	ATP	C2'-C1'	-2.26	1.46	1.53
6	C	5103	ATP	C2'-C1'	-2.26	1.46	1.53
6	D	5103	ATP	C2'-C1'	-2.26	1.46	1.53
6	B	5103	ATP	O3'-C3'	2.25	1.48	1.43
7	D	5104	CFF	C8-N9	2.25	1.38	1.32
7	A	5104	CFF	C8-N9	2.25	1.38	1.32
7	C	5104	CFF	C8-N9	2.25	1.38	1.32
7	B	5104	CFF	C8-N9	2.23	1.38	1.32
7	C	5104	CFF	C10-N1	-2.18	1.43	1.47
6	A	5103	ATP	C5-C4	2.18	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5103	ATP	C5-C4	2.15	1.42	1.39
6	C	5103	ATP	C5-C4	2.15	1.42	1.39
6	D	5103	ATP	C5-C4	2.15	1.42	1.39
7	A	5104	CFF	C10-N1	-2.13	1.43	1.47
7	D	5104	CFF	C10-N1	-2.13	1.43	1.47
7	B	5104	CFF	C10-N1	-2.09	1.43	1.47
6	C	5103	ATP	PA-O2A	-2.05	1.45	1.55
6	A	5103	ATP	C2-N3	-2.05	1.30	1.33
6	B	5103	ATP	C2-N3	-2.05	1.30	1.33
6	C	5103	ATP	C2-N3	-2.05	1.30	1.33
6	D	5103	ATP	C2-N3	-2.05	1.30	1.33
6	A	5103	ATP	PA-O2A	-2.05	1.45	1.55
6	B	5103	ATP	PA-O2A	-2.05	1.45	1.55
6	D	5103	ATP	PA-O2A	-2.05	1.45	1.55
6	A	5103	ATP	PB-O2B	-2.03	1.45	1.55
6	B	5103	ATP	PB-O2B	-2.03	1.45	1.55
6	C	5103	ATP	PB-O2B	-2.03	1.45	1.55
6	D	5103	ATP	PB-O2B	-2.03	1.45	1.55
6	A	5103	ATP	C4-N9	-2.01	1.33	1.37
6	C	5103	ATP	C4-N9	-2.01	1.33	1.37

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	ATP	C4-N9-C8	10.36	116.62	105.74
6	C	5103	ATP	C4-N9-C8	10.36	116.62	105.74
6	D	5103	ATP	C4-N9-C8	10.35	116.61	105.74
6	B	5103	ATP	C4-N9-C8	10.32	116.57	105.74
6	B	5103	ATP	C4'-O4'-C1'	-9.47	88.56	109.47
6	C	5103	ATP	C4'-O4'-C1'	-9.47	88.57	109.47
6	A	5103	ATP	C4'-O4'-C1'	-9.46	88.58	109.47
6	D	5103	ATP	C4'-O4'-C1'	-9.45	88.61	109.47
7	A	5104	CFF	C14-N7-C8	-7.53	112.19	126.28
7	D	5104	CFF	C14-N7-C8	-7.53	112.19	126.28
7	B	5104	CFF	C14-N7-C8	-7.51	112.22	126.28
7	C	5104	CFF	C14-N7-C8	-7.51	112.23	126.28
7	B	5104	CFF	C6-C5-C4	-6.13	115.20	122.92
7	C	5104	CFF	C6-C5-C4	-6.13	115.20	122.92
7	A	5104	CFF	C6-C5-C4	-6.10	115.24	122.92
7	D	5104	CFF	C6-C5-C4	-6.08	115.26	122.92
6	A	5103	ATP	N9-C8-N7	-5.62	105.97	113.94
6	C	5103	ATP	N9-C8-N7	-5.61	105.97	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5103	ATP	N9-C8-N7	-5.61	105.97	113.94
6	B	5103	ATP	N9-C8-N7	-5.59	106.01	113.94
6	B	5103	ATP	C4-C5-N7	-5.48	104.32	110.58
6	D	5103	ATP	C4-C5-N7	-5.48	104.32	110.58
6	A	5103	ATP	C4-C5-N7	-5.47	104.32	110.58
6	C	5103	ATP	C4-C5-N7	-5.46	104.34	110.58
7	A	5104	CFF	C8-N7-C5	5.02	115.03	105.59
7	D	5104	CFF	C8-N7-C5	5.02	115.03	105.59
7	C	5104	CFF	C8-N7-C5	5.00	114.98	105.59
7	B	5104	CFF	C8-N7-C5	4.99	114.98	105.59
7	B	5104	CFF	C12-N3-C2	4.92	125.91	117.33
7	D	5104	CFF	C12-N3-C2	4.92	125.91	117.33
7	C	5104	CFF	C12-N3-C2	4.91	125.88	117.33
7	A	5104	CFF	C12-N3-C2	4.89	125.85	117.33
7	C	5104	CFF	C5-C6-N1	4.70	120.67	112.06
7	D	5104	CFF	C5-C6-N1	4.68	120.64	112.06
7	B	5104	CFF	C5-C6-N1	4.68	120.63	112.06
7	A	5104	CFF	C5-C6-N1	4.67	120.62	112.06
7	A	5104	CFF	C6-C5-N7	4.66	140.47	131.10
7	B	5104	CFF	C6-C5-N7	4.66	140.47	131.10
7	C	5104	CFF	C6-C5-N7	4.66	140.47	131.10
7	D	5104	CFF	C6-C5-N7	4.65	140.44	131.10
6	A	5103	ATP	C5-C4-N3	-4.57	120.42	126.72
6	B	5103	ATP	C5-C4-N3	-4.56	120.44	126.72
6	C	5103	ATP	C5-C4-N3	-4.56	120.44	126.72
6	D	5103	ATP	C5-C4-N3	-4.56	120.44	126.72
6	B	5103	ATP	N3-C2-N1	-4.50	121.76	128.58
6	D	5103	ATP	N3-C2-N1	-4.50	121.76	128.58
6	C	5103	ATP	N3-C2-N1	-4.49	121.78	128.58
6	A	5103	ATP	N3-C2-N1	-4.47	121.81	128.58
6	A	5103	ATP	N3-C4-N9	4.43	134.71	127.17
6	C	5103	ATP	N3-C4-N9	4.43	134.71	127.17
6	D	5103	ATP	N3-C4-N9	4.43	134.70	127.17
6	B	5103	ATP	N3-C4-N9	4.41	134.66	127.17
7	C	5104	CFF	C12-N3-C4	-4.38	114.30	120.75
7	A	5104	CFF	C12-N3-C4	-4.35	114.34	120.75
7	B	5104	CFF	C12-N3-C4	-4.35	114.34	120.75
7	D	5104	CFF	C12-N3-C4	-4.35	114.34	120.75
6	B	5103	ATP	C6-C5-N7	4.31	140.39	132.09
6	A	5103	ATP	C6-C5-N7	4.29	140.37	132.09
6	D	5103	ATP	C6-C5-N7	4.28	140.35	132.09
6	C	5103	ATP	C6-C5-N7	4.27	140.33	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5103	ATP	O4'-C1'-N9	3.80	115.38	108.09
6	A	5103	ATP	O4'-C1'-N9	3.78	115.35	108.09
6	B	5103	ATP	O4'-C1'-N9	3.78	115.35	108.09
6	C	5103	ATP	O4'-C1'-N9	3.77	115.33	108.09
6	A	5103	ATP	C2-N3-C4	3.27	119.82	111.83
6	B	5103	ATP	C2-N3-C4	3.27	119.82	111.83
6	C	5103	ATP	C2-N3-C4	3.27	119.82	111.83
6	D	5103	ATP	C2-N3-C4	3.27	119.82	111.83
6	D	5103	ATP	C3'-C2'-C1'	3.20	107.52	101.46
6	A	5103	ATP	C3'-C2'-C1'	3.19	107.50	101.46
6	B	5103	ATP	C3'-C2'-C1'	3.19	107.50	101.46
6	C	5103	ATP	C3'-C2'-C1'	3.18	107.47	101.46
6	D	5103	ATP	C5-N7-C8	3.04	108.23	103.45
6	A	5103	ATP	C5-N7-C8	3.03	108.21	103.45
6	C	5103	ATP	C5-N7-C8	3.03	108.21	103.45
7	D	5104	CFF	O13-C6-N1	-3.02	114.83	120.36
6	B	5103	ATP	C5-N7-C8	3.02	108.19	103.45
7	C	5104	CFF	O13-C6-N1	-3.00	114.87	120.36
7	B	5104	CFF	O13-C6-N1	-3.00	114.87	120.36
7	A	5104	CFF	O13-C6-N1	-3.00	114.88	120.36
7	C	5104	CFF	C5-C4-N9	-2.86	106.44	112.10
7	B	5104	CFF	C5-C4-N9	-2.86	106.44	112.10
7	D	5104	CFF	C5-C4-N9	-2.84	106.48	112.10
7	A	5104	CFF	C5-C4-N9	-2.83	106.49	112.10
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
6	D	5103	ATP	C2-N1-C6	2.75	123.25	118.73
6	A	5103	ATP	O2G-PG-O3B	2.75	113.85	104.64
6	B	5103	ATP	C2-N1-C6	2.74	123.23	118.73
6	D	5103	ATP	O2G-PG-O3B	2.73	113.80	104.64
6	A	5103	ATP	C2-N1-C6	2.72	123.20	118.73
6	C	5103	ATP	C2-N1-C6	2.72	123.20	118.73
7	C	5104	CFF	C10-N1-C2	2.72	122.07	117.33
7	B	5104	CFF	C10-N1-C2	2.70	122.04	117.33
7	A	5104	CFF	C10-N1-C2	2.70	122.03	117.33
7	D	5104	CFF	C10-N1-C2	2.70	122.03	117.33
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
6	C	5103	ATP	C4-N9-C1'	-2.43	120.94	126.63
6	A	5103	ATP	C4-N9-C1'	-2.42	120.97	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5103	ATP	C4-N9-C1'	-2.42	120.98	126.63
6	B	5103	ATP	C4-N9-C1'	-2.40	121.02	126.63
6	C	5103	ATP	O2A-PA-O1A	-2.33	101.59	112.44
7	A	5104	CFF	C14-N7-C5	-2.33	122.22	127.77
7	C	5104	CFF	C14-N7-C5	-2.33	122.22	127.77
7	D	5104	CFF	C14-N7-C5	-2.33	122.22	127.77
6	D	5103	ATP	O2A-PA-O1A	-2.33	101.61	112.44
6	A	5103	ATP	O2A-PA-O1A	-2.33	101.63	112.44
6	B	5103	ATP	O2A-PA-O1A	-2.33	101.63	112.44
7	B	5104	CFF	C14-N7-C5	-2.32	122.25	127.77
7	C	5104	CFF	C6-N1-C2	-2.27	121.97	125.66
7	D	5104	CFF	C6-N1-C2	-2.27	121.97	125.66
7	A	5104	CFF	C6-N1-C2	-2.24	122.02	125.66
7	B	5104	CFF	C6-N1-C2	-2.24	122.03	125.66
6	D	5103	ATP	O2B-PB-O1B	-2.23	102.06	112.44
6	A	5103	ATP	O2B-PB-O1B	-2.23	102.08	112.44
6	B	5103	ATP	O2B-PB-O1B	-2.23	102.08	112.44
6	C	5103	ATP	O2B-PB-O1B	-2.23	102.08	112.44
6	A	5103	ATP	C1'-N9-C8	-2.13	122.38	127.09
6	B	5103	ATP	C1'-N9-C8	-2.13	122.38	127.09
6	D	5103	ATP	C1'-N9-C8	-2.13	122.38	127.09
6	C	5103	ATP	C1'-N9-C8	-2.11	122.41	127.09
6	B	5103	ATP	O4'-C4'-C5'	2.03	115.85	109.33
6	C	5103	ATP	O4'-C4'-C5'	2.03	115.85	109.33
6	A	5103	ATP	O4'-C4'-C5'	2.03	115.84	109.33
6	D	5103	ATP	O4'-C4'-C5'	2.03	115.83	109.33

There are no chirality outliers.

All (20) 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	C5'-O5'-PA-O1A
6	B	5103	ATP	C5'-O5'-PA-O1A
6	C	5103	ATP	C5'-O5'-PA-O1A

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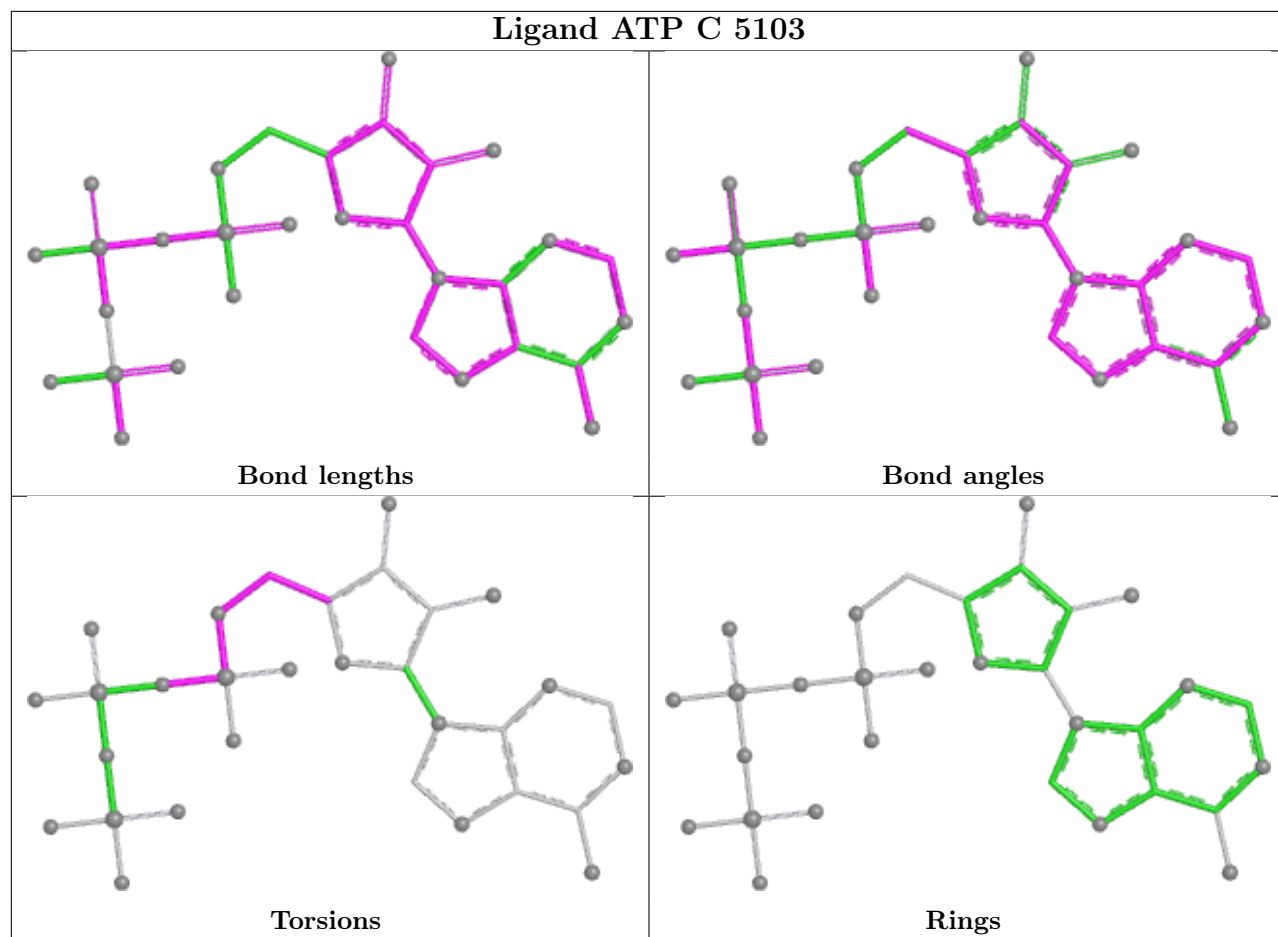
Mol	Chain	Res	Type	Atoms
6	D	5103	ATP	C5'-O5'-PA-O1A
6	A	5103	ATP	O4'-C4'-C5'-O5'
6	B	5103	ATP	O4'-C4'-C5'-O5'
6	C	5103	ATP	O4'-C4'-C5'-O5'
6	D	5103	ATP	O4'-C4'-C5'-O5'
6	A	5103	ATP	PB-O3A-PA-O2A
6	B	5103	ATP	PB-O3A-PA-O2A
6	C	5103	ATP	PB-O3A-PA-O2A
6	D	5103	ATP	PB-O3A-PA-O2A

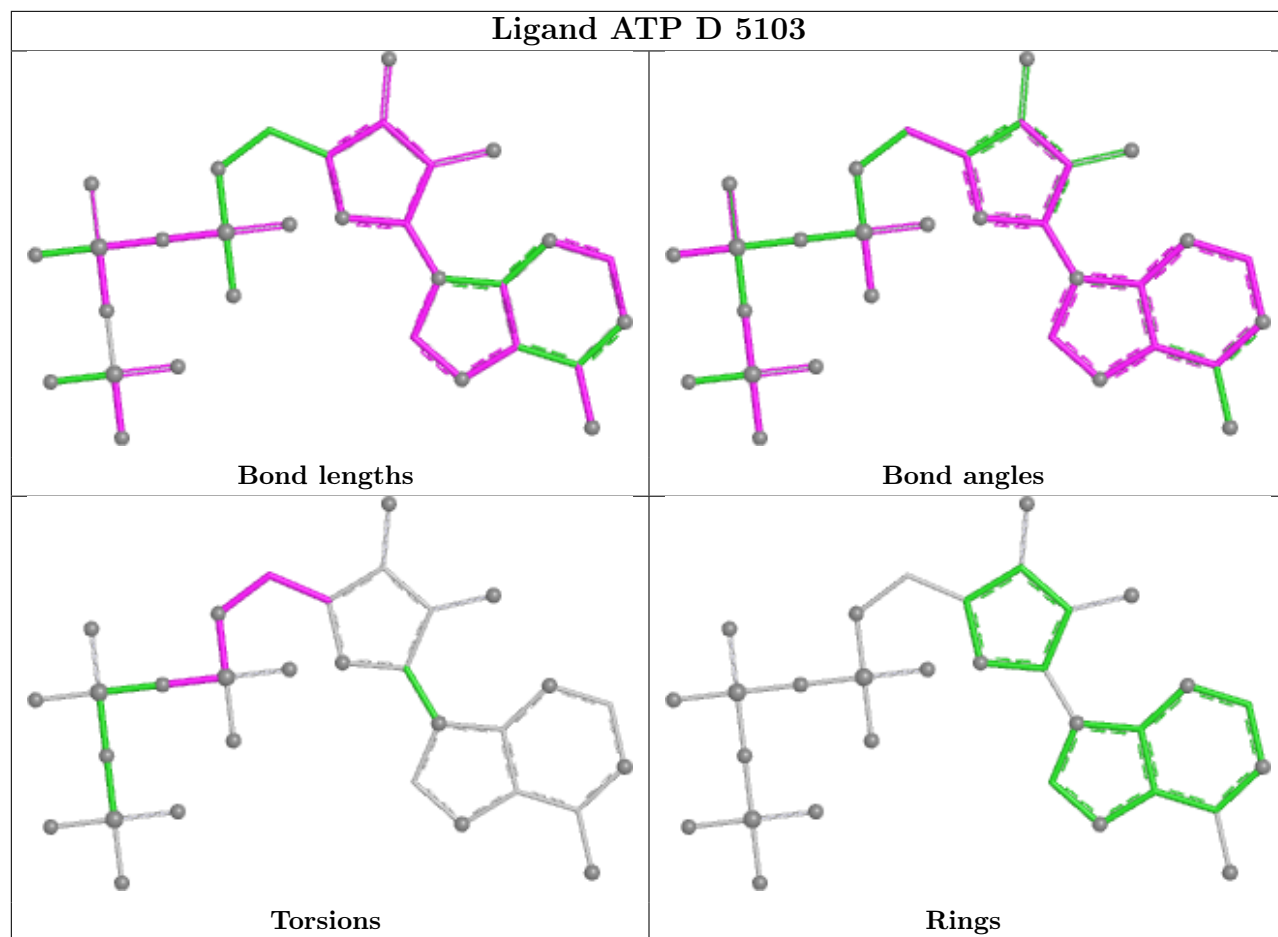
There are no ring outliers.

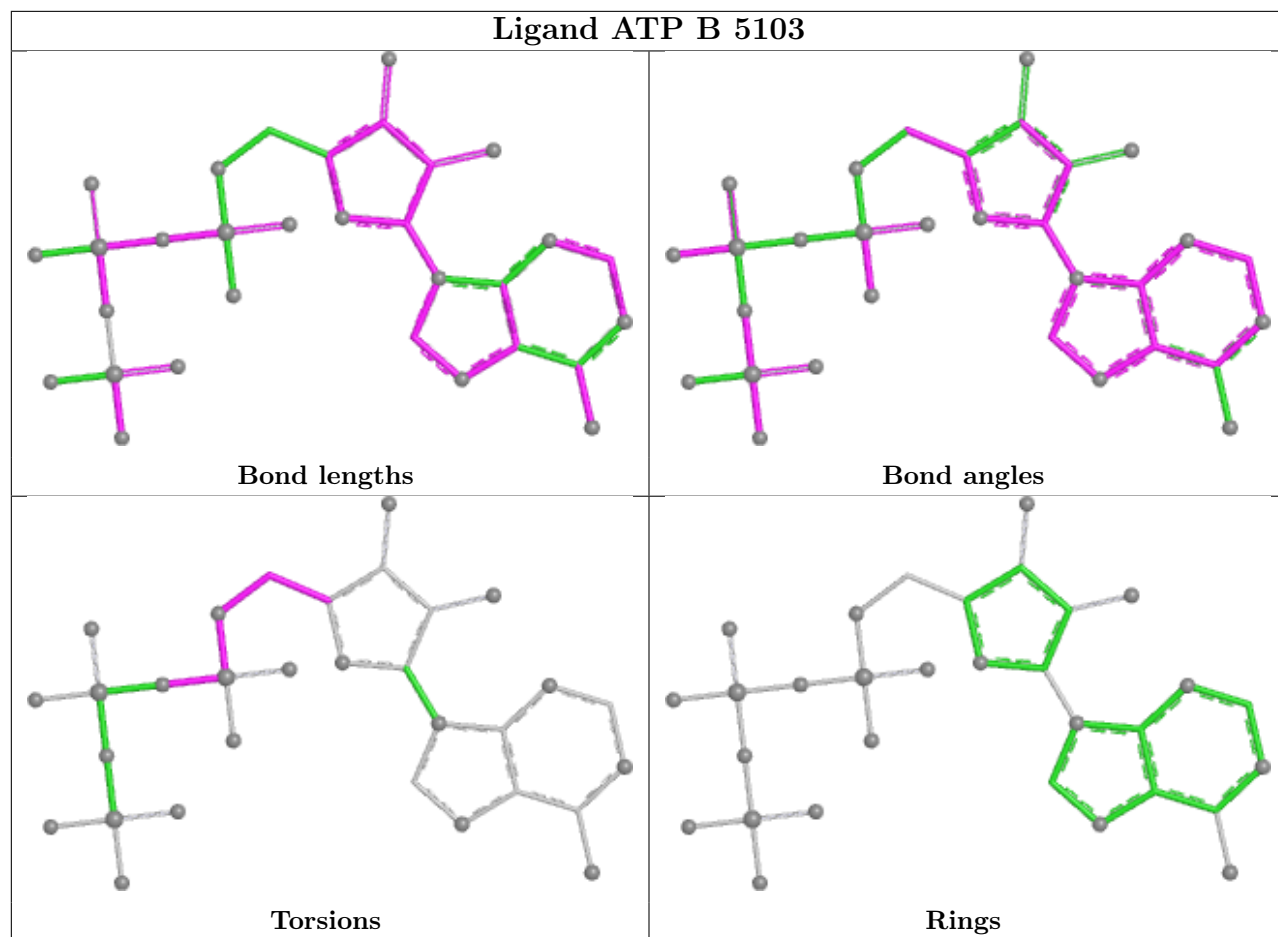
8 monomers are involved in 8 short contacts:

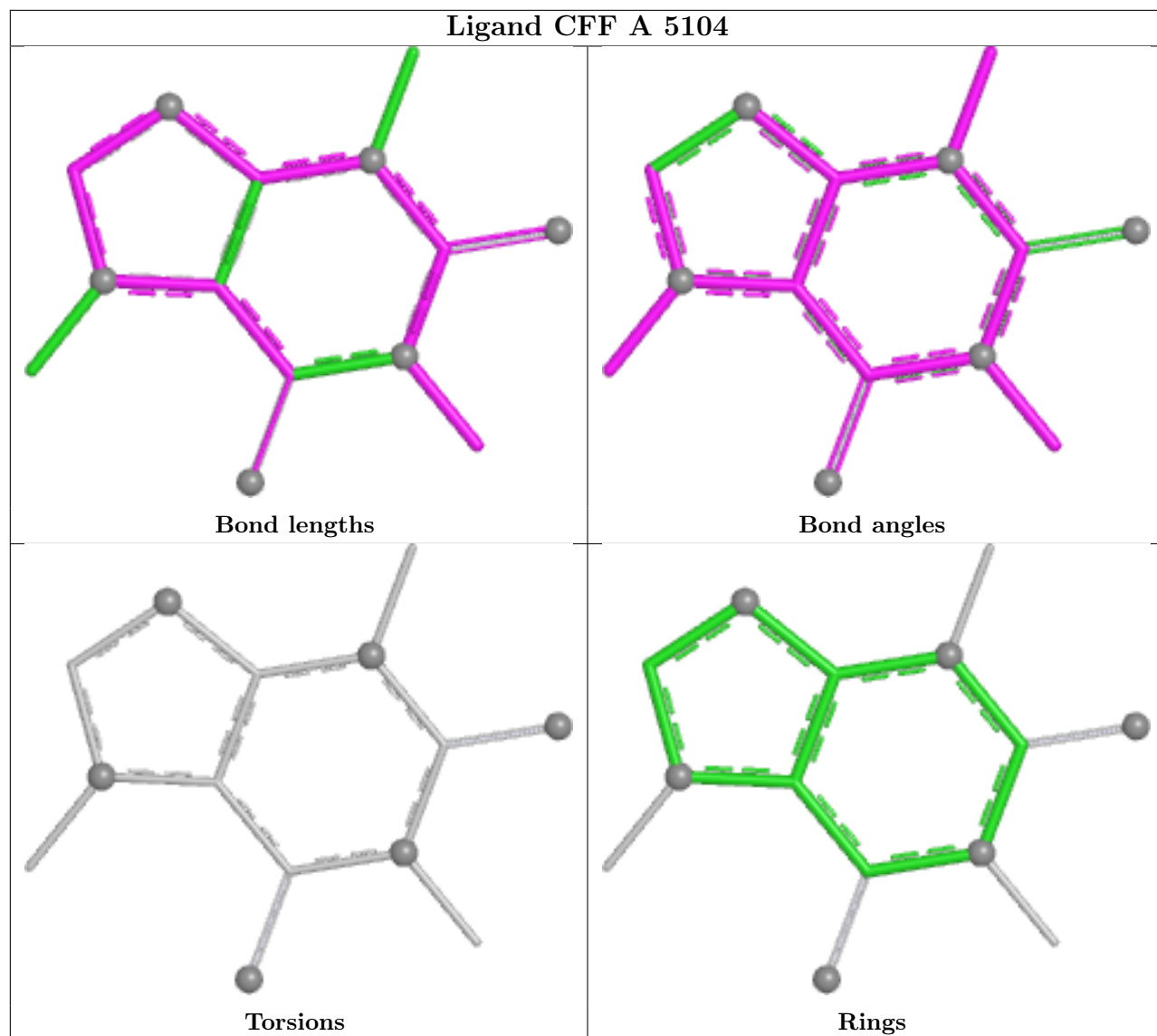
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5103	ATP	1	0
6	D	5103	ATP	1	0
6	B	5103	ATP	1	0
7	A	5104	CFF	1	0
7	B	5104	CFF	1	0
6	A	5103	ATP	1	0
7	C	5104	CFF	1	0
7	D	5104	CFF	1	0

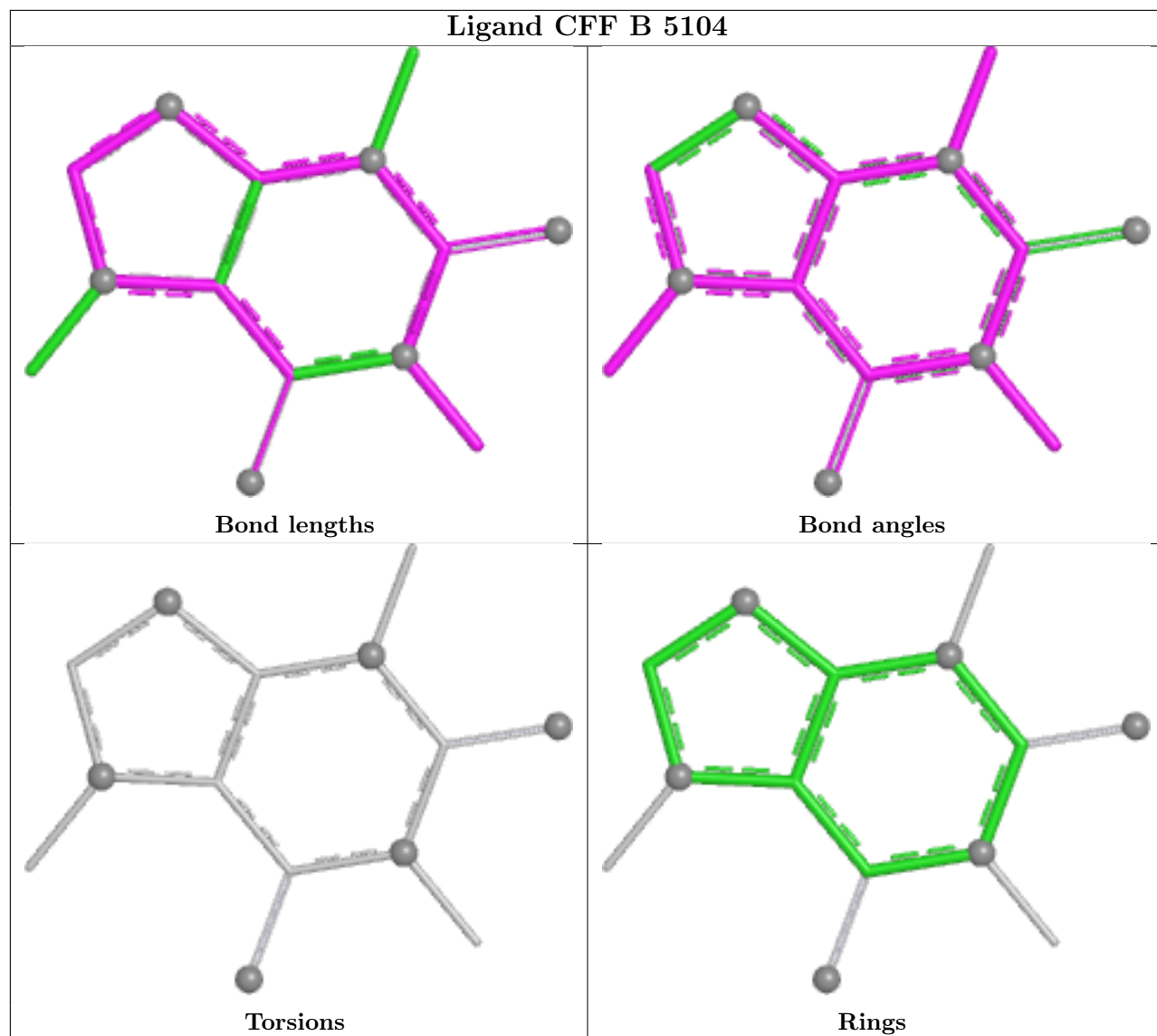
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

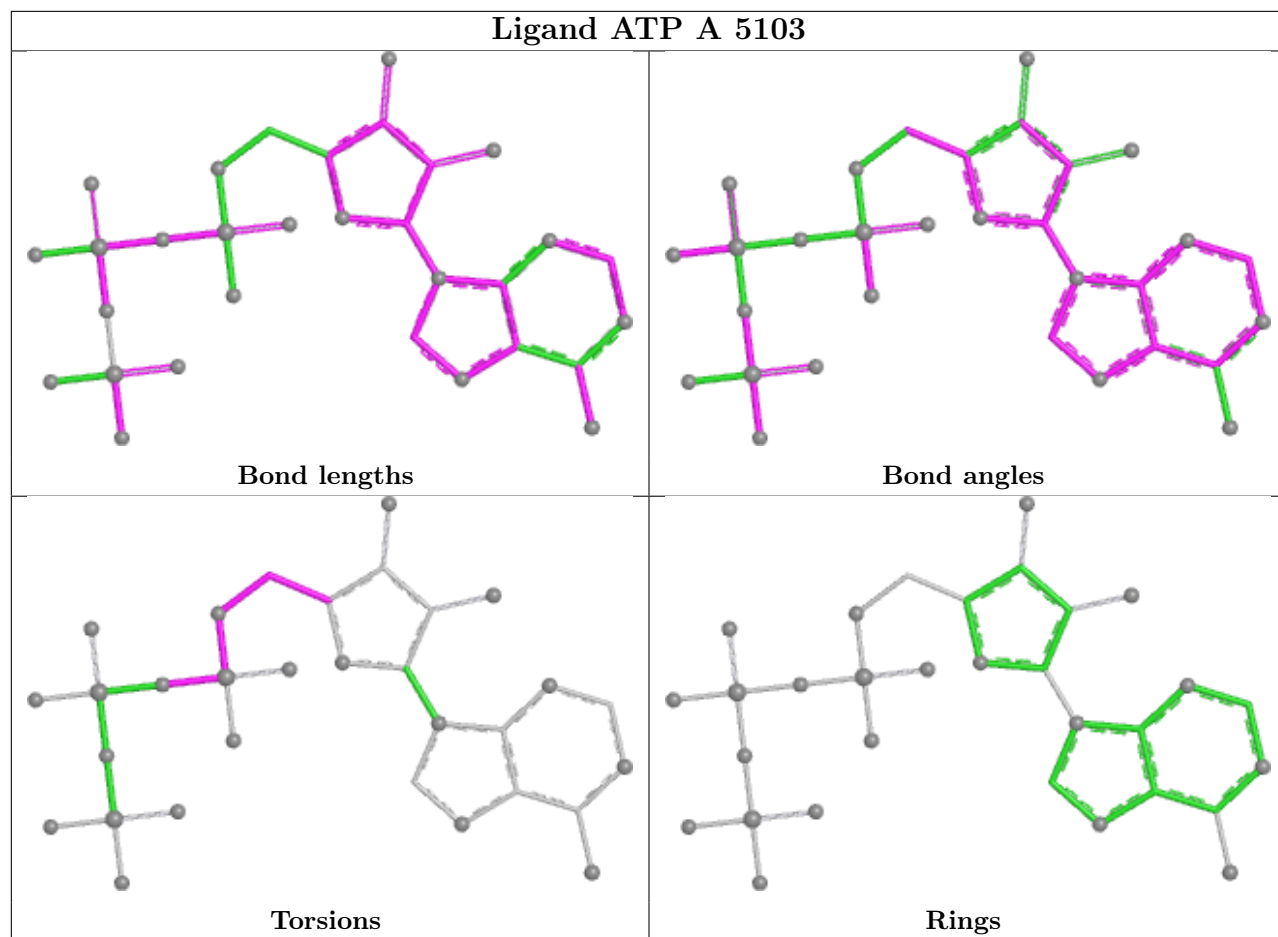


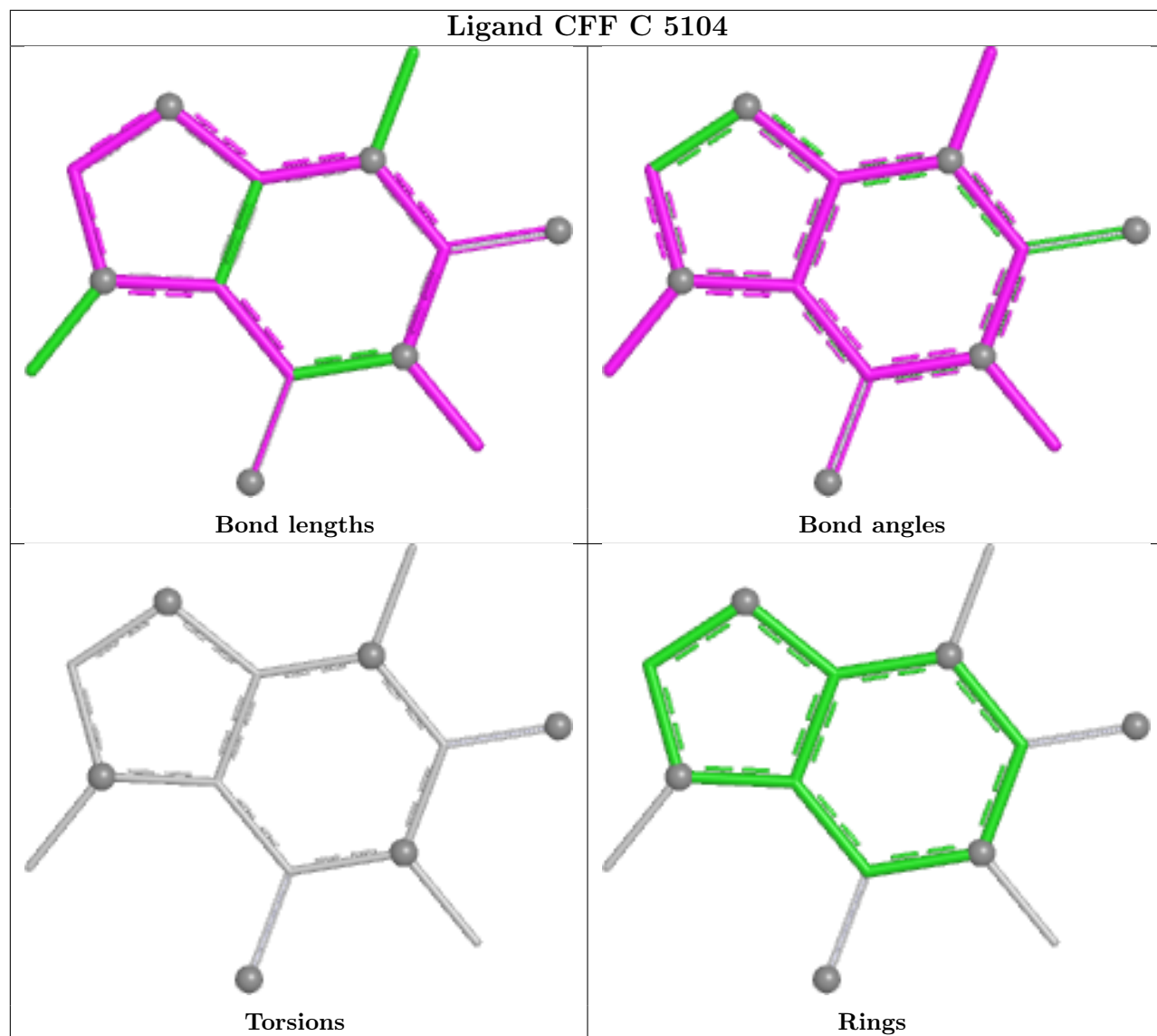


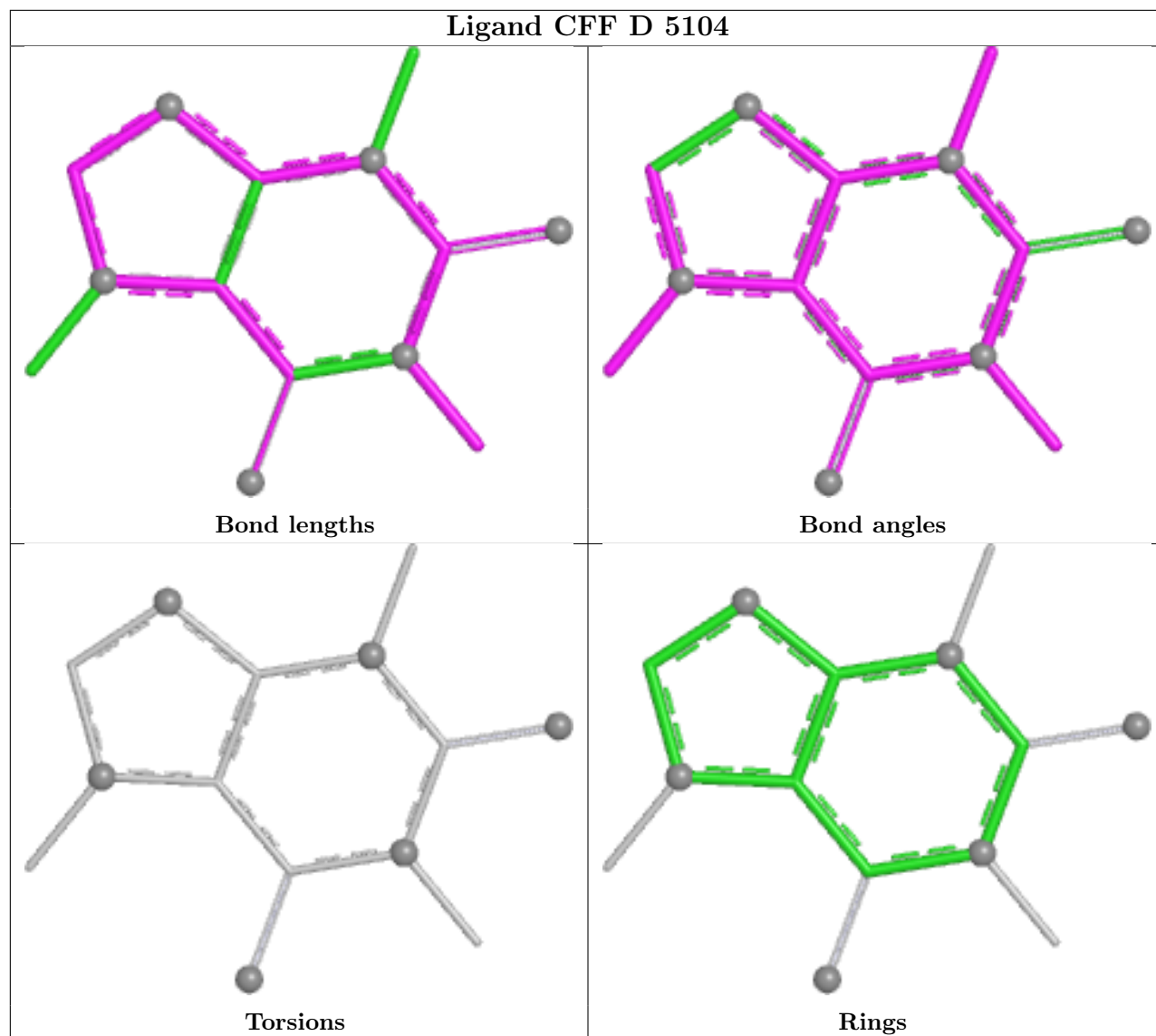












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

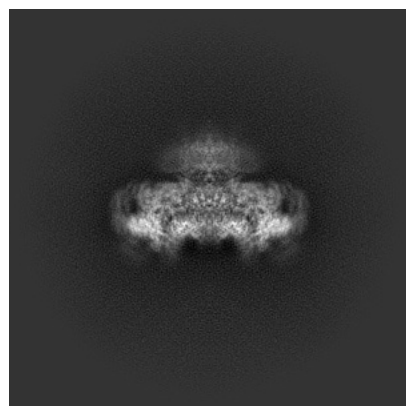
6 Map visualisation [i](#)

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

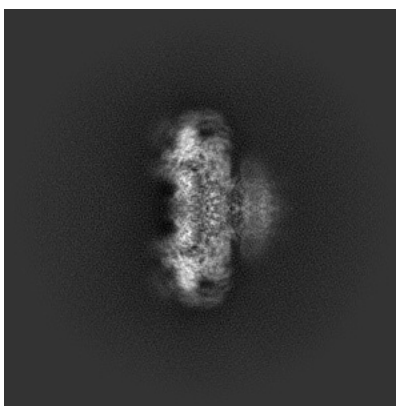
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

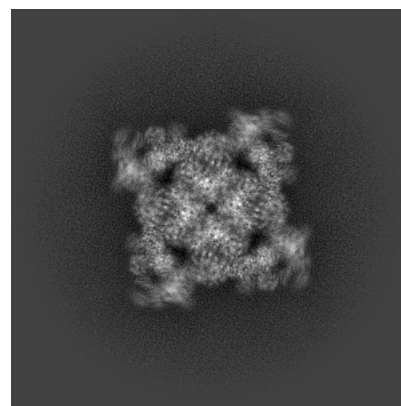
6.1.1 Primary map



X

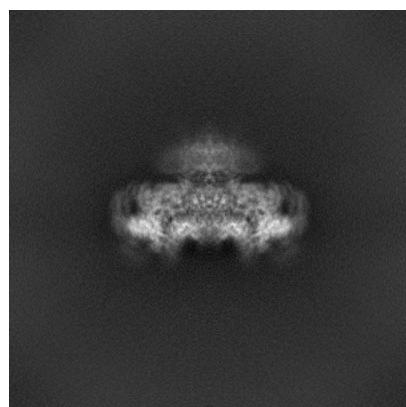


Y

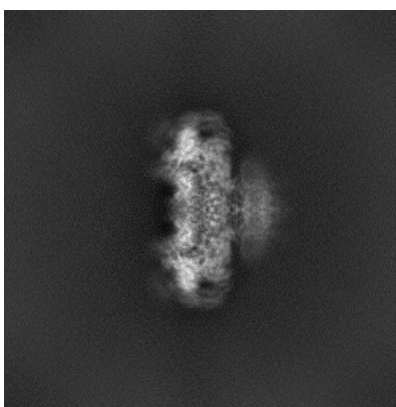


Z

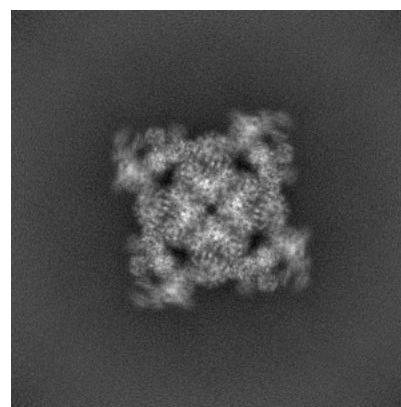
6.1.2 Raw map



X



Y

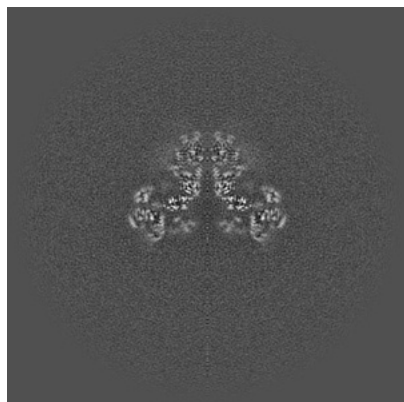


Z

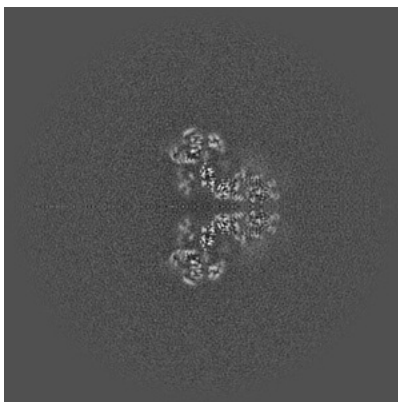
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

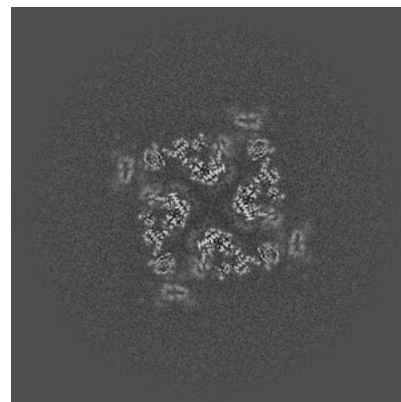
6.2.1 Primary map



X Index: 240

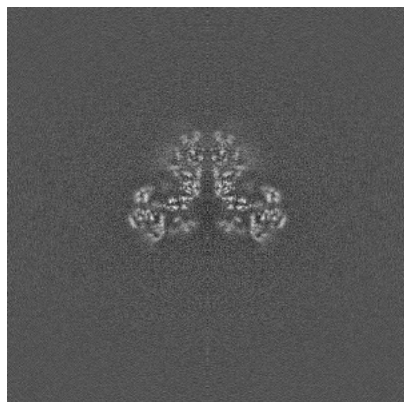


Y Index: 240

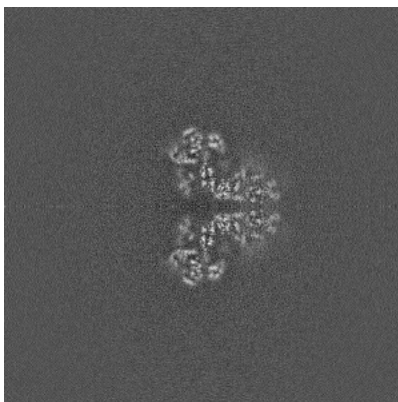


Z Index: 240

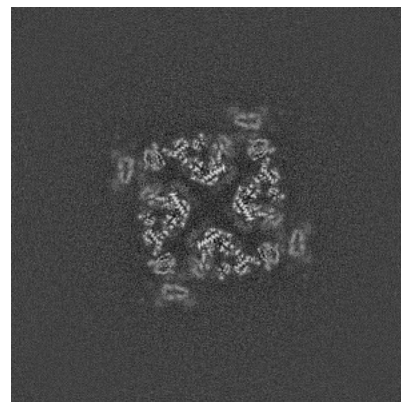
6.2.2 Raw map



X Index: 240



Y Index: 240

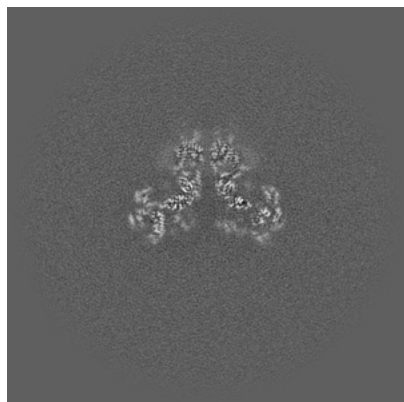


Z Index: 240

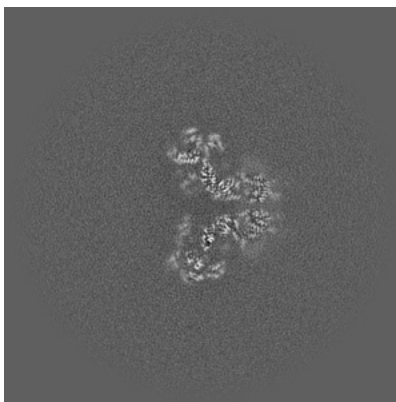
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

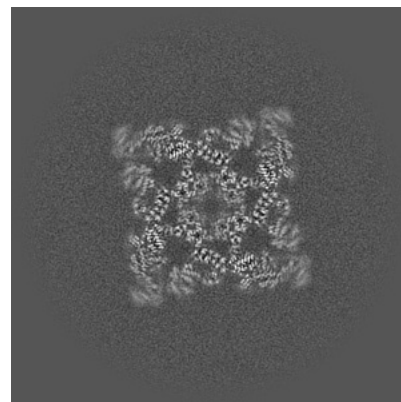
6.3.1 Primary map



X Index: 238

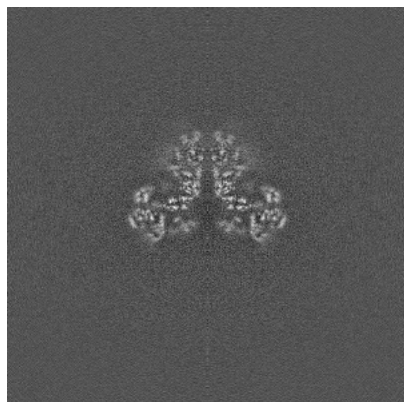


Y Index: 238

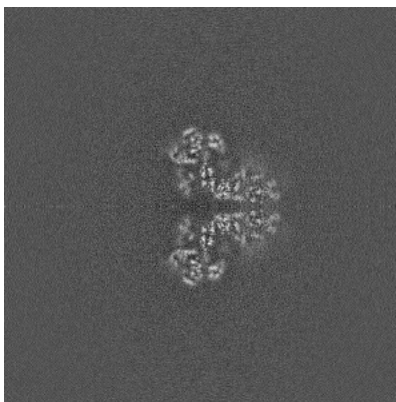


Z Index: 223

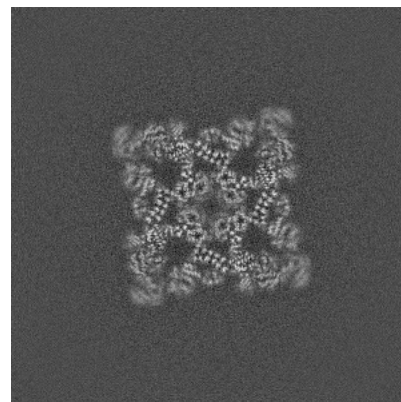
6.3.2 Raw map



X Index: 240



Y Index: 240

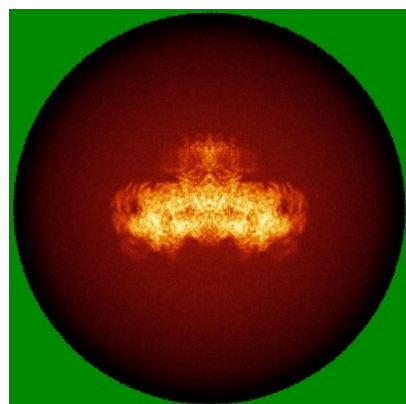


Z Index: 222

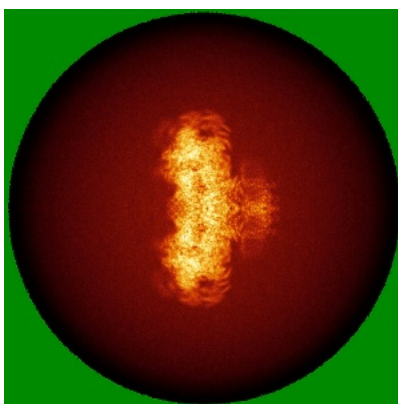
The images above show the largest variance slices of the map in three orthogonal directions.

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

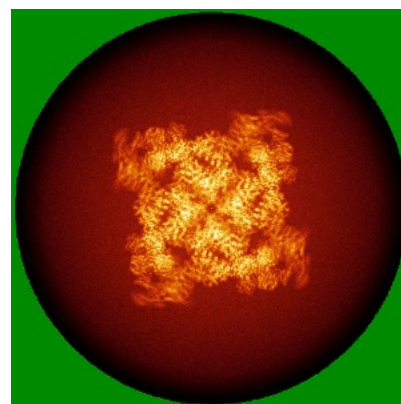
6.4.1 Primary map



X

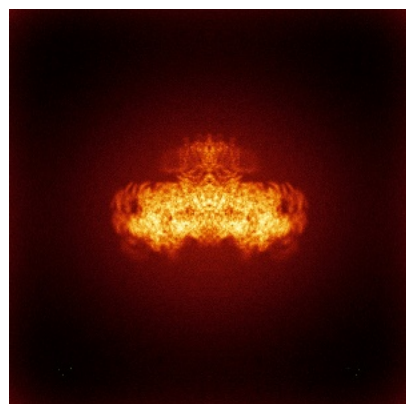


Y

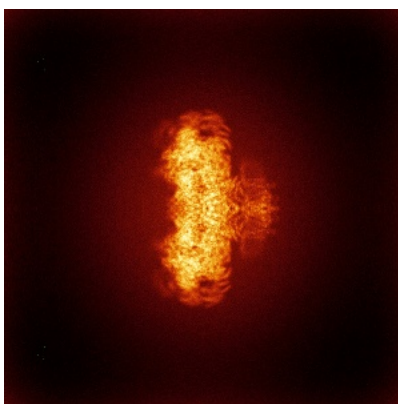


Z

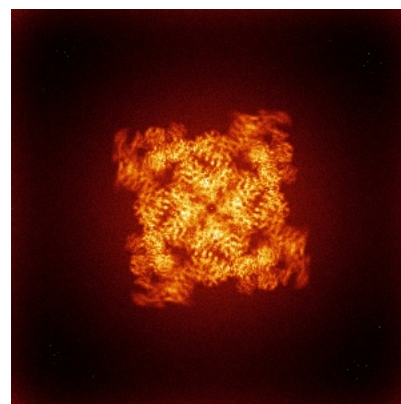
6.4.2 Raw map



X



Y

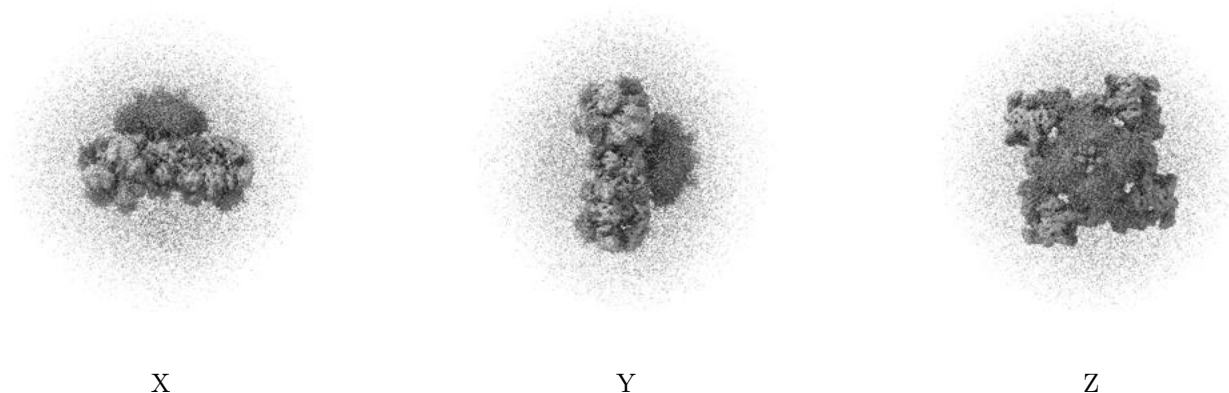


Z

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.

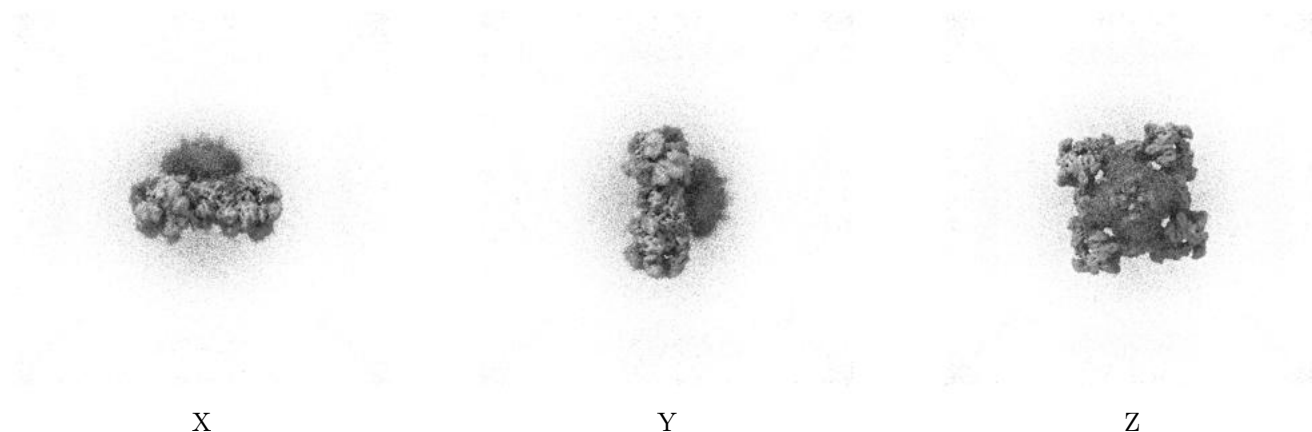
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

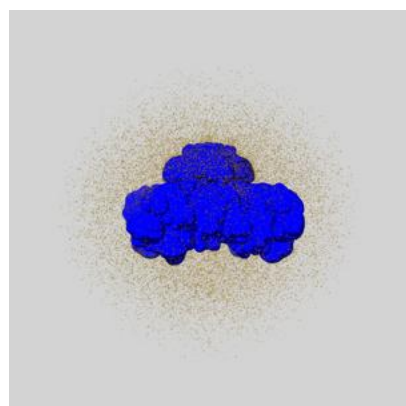
6.6 Mask visualisation [i](#)

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

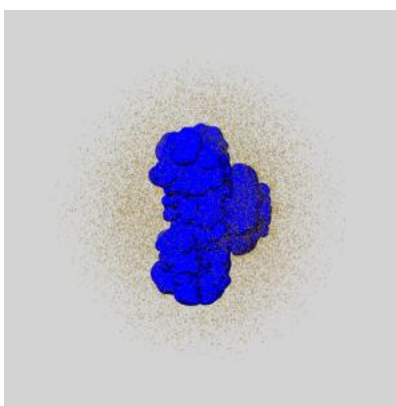
A mask typically either:

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

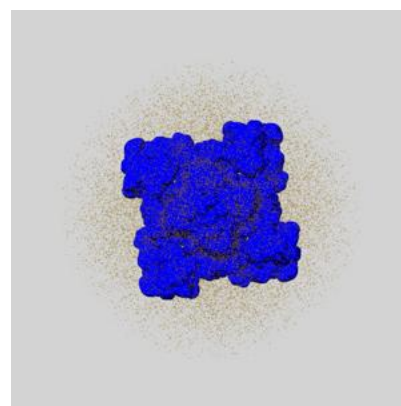
6.6.1 emd_38447_msk_1.map [i](#)



X



Y

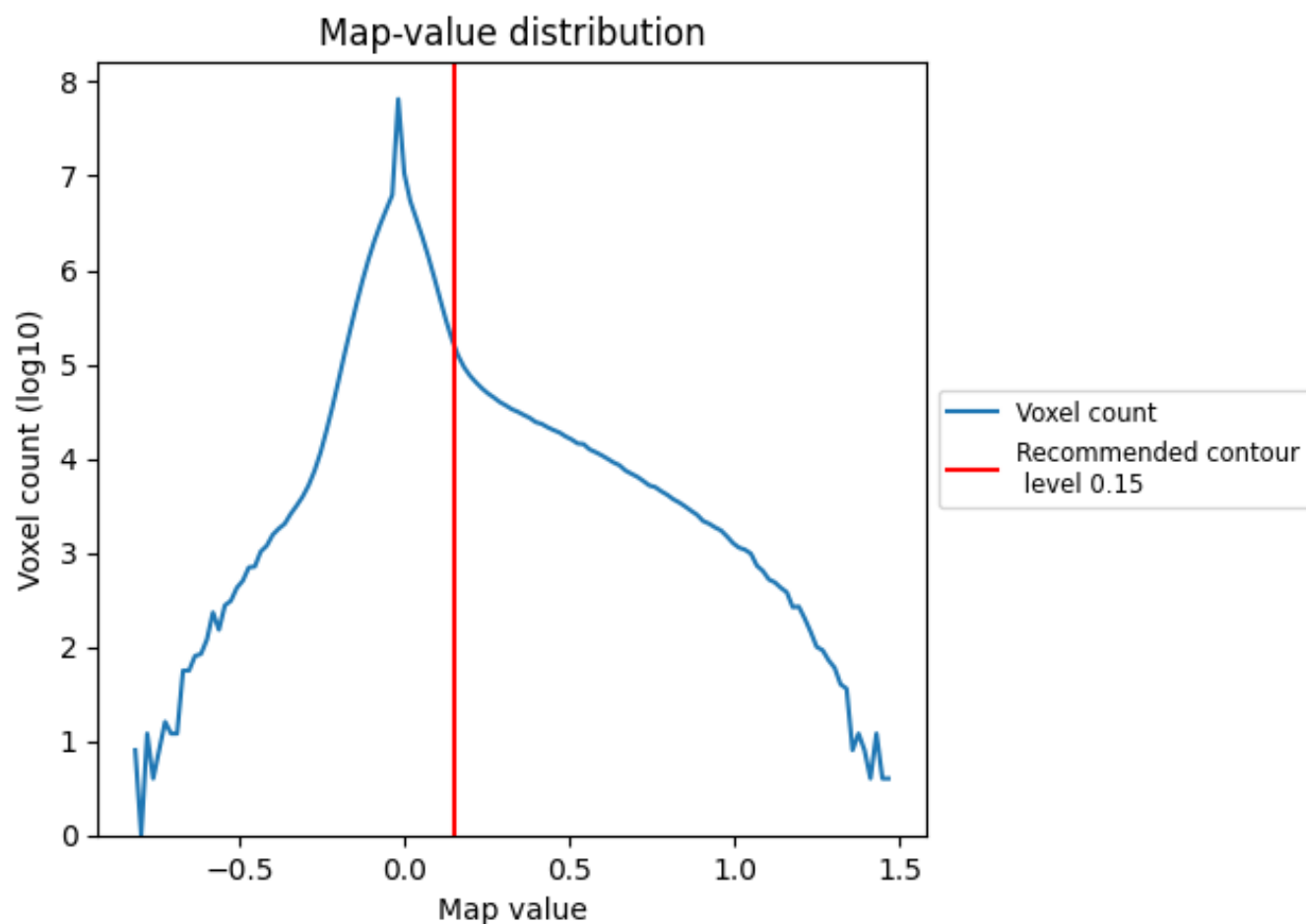


Z

7 Map analysis [i](#)

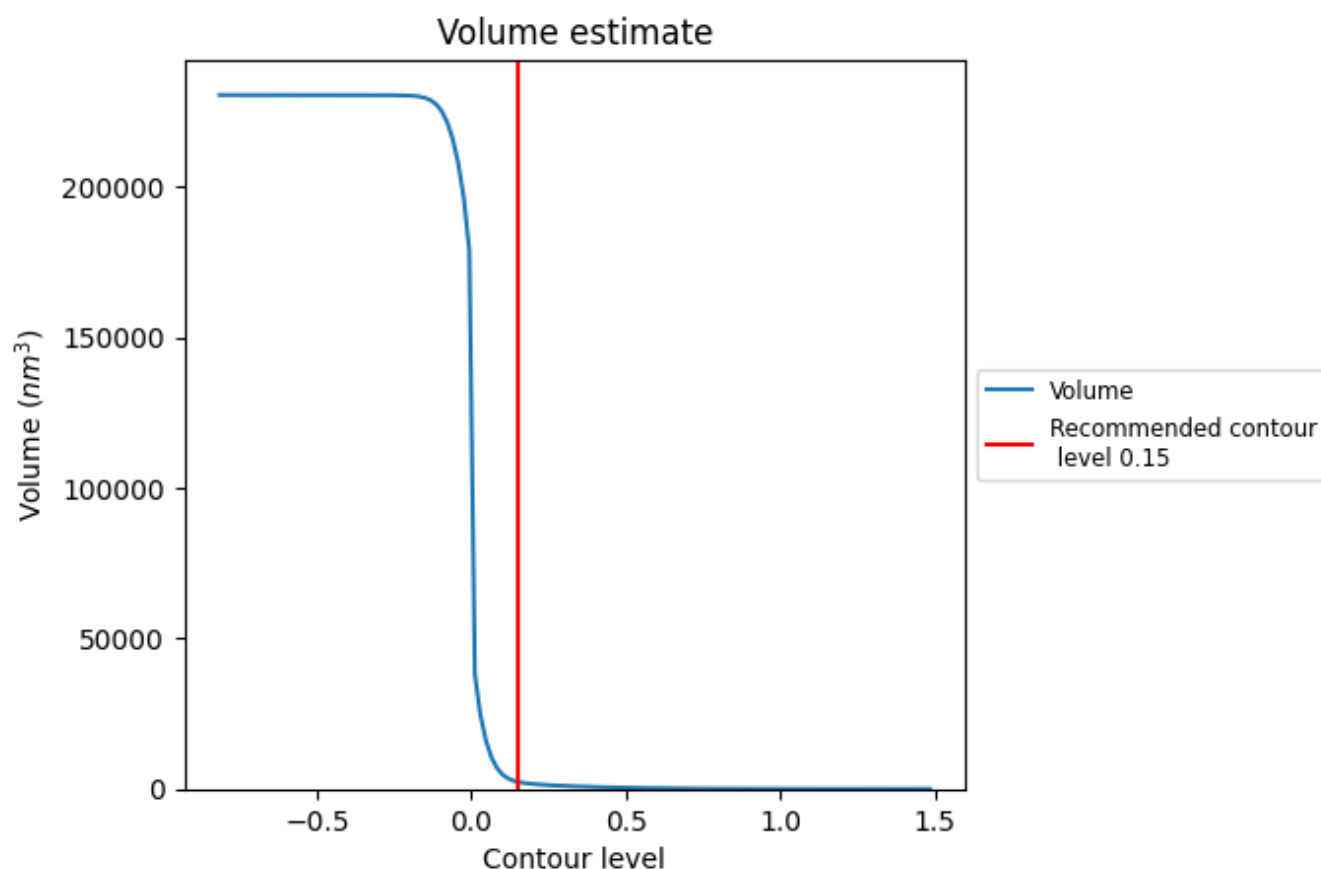
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

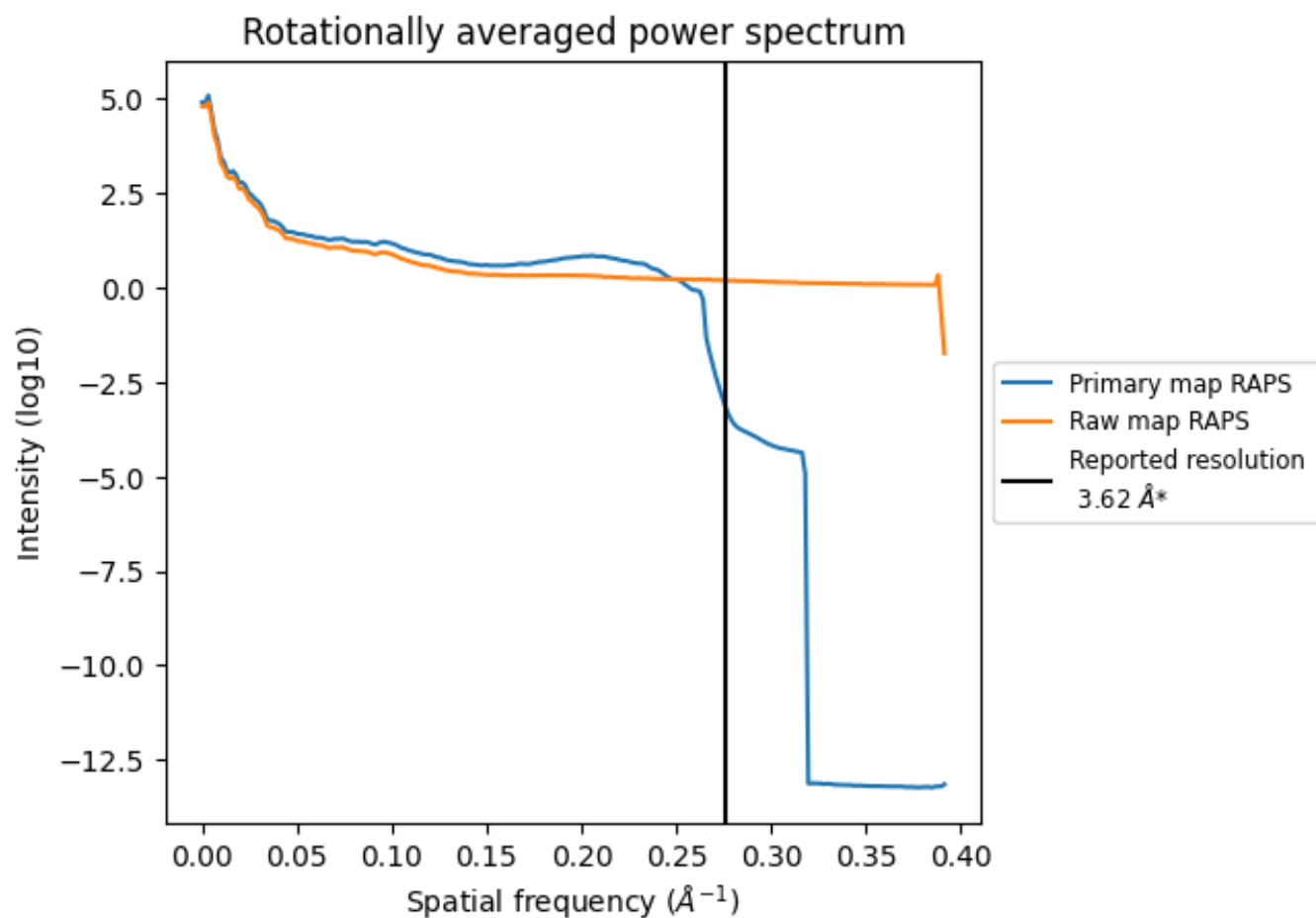
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

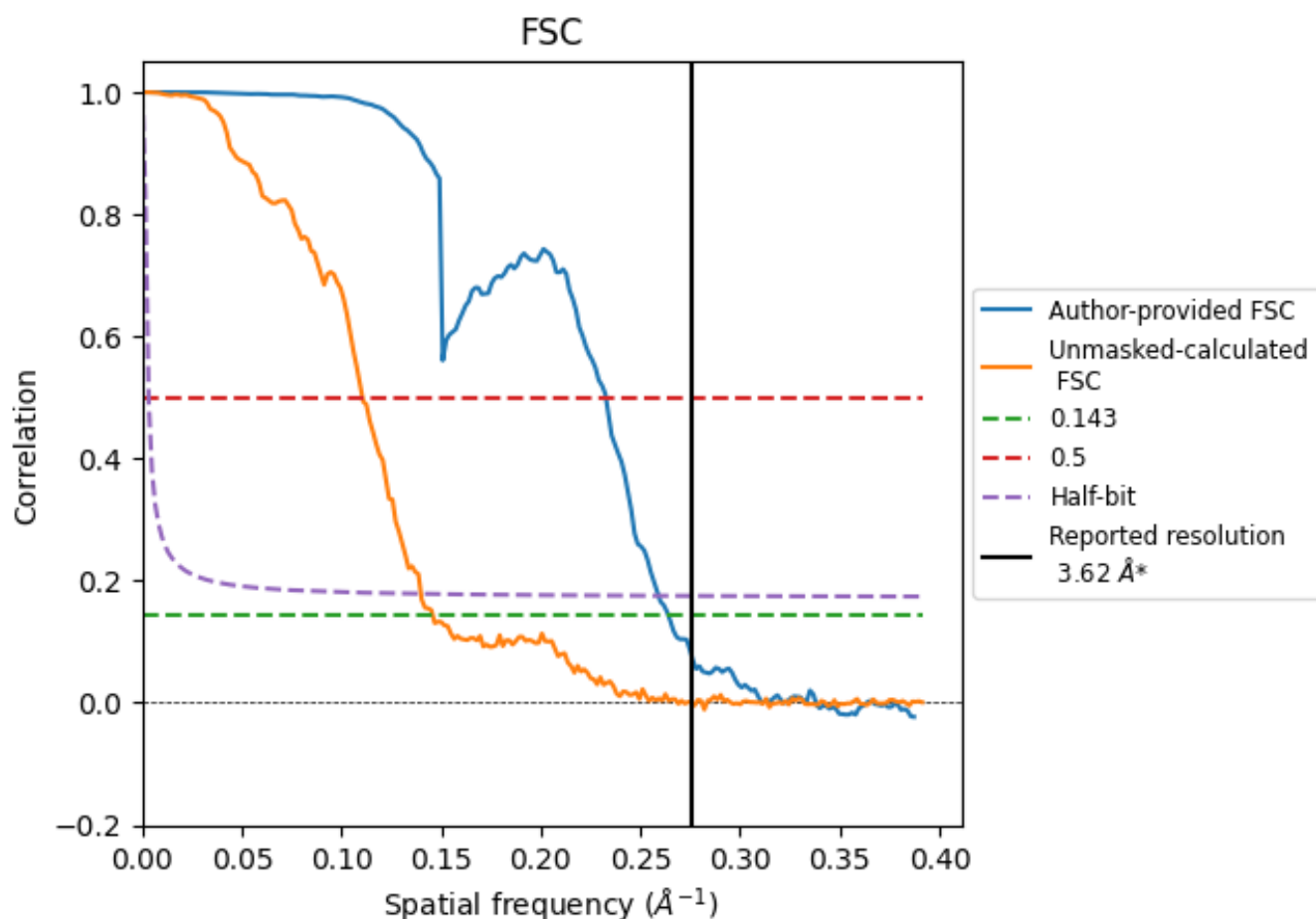


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.276 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

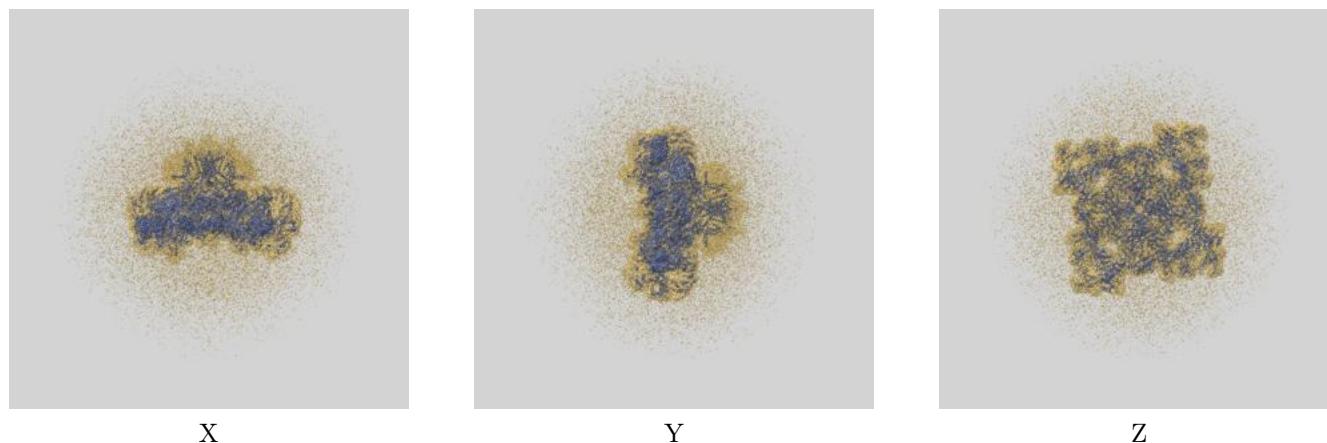
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.79	4.30	3.86
Unmasked-calculated*	6.86	9.05	7.15

*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 [i](#)

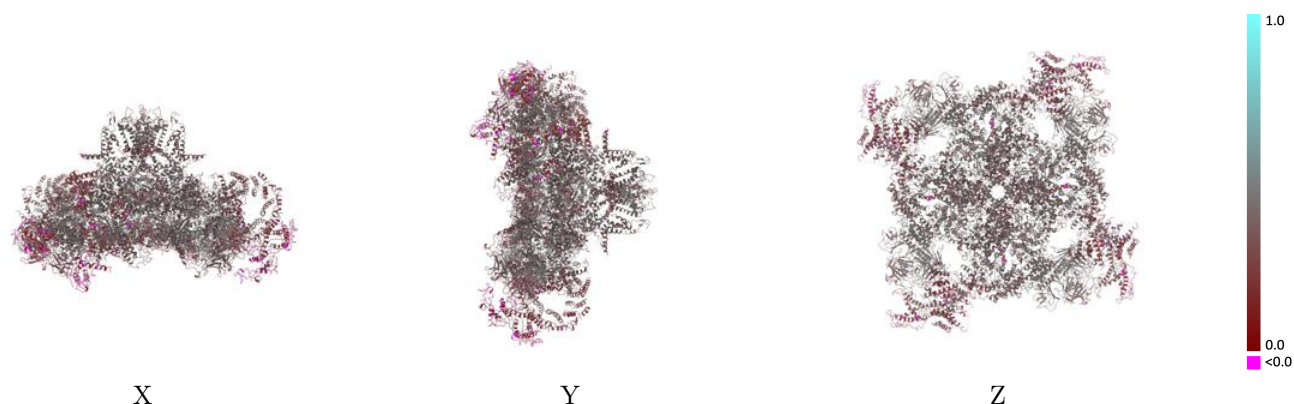
This section contains information regarding the fit between EMDB map EMD-38447 and PDB model 8XLF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



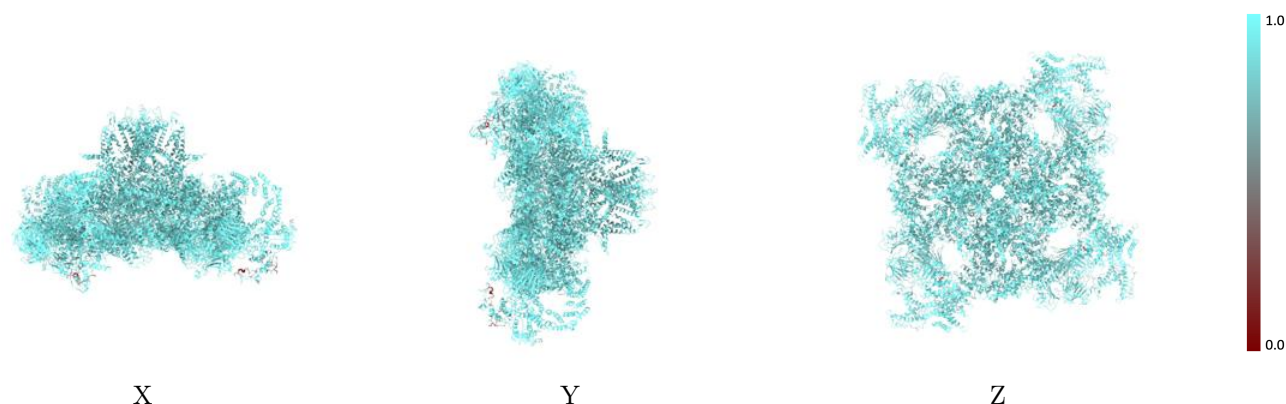
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



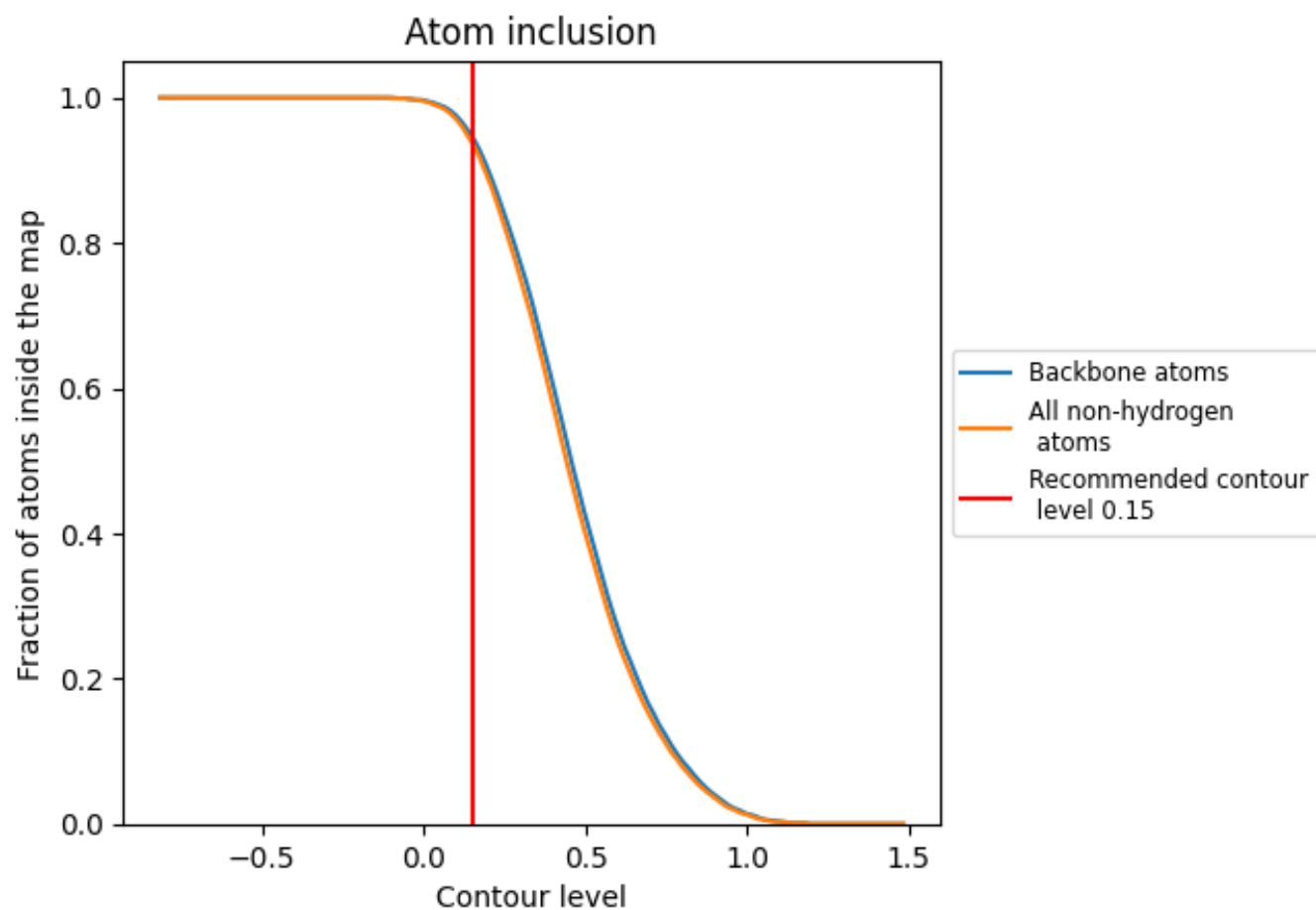
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

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

