



## Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 04:46 PM JST

PDB ID : 8X49  
EMDB ID : EMD-38043  
Title : Cryo-EM structure of Ryanodine receptor 1 (100 nM Ca<sup>2+</sup>)  
Authors : Chen, Q.; Hu, H.  
Deposited on : 2023-11-15  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

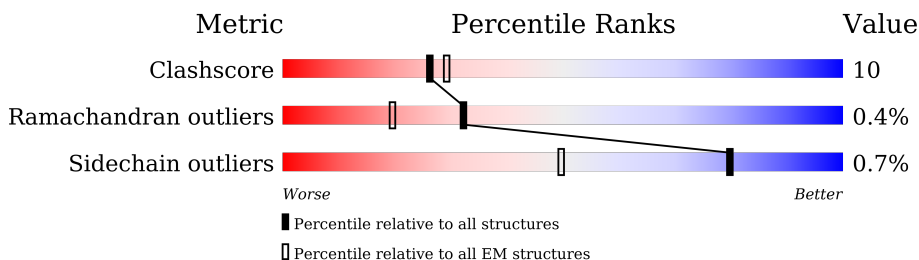
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	 5% 63% 15% 22%
1	B	5037	 5% 63% 15% 22%
1	C	5037	 5% 63% 15% 22%
1	D	5037	 5% 63% 15% 22%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 117356 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3952	Total	C	N	O	S	0	0
			29337	18674	5081	5394	188		
1	B	3952	Total	C	N	O	S	0	0
			29337	18674	5081	5394	188		
1	C	3952	Total	C	N	O	S	0	0
			29337	18674	5081	5394	188		
1	D	3952	Total	C	N	O	S	0	0
			29337	18674	5081	5394	188		

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

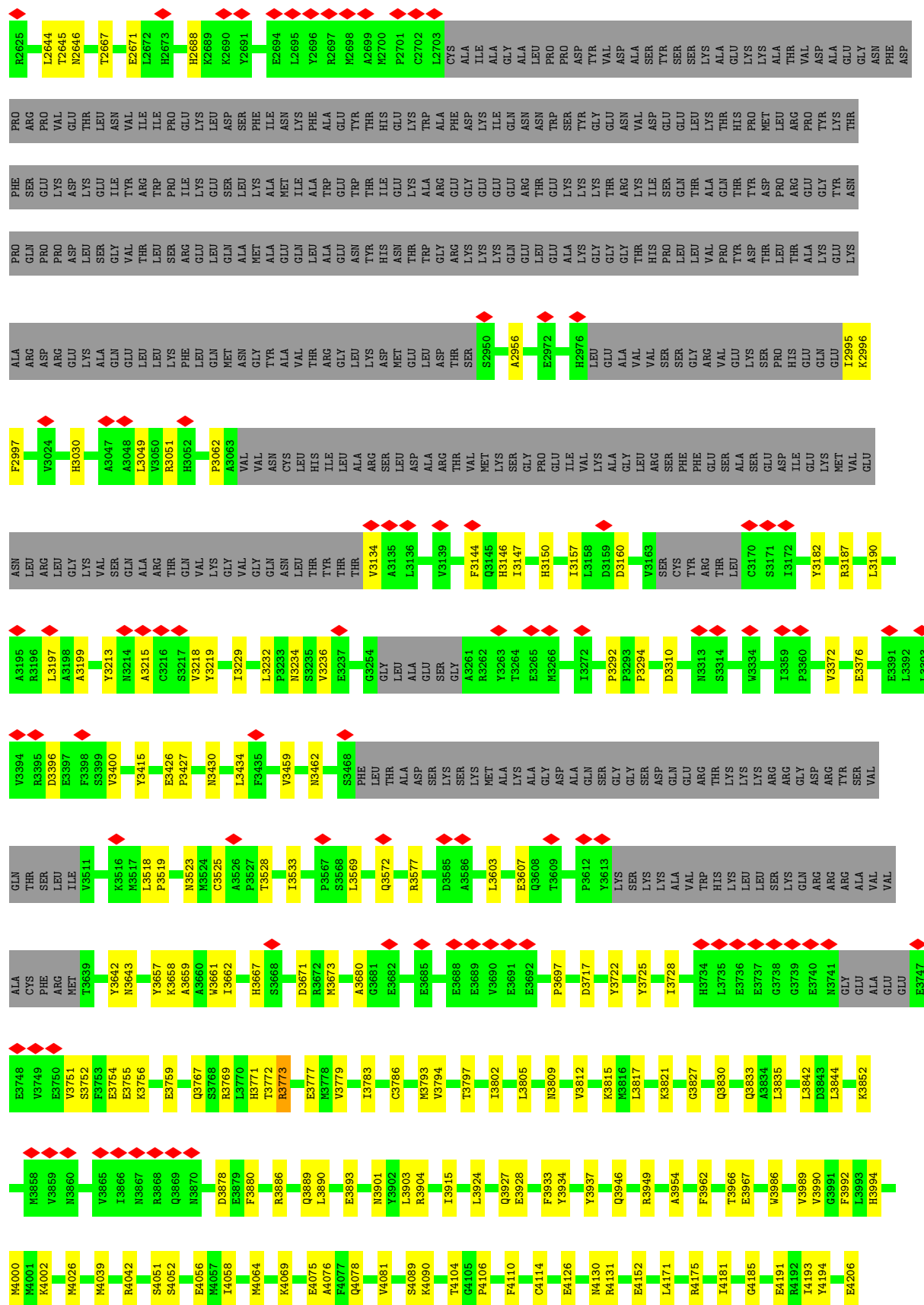
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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





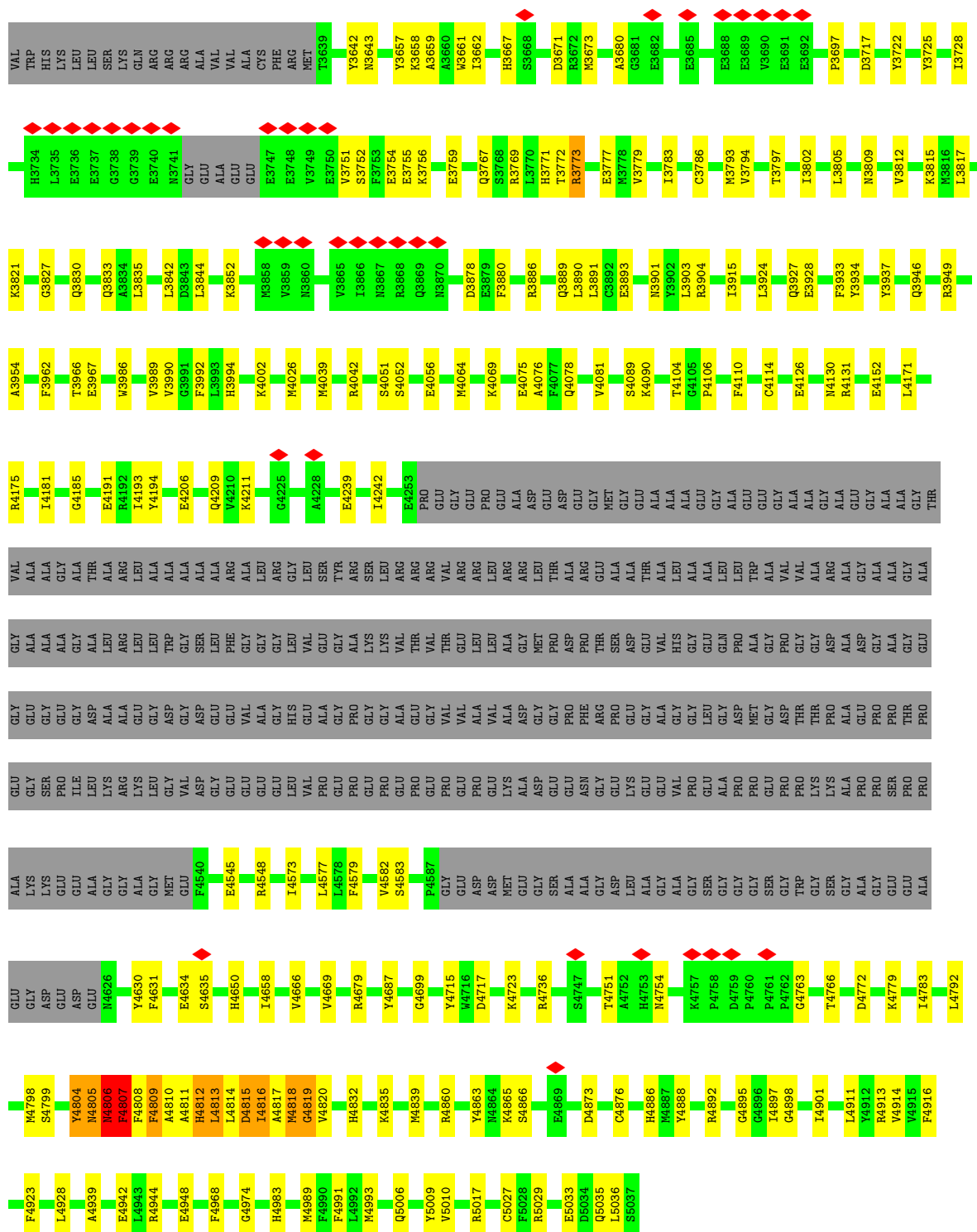




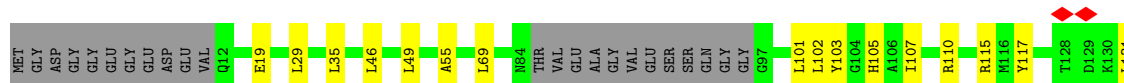
GLU	GLU	ALA	PRO	GLU	GLY	LYS	ASP	L1922	L1926	V1935	C1947	Y1965	L1969	N1972	R1976	Q2003	N2007	M2008	L2009	L2010	K2013	C2021	P2022	L2023	R2028	Q2029	D2030	L2031	I2044	Q2045	L2046	E2047	G2048	GLU	GLU	GLU	GLU	PRO	GLU	GLU	GLU	GLU	GLU	THR	SER	LEU				
P1840	V1841	L1842	K1843	L1844	V1845	S1846	T1847	L1848	L1849	V1850	M1851	V1859	I1862	L1863	K1864	M1865	V1870	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
S1726	R1727	L1728	S1729	M1730	L1731	S1732	R1752	R1758	L1762	V1765	R1772	P1773	P1774	F1782	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1796	R1797	E1805	R1808	A1811	M1814	V1819	A1826	R1827	D1828	P1829	V1830	G1831	G1832	S1833	V1834	E1835	F1836	Q1837	F1838	V1839				
L1575	F1580	E1583	P1592	F1593	L1594	L1595	M1600	M1601	P1602	R1607	N1610	V1615	GLU	THR	ARG	ALA	GLY	E1622	W1626	C1630	L1634	M1637	A1638	L1639	E1643	L1653	R1656	Q1660	T1666	C1674	S1687	P1704	L1707	T1716	S1717	I1718	Y1573	P1574												
M1482	V1483	S1486	C1489	S1490	C1492	M1493	M1494	V1495	W1496	V1501	S1502	P1503	Q1506	G1507	R1508	V1515	L1522	A1523	T1524	G1525	L1526	M1527	T1530	A1531	M1532	N1537	T1538	F1539	F1540	N1545	V1552	F1553	V1554	L1555	P1556	Q1563	F1564	GLU	LEU	GLY	LYS	GLN	LYS	ASN	ILE	M1573	P1574			
MET	THR	GLN	PRO	PRO	ALA	THR	PRO	ALA	LEU	ARG	PRO	HIS	ASP	ASN	ARG	ASP	PRO	GLY	ILE	ILE	LEU	ASN	T1430	V1450	G1451	W1452	V1453	T1454	Y1457	H1458	Q1459	N1463	F1464	D1465	L1466	S1467	K1468	Y1469	R1470	A1471	V1472	T1473	V1474	T1475	D1478	E1479	Y1480			
ALA	GLY	TRP	GLY	ALA	GLU	GLY	GLY	LYS	GLU	THR	ALA	LYS	GLY	THR	GLY	THR	GLY	PRO	VAL	ALA	GLN	PRO	THR	ALA	ARG	ALA	ASN	GLU	LYS	ASP	ALA	THR	GLY	LYS	ASN	ARG	GLY	PHE	LEU	PHE	LYS	ALA	ALA	ALA	MET					
C1289	L1270	R1271	L1272	T1276	L1283	V1284	E1285	M1286	L1287	F1288	L1289	Q1295	V1296	F1297	HIS	HIS	PHE	ARG	CYS	THR	ALA	GLY	ALA	THR	PRO	LEU	ALA	PRO	GLY	GLN	PRO	ASP	GLU	ALA	ARG	ALA	PRO	ASP	THR	LYS	ASN	ARG	GLY	THR	SER					
D1147	V1148	C1151	M1152	I1153	L1154	T1155	E1157	N1158	T1159	D1172	A1178	F1179	R1180	E1181	L1182	D1186	L1189	Q1198	L1202	N1203	Q1206	L1207	V1208	S1209	R1212	E1221	G1222	F1223	E1224	P1225	F1226	I1228	M1229	Q1231	W1237	P1243	E1246	H1252	Y1255	E1256	V1257									
A1042	L1047	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	E1078	R1087	W1088	Y1089	F1090	E1091	F1092	T1096	E1099	M1100	W1104	P1107	L1115	G1116	V1123	F1124	N1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	S1136	Q1144				
A942	D943	E944	A946	E947	D948	H949	L950	K951	K952	K953	T953	L955	P956	K957	T958	Y959	M960	M961	S962	G964	Y965	K966	P967	D971	L972	S973	H974	V975	R976	L977	T978	A997	A1002	Q1003	G1004	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	P1023	D1037		
I861	V862	L863	P864	P865	E868	K873	L874	N877	I878	L884	E888	G894	P895	V896	R897	D898	D899	N900	K901	R902	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	G926	E927	T928	L929	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941
D774	G775	L776	F777	P778	V779	V780	S781	G786	F791	L792	G793	G794	G795	G798	C811	L821	R822	L823	K827	GLU	TYR	ARG	ARG	GLU	GLY	PRO	ARG	GLY	PRO	HIS	LEU	VAL	GLY	PRO	SER	ARG	CYS	PRO	VAL	ASP	THR	THR	VAL	GLN						
F664	E665	V668	V671	L675	T676	A677	L682	R683	V684	G685	G794	W686	A687	L688	G697	G704	D710	L711	Y714	D717	G718	L719	H720	L721	L722	R728	H736	L737	V744	S745	C746	C747	L748	D749	L750	I755	S756	F757	R758	I759	C762	P763	F768	L773						

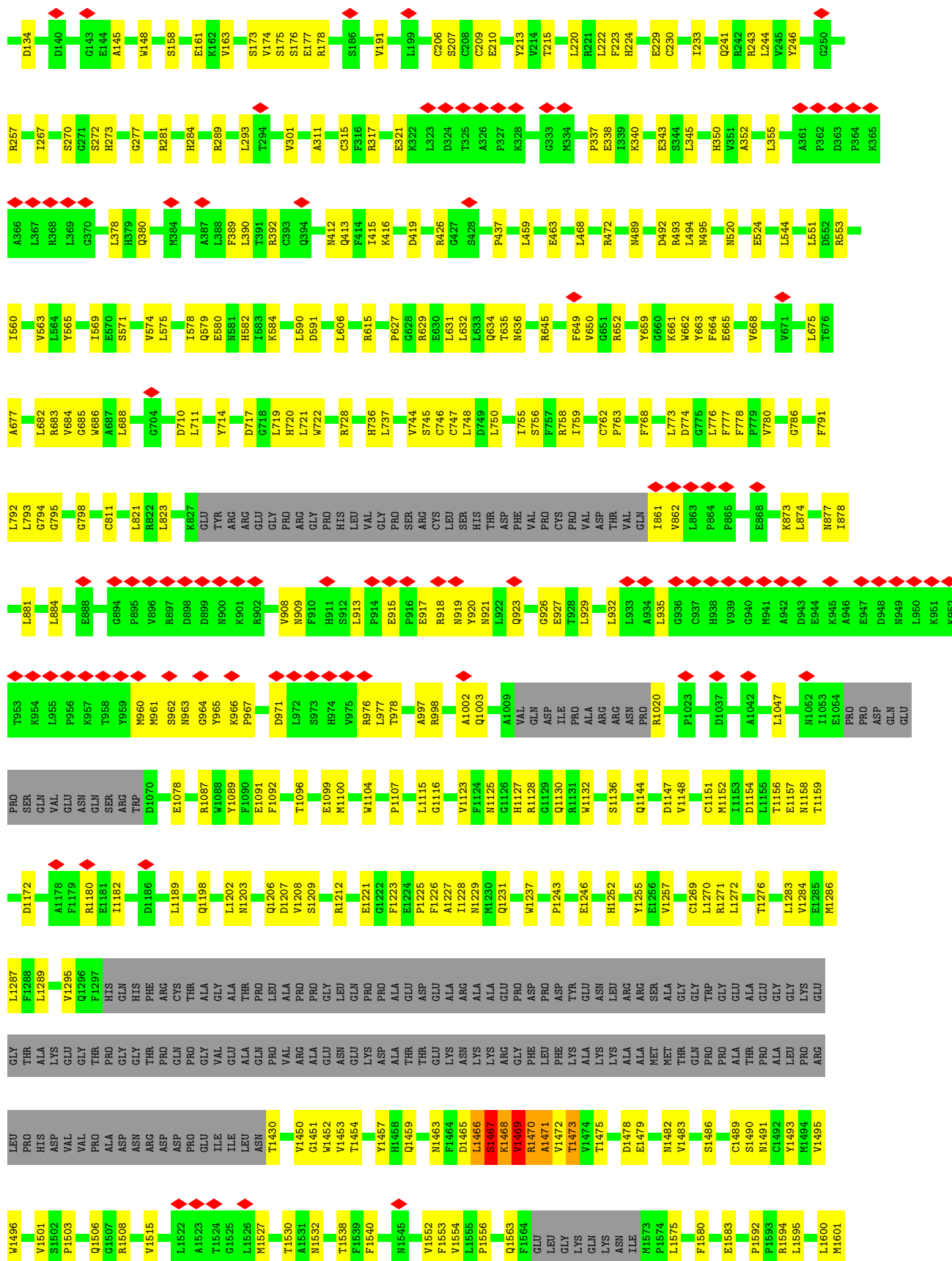






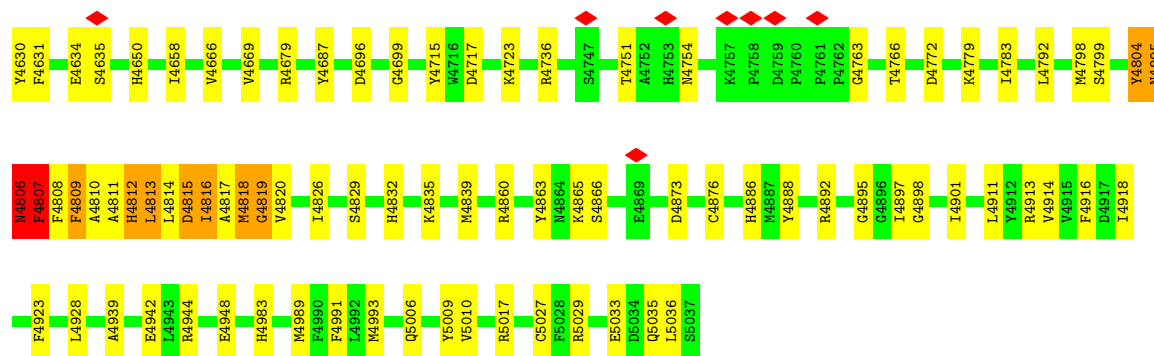
• Molecule 1: Ryanodine receptor 1



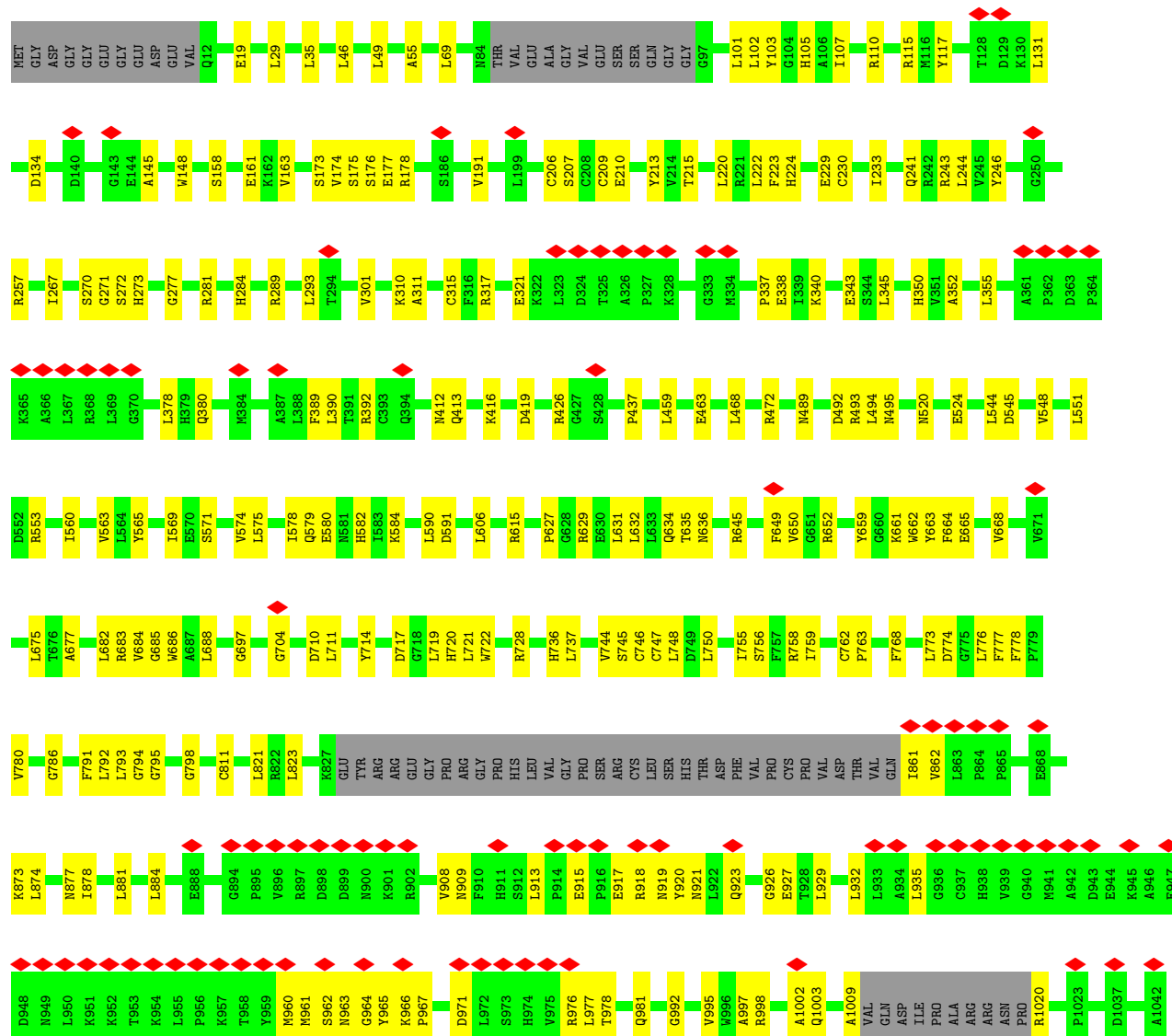








• Molecule 1: Ryanodine receptor 1





A3954	G3827	L3735	HIS	P3360	R3187	ILE	SER	PRO	THR	GLN	THR	ALA	V2586
F3962	Q3830	E3736	LYS	V3372	L3190	GLU	PRO	TYR	HIS	THR	THR	THR	Y2587
T3966	Q3833	G3738	SER	E3376	A3195	VAL	GLN	ASP	ASP	PRO	MET	ALA	S2590
E3967	A3834	G3739	LYS	E3391	R3196	GLU	GLU	THR	GLN	PRO	ARG	GLU	R2591
W3966	L3835	E3740	GLN	L3392	L3197	ASN	GLU	ALA	ARG	GLY	PRO	GLY	Y2613
L3842	L3842	N3741	ARG	L3393	A3199	LEU	LYS	LYS	TYR	GLY	TYR	ASN	P2616
V3989	D3843	GLY	ARG	V3394	A3199	LEU	GLY	ALA	PRO	ASN	THR	ASP	R2625
V3990	L3844	ALA	VAL	R3395	Y3213	LYS	VAL	ASP	SER	GLN	ARG	PRO	L2644
G3991	K3852	VAL	VAL	D3396	N3214	SER	SER	ARG	GLU	PRO	GLY	VAL	T2645
L3953	M3858	ALA	ALA	E3397	C3216	GLN	A3047	GLU	LYS	ASP	LYS	THR	T2646
H3994	V3859	CYS	PHE	F3398	A3215	ALA	A3049	LYS	GLY	LEU	LYS	THR	T2667
M4001	N3860	ARG	ARG	S3399	ARG	THR	R3051	ALA	SER	GLY	ILE	ASN	T2671
M4002	N3870	ILE	ILE	V3400	S3217	GLN	H3052	GLU	VAL	THR	ARG	ILE	L2672
M4026	V3865	V3511	V3511	Y3415	Y3219	VAL	P3062	LEU	THR	THR	ARG	ILE	H2673
M4039	I3866	K3516	K3516	E3426	T3229	LYS	A3063	LYS	LEU	THR	THR	PRO	R2688
R3868	N3867	M3517	M3517	P3427	L3232	VAL	VAL	PHE	ARG	ILE	GLU	PRO	K2690
R3869	K3657	L3518	L3518	N3430	L3233	GLY	VAL	GLN	GLY	GLU	GLY	LEU	T2691
Q3869	K3658	P3519	P3519	M3434	N3234	ASN	ASN	GLN	GLY	SER	ASP	ASP	E2694
N3870	A3659	N3523	N3523	F3435	S3285	LEU	LEU	ALA	ALA	ALA	ILE	ASN	L2695
D3878	A3660	C3525	C3525	S3446	V3236	THR	ILE	TYR	GLY	GLY	MET	ASN	R2697
E3879	I3662	A3526	A3526	H3449	E3237	THR	ALA	VAL	ALA	THR	ILE	LYS	R2698
F3880	H3667	T3528	T3528	V3459	G3254	THR	ARG	THR	ARG	GLU	ALA	ALA	R2699
R3886	S3668	L3533	L3533	N3462	GLY	GLY	THR	THR	THR	GLY	ALA	ALA	R2699
Q3888	D3671	P3567	P3567	S3468	A3261	GLY	THR	THR	THR	GLY	ALA	ALA	R2701
L3890	R3672	S3568	S3568	PHE	R3262	LEU	VAL	VAL	VAL	GLY	ALA	ALA	C2702
L3891	K3673	Q3572	Q3572	THR	Y3263	GLU	LYS	LYS	THR	GLY	ALA	ALA	L2703
C3892	M3673	L3569	L3569	ALA	T3264	ASP	SER	THR	THR	ARG	GLY	ALA	CYS
E3777	A3680	R3577	R3577	ASP	E3265	LYS	GLY	SER	GLY	LYS	ASP	ALA	ILE
R3778	G3681	D3585	D3585	SER	M3266	PRO	PRO	GLY	GLY	LYS	ASP	ALA	ALA
V3779	E3682	A3586	A3586	LYS	I3272	ILE	ILE	GLU	GLU	LYS	ILE	GLY	ALA
I3783	E3685	L3603	L3603	MET	P3292	LYS	LYS	GLN	GLU	GLY	GLN	GLY	ALA
C3786	E3688	Q3607	Q3607	ALA	P3293	CYS	VAL	GLU	GLY	ARG	ASN	ASN	ALA
M3793	E3689	T3609	T3609	ALA	P3294	TYR	SER	LEU	THR	THR	THR	THR	PRO
V3794	V3690	P3612	P3612	ASP	D3310	ARG	PHE	ALA	GLY	GLY	GLY	GLY	ASP
T3797	E3691	Y3613	Y3613	GLN	N3313	THR	PHE	VAL	SER	THR	THR	THR	VAL
T3802	E3692	LYS	LYS	ALA	S3314	LEU	GLU	VAL	GLY	GLY	GLY	GLY	ALA
L3805	P3697	SER	SER	GLY	G3317	GLY	SER	GLY	GLY	GLY	GLY	GLY	ASP
L3809	D3717	LYS	LYS	GLN	L3320	ASP	GLU	VAL	VAL	VAL	VAL	VAL	TYR
V3812	Y3722	LYS	LYS	GLN	H3334	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL
K3815	Y3725	SER	SER	GLY	G3317	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL
M3816	I3728	LYS	LYS	GLY	L3320	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL
L3817	H3734	ALA	ALA	ASP	H3334	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL
K3821		TRP	TRP	GLU	I3359	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183859	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)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.737	Depositor
Minimum map value	-2.523	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.466	Depositor
Map size (Å)	516.72003, 516.72003, 516.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0765, 1.0765, 1.0765	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/29956	0.47	0/40772
1	B	0.30	0/29956	0.47	0/40772
1	C	0.30	0/29956	0.47	0/40772
1	D	0.30	0/29956	0.47	0/40772
All	All	0.30	0/119824	0.47	0/163088

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29337	0	27528	579	0
1	B	29337	0	27528	585	0
1	C	29337	0	27528	579	0
1	D	29337	0	27528	580	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	117356	0	110112	2250	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 10.

All (2250) 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:C:1965:TYR:CE2	1:C:1969:LEU:HD11	2.12	0.85
1:D:1965:TYR:CE2	1:D:1969:LEU:HD11	2.12	0.84
1:B:1965:TYR:CE2	1:B:1969:LEU:HD11	2.12	0.84
1:A:1965:TYR:CE2	1:A:1969:LEU:HD11	2.12	0.84
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.61	0.82
1:A:3990:VAL:HG23	1:A:4051:SER:HB3	1.61	0.81
1:B:1830:VAL:O	1:B:1832:GLY:N	2.13	0.81
1:B:3990:VAL:HG23	1:B:4051:SER:HB3	1.61	0.81
1:D:3990:VAL:HG23	1:D:4051:SER:HB3	1.61	0.81
1:A:1830:VAL:O	1:A:1832:GLY:N	2.13	0.80
1:C:1830:VAL:O	1:C:1832:GLY:N	2.13	0.80
1:D:1830:VAL:O	1:D:1832:GLY:N	2.13	0.80
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.56	0.79
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.56	0.79
1:C:2170:MET:HG3	1:C:2214:VAL:HG12	1.65	0.79
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.56	0.79
1:B:2170:MET:HG3	1:B:2214:VAL:HG12	1.65	0.79
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.56	0.78
1:A:3134:VAL:N	1:D:978:THR:HG1	1.81	0.78
1:B:978:THR:HG1	1:C:3134:VAL:N	1.81	0.78
1:A:4901:ILE:HD12	1:A:4913:ARG:HH22	1.48	0.78
1:D:2170:MET:HG3	1:D:2214:VAL:HG12	1.65	0.78
1:D:4901:ILE:HD12	1:D:4913:ARG:HH22	1.48	0.78
1:B:220:LEU:HD11	1:B:390:LEU:HD23	1.66	0.78
1:C:4901:ILE:HD12	1:C:4913:ARG:HH22	1.48	0.77
1:C:978:THR:HG1	1:D:3134:VAL:N	1.82	0.77
1:A:2170:MET:HG3	1:A:2214:VAL:HG12	1.65	0.77
1:C:220:LEU:HD11	1:C:390:LEU:HD23	1.66	0.77
1:C:1471:ALA:O	1:C:1473:THR:N	2.18	0.77
1:D:220:LEU:HD11	1:D:390:LEU:HD23	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1471:ALA:O	1:A:1473:THR:N	2.18	0.77
1:A:220:LEU:HD11	1:A:390:LEU:HD23	1.66	0.77
1:B:4901:ILE:HD12	1:B:4913:ARG:HH22	1.48	0.77
1:C:1839:VAL:HG23	1:C:1935:VAL:HG12	1.67	0.77
1:B:1471:ALA:O	1:B:1473:THR:N	2.18	0.76
1:B:1839:VAL:HG23	1:B:1935:VAL:HG12	1.67	0.76
1:D:1471:ALA:O	1:D:1473:THR:N	2.18	0.76
1:A:1839:VAL:HG23	1:A:1935:VAL:HG12	1.67	0.75
1:B:213:TYR:HB3	1:B:273:HIS:HE1	1.52	0.75
1:D:1835:GLU:O	1:D:1837:GLN:N	2.20	0.75
1:D:1839:VAL:HG23	1:D:1935:VAL:HG12	1.67	0.75
1:A:1835:GLU:O	1:A:1837:GLN:N	2.20	0.75
1:B:1835:GLU:O	1:B:1837:GLN:N	2.20	0.75
1:A:747:CYS:SG	1:A:756:SER:OG	2.45	0.74
1:A:2336:ARG:O	1:A:2340:PHE:HB2	1.88	0.74
1:C:213:TYR:HB3	1:C:273:HIS:HE1	1.52	0.74
1:D:747:CYS:SG	1:D:756:SER:OG	2.45	0.74
1:A:4679:ARG:NH1	1:A:4715:TYR:OH	2.20	0.74
1:C:2336:ARG:O	1:C:2340:PHE:HB2	1.88	0.74
1:B:747:CYS:SG	1:B:756:SER:OG	2.45	0.74
1:B:2336:ARG:O	1:B:2340:PHE:HB2	1.88	0.74
1:D:4679:ARG:NH1	1:D:4715:TYR:OH	2.20	0.74
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.20	0.74
1:C:1835:GLU:O	1:C:1837:GLN:N	2.20	0.74
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.20	0.74
1:C:747:CYS:SG	1:C:756:SER:OG	2.45	0.74
1:C:1965:TYR:CZ	1:C:1969:LEU:HD11	2.23	0.74
1:D:213:TYR:HB3	1:D:273:HIS:HE1	1.52	0.74
1:A:1965:TYR:CZ	1:A:1969:LEU:HD11	2.23	0.74
1:B:1965:TYR:CE2	1:B:1969:LEU:CD1	2.71	0.73
1:A:213:TYR:HB3	1:A:273:HIS:HE1	1.52	0.73
1:B:1965:TYR:CZ	1:B:1969:LEU:HD11	2.23	0.73
1:D:145:ALA:HA	1:D:175:SER:HB2	1.70	0.73
1:D:1284:VAL:HG22	1:D:1463:ASN:HB2	1.70	0.73
1:D:1965:TYR:CE2	1:D:1969:LEU:CD1	2.71	0.73
1:D:2336:ARG:O	1:D:2340:PHE:HB2	1.88	0.73
1:C:1965:TYR:CE2	1:C:1969:LEU:CD1	2.71	0.73
1:D:2584:HIS:CD2	1:D:2585:THR:H	2.07	0.73
1:D:1965:TYR:CZ	1:D:1969:LEU:HD11	2.23	0.73
1:C:2584:HIS:CD2	1:C:2585:THR:H	2.07	0.73
1:B:1284:VAL:HG22	1:B:1463:ASN:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:O	1:B:2452:ARG:NH1	2.22	0.72
1:A:1965:TYR:CE2	1:A:1969:LEU:CD1	2.71	0.72
1:B:686:TRP:HE1	1:B:746:CYS:HG	1.31	0.72
1:C:1284:VAL:HG22	1:C:1463:ASN:HB2	1.70	0.72
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.72	0.72
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.72	0.72
1:A:1284:VAL:HG22	1:A:1463:ASN:HB2	1.70	0.72
1:A:2452:ARG:NH1	1:D:174:VAL:O	2.22	0.72
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.72	0.72
1:A:145:ALA:HA	1:A:175:SER:HB2	1.70	0.72
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.72	0.72
1:C:174:VAL:O	1:D:2452:ARG:NH1	2.22	0.72
1:B:174:VAL:O	1:C:2452:ARG:NH1	2.22	0.72
1:B:2584:HIS:CD2	1:B:2585:THR:H	2.07	0.71
1:D:209:CYS:SG	1:D:210:GLU:N	2.63	0.71
1:A:978:THR:HG1	1:B:3134:VAL:N	1.88	0.71
1:A:2584:HIS:CD2	1:A:2585:THR:H	2.07	0.71
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.73	0.71
1:B:145:ALA:HA	1:B:175:SER:HB2	1.70	0.71
1:A:209:CYS:SG	1:A:210:GLU:N	2.63	0.71
1:C:145:ALA:HA	1:C:175:SER:HB2	1.70	0.71
1:B:209:CYS:SG	1:B:210:GLU:N	2.63	0.71
1:B:997:ALA:HB1	1:B:1002:ALA:HB3	1.72	0.71
1:C:209:CYS:SG	1:C:210:GLU:N	2.63	0.71
1:C:997:ALA:HB1	1:C:1002:ALA:HB3	1.72	0.71
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.24	0.71
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.24	0.71
1:D:4126:GLU:O	1:D:4130:ASN:ND2	2.23	0.71
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.73	0.71
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.24	0.70
1:A:4126:GLU:O	1:A:4130:ASN:ND2	2.23	0.70
1:B:4126:GLU:O	1:B:4130:ASN:ND2	2.23	0.70
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.24	0.70
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.73	0.70
1:C:4126:GLU:O	1:C:4130:ASN:ND2	2.23	0.70
1:A:551:LEU:HB3	1:A:553:ARG:HH22	1.56	0.70
1:D:3049:LEU:HB3	1:D:3051:ARG:HG2	1.74	0.70
1:D:627:PRO:O	1:D:629:ARG:NH1	2.25	0.70
1:B:3049:LEU:HB3	1:B:3051:ARG:HG2	1.74	0.70
1:C:551:LEU:HB3	1:C:553:ARG:HH22	1.56	0.70
1:D:551:LEU:HB3	1:D:553:ARG:HH22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:ALA:HB1	1:A:1002:ALA:HB3	1.72	0.69
1:C:3049:LEU:HB3	1:C:3051:ARG:HG2	1.74	0.69
1:C:3671:ASP:OD1	1:C:3769:ARG:NH2	2.24	0.69
1:D:997:ALA:HB1	1:D:1002:ALA:HB3	1.72	0.69
1:D:3671:ASP:OD1	1:D:3769:ARG:NH2	2.24	0.69
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.73	0.69
1:B:551:LEU:HB3	1:B:553:ARG:HH22	1.56	0.69
1:B:627:PRO:O	1:B:629:ARG:NH1	2.25	0.69
1:A:627:PRO:O	1:A:629:ARG:NH1	2.25	0.69
1:B:3772:THR:OG1	1:B:3815:LYS:NZ	2.26	0.69
1:C:627:PRO:O	1:C:629:ARG:NH1	2.25	0.69
1:A:3049:LEU:HB3	1:A:3051:ARG:HG2	1.74	0.69
1:C:3772:THR:OG1	1:C:3815:LYS:NZ	2.26	0.69
1:B:1863:LEU:HD21	1:B:1870:VAL:HG11	1.76	0.68
1:B:110:ARG:HE	1:B:115:ARG:HE	1.42	0.68
1:C:686:TRP:HE1	1:C:746:CYS:HG	1.37	0.68
1:A:4069:LYS:NZ	1:A:4130:ASN:OD1	2.27	0.68
1:B:4242:ILE:HG13	1:B:4989:MET:HE1	1.76	0.68
1:D:1863:LEU:HD21	1:D:1870:VAL:HG11	1.76	0.68
1:D:3772:THR:OG1	1:D:3815:LYS:NZ	2.26	0.68
1:A:459:LEU:HD21	1:A:463:GLU:HG2	1.76	0.67
1:C:459:LEU:HD21	1:C:463:GLU:HG2	1.76	0.67
1:B:3671:ASP:OD1	1:B:3769:ARG:NH2	2.24	0.67
1:C:110:ARG:HE	1:C:115:ARG:HE	1.42	0.67
1:C:1863:LEU:HD21	1:C:1870:VAL:HG11	1.76	0.67
1:A:110:ARG:HE	1:A:115:ARG:HE	1.42	0.67
1:B:277:GLY:HA2	1:B:315:CYS:HB2	1.77	0.67
1:D:1269:CYS:SG	1:D:1471:ALA:HB1	2.35	0.67
1:D:4242:ILE:HG13	1:D:4989:MET:HE1	1.77	0.67
1:B:19:GLU:HB3	1:B:206:CYS:HB3	1.77	0.67
1:C:1269:CYS:SG	1:C:1471:ALA:HB1	2.35	0.67
1:D:277:GLY:HA2	1:D:315:CYS:HB2	1.77	0.67
1:C:19:GLU:HB3	1:C:206:CYS:HB3	1.77	0.66
1:A:1276:THR:HA	1:A:1466:LEU:HD22	1.77	0.66
1:A:3772:THR:OG1	1:A:3815:LYS:NZ	2.26	0.66
1:A:4242:ILE:HG13	1:A:4989:MET:HE1	1.77	0.66
1:B:459:LEU:HD21	1:B:463:GLU:HG2	1.76	0.66
1:D:2205:GLU:O	1:D:2209:GLU:HG2	1.96	0.66
1:C:786:GLY:N	1:C:1630:CYS:O	2.29	0.66
1:D:675:LEU:HD23	1:D:677:ALA:H	1.60	0.66
1:B:675:LEU:HD23	1:B:677:ALA:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:LEU:HD21	1:D:463:GLU:HG2	1.76	0.66
1:D:3146:HIS:O	1:D:3150:HIS:ND1	2.25	0.66
1:A:1269:CYS:SG	1:A:1471:ALA:HB1	2.35	0.66
1:D:19:GLU:HB3	1:D:206:CYS:HB3	1.77	0.66
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.13	0.66
1:A:4573:ILE:O	1:A:4577:LEU:HD12	1.96	0.66
1:B:1269:CYS:SG	1:B:1471:ALA:HB1	2.35	0.66
1:B:1501:VAL:HG22	1:B:1503:PRO:HD3	1.78	0.66
1:B:3146:HIS:O	1:B:3150:HIS:ND1	2.25	0.66
1:C:1501:VAL:HG22	1:C:1503:PRO:HD3	1.78	0.66
1:A:19:GLU:HB3	1:A:206:CYS:HB3	1.77	0.66
1:A:3146:HIS:O	1:A:3150:HIS:ND1	2.25	0.66
1:A:3671:ASP:OD1	1:A:3769:ARG:NH2	2.24	0.66
1:B:4069:LYS:NZ	1:B:4130:ASN:OD1	2.27	0.66
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.13	0.66
1:A:2205:GLU:O	1:A:2209:GLU:HG2	1.96	0.66
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.13	0.66
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.29	0.66
1:C:675:LEU:HD23	1:C:677:ALA:H	1.60	0.66
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.29	0.66
1:C:3751:VAL:O	1:C:3756:LYS:NZ	2.29	0.66
1:B:786:GLY:N	1:B:1630:CYS:O	2.29	0.65
1:C:1276:THR:HA	1:C:1466:LEU:HD22	1.77	0.65
1:D:786:GLY:N	1:D:1630:CYS:O	2.29	0.65
1:D:4069:LYS:NZ	1:D:4130:ASN:OD1	2.27	0.65
1:D:4573:ILE:O	1:D:4577:LEU:HD12	1.96	0.65
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.29	0.65
1:A:4817:ALA:C	1:A:4819:GLY:H	2.00	0.65
1:C:257:ARG:O	1:C:284:HIS:NE2	2.30	0.65
1:C:2205:GLU:O	1:C:2209:GLU:HG2	1.96	0.65
1:D:110:ARG:HE	1:D:115:ARG:HE	1.42	0.65
1:D:794:GLY:H	1:D:798:GLY:HA3	1.62	0.65
1:D:4817:ALA:C	1:D:4819:GLY:H	2.00	0.65
1:A:277:GLY:HA2	1:A:315:CYS:HB2	1.77	0.65
1:A:1863:LEU:HD21	1:A:1870:VAL:HG11	1.76	0.65
1:A:3751:VAL:O	1:A:3756:LYS:NZ	2.29	0.65
1:A:3434:LEU:HD21	1:A:3533:ILE:HG12	1.78	0.65
1:D:1276:THR:HA	1:D:1466:LEU:HD22	1.77	0.65
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.29	0.65
1:A:675:LEU:HD23	1:A:677:ALA:H	1.60	0.65
1:A:786:GLY:N	1:A:1630:CYS:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3459:VAL:O	1:B:3462:ASN:ND2	2.30	0.65
1:A:2495:VAL:HG12	1:A:2497:ASP:H	1.62	0.65
1:B:3434:LEU:HD21	1:B:3533:ILE:HG12	1.78	0.65
1:B:4573:ILE:O	1:B:4577:LEU:HD12	1.96	0.65
1:C:3146:HIS:O	1:C:3150:HIS:ND1	2.25	0.65
1:D:2495:VAL:HG12	1:D:2497:ASP:H	1.62	0.65
1:B:1276:THR:HA	1:B:1466:LEU:HD22	1.77	0.65
1:B:3751:VAL:O	1:B:3756:LYS:NZ	2.29	0.65
1:D:1501:VAL:HG22	1:D:1503:PRO:HD3	1.78	0.65
1:A:1501:VAL:HG22	1:A:1503:PRO:HD3	1.78	0.65
1:B:2205:GLU:O	1:B:2209:GLU:HG2	1.96	0.65
1:C:3434:LEU:HD21	1:C:3533:ILE:HG12	1.78	0.65
1:C:4573:ILE:O	1:C:4577:LEU:HD12	1.96	0.65
1:D:3751:VAL:O	1:D:3756:LYS:NZ	2.29	0.65
1:A:257:ARG:O	1:A:284:HIS:NE2	2.30	0.65
1:A:1159:THR:HG22	1:A:1180:ARG:HH21	1.62	0.65
1:C:794:GLY:H	1:C:798:GLY:HA3	1.62	0.65
1:D:1159:THR:HG22	1:D:1180:ARG:HH21	1.62	0.65
1:B:1159:THR:HG22	1:B:1180:ARG:HH21	1.62	0.64
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.79	0.64
1:C:1159:THR:HG22	1:C:1180:ARG:HH21	1.62	0.64
1:D:257:ARG:O	1:D:284:HIS:NE2	2.30	0.64
1:A:3459:VAL:O	1:A:3462:ASN:ND2	2.30	0.64
1:B:257:ARG:O	1:B:284:HIS:NE2	2.30	0.64
1:C:277:GLY:HA2	1:C:315:CYS:HB2	1.77	0.64
1:A:794:GLY:H	1:A:798:GLY:HA3	1.62	0.64
1:B:635:THR:CG2	1:B:1637:MET:HG2	2.28	0.64
1:B:4817:ALA:C	1:B:4819:GLY:H	2.00	0.64
1:C:635:THR:CG2	1:C:1637:MET:HG2	2.28	0.64
1:C:2500:ALA:O	1:C:2551:ASN:ND2	2.30	0.64
1:C:4817:ALA:C	1:C:4819:GLY:H	2.00	0.64
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.79	0.64
1:D:635:THR:CG2	1:D:1637:MET:HG2	2.28	0.64
1:D:3434:LEU:HD21	1:D:3533:ILE:HG12	1.78	0.64
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.66	0.64
1:D:3459:VAL:O	1:D:3462:ASN:ND2	2.30	0.64
1:A:1728:ARG:HA	1:A:1731:LEU:HD12	1.80	0.64
1:A:2500:ALA:O	1:A:2551:ASN:ND2	2.30	0.64
1:C:3901:ASN:OD1	1:C:3904:ARG:NH2	2.29	0.64
1:C:1453:VAL:HG23	1:C:1454:THR:H	1.63	0.64
1:C:3459:VAL:O	1:C:3462:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4069:LYS:NZ	1:C:4130:ASN:OD1	2.27	0.64
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.79	0.64
1:A:635:THR:CG2	1:A:1637:MET:HG2	2.28	0.64
1:B:1728:ARG:HA	1:B:1731:LEU:HD12	1.80	0.64
1:B:2495:VAL:HG12	1:B:2497:ASP:H	1.62	0.64
1:B:2500:ALA:O	1:B:2551:ASN:ND2	2.30	0.64
1:B:1271:ARG:NH2	1:B:1469:VAL:O	2.31	0.64
1:C:908:VAL:HG22	1:C:909:ASN:H	1.63	0.64
1:C:2340:PHE:HA	1:C:2435:ARG:HE	1.62	0.64
1:C:2495:VAL:HG12	1:C:2497:ASP:H	1.62	0.63
1:A:1271:ARG:NH2	1:A:1469:VAL:O	2.31	0.63
1:A:3901:ASN:OD1	1:A:3904:ARG:NH2	2.29	0.63
1:C:1271:ARG:NH2	1:C:1469:VAL:O	2.31	0.63
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.13	0.63
1:D:1271:ARG:NH2	1:D:1469:VAL:O	2.31	0.63
1:D:1453:VAL:HG23	1:D:1454:THR:H	1.63	0.63
1:D:2500:ALA:O	1:D:2551:ASN:ND2	2.30	0.63
1:B:794:GLY:H	1:B:798:GLY:HA3	1.62	0.63
1:D:4805:ASN:O	1:D:4806:ASN:C	2.36	0.63
1:A:2340:PHE:HA	1:A:2435:ARG:HE	1.62	0.63
1:C:1289:LEU:HD12	1:C:1595:LEU:HD12	1.80	0.63
1:C:1728:ARG:HA	1:C:1731:LEU:HD12	1.80	0.63
1:D:2340:PHE:HA	1:D:2435:ARG:HE	1.62	0.63
1:B:1453:VAL:HG23	1:B:1454:THR:H	1.63	0.63
1:B:4805:ASN:O	1:B:4806:ASN:C	2.36	0.63
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.79	0.63
1:B:908:VAL:HG22	1:B:909:ASN:H	1.63	0.63
1:C:635:THR:CG2	1:C:1637:MET:CG	2.77	0.63
1:C:1228:ILE:HG13	1:D:3572:GLN:HE21	1.63	0.63
1:A:3572:GLN:HE21	1:D:1228:ILE:HG13	1.63	0.63
1:A:4805:ASN:O	1:A:4806:ASN:C	2.36	0.63
1:A:1289:LEU:HD12	1:A:1595:LEU:HD12	1.80	0.63
1:A:2044:ILE:HG22	1:A:2046:LEU:H	1.64	0.63
1:A:3430:ASN:ND2	1:A:3525:CYS:SG	2.72	0.63
1:B:1289:LEU:HD12	1:B:1595:LEU:HD12	1.80	0.63
1:B:2340:PHE:HA	1:B:2435:ARG:HE	1.62	0.63
1:C:2044:ILE:HG22	1:C:2046:LEU:H	1.64	0.63
1:D:635:THR:CG2	1:D:1637:MET:CG	2.77	0.63
1:D:908:VAL:HG22	1:D:909:ASN:H	1.63	0.63
1:D:2044:ILE:HG22	1:D:2046:LEU:H	1.64	0.63
1:A:1453:VAL:HG23	1:A:1454:THR:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:THR:CG2	1:B:1637:MET:CG	2.77	0.62
1:B:224:HIS:N	1:B:229:GLU:O	2.27	0.62
1:D:1728:ARG:HA	1:D:1731:LEU:HD12	1.80	0.62
1:A:1231:GLN:HE22	1:A:1826:ALA:HB2	1.65	0.62
1:B:35:LEU:HB3	1:B:49:LEU:HD23	1.82	0.62
1:D:3901:ASN:OD1	1:D:3904:ARG:NH2	2.29	0.62
1:D:4814:LEU:O	1:D:4816:ILE:N	2.33	0.62
1:A:35:LEU:HB3	1:A:49:LEU:HD23	1.82	0.62
1:A:1228:ILE:HG13	1:B:3572:GLN:HE21	1.63	0.62
1:D:1289:LEU:HD12	1:D:1595:LEU:HD12	1.80	0.62
1:D:3430:ASN:ND2	1:D:3525:CYS:SG	2.72	0.62
1:D:35:LEU:HB3	1:D:49:LEU:HD23	1.82	0.62
1:A:635:THR:CG2	1:A:1637:MET:CG	2.77	0.62
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.33	0.62
1:A:3577:ARG:HH22	1:D:1209:SER:HA	1.65	0.62
1:B:3234:ASN:ND2	1:B:3310:ASP:OD2	2.33	0.62
1:B:3430:ASN:ND2	1:B:3525:CYS:SG	2.72	0.62
1:C:3430:ASN:ND2	1:C:3525:CYS:SG	2.72	0.62
1:B:1228:ILE:HG13	1:C:3572:GLN:HE21	1.63	0.62
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.33	0.62
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.33	0.62
1:A:4814:LEU:O	1:A:4816:ILE:N	2.33	0.62
1:A:4835:LYS:O	1:A:4839:MET:HG2	2.00	0.62
1:A:908:VAL:HG22	1:A:909:ASN:H	1.63	0.62
1:B:2044:ILE:HG22	1:B:2046:LEU:H	1.64	0.62
1:C:3234:ASN:ND2	1:C:3310:ASP:OD2	2.33	0.62
1:C:35:LEU:HB3	1:C:49:LEU:HD23	1.82	0.61
1:D:665:GLU:HG2	1:D:792:LEU:HD12	1.82	0.61
1:A:1209:SER:HA	1:B:3577:ARG:HH22	1.65	0.61
1:C:4814:LEU:O	1:C:4816:ILE:N	2.33	0.61
1:C:4835:LYS:O	1:C:4839:MET:HG2	2.00	0.61
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.66	0.61
1:C:1231:GLN:HE22	1:C:1826:ALA:HB2	1.65	0.61
1:C:1209:SER:HA	1:D:3577:ARG:HH22	1.65	0.61
1:A:3234:ASN:ND2	1:A:3310:ASP:OD2	2.33	0.61
1:C:578:ILE:HG23	1:C:582:HIS:HD2	1.65	0.61
1:D:578:ILE:HG23	1:D:582:HIS:HD2	1.65	0.61
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.33	0.61
1:D:4835:LYS:O	1:D:4839:MET:HG2	2.00	0.61
1:B:1209:SER:HA	1:C:3577:ARG:HH22	1.65	0.61
1:C:645:ARG:HB2	1:C:780:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4805:ASN:O	1:C:4806:ASN:C	2.36	0.61
1:B:4814:LEU:O	1:B:4816:ILE:N	2.33	0.61
1:D:645:ARG:HB2	1:D:780:VAL:HG12	1.83	0.61
1:B:1231:GLN:HE22	1:B:1826:ALA:HB2	1.65	0.61
1:D:580:GLU:OE1	1:D:584:LYS:NZ	2.33	0.61
1:D:590:LEU:HD22	1:D:631:LEU:HD21	1.82	0.61
1:A:665:GLU:HG2	1:A:792:LEU:HD12	1.82	0.61
1:B:590:LEU:HD22	1:B:631:LEU:HD21	1.82	0.61
1:B:645:ARG:HB2	1:B:780:VAL:HG12	1.83	0.61
1:A:5029:ARG:O	1:A:5033:GLU:HB2	2.01	0.60
1:B:2185:ILE:O	1:B:2188:ASN:ND2	2.34	0.60
1:B:4835:LYS:O	1:B:4839:MET:HG2	2.00	0.60
1:D:267:ILE:O	1:D:270:SER:OG	2.19	0.60
1:D:2185:ILE:O	1:D:2188:ASN:ND2	2.34	0.60
1:A:590:LEU:HD22	1:A:631:LEU:HD21	1.82	0.60
1:A:645:ARG:HB2	1:A:780:VAL:HG12	1.83	0.60
1:A:1540:PHE:HE1	1:A:1552:VAL:HG11	1.66	0.60
1:A:4983:HIS:ND1	1:A:4983:HIS:O	2.34	0.60
1:C:590:LEU:HD22	1:C:631:LEU:HD21	1.82	0.60
1:C:5029:ARG:O	1:C:5033:GLU:HB2	2.01	0.60
1:D:1842:LEU:O	1:D:1843:LYS:C	2.40	0.60
1:D:3234:ASN:ND2	1:D:3310:ASP:OD2	2.33	0.60
1:D:5029:ARG:O	1:D:5033:GLU:HB2	2.01	0.60
1:A:3786:CYS:SG	1:A:3794:VAL:HG22	2.41	0.60
1:A:3903:LEU:HD13	1:A:3915:ILE:HD11	1.84	0.60
1:B:3901:ASN:OD1	1:B:3904:ARG:NH2	2.29	0.60
1:D:1540:PHE:HE1	1:D:1552:VAL:HG11	1.66	0.60
1:A:2185:ILE:O	1:A:2188:ASN:ND2	2.34	0.60
1:D:3786:CYS:SG	1:D:3794:VAL:HG22	2.41	0.60
1:A:1270:LEU:O	1:A:1471:ALA:HA	2.01	0.60
1:A:2010:LEU:HG	1:A:3659:ALA:HB3	1.84	0.60
1:A:2452:ARG:NH2	1:D:175:SER:O	2.35	0.60
1:B:578:ILE:HG23	1:B:582:HIS:HD2	1.65	0.60
1:B:2010:LEU:HG	1:B:3659:ALA:HB3	1.84	0.60
1:B:4983:HIS:ND1	1:B:4983:HIS:O	2.34	0.60
1:D:1231:GLN:HE22	1:D:1826:ALA:HB2	1.65	0.60
1:D:3903:LEU:HD13	1:D:3915:ILE:HD11	1.84	0.60
1:A:175:SER:O	1:B:2452:ARG:NH2	2.35	0.60
1:A:224:HIS:N	1:A:229:GLU:O	2.27	0.60
1:A:580:GLU:OE1	1:A:584:LYS:NZ	2.33	0.60
1:B:3199:ALA:HB2	1:B:3236:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2185:ILE:O	1:C:2188:ASN:ND2	2.34	0.60
1:D:1270:LEU:O	1:D:1471:ALA:HA	2.01	0.60
1:A:3199:ALA:HB2	1:A:3236:VAL:HG11	1.84	0.60
1:B:1270:LEU:O	1:B:1471:ALA:HA	2.01	0.60
1:C:175:SER:O	1:D:2452:ARG:NH2	2.35	0.60
1:C:1270:LEU:O	1:C:1471:ALA:HA	2.01	0.60
1:C:4983:HIS:ND1	1:C:4983:HIS:O	2.34	0.60
1:A:1653:LEU:HB3	1:A:1660:GLN:HB2	1.84	0.60
1:A:4808:PHE:C	1:A:4810:ALA:H	2.05	0.60
1:B:3903:LEU:HD13	1:B:3915:ILE:HD11	1.84	0.60
1:B:4817:ALA:O	1:B:4819:GLY:N	2.34	0.60
1:C:2010:LEU:HG	1:C:3659:ALA:HB3	1.84	0.60
1:D:4808:PHE:C	1:D:4810:ALA:H	2.05	0.60
1:A:578:ILE:HG23	1:A:582:HIS:HD2	1.65	0.60
1:C:3903:LEU:HD13	1:C:3915:ILE:HD11	1.84	0.60
1:D:4983:HIS:ND1	1:D:4983:HIS:O	2.34	0.60
1:C:267:ILE:O	1:C:270:SER:OG	2.19	0.60
1:C:4817:ALA:O	1:C:4819:GLY:N	2.34	0.60
1:D:2010:LEU:HG	1:D:3659:ALA:HB3	1.84	0.60
1:D:4817:ALA:O	1:D:4819:GLY:N	2.34	0.60
1:A:645:ARG:HD2	1:A:778:PHE:CD2	2.37	0.59
1:C:206:CYS:SG	1:C:207:SER:N	2.75	0.59
1:D:645:ARG:HD2	1:D:778:PHE:CD2	2.37	0.59
1:A:267:ILE:O	1:A:270:SER:OG	2.19	0.59
1:B:645:ARG:HD2	1:B:778:PHE:CD2	2.37	0.59
1:B:665:GLU:HG2	1:B:792:LEU:HD12	1.82	0.59
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.84	0.59
1:C:3199:ALA:HB2	1:C:3236:VAL:HG11	1.84	0.59
1:A:4751:THR:O	1:A:4754:ASN:ND2	2.36	0.59
1:B:267:ILE:O	1:B:270:SER:OG	2.19	0.59
1:D:3199:ALA:HB2	1:D:3236:VAL:HG11	1.84	0.59
1:A:2347:GLU:OE2	1:A:3852:LYS:NZ	2.36	0.59
1:B:1272:LEU:HD21	1:B:1287:LEU:HD21	1.85	0.59
1:B:3786:CYS:SG	1:B:3794:VAL:HG22	2.41	0.59
1:C:684:VAL:HG21	1:C:744:VAL:HG11	1.85	0.59
1:D:2347:GLU:OE2	1:D:3852:LYS:NZ	2.36	0.59
1:B:4751:THR:O	1:B:4754:ASN:ND2	2.36	0.59
1:B:5029:ARG:O	1:B:5033:GLU:HB2	2.01	0.59
1:C:1272:LEU:HD21	1:C:1287:LEU:HD21	1.85	0.59
1:D:2644:LEU:HG	1:D:2645:THR:HG23	1.83	0.59
1:A:1272:LEU:HD21	1:A:1287:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:GLU:OE1	1:C:584:LYS:NZ	2.33	0.59
1:C:645:ARG:HD2	1:C:778:PHE:CD2	2.37	0.59
1:D:684:VAL:HG21	1:D:744:VAL:HG11	1.85	0.59
1:D:1272:LEU:HD21	1:D:1287:LEU:HD21	1.85	0.59
1:A:659:TYR:OH	1:A:1020:ARG:NH2	2.35	0.59
1:B:1540:PHE:HE1	1:B:1552:VAL:HG11	1.66	0.59
1:B:2644:LEU:HG	1:B:2645:THR:HG23	1.83	0.59
1:C:224:HIS:N	1:C:229:GLU:O	2.27	0.59
1:A:2023:LEU:O	1:A:2028:ARG:NH1	2.36	0.59
1:B:1842:LEU:O	1:B:1843:LYS:C	2.40	0.59
1:B:2347:GLU:OE2	1:B:3852:LYS:NZ	2.36	0.59
1:C:2347:GLU:OE2	1:C:3852:LYS:NZ	2.36	0.59
1:C:1540:PHE:HE1	1:C:1552:VAL:HG11	1.66	0.59
1:C:1972:ASN:OD1	1:C:1976:ARG:NH1	2.36	0.59
1:C:3786:CYS:SG	1:C:3794:VAL:HG22	2.41	0.59
1:D:206:CYS:SG	1:D:207:SER:N	2.75	0.59
1:A:2644:LEU:HG	1:A:2645:THR:HG23	1.83	0.59
1:B:206:CYS:SG	1:B:207:SER:N	2.75	0.59
1:C:4808:PHE:C	1:C:4810:ALA:H	2.05	0.59
1:D:1540:PHE:HZ	1:D:1552:VAL:HG21	1.68	0.59
1:D:1835:GLU:C	1:D:1837:GLN:H	2.06	0.59
1:D:2023:LEU:O	1:D:2028:ARG:NH1	2.36	0.59
1:A:206:CYS:SG	1:A:207:SER:N	2.75	0.58
1:C:665:GLU:HG2	1:C:792:LEU:HD12	1.82	0.58
1:C:4751:THR:O	1:C:4754:ASN:ND2	2.36	0.58
1:D:4751:THR:O	1:D:4754:ASN:ND2	2.36	0.58
1:A:913:LEU:HD13	1:A:917:GLU:HG3	1.86	0.58
1:B:1972:ASN:OD1	1:B:1976:ARG:NH1	2.36	0.58
1:C:759:ILE:HD11	1:C:762:CYS:HB2	1.85	0.58
1:D:1972:ASN:OD1	1:D:1976:ARG:NH1	2.36	0.58
1:C:2644:LEU:HG	1:C:2645:THR:HG23	1.83	0.58
1:D:1653:LEU:HB3	1:D:1660:GLN:HB2	1.84	0.58
1:B:175:SER:O	1:C:2452:ARG:NH2	2.35	0.58
1:D:759:ILE:HD11	1:D:762:CYS:HB2	1.85	0.58
1:D:913:LEU:HD13	1:D:917:GLU:HG3	1.86	0.58
1:A:1972:ASN:OD1	1:A:1976:ARG:NH1	2.36	0.58
1:B:3187:ARG:NH2	1:B:3190:LEU:O	2.36	0.58
1:C:998:ARG:HA	1:C:1003:GLN:HB3	1.86	0.58
1:C:3187:ARG:NH2	1:C:3190:LEU:O	2.36	0.58
1:C:4075:GLU:HA	1:C:4078:GLN:HB3	1.86	0.58
1:A:220:LEU:HB2	1:A:392:ARG:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:HIS:HD2	1:A:352:ALA:H	1.52	0.58
1:B:580:GLU:OE1	1:B:584:LYS:NZ	2.33	0.58
1:C:1653:LEU:HB3	1:C:1660:GLN:HB2	1.84	0.58
1:C:1835:GLU:C	1:C:1837:GLN:H	2.06	0.58
1:A:1835:GLU:C	1:A:1837:GLN:H	2.06	0.58
1:A:4075:GLU:HA	1:A:4078:GLN:HB3	1.86	0.58
1:B:220:LEU:HB2	1:B:392:ARG:HA	1.86	0.58
1:B:684:VAL:HG21	1:B:744:VAL:HG11	1.85	0.58
1:B:759:ILE:HD11	1:B:762:CYS:HB2	1.85	0.58
1:C:1540:PHE:HZ	1:C:1552:VAL:HG21	1.68	0.58
1:C:4897:ILE:HD11	1:C:4916:PHE:CE2	2.39	0.58
1:D:4075:GLU:HA	1:D:4078:GLN:HB3	1.86	0.58
1:A:1540:PHE:HZ	1:A:1552:VAL:HG21	1.68	0.58
1:D:659:TYR:OH	1:D:1020:ARG:NH2	2.35	0.58
1:B:1540:PHE:HZ	1:B:1552:VAL:HG21	1.68	0.58
1:B:1842:LEU:HA	1:B:1845:VAL:HG12	1.86	0.58
1:B:4075:GLU:HA	1:B:4078:GLN:HB3	1.86	0.58
1:B:4808:PHE:C	1:B:4810:ALA:H	2.05	0.58
1:D:1969:LEU:HD22	1:D:2009:LEU:HD21	1.86	0.58
1:D:3232:LEU:HD11	1:D:3236:VAL:HG13	1.86	0.58
1:A:419:ASP:OD2	1:A:493:ARG:NH1	2.37	0.58
1:A:1842:LEU:HA	1:A:1845:VAL:HG12	1.86	0.58
1:C:1842:LEU:HA	1:C:1845:VAL:HG12	1.86	0.58
1:A:684:VAL:HG21	1:A:744:VAL:HG11	1.85	0.57
1:B:350:HIS:HD2	1:B:352:ALA:H	1.52	0.57
1:D:3187:ARG:NH2	1:D:3190:LEU:O	2.36	0.57
1:D:4897:ILE:HD11	1:D:4916:PHE:CE2	2.39	0.57
1:A:1969:LEU:HD22	1:A:2009:LEU:HD21	1.86	0.57
1:A:3187:ARG:NH2	1:A:3190:LEU:O	2.36	0.57
1:A:3232:LEU:HD11	1:A:3236:VAL:HG13	1.86	0.57
1:A:3802:ILE:HD12	1:A:3886:ARG:HG2	1.85	0.57
1:B:913:LEU:HD13	1:B:917:GLU:HG3	1.86	0.57
1:B:998:ARG:HA	1:B:1003:GLN:HB3	1.86	0.57
1:B:1835:GLU:C	1:B:1837:GLN:H	2.06	0.57
1:B:1969:LEU:HD22	1:B:2009:LEU:HD21	1.86	0.57
1:C:213:TYR:HB3	1:C:273:HIS:CE1	2.38	0.57
1:C:791:PHE:HE2	1:C:823:LEU:HD11	1.70	0.57
1:B:3232:LEU:HD11	1:B:3236:VAL:HG13	1.86	0.57
1:B:4897:ILE:HD11	1:B:4916:PHE:CE2	2.39	0.57
1:C:913:LEU:HD13	1:C:917:GLU:HG3	1.86	0.57
1:C:3232:LEU:HD11	1:C:3236:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASP:OD2	1:B:493:ARG:NH1	2.37	0.57
1:B:961:MET:SD	1:B:962:SER:N	2.78	0.57
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.66	0.57
1:C:961:MET:SD	1:C:962:SER:N	2.78	0.57
1:C:4810:ALA:O	1:C:4811:ALA:C	2.42	0.57
1:D:213:TYR:HB3	1:D:273:HIS:CE1	2.38	0.57
1:D:1842:LEU:HA	1:D:1845:VAL:HG12	1.86	0.57
1:C:1969:LEU:HD22	1:C:2009:LEU:HD21	1.86	0.57
1:C:2023:LEU:O	1:C:2028:ARG:NH1	2.36	0.57
1:A:961:MET:SD	1:A:962:SER:N	2.78	0.57
1:A:4039:MET:SD	1:A:4042:ARG:NH1	2.78	0.57
1:B:4039:MET:SD	1:B:4042:ARG:NH1	2.78	0.57
1:D:220:LEU:HB2	1:D:392:ARG:HA	1.86	0.57
1:D:961:MET:SD	1:D:962:SER:N	2.78	0.57
1:A:998:ARG:HA	1:A:1003:GLN:HB3	1.86	0.57
1:A:2158:CYS:SG	1:A:2184:ASN:ND2	2.78	0.57
1:D:241:GLN:HB3	1:D:243:ARG:HE	1.69	0.57
1:D:3802:ILE:HD12	1:D:3886:ARG:HG2	1.85	0.57
1:A:1842:LEU:O	1:A:1843:LYS:C	2.40	0.57
1:A:4897:ILE:HD11	1:A:4916:PHE:CE2	2.39	0.57
1:B:791:PHE:HE2	1:B:823:LEU:HD11	1.70	0.57
1:C:241:GLN:HB3	1:C:243:ARG:HE	1.69	0.57
1:C:350:HIS:HD2	1:C:352:ALA:H	1.52	0.57
1:D:350:HIS:HD2	1:D:352:ALA:H	1.52	0.57
1:A:2466:LEU:O	1:A:2470:ILE:HD12	2.05	0.57
1:A:791:PHE:HE2	1:A:823:LEU:HD11	1.70	0.56
1:B:1465:ASP:OD2	1:B:1490:SER:OG	2.23	0.56
1:C:220:LEU:HB2	1:C:392:ARG:HA	1.86	0.56
1:C:2158:CYS:SG	1:C:2184:ASN:ND2	2.78	0.56
1:C:3802:ILE:HD12	1:C:3886:ARG:HG2	1.85	0.56
1:C:4816:ILE:O	1:C:4820:VAL:HG23	2.05	0.56
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.87	0.56
1:A:4817:ALA:O	1:A:4819:GLY:N	2.34	0.56
1:B:1850:VAL:HG12	1:B:1851:MET:N	2.21	0.56
1:B:4816:ILE:O	1:B:4820:VAL:HG23	2.05	0.56
1:D:419:ASP:OD2	1:D:493:ARG:NH1	2.37	0.56
1:D:4039:MET:SD	1:D:4042:ARG:NH1	2.78	0.56
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.87	0.56
1:A:759:ILE:HD11	1:A:762:CYS:HB2	1.85	0.56
1:A:1639:LEU:HD11	1:A:1653:LEU:HD11	1.87	0.56
1:A:3642:TYR:O	1:A:3643:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:LEU:HD23	1:B:1626:TRP:HE1	1.70	0.56
1:B:932:LEU:HD12	1:B:935:LEU:HD12	1.86	0.56
1:B:2158:CYS:SG	1:B:2184:ASN:ND2	2.78	0.56
1:B:2339:VAL:HG23	1:B:2435:ARG:HG3	1.87	0.56
1:B:3802:ILE:HD12	1:B:3886:ARG:HG2	1.85	0.56
1:C:1158:ASN:HB3	1:C:1182:ILE:H	1.71	0.56
1:C:1465:ASP:OD2	1:C:1490:SER:OG	2.23	0.56
1:C:2466:LEU:O	1:C:2470:ILE:HD12	2.05	0.56
1:D:1158:ASN:HB3	1:D:1182:ILE:H	1.71	0.56
1:D:2158:CYS:SG	1:D:2184:ASN:ND2	2.78	0.56
1:D:2466:LEU:O	1:D:2470:ILE:HD12	2.05	0.56
1:D:3642:TYR:O	1:D:3643:ASN:ND2	2.38	0.56
1:D:4811:ALA:O	1:D:4813:LEU:N	2.38	0.56
1:A:932:LEU:HD12	1:A:935:LEU:HD12	1.86	0.56
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.87	0.56
1:C:3062:PRO:HA	1:C:3187:ARG:HH22	1.70	0.56
1:C:3817:LEU:HD11	1:C:3821:LYS:HE3	1.88	0.56
1:D:224:HIS:N	1:D:229:GLU:O	2.27	0.56
1:D:3817:LEU:HD11	1:D:3821:LYS:HE3	1.88	0.56
1:A:4810:ALA:O	1:A:4811:ALA:C	2.42	0.56
1:B:213:TYR:HB3	1:B:273:HIS:CE1	2.38	0.56
1:B:2466:LEU:O	1:B:2470:ILE:HD12	2.05	0.56
1:B:4810:ALA:O	1:B:4811:ALA:C	2.42	0.56
1:C:932:LEU:HD12	1:C:935:LEU:HD12	1.86	0.56
1:C:4039:MET:SD	1:C:4042:ARG:NH1	2.78	0.56
1:D:791:PHE:HE2	1:D:823:LEU:HD11	1.70	0.56
1:D:998:ARG:HA	1:D:1003:GLN:HB3	1.86	0.56
1:D:3062:PRO:HA	1:D:3187:ARG:HH22	1.70	0.56
1:A:3062:PRO:HA	1:A:3187:ARG:HH22	1.70	0.56
1:A:3817:LEU:HD11	1:A:3821:LYS:HE3	1.88	0.56
1:B:1158:ASN:HB3	1:B:1182:ILE:H	1.71	0.56
1:B:3062:PRO:HA	1:B:3187:ARG:HH22	1.70	0.56
1:C:419:ASP:OD2	1:C:493:ARG:NH1	2.37	0.56
1:D:1850:VAL:HG12	1:D:1851:MET:N	2.21	0.56
1:D:4816:ILE:O	1:D:4820:VAL:HG23	2.05	0.56
1:A:1158:ASN:HB3	1:A:1182:ILE:H	1.71	0.56
1:A:1207:ASP:OD2	1:A:1209:SER:OG	2.19	0.56
1:B:1639:LEU:HD11	1:B:1653:LEU:HD11	1.87	0.56
1:B:2023:LEU:O	1:B:2028:ARG:NH1	2.36	0.56
1:B:3657:TYR:HE2	1:B:3662:ILE:HG23	1.71	0.56
1:B:4811:ALA:O	1:B:4813:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:LEU:HG	1:D:795:GLY:H	1.71	0.56
1:D:932:LEU:HD12	1:D:935:LEU:HD12	1.86	0.56
1:C:1842:LEU:O	1:C:1843:LYS:C	2.40	0.56
1:A:213:TYR:HB3	1:A:273:HIS:CE1	2.38	0.56
1:A:4811:ALA:O	1:A:4813:LEU:N	2.38	0.56
1:B:3817:LEU:HD11	1:B:3821:LYS:HE3	1.88	0.56
1:C:821:LEU:HD23	1:C:1626:TRP:HE1	1.70	0.56
1:D:1468:LYS:C	1:D:1469:VAL:HG22	2.27	0.56
1:A:4816:ILE:O	1:A:4820:VAL:HG23	2.05	0.56
1:C:2339:VAL:HG23	1:C:2435:ARG:HG3	1.87	0.56
1:C:3642:TYR:O	1:C:3643:ASN:ND2	2.38	0.56
1:C:3657:TYR:HE2	1:C:3662:ILE:HG23	1.71	0.56
1:C:4811:ALA:O	1:C:4813:LEU:N	2.38	0.56
1:D:1159:THR:CG2	1:D:1180:ARG:HH21	2.19	0.56
1:D:3754:GLU:OE1	1:D:3754:GLU:N	2.37	0.56
1:A:2339:VAL:HG23	1:A:2435:ARG:HG3	1.87	0.55
1:B:1465:ASP:O	1:B:1466:LEU:HB2	2.06	0.55
1:C:3533:ILE:H	1:C:3533:ILE:HD12	1.71	0.55
1:A:793:LEU:HG	1:A:795:GLY:H	1.71	0.55
1:A:821:LEU:HD23	1:A:1626:TRP:HE1	1.70	0.55
1:A:3533:ILE:H	1:A:3533:ILE:HD12	1.71	0.55
1:A:3657:TYR:HE2	1:A:3662:ILE:HG23	1.71	0.55
1:B:241:GLN:HB3	1:B:243:ARG:HE	1.69	0.55
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.87	0.55
1:D:1207:ASP:OD2	1:D:1209:SER:OG	2.19	0.55
1:A:241:GLN:HB3	1:A:243:ARG:HE	1.69	0.55
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.40	0.55
1:C:793:LEU:HG	1:C:795:GLY:H	1.71	0.55
1:C:1159:THR:CG2	1:C:1180:ARG:HH21	2.19	0.55
1:C:1850:VAL:HG12	1:C:1851:MET:N	2.21	0.55
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.66	0.55
1:D:3937:TYR:O	1:D:4002:LYS:NZ	2.40	0.55
1:A:1465:ASP:OD2	1:A:1490:SER:OG	2.23	0.55
1:A:1850:VAL:HG12	1:A:1851:MET:N	2.21	0.55
1:B:3642:TYR:O	1:B:3643:ASN:ND2	2.38	0.55
1:C:1639:LEU:HD11	1:C:1653:LEU:HD11	1.87	0.55
1:C:3937:TYR:O	1:C:4002:LYS:NZ	2.40	0.55
1:D:1465:ASP:OD2	1:D:1490:SER:OG	2.23	0.55
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.40	0.55
1:B:3533:ILE:HD12	1:B:3533:ILE:H	1.71	0.55
1:D:652:ARG:HB2	1:D:750:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2339:VAL:HG23	1:D:2435:ARG:HG3	1.87	0.55
1:A:177:GLU:HG2	1:B:2452:ARG:NH1	2.22	0.55
1:C:1515:VAL:HG23	1:C:1530:THR:HA	1.89	0.55
1:A:3842:LEU:HB3	1:A:3933:PHE:CE2	2.42	0.55
1:B:177:GLU:HG2	1:C:2452:ARG:NH1	2.22	0.55
1:B:1583:GLU:OE1	1:B:1583:GLU:N	2.40	0.55
1:B:2532:ALA:HB2	1:B:2578:MET:HG2	1.88	0.55
1:C:4886:HIS:HD2	1:C:4897:ILE:HG21	1.72	0.55
1:D:3533:ILE:H	1:D:3533:ILE:HD12	1.71	0.55
1:D:4810:ALA:O	1:D:4811:ALA:C	2.42	0.55
1:A:1468:LYS:C	1:A:1469:VAL:HG22	2.27	0.55
1:A:4815:ASP:O	1:A:4816:ILE:C	2.44	0.55
1:C:1465:ASP:O	1:C:1466:LEU:HB2	2.06	0.55
1:A:652:ARG:HB3	1:A:773:LEU:HD13	1.88	0.55
1:A:1159:THR:CG2	1:A:1180:ARG:HH21	2.19	0.55
1:B:3842:LEU:HB3	1:B:3933:PHE:CE2	2.42	0.55
1:D:1583:GLU:OE1	1:D:1583:GLU:N	2.40	0.55
1:D:1639:LEU:HD11	1:D:1653:LEU:HD11	1.87	0.55
1:D:3842:LEU:HB3	1:D:3933:PHE:CE2	2.42	0.55
1:A:176:SER:N	1:B:2452:ARG:HH12	2.05	0.55
1:B:176:SER:N	1:C:2452:ARG:HH12	2.05	0.55
1:D:652:ARG:HB3	1:D:773:LEU:HD13	1.88	0.55
1:B:4814:LEU:O	1:B:4815:ASP:C	2.45	0.54
1:B:4886:HIS:HD2	1:B:4897:ILE:HG21	1.72	0.54
1:C:3842:LEU:HB3	1:C:3933:PHE:CE2	2.42	0.54
1:D:1104:TRP:NE1	1:D:1151:CYS:SG	2.80	0.54
1:D:1515:VAL:HG23	1:D:1530:THR:HA	1.89	0.54
1:D:2532:ALA:HB2	1:D:2578:MET:HG2	1.88	0.54
1:A:652:ARG:HB2	1:A:750:LEU:HD11	1.89	0.54
1:B:793:LEU:HG	1:B:795:GLY:H	1.71	0.54
1:B:1159:THR:CG2	1:B:1180:ARG:HH21	2.19	0.54
1:C:176:SER:N	1:D:2452:ARG:HH12	2.05	0.54
1:C:177:GLU:HG2	1:D:2452:ARG:NH1	2.22	0.54
1:C:884:LEU:HD13	1:C:967:PRO:HA	1.89	0.54
1:C:4815:ASP:O	1:C:4816:ILE:C	2.44	0.54
1:D:821:LEU:HD23	1:D:1626:TRP:HE1	1.70	0.54
1:D:1479:GLU:O	1:D:1563:GLN:NE2	2.40	0.54
1:D:3657:TYR:HE2	1:D:3662:ILE:HG23	1.71	0.54
1:A:1104:TRP:NE1	1:A:1151:CYS:SG	2.80	0.54
1:A:1515:VAL:HG23	1:A:1530:THR:HA	1.89	0.54
1:A:2532:ALA:HB2	1:A:2578:MET:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:TRP:NE1	1:B:1151:CYS:SG	2.80	0.54
1:B:1515:VAL:HG23	1:B:1530:THR:HA	1.89	0.54
1:A:1465:ASP:O	1:A:1466:LEU:HB2	2.06	0.54
1:C:2272:PRO:HA	1:C:2275:VAL:HG12	1.90	0.54
1:D:884:LEU:HD13	1:D:967:PRO:HA	1.89	0.54
1:A:4886:HIS:HD2	1:A:4897:ILE:HG21	1.72	0.54
1:B:652:ARG:HB3	1:B:773:LEU:HD13	1.88	0.54
1:B:1468:LYS:C	1:B:1469:VAL:HG22	2.27	0.54
1:B:1479:GLU:O	1:B:1563:GLN:NE2	2.40	0.54
1:C:652:ARG:HB2	1:C:750:LEU:HD11	1.89	0.54
1:D:1465:ASP:O	1:D:1466:LEU:HB2	2.06	0.54
1:A:2452:ARG:NH1	1:D:177:GLU:HG2	2.22	0.54
1:B:884:LEU:HD13	1:B:967:PRO:HA	1.89	0.54
1:C:1468:LYS:C	1:C:1469:VAL:HG22	2.27	0.54
1:C:1479:GLU:O	1:C:1563:GLN:NE2	2.40	0.54
1:C:2532:ALA:HB2	1:C:2578:MET:HG2	1.88	0.54
1:A:1479:GLU:O	1:A:1563:GLN:NE2	2.40	0.54
1:A:1583:GLU:OE1	1:A:1583:GLU:N	2.40	0.54
1:A:2272:PRO:HA	1:A:2275:VAL:HG12	1.90	0.54
1:B:652:ARG:HB2	1:B:750:LEU:HD11	1.89	0.54
1:C:1104:TRP:NE1	1:C:1151:CYS:SG	2.80	0.54
1:A:472:ARG:HH21	1:A:472:ARG:HG3	1.73	0.54
1:A:884:LEU:HD13	1:A:967:PRO:HA	1.89	0.54
1:B:774:ASP:OD1	1:B:774:ASP:N	2.41	0.54
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	1.90	0.54
1:C:1495:VAL:HG21	1:C:1538:THR:HG23	1.90	0.54
1:D:774:ASP:OD1	1:D:774:ASP:N	2.41	0.54
1:B:4815:ASP:O	1:B:4816:ILE:C	2.44	0.54
1:D:1495:VAL:HG21	1:D:1538:THR:HG23	1.90	0.54
1:D:2272:PRO:HA	1:D:2275:VAL:HG12	1.90	0.54
1:D:4886:HIS:HD2	1:D:4897:ILE:HG21	1.72	0.54
1:A:1732:SER:O	1:A:2140:ARG:HD2	2.09	0.54
1:A:2452:ARG:HH12	1:D:176:SER:N	2.05	0.54
1:A:4814:LEU:O	1:A:4815:ASP:C	2.45	0.54
1:B:1495:VAL:HG21	1:B:1538:THR:HG23	1.90	0.54
1:C:1207:ASP:OD2	1:C:1209:SER:OG	2.19	0.54
1:C:1583:GLU:N	1:C:1583:GLU:OE1	2.40	0.54
1:D:4815:ASP:O	1:D:4816:ILE:C	2.44	0.54
1:A:551:LEU:HB3	1:A:553:ARG:NH2	2.24	0.53
1:A:1468:LYS:O	1:A:1469:VAL:HG13	2.08	0.53
1:C:652:ARG:HB3	1:C:773:LEU:HD13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:LEU:O	1:C:720:HIS:ND1	2.42	0.53
1:A:222:LEU:HG	1:A:390:LEU:HG	1.91	0.53
1:A:1527:MET:N	1:A:1527:MET:SD	2.82	0.53
1:B:1468:LYS:O	1:B:1469:VAL:HG13	2.08	0.53
1:C:960:MET:HE1	1:C:966:LYS:HG3	1.89	0.53
1:A:719:LEU:O	1:A:720:HIS:ND1	2.42	0.53
1:A:4814:LEU:C	1:A:4816:ILE:N	2.62	0.53
1:D:719:LEU:O	1:D:720:HIS:ND1	2.42	0.53
1:B:222:LEU:HG	1:B:390:LEU:HG	1.91	0.53
1:B:3755:GLU:O	1:B:3759:GLU:HG2	2.08	0.53
1:C:3755:GLU:O	1:C:3759:GLU:HG2	2.08	0.53
1:D:1732:SER:O	1:D:2140:ARG:HD2	2.09	0.53
1:D:2368:LEU:HD21	1:D:2376:LEU:HD12	1.90	0.53
1:D:2688:HIS:ND1	1:D:2688:HIS:O	2.42	0.53
1:A:1495:VAL:HG21	1:A:1538:THR:HG23	1.90	0.53
1:B:551:LEU:HB3	1:B:553:ARG:NH2	2.24	0.53
1:D:1468:LYS:O	1:D:1469:VAL:HG13	2.08	0.53
1:B:719:LEU:O	1:B:720:HIS:ND1	2.42	0.53
1:B:1527:MET:SD	1:B:1527:MET:N	2.82	0.53
1:B:1834:VAL:O	1:B:1834:VAL:HG22	2.09	0.53
1:C:659:TYR:OH	1:C:1020:ARG:NH2	2.35	0.53
1:D:3755:GLU:O	1:D:3759:GLU:HG2	2.08	0.53
1:A:2688:HIS:ND1	1:A:2688:HIS:O	2.42	0.53
1:B:977:LEU:HD13	1:B:1047:LEU:HD22	1.91	0.53
1:B:960:MET:HE1	1:B:966:LYS:HG3	1.90	0.53
1:B:2171:GLY:H	1:B:2174:GLU:HB2	1.74	0.53
1:B:2368:LEU:HD21	1:B:2376:LEU:HD12	1.90	0.53
1:C:1527:MET:N	1:C:1527:MET:SD	2.82	0.53
1:D:472:ARG:HH21	1:D:472:ARG:HG3	1.73	0.53
1:D:649:PHE:HA	1:D:778:PHE:HE1	1.74	0.53
1:B:4895:GLY:O	1:C:4892:ARG:NH2	2.41	0.53
1:C:1468:LYS:O	1:C:1469:VAL:HG13	2.08	0.53
1:C:2688:HIS:ND1	1:C:2688:HIS:O	2.42	0.53
1:D:222:LEU:HG	1:D:390:LEU:HG	1.91	0.53
1:D:4814:LEU:O	1:D:4815:ASP:C	2.45	0.53
1:A:2368:LEU:HD21	1:A:2376:LEU:HD12	1.90	0.53
1:B:1092:PHE:HD1	1:B:1202:LEU:HB3	1.74	0.53
1:B:4866:SER:N	1:B:4873:ASP:OD2	2.42	0.53
1:C:551:LEU:HB3	1:C:553:ARG:NH2	2.24	0.53
1:C:2171:GLY:H	1:C:2174:GLU:HB2	1.74	0.53
1:B:472:ARG:HH21	1:B:472:ARG:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2437:ALA:HB3	1:C:2508:ARG:HH11	1.74	0.52
1:D:1144:GLN:HG2	1:D:1147:ASP:HB2	1.92	0.52
1:D:1527:MET:N	1:D:1527:MET:SD	2.82	0.52
1:D:4866:SER:N	1:D:4873:ASP:OD2	2.42	0.52
1:A:1092:PHE:HD1	1:A:1202:LEU:HB3	1.74	0.52
1:A:1144:GLN:HG2	1:A:1147:ASP:HB2	1.92	0.52
1:A:2171:GLY:H	1:A:2174:GLU:HB2	1.74	0.52
1:C:222:LEU:HG	1:C:390:LEU:HG	1.91	0.52
1:C:2368:LEU:HD21	1:C:2376:LEU:HD12	1.90	0.52
1:D:2437:ALA:HB3	1:D:2508:ARG:HH11	1.74	0.52
1:D:4873:ASP:OD1	1:D:4873:ASP:N	2.40	0.52
1:A:1130:GLN:OE1	1:A:1136:SER:OG	2.28	0.52
1:A:1834:VAL:HG22	1:A:1834:VAL:O	2.09	0.52
1:A:3754:GLU:OE1	1:A:3754:GLU:N	2.37	0.52
1:A:3755:GLU:O	1:A:3759:GLU:HG2	2.08	0.52
1:B:643:SER:HG	1:B:782:SER:HG	1.56	0.52
1:B:649:PHE:HA	1:B:778:PHE:HE1	1.74	0.52
1:C:544:LEU:HD22	1:C:574:VAL:HG22	1.92	0.52
1:C:649:PHE:HA	1:C:778:PHE:HE1	1.74	0.52
1:C:1554:VAL:HG12	1:C:1556:PRO:HD3	1.90	0.52
1:C:4942:GLU:OE1	1:D:4944:ARG:HD3	2.10	0.52
1:B:1144:GLN:HG2	1:B:1147:ASP:HB2	1.92	0.52
1:B:2688:HIS:ND1	1:B:2688:HIS:O	2.42	0.52
1:C:1834:VAL:HG22	1:C:1834:VAL:O	2.09	0.52
1:D:1834:VAL:O	1:D:1834:VAL:HG22	2.09	0.52
1:D:4191:GLU:OE2	1:D:5006:GLN:NE2	2.41	0.52
1:A:3519:PRO:O	1:A:3523:ASN:N	2.43	0.52
1:B:544:LEU:HD22	1:B:574:VAL:HG22	1.92	0.52
1:B:4191:GLU:OE2	1:B:5006:GLN:NE2	2.41	0.52
1:B:4942:GLU:OE1	1:C:4944:ARG:HD3	2.10	0.52
1:C:1493:TYR:OH	1:C:1508:ARG:NE	2.43	0.52
1:C:1732:SER:O	1:C:2140:ARG:HD2	2.09	0.52
1:D:977:LEU:HD13	1:D:1047:LEU:HD22	1.91	0.52
1:A:4892:ARG:NH2	1:D:4895:GLY:O	2.41	0.52
1:A:4895:GLY:O	1:B:4892:ARG:NH2	2.41	0.52
1:B:1493:TYR:OH	1:B:1508:ARG:NE	2.43	0.52
1:C:472:ARG:HH21	1:C:472:ARG:HG3	1.73	0.52
1:C:4814:LEU:O	1:C:4815:ASP:C	2.45	0.52
1:D:233:ILE:O	1:D:257:ARG:NH1	2.43	0.52
1:D:544:LEU:HD22	1:D:574:VAL:HG22	1.92	0.52
1:D:3680:ALA:HB3	1:D:3697:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4942:GLU:OE1	1:B:4944:ARG:HD3	2.10	0.52
1:B:659:TYR:OH	1:B:1020:ARG:NH2	2.35	0.52
1:C:233:ILE:O	1:C:257:ARG:NH1	2.43	0.52
1:C:1144:GLN:HG2	1:C:1147:ASP:HB2	1.92	0.52
1:C:4895:GLY:O	1:D:4892:ARG:NH2	2.41	0.52
1:D:2171:GLY:H	1:D:2174:GLU:HB2	1.74	0.52
1:A:1839:VAL:O	1:A:1841:VAL:N	2.43	0.52
1:B:1130:GLN:OE1	1:B:1136:SER:OG	2.28	0.52
1:B:1226:PHE:O	1:B:1827:ARG:NH1	2.39	0.52
1:B:1554:VAL:HG12	1:B:1556:PRO:HD3	1.90	0.52
1:B:1732:SER:O	1:B:2140:ARG:HD2	2.09	0.52
1:C:1092:PHE:HD1	1:C:1202:LEU:HB3	1.74	0.52
1:D:3519:PRO:O	1:D:3523:ASN:N	2.43	0.52
1:D:4763:GLY:O	1:D:4766:THR:OG1	2.26	0.52
1:A:4634:GLU:HG2	1:A:4635:SER:H	1.75	0.52
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.92	0.52
1:D:1493:TYR:OH	1:D:1508:ARG:NE	2.43	0.52
1:D:4814:LEU:C	1:D:4816:ILE:N	2.62	0.52
1:A:649:PHE:HA	1:A:778:PHE:HE1	1.74	0.52
1:B:233:ILE:O	1:B:257:ARG:NH1	2.43	0.52
1:B:3519:PRO:O	1:B:3523:ASN:N	2.43	0.52
1:A:233:ILE:O	1:A:257:ARG:NH1	2.43	0.51
1:A:544:LEU:HD22	1:A:574:VAL:HG22	1.92	0.51
1:C:977:LEU:HD13	1:C:1047:LEU:HD22	1.91	0.51
1:D:3446:SER:HA	1:D:3449:HIS:HD1	1.75	0.51
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.92	0.51
1:A:4944:ARG:HD3	1:D:4942:GLU:OE1	2.10	0.51
1:B:102:LEU:HB2	1:B:105:HIS:CD2	2.46	0.51
1:B:1839:VAL:O	1:B:1841:VAL:N	2.43	0.51
1:B:4863:TYR:HD2	1:B:4876:CYS:HB3	1.75	0.51
1:C:774:ASP:N	1:C:774:ASP:OD1	2.41	0.51
1:C:4863:TYR:HD2	1:C:4876:CYS:HB3	1.75	0.51
1:D:4634:GLU:HG2	1:D:4635:SER:H	1.75	0.51
1:D:4863:TYR:HD2	1:D:4876:CYS:HB3	1.75	0.51
1:A:977:LEU:HD13	1:A:1047:LEU:HD22	1.91	0.51
1:C:3147:ILE:HD13	1:C:3197:LEU:HD11	1.92	0.51
1:C:4634:GLU:HG2	1:C:4635:SER:H	1.75	0.51
1:D:1092:PHE:HD1	1:D:1202:LEU:HB3	1.74	0.51
1:D:1839:VAL:O	1:D:1841:VAL:N	2.43	0.51
1:A:4804:TYR:CG	1:A:4804:TYR:O	2.63	0.51
1:B:2437:ALA:HB3	1:B:2508:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3446:SER:HA	1:B:3449:HIS:HD1	1.75	0.51
1:B:4171:LEU:O	1:B:4175:ARG:HG3	2.10	0.51
1:B:4814:LEU:C	1:B:4816:ILE:N	2.62	0.51
1:C:3519:PRO:O	1:C:3523:ASN:N	2.43	0.51
1:D:1554:VAL:HG12	1:D:1556:PRO:HD3	1.90	0.51
1:A:4901:ILE:HD12	1:A:4913:ARG:NH2	2.23	0.51
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.92	0.51
1:C:492:ASP:HA	1:C:495:ASN:ND2	2.26	0.51
1:C:971:ASP:OD1	1:C:971:ASP:N	2.44	0.51
1:C:1828:ASP:O	1:C:1829:PRO:C	2.48	0.51
1:D:102:LEU:HB2	1:D:105:HIS:CD2	2.46	0.51
1:A:102:LEU:HB2	1:A:105:HIS:CD2	2.46	0.51
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.92	0.51
1:B:3754:GLU:OE1	1:B:3754:GLU:N	2.37	0.51
1:B:4579:PHE:HB2	1:B:4631:PHE:HE1	1.76	0.51
1:C:1226:PHE:O	1:C:1827:ARG:NH1	2.39	0.51
1:C:1276:THR:CB	1:C:1466:LEU:HD22	2.41	0.51
1:C:1450:VAL:HG21	1:C:1454:THR:HG21	1.92	0.51
1:A:1554:VAL:HG12	1:A:1556:PRO:HD3	1.90	0.51
1:A:4763:GLY:O	1:A:4766:THR:OG1	2.26	0.51
1:B:4634:GLU:HG2	1:B:4635:SER:H	1.75	0.51
1:C:736:HIS:ND1	1:C:737:LEU:O	2.43	0.51
1:D:960:MET:HE1	1:D:966:LYS:HG3	1.93	0.51
1:D:4804:TYR:CG	1:D:4804:TYR:O	2.63	0.51
1:A:961:MET:HE1	1:A:963:ASN:HB3	1.93	0.51
1:A:3680:ALA:HB3	1:A:3697:PRO:HG2	1.92	0.51
1:B:1486:SER:HB2	1:B:1553:PHE:CE1	2.46	0.51
1:B:2587:TYR:O	1:B:2590:SER:N	2.44	0.51
1:C:3680:ALA:HB3	1:C:3697:PRO:HG2	1.92	0.51
1:C:4579:PHE:HB2	1:C:4631:PHE:HE1	1.76	0.51
1:C:4866:SER:N	1:C:4873:ASP:OD2	2.42	0.51
1:A:55:ALA:O	1:A:281:ARG:NH2	2.39	0.51
1:A:960:MET:HE1	1:A:966:LYS:HG3	1.92	0.51
1:D:4579:PHE:HB2	1:D:4631:PHE:HE1	1.76	0.51
1:A:1486:SER:HB2	1:A:1553:PHE:CE1	2.46	0.51
1:A:2437:ALA:HB3	1:A:2508:ARG:HH11	1.74	0.51
1:A:4171:LEU:O	1:A:4175:ARG:HG3	2.10	0.51
1:A:4579:PHE:HB2	1:A:4631:PHE:HE1	1.76	0.51
1:C:102:LEU:HB2	1:C:105:HIS:CD2	2.46	0.51
1:C:4171:LEU:O	1:C:4175:ARG:HG3	2.10	0.51
1:D:492:ASP:HA	1:D:495:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:TYR:OH	1:A:1508:ARG:NE	2.43	0.50
1:A:2310:CYS:HB2	1:A:2324:ASN:ND2	2.26	0.50
1:B:736:HIS:ND1	1:B:737:LEU:O	2.43	0.50
1:B:1276:THR:CB	1:B:1466:LEU:HD22	2.41	0.50
1:B:3147:ILE:HD13	1:B:3197:LEU:HD11	1.92	0.50
1:C:1130:GLN:OE1	1:C:1136:SER:OG	2.28	0.50
1:C:1839:VAL:O	1:C:1841:VAL:N	2.43	0.50
1:C:4804:TYR:CG	1:C:4804:TYR:O	2.63	0.50
1:D:1486:SER:HB2	1:D:1553:PHE:CE1	2.46	0.50
1:A:1276:THR:CB	1:A:1466:LEU:HD22	2.41	0.50
1:A:1450:VAL:HG21	1:A:1454:THR:HG21	1.92	0.50
1:A:2587:TYR:O	1:A:2590:SER:N	2.44	0.50
1:A:3147:ILE:HD13	1:A:3197:LEU:HD11	1.92	0.50
1:A:4863:TYR:HD2	1:A:4876:CYS:HB3	1.75	0.50
1:A:4944:ARG:O	1:A:4948:GLU:HG2	2.12	0.50
1:B:492:ASP:HA	1:B:495:ASN:ND2	2.26	0.50
1:B:1450:VAL:HG21	1:B:1454:THR:HG21	1.92	0.50
1:B:4804:TYR:O	1:B:4804:TYR:CG	2.63	0.50
1:C:721:LEU:HB2	1:C:728:ARG:HB2	1.93	0.50
1:C:1486:SER:HB2	1:C:1553:PHE:CE1	2.46	0.50
1:C:2310:CYS:HB2	1:C:2324:ASN:ND2	2.26	0.50
1:D:1450:VAL:HG21	1:D:1454:THR:HG21	1.92	0.50
1:D:3147:ILE:HD13	1:D:3197:LEU:HD11	1.92	0.50
1:A:1828:ASP:O	1:A:1829:PRO:C	2.48	0.50
1:B:55:ALA:O	1:B:281:ARG:NH2	2.39	0.50
1:C:1839:VAL:N	1:C:1840:PRO:HD2	2.27	0.50
1:D:1276:THR:CB	1:D:1466:LEU:HD22	2.41	0.50
1:D:2587:TYR:O	1:D:2590:SER:N	2.44	0.50
1:A:1839:VAL:N	1:A:1840:PRO:HD2	2.27	0.50
1:A:4866:SER:N	1:A:4873:ASP:OD2	2.42	0.50
1:B:961:MET:HE1	1:B:963:ASN:HB3	1.93	0.50
1:B:1257:VAL:HG12	1:B:1272:LEU:HG	1.93	0.50
1:C:1257:VAL:HG12	1:C:1272:LEU:HG	1.93	0.50
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.26	0.50
1:D:4171:LEU:O	1:D:4175:ARG:HG3	2.10	0.50
1:B:3680:ALA:HB3	1:B:3697:PRO:HG2	1.92	0.50
1:B:4832:HIS:CD2	1:B:4942:GLU:HG3	2.47	0.50
1:C:758:ARG:HG3	1:C:763:PRO:HA	1.93	0.50
1:C:1844:LEU:O	1:C:1845:VAL:C	2.48	0.50
1:D:2030:ASP:OD1	1:D:2031:LEU:N	2.45	0.50
1:D:4983:HIS:NE2	1:D:5027:CYS:SG	2.82	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2103:VAL:O	1:B:2107:GLN:HG3	2.12	0.50
1:C:961:MET:HE1	1:C:963:ASN:HB3	1.94	0.50
1:D:1828:ASP:O	1:D:1829:PRO:C	2.48	0.50
1:D:1839:VAL:N	1:D:1840:PRO:HD2	2.27	0.50
1:D:2103:VAL:O	1:D:2107:GLN:HG3	2.12	0.50
1:A:2503:VAL:HB	1:A:2551:ASN:ND2	2.27	0.50
1:B:4944:ARG:O	1:B:4948:GLU:HG2	2.12	0.50
1:C:2579:VAL:O	1:C:2591:ARG:NH1	2.39	0.50
1:D:758:ARG:HG3	1:D:763:PRO:HA	1.93	0.50
1:D:3717:ASP:OD1	1:D:3717:ASP:N	2.45	0.50
1:D:4944:ARG:O	1:D:4948:GLU:HG2	2.12	0.50
1:A:662:TRP:HZ3	1:A:811:CYS:HA	1.77	0.50
1:A:758:ARG:HG3	1:A:763:PRO:HA	1.93	0.50
1:A:963:ASN:OD1	1:A:965:TYR:N	2.45	0.50
1:A:1115:LEU:HB3	1:A:1123:VAL:HG11	1.94	0.50
1:B:4817:ALA:C	1:B:4819:GLY:N	2.65	0.50
1:C:2030:ASP:OD1	1:C:2031:LEU:N	2.45	0.50
1:C:2587:TYR:O	1:C:2590:SER:N	2.44	0.50
1:C:4814:LEU:C	1:C:4816:ILE:N	2.62	0.50
1:D:662:TRP:HZ3	1:D:811:CYS:HA	1.77	0.50
1:D:721:LEU:HB2	1:D:728:ARG:HB2	1.93	0.50
1:D:2394:GLY:H	1:D:2418:LEU:HG	1.77	0.50
1:A:158:SER:N	1:A:161:GLU:OE2	2.43	0.50
1:A:721:LEU:HB2	1:A:728:ARG:HB2	1.93	0.50
1:B:662:TRP:HZ3	1:B:811:CYS:HA	1.77	0.50
1:B:758:ARG:HG3	1:B:763:PRO:HA	1.93	0.50
1:C:4944:ARG:O	1:C:4948:GLU:HG2	2.12	0.50
1:D:1115:LEU:HB3	1:D:1123:VAL:HG11	1.94	0.50
1:D:2310:CYS:HB2	1:D:2324:ASN:ND2	2.26	0.50
1:A:492:ASP:HA	1:A:495:ASN:ND2	2.26	0.49
1:A:736:HIS:ND1	1:A:737:LEU:O	2.43	0.49
1:B:971:ASP:N	1:B:971:ASP:OD1	2.44	0.49
1:B:2030:ASP:OD1	1:B:2031:LEU:N	2.45	0.49
1:B:2310:CYS:HB2	1:B:2324:ASN:ND2	2.26	0.49
1:B:2503:VAL:HB	1:B:2551:ASN:ND2	2.27	0.49
1:C:662:TRP:HZ3	1:C:811:CYS:HA	1.77	0.49
1:C:963:ASN:OD1	1:C:965:TYR:N	2.45	0.49
1:C:2103:VAL:O	1:C:2107:GLN:HG3	2.12	0.49
1:C:2394:GLY:H	1:C:2418:LEU:HG	1.77	0.49
1:A:2394:GLY:H	1:A:2418:LEU:HG	1.77	0.49
1:A:3717:ASP:OD1	1:A:3717:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:LEU:HB3	1:B:1123:VAL:HG11	1.94	0.49
1:B:1653:LEU:HA	1:B:1656:ARG:HB2	1.94	0.49
1:C:560:ILE:HA	1:C:563:VAL:HG12	1.95	0.49
1:C:4239:GLU:OE1	1:C:4679:ARG:NH2	2.45	0.49
1:D:1257:VAL:HG12	1:D:1272:LEU:HG	1.93	0.49
1:D:1653:LEU:HA	1:D:1656:ARG:HB2	1.94	0.49
1:A:2030:ASP:OD1	1:A:2031:LEU:N	2.45	0.49
1:A:2495:VAL:HB	1:A:2498:HIS:ND1	2.27	0.49
1:A:4832:HIS:CD2	1:A:4942:GLU:HG3	2.47	0.49
1:B:1844:LEU:O	1:B:1845:VAL:C	2.48	0.49
1:B:4805:ASN:O	1:B:4807:PHE:N	2.46	0.49
1:C:4832:HIS:CD2	1:C:4942:GLU:HG3	2.47	0.49
1:D:412:ASN:O	1:D:416:LYS:HG2	2.13	0.49
1:D:3890:LEU:HA	1:D:3893:GLU:HB2	1.95	0.49
1:A:1257:VAL:HG12	1:A:1272:LEU:HG	1.93	0.49
1:B:721:LEU:HB2	1:B:728:ARG:HB2	1.93	0.49
1:B:2495:VAL:HB	1:B:2498:HIS:ND1	2.27	0.49
1:C:3890:LEU:HA	1:C:3893:GLU:HB2	1.95	0.49
1:D:961:MET:HE1	1:D:963:ASN:HB3	1.94	0.49
1:D:2503:VAL:HB	1:D:2551:ASN:ND2	2.27	0.49
1:D:4832:HIS:CD2	1:D:4942:GLU:HG3	2.47	0.49
1:A:1226:PHE:O	1:A:1827:ARG:NH1	2.39	0.49
1:A:2103:VAL:O	1:A:2107:GLN:HG3	2.12	0.49
1:B:2579:VAL:O	1:B:2591:ARG:NH1	2.39	0.49
1:B:3777:GLU:N	1:B:3777:GLU:OE1	2.45	0.49
1:C:1653:LEU:HA	1:C:1656:ARG:HB2	1.94	0.49
1:C:2495:VAL:HB	1:C:2498:HIS:ND1	2.27	0.49
1:D:2495:VAL:HB	1:D:2498:HIS:ND1	2.27	0.49
1:B:1839:VAL:N	1:B:1840:PRO:HD2	2.27	0.49
1:C:2302:LEU:HD23	1:C:2363:CYS:HB3	1.95	0.49
1:C:3754:GLU:OE1	1:C:3754:GLU:N	2.37	0.49
1:C:4191:GLU:OE2	1:C:5006:GLN:NE2	2.41	0.49
1:D:69:LEU:HD22	1:D:107:ILE:HD11	1.95	0.49
1:D:1844:LEU:O	1:D:1845:VAL:C	2.48	0.49
1:B:685:GLY:HA3	1:B:714:TYR:O	2.13	0.49
1:C:685:GLY:HA3	1:C:714:TYR:O	2.13	0.49
1:C:2503:VAL:HB	1:C:2551:ASN:ND2	2.27	0.49
1:A:1704:PRO:HG2	1:A:1707:LEU:HD12	1.95	0.49
1:A:3890:LEU:HA	1:A:3893:GLU:HB2	1.95	0.49
1:B:963:ASN:OD1	1:B:965:TYR:N	2.45	0.49
1:B:4798:MET:HB3	1:B:4812:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ALA:O	1:C:281:ARG:NH2	2.39	0.49
1:C:1704:PRO:HG2	1:C:1707:LEU:HD12	1.95	0.49
1:C:3777:GLU:OE1	1:C:3777:GLU:N	2.45	0.49
1:C:4736:ARG:HH22	1:D:4076:ALA:HA	1.77	0.49
1:D:963:ASN:OD1	1:D:965:TYR:N	2.45	0.49
1:D:4805:ASN:O	1:D:4807:PHE:N	2.46	0.49
1:A:1096:THR:OG1	1:A:1198:GLN:OE1	2.25	0.49
1:A:3924:LEU:O	1:A:3927:GLN:HG3	2.13	0.49
1:A:4076:ALA:HA	1:D:4736:ARG:HH22	1.77	0.49
1:C:1099:GLU:OE2	1:C:1128:ARG:NH2	2.46	0.49
1:D:1099:GLU:OE1	1:D:1125:ASN:ND2	2.46	0.49
1:A:560:ILE:HA	1:A:563:VAL:HG12	1.95	0.49
1:A:4239:GLU:OE1	1:A:4679:ARG:NH2	2.45	0.49
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.95	0.49
1:B:3842:LEU:HD21	1:B:3954:ALA:HB2	1.95	0.49
1:C:412:ASN:O	1:C:416:LYS:HG2	2.13	0.49
1:C:1107:PRO:HA	1:C:1189:LEU:HD12	1.95	0.49
1:C:1115:LEU:HB3	1:C:1123:VAL:HG11	1.94	0.49
1:D:685:GLY:HA3	1:D:714:TYR:O	2.13	0.49
1:D:1107:PRO:HA	1:D:1189:LEU:HD12	1.95	0.49
1:D:1157:GLU:HG2	1:D:1159:THR:HG23	1.95	0.49
1:D:2302:LEU:HD23	1:D:2363:CYS:HB3	1.95	0.49
1:D:4798:MET:HB3	1:D:4812:HIS:NE2	2.28	0.49
1:A:412:ASN:O	1:A:416:LYS:HG2	2.13	0.48
1:A:3842:LEU:HD21	1:A:3954:ALA:HB2	1.95	0.48
1:A:4798:MET:HB3	1:A:4812:HIS:NE2	2.28	0.48
1:A:4805:ASN:O	1:A:4807:PHE:N	2.46	0.48
1:A:4817:ALA:C	1:A:4819:GLY:N	2.65	0.48
1:B:1091:GLU:HG3	1:B:1203:ASN:HB2	1.95	0.48
1:B:1099:GLU:OE1	1:B:1125:ASN:ND2	2.46	0.48
1:B:3890:LEU:HA	1:B:3893:GLU:HB2	1.95	0.48
1:D:736:HIS:ND1	1:D:737:LEU:O	2.43	0.48
1:D:1130:GLN:OE1	1:D:1136:SER:OG	2.28	0.48
1:D:3182:TYR:HA	1:D:3229:ILE:HG21	1.95	0.48
1:D:3415:TYR:CD2	1:D:3518:LEU:HD22	2.48	0.48
1:D:4897:ILE:HD11	1:D:4916:PHE:HE2	1.78	0.48
1:A:861:ILE:HG23	1:A:862:VAL:HG23	1.95	0.48
1:A:1157:GLU:HG2	1:A:1159:THR:HG23	1.95	0.48
1:A:1653:LEU:HA	1:A:1656:ARG:HB2	1.94	0.48
1:A:3182:TYR:HA	1:A:3229:ILE:HG21	1.95	0.48
1:A:4736:ARG:HH22	1:B:4076:ALA:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:ILE:HG23	1:B:862:VAL:HG23	1.95	0.48
1:B:2310:CYS:HB2	1:B:2324:ASN:HD22	1.79	0.48
1:B:4736:ARG:HH22	1:C:4076:ALA:HA	1.77	0.48
1:C:659:TYR:HB3	1:C:661:LYS:HE2	1.96	0.48
1:C:3415:TYR:CD2	1:C:3518:LEU:HD22	2.48	0.48
1:D:551:LEU:HB3	1:D:553:ARG:NH2	2.24	0.48
1:D:1839:VAL:HG12	1:D:1840:PRO:N	2.28	0.48
1:A:1091:GLU:HG3	1:A:1203:ASN:HB2	1.95	0.48
1:A:1099:GLU:OE1	1:A:1125:ASN:ND2	2.46	0.48
1:B:412:ASN:O	1:B:416:LYS:HG2	2.13	0.48
1:B:1157:GLU:HG2	1:B:1159:THR:HG23	1.95	0.48
1:C:1091:GLU:HG3	1:C:1203:ASN:HB2	1.95	0.48
1:C:1295:VAL:O	1:C:1453:VAL:HA	2.14	0.48
1:C:4798:MET:HB3	1:C:4812:HIS:NE2	2.28	0.48
1:D:1830:VAL:HG12	1:D:1831:GLY:H	1.78	0.48
1:D:3777:GLU:OE1	1:D:3777:GLU:N	2.45	0.48
1:A:3372:VAL:O	1:A:3376:GLU:HG2	2.13	0.48
1:B:659:TYR:HB3	1:B:661:LYS:HE2	1.96	0.48
1:B:1099:GLU:OE2	1:B:1128:ARG:NH2	2.46	0.48
1:B:1704:PRO:HG2	1:B:1707:LEU:HD12	1.95	0.48
1:B:3372:VAL:O	1:B:3376:GLU:HG2	2.13	0.48
1:C:1099:GLU:OE1	1:C:1125:ASN:ND2	2.46	0.48
1:C:4114:CYS:SG	1:C:4131:ARG:NH2	2.86	0.48
1:D:1704:PRO:HG2	1:D:1707:LEU:HD12	1.95	0.48
1:D:3372:VAL:O	1:D:3376:GLU:HG2	2.13	0.48
1:D:4901:ILE:CD1	1:D:4913:ARG:HH22	2.24	0.48
1:A:591:ASP:O	1:A:1594:ARG:NH2	2.47	0.48
1:A:659:TYR:HB3	1:A:661:LYS:HE2	1.96	0.48
1:A:1469:VAL:HB	1:A:1470:ARG:H	1.50	0.48
1:A:1839:VAL:H	1:A:1840:PRO:HD2	1.78	0.48
1:A:2463:LEU:HG	1:A:2464:ASP:H	1.78	0.48
1:A:3777:GLU:OE1	1:A:3777:GLU:N	2.45	0.48
1:B:1450:VAL:HG22	1:B:1452:TRP:HE3	1.79	0.48
1:B:1839:VAL:H	1:B:1840:PRO:HD2	1.78	0.48
1:B:2302:LEU:HD23	1:B:2363:CYS:HB3	1.95	0.48
1:B:2394:GLY:H	1:B:2418:LEU:HG	1.77	0.48
1:B:3415:TYR:CD2	1:B:3518:LEU:HD22	2.48	0.48
1:B:3924:LEU:O	1:B:3927:GLN:HG3	2.13	0.48
1:B:4583:SER:HB3	1:B:4630:TYR:HE1	1.78	0.48
1:C:345:LEU:HD23	1:C:389:PHE:HB3	1.96	0.48
1:C:1830:VAL:HG12	1:C:1831:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2257:LEU:HD23	1:C:2275:VAL:HG13	1.96	0.48
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.14	0.48
1:D:1091:GLU:HG3	1:D:1203:ASN:HB2	1.95	0.48
1:D:1099:GLU:OE2	1:D:1128:ARG:NH2	2.46	0.48
1:D:4865:LYS:N	1:D:4873:ASP:OD2	2.47	0.48
1:A:3415:TYR:CD2	1:A:3518:LEU:HD22	2.48	0.48
1:A:4191:GLU:OE2	1:A:5006:GLN:NE2	2.41	0.48
1:B:1148:VAL:HG21	1:B:1212:ARG:HG3	1.96	0.48
1:B:1295:VAL:O	1:B:1453:VAL:HA	2.14	0.48
1:B:1475:THR:OG1	1:B:1482:ASN:O	2.32	0.48
1:B:1839:VAL:HG12	1:B:1840:PRO:N	2.28	0.48
1:B:3722:TYR:OH	1:B:3797:THR:HG22	2.14	0.48
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.14	0.48
1:C:1157:GLU:HG2	1:C:1159:THR:HG23	1.95	0.48
1:C:2424:SER:HA	1:C:2498:HIS:CD2	2.49	0.48
1:C:3722:TYR:OH	1:C:3797:THR:HG22	2.14	0.48
1:D:635:THR:HG22	1:D:636:ASN:N	2.29	0.48
1:D:659:TYR:HB3	1:D:661:LYS:HE2	1.96	0.48
1:D:861:ILE:HG23	1:D:862:VAL:HG23	1.95	0.48
1:D:1295:VAL:O	1:D:1453:VAL:HA	2.14	0.48
1:D:2424:SER:HA	1:D:2498:HIS:CD2	2.49	0.48
1:D:2463:LEU:HG	1:D:2464:ASP:H	1.78	0.48
1:A:2257:LEU:HD23	1:A:2275:VAL:HG13	1.96	0.48
1:A:2310:CYS:HB2	1:A:2324:ASN:HD22	1.79	0.48
1:A:2424:SER:HA	1:A:2498:HIS:CD2	2.49	0.48
1:A:4114:CYS:SG	1:A:4131:ARG:NH2	2.86	0.48
1:A:4583:SER:HB3	1:A:4630:TYR:HE1	1.78	0.48
1:B:345:LEU:HD23	1:B:389:PHE:HB3	1.96	0.48
1:B:635:THR:HG21	1:B:1637:MET:HG2	1.95	0.48
1:B:710:ASP:OD1	1:B:710:ASP:N	2.47	0.48
1:C:861:ILE:HG23	1:C:862:VAL:HG23	1.95	0.48
1:C:2310:CYS:HB2	1:C:2324:ASN:HD22	1.79	0.48
1:C:4805:ASN:O	1:C:4807:PHE:N	2.46	0.48
1:D:2257:LEU:HD23	1:D:2275:VAL:HG13	1.96	0.48
1:A:1839:VAL:HG12	1:A:1840:PRO:N	2.28	0.48
1:A:1844:LEU:O	1:A:1845:VAL:C	2.48	0.48
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.14	0.48
1:B:2292:GLU:O	1:B:2295:LEU:N	2.47	0.48
1:B:2463:LEU:HG	1:B:2464:ASP:H	1.78	0.48
1:C:635:THR:HG22	1:C:636:ASN:N	2.29	0.48
1:C:710:ASP:OD1	1:C:710:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:VAL:HG21	1:C:1212:ARG:HG3	1.96	0.48
1:D:55:ALA:O	1:D:281:ARG:NH2	2.39	0.48
1:D:4114:CYS:SG	1:D:4131:ARG:NH2	2.86	0.48
1:D:4545:GLU:OE1	1:D:4548:ARG:NH1	2.47	0.48
1:A:293:LEU:HD23	1:A:311:ALA:HB1	1.96	0.48
1:A:635:THR:HG21	1:A:1637:MET:HG2	1.95	0.48
1:A:710:ASP:N	1:A:710:ASP:OD1	2.47	0.48
1:A:1450:VAL:HG22	1:A:1452:TRP:HE3	1.79	0.48
1:A:4545:GLU:OE1	1:A:4548:ARG:NH1	2.47	0.48
1:A:4983:HIS:CD2	1:A:5027:CYS:HG	2.31	0.48
1:B:591:ASP:O	1:B:1594:ARG:NH2	2.47	0.48
1:B:1830:VAL:HG12	1:B:1831:GLY:H	1.78	0.48
1:B:4114:CYS:SG	1:B:4131:ARG:NH2	2.86	0.48
1:B:4545:GLU:OE1	1:B:4548:ARG:NH1	2.47	0.48
1:B:4763:GLY:O	1:B:4766:THR:OG1	2.26	0.48
1:B:4865:LYS:N	1:B:4873:ASP:OD2	2.47	0.48
1:C:1839:VAL:HG12	1:C:1840:PRO:N	2.28	0.48
1:D:635:THR:HG21	1:D:1637:MET:HG2	1.95	0.48
1:A:69:LEU:HD22	1:A:107:ILE:HD11	1.95	0.48
1:A:685:GLY:HA3	1:A:714:TYR:O	2.13	0.48
1:A:1148:VAL:HG21	1:A:1212:ARG:HG3	1.96	0.48
1:A:2302:LEU:HD23	1:A:2363:CYS:HB3	1.95	0.48
1:A:3722:TYR:OH	1:A:3797:THR:HG22	2.14	0.48
1:B:69:LEU:HD22	1:B:107:ILE:HD11	1.95	0.48
1:B:103:TYR:CE1	1:B:163:VAL:HG22	2.49	0.48
1:B:131:LEU:CD2	1:B:178:ARG:HG3	2.44	0.48
1:B:635:THR:HG22	1:B:636:ASN:N	2.29	0.48
1:B:1252:HIS:ND1	1:B:1255:TYR:HB2	2.29	0.48
1:B:1828:ASP:O	1:B:1829:PRO:C	2.48	0.48
1:B:2424:SER:HA	1:B:2498:HIS:CD2	2.49	0.48
1:C:69:LEU:HD22	1:C:107:ILE:HD11	1.95	0.48
1:C:3372:VAL:O	1:C:3376:GLU:HG2	2.13	0.48
1:C:4897:ILE:HD11	1:C:4916:PHE:HE2	1.78	0.48
1:D:3722:TYR:OH	1:D:3797:THR:HG22	2.14	0.48
1:D:3924:LEU:O	1:D:3927:GLN:HG3	2.13	0.48
1:A:131:LEU:CD2	1:A:178:ARG:HG3	2.44	0.47
1:A:2292:GLU:O	1:A:2295:LEU:N	2.47	0.47
1:A:3830:GLN:HA	1:A:3833:GLN:HG2	1.97	0.47
1:B:3396:ASP:O	1:B:3400:VAL:HG23	2.14	0.47
1:C:635:THR:HG21	1:C:1637:MET:HG2	1.95	0.47
1:D:710:ASP:N	1:D:710:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2310:CYS:HB2	1:D:2324:ASN:HD22	1.79	0.47
1:A:289:ARG:HB2	1:A:301:VAL:HG12	1.96	0.47
1:A:4865:LYS:N	1:A:4873:ASP:OD2	2.47	0.47
1:B:317:ARG:NH2	1:B:321:GLU:O	2.47	0.47
1:B:1283:LEU:HD23	1:B:1284:VAL:N	2.30	0.47
1:B:1592:PRO:HD2	1:B:1595:LEU:HD23	1.97	0.47
1:B:4239:GLU:OE1	1:B:4679:ARG:NH2	2.45	0.47
1:C:4545:GLU:OE1	1:C:4548:ARG:NH1	2.47	0.47
1:C:4583:SER:HB3	1:C:4630:TYR:HE1	1.78	0.47
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.95	0.47
1:D:711:LEU:HA	1:D:1532:ASN:HD21	1.80	0.47
1:D:1601:MET:HE3	1:D:1602:PRO:HD2	1.95	0.47
1:D:4983:HIS:CD2	1:D:5027:CYS:HG	2.32	0.47
1:A:1295:VAL:O	1:A:1453:VAL:HA	2.14	0.47
1:A:1830:VAL:HG12	1:A:1831:GLY:H	1.78	0.47
1:A:3396:ASP:O	1:A:3400:VAL:HG23	2.14	0.47
1:A:4799:SER:CA	1:A:4812:HIS:HE1	2.27	0.47
1:B:1228:ILE:O	1:C:3572:GLN:NE2	2.48	0.47
1:B:2257:LEU:HD23	1:B:2275:VAL:HG13	1.96	0.47
1:B:4901:ILE:HD12	1:B:4913:ARG:NH2	2.23	0.47
1:C:293:LEU:HD23	1:C:311:ALA:HB1	1.96	0.47
1:D:1243:PRO:HB2	1:D:1600:LEU:HD12	1.96	0.47
1:D:1271:ARG:NH2	1:D:1470:ARG:O	2.45	0.47
1:A:1099:GLU:OE2	1:A:1128:ARG:NH2	2.46	0.47
1:A:4064:MET:HE1	1:A:4110:PHE:CD2	2.49	0.47
1:C:317:ARG:NH2	1:C:321:GLU:O	2.47	0.47
1:C:3842:LEU:HD21	1:C:3954:ALA:HB2	1.95	0.47
1:C:3924:LEU:O	1:C:3927:GLN:HG3	2.13	0.47
1:D:244:LEU:HB3	1:D:246:TYR:CE1	2.50	0.47
1:D:289:ARG:HB2	1:D:301:VAL:HG12	1.96	0.47
1:D:293:LEU:HD23	1:D:311:ALA:HB1	1.96	0.47
1:D:468:LEU:O	1:D:472:ARG:HG2	2.15	0.47
1:D:591:ASP:O	1:D:1594:ARG:NH2	2.47	0.47
1:A:489:ASN:O	1:A:493:ARG:HG2	2.14	0.47
1:A:4807:PHE:C	1:A:4809:PHE:N	2.68	0.47
1:B:3182:TYR:HA	1:B:3229:ILE:HG21	1.95	0.47
1:B:4064:MET:HE1	1:B:4110:PHE:CD2	2.49	0.47
1:C:489:ASN:O	1:C:493:ARG:HG2	2.14	0.47
1:C:1592:PRO:HD2	1:C:1595:LEU:HD23	1.97	0.47
1:C:1839:VAL:H	1:C:1840:PRO:HD2	1.78	0.47
1:C:3182:TYR:HA	1:C:3229:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3830:GLN:HA	1:C:3833:GLN:HG2	1.97	0.47
1:C:4865:LYS:N	1:C:4873:ASP:OD2	2.47	0.47
1:D:110:ARG:NH1	1:D:117:TYR:OH	2.48	0.47
1:D:1475:THR:OG1	1:D:1482:ASN:O	2.32	0.47
1:D:1839:VAL:H	1:D:1840:PRO:HD2	1.78	0.47
1:D:2340:PHE:HD1	1:D:2435:ARG:HG2	1.80	0.47
1:D:3830:GLN:HA	1:D:3833:GLN:HG2	1.97	0.47
1:D:4583:SER:HB3	1:D:4630:TYR:HE1	1.78	0.47
1:A:1252:HIS:ND1	1:A:1255:TYR:HB2	2.29	0.47
1:B:46:LEU:HD11	1:B:134:ASP:OD2	2.15	0.47
1:C:103:TYR:CE1	1:C:163:VAL:HG22	2.49	0.47
1:C:649:PHE:HA	1:C:778:PHE:CE1	2.50	0.47
1:C:663:TYR:CE1	1:C:745:SER:HB2	2.50	0.47
1:C:1450:VAL:HG22	1:C:1452:TRP:HE3	1.79	0.47
1:C:2292:GLU:O	1:C:2295:LEU:N	2.47	0.47
1:C:4206:GLU:HA	1:C:4211:LYS:NZ	2.30	0.47
1:C:4808:PHE:C	1:C:4810:ALA:N	2.68	0.47
1:D:103:TYR:CE1	1:D:163:VAL:HG22	2.49	0.47
1:D:971:ASP:OD1	1:D:971:ASP:N	2.44	0.47
1:D:1592:PRO:HD2	1:D:1595:LEU:HD23	1.97	0.47
1:D:3184:GLU:OE1	1:D:3184:GLU:N	2.45	0.47
1:D:4805:ASN:O	1:D:4807:PHE:HB2	2.15	0.47
1:A:215:THR:OG1	1:A:271:GLY:O	2.30	0.47
1:A:345:LEU:HD23	1:A:389:PHE:HB3	1.96	0.47
1:A:1107:PRO:HA	1:A:1189:LEU:HD12	1.95	0.47
1:A:3927:GLN:HB3	1:A:3992:PHE:CE2	2.50	0.47
1:A:4808:PHE:C	1:A:4810:ALA:N	2.68	0.47
1:A:4897:ILE:HD11	1:A:4916:PHE:HE2	1.78	0.47
1:B:489:ASN:O	1:B:493:ARG:HG2	2.14	0.47
1:B:711:LEU:HA	1:B:1532:ASN:HD21	1.80	0.47
1:B:1243:PRO:HB2	1:B:1600:LEU:HD12	1.96	0.47
1:B:4799:SER:CA	1:B:4812:HIS:HE1	2.27	0.47
1:B:4808:PHE:C	1:B:4810:ALA:N	2.68	0.47
1:C:46:LEU:HD11	1:C:134:ASP:OD2	2.15	0.47
1:C:244:LEU:HB3	1:C:246:TYR:CE1	2.50	0.47
1:C:629:ARG:HB3	1:C:634:GLN:CD	2.35	0.47
1:C:1601:MET:HE3	1:C:1602:PRO:HD2	1.96	0.47
1:C:2463:LEU:HG	1:C:2464:ASP:H	1.78	0.47
1:C:3396:ASP:O	1:C:3400:VAL:HG23	2.14	0.47
1:C:4817:ALA:C	1:C:4819:GLY:N	2.65	0.47
1:C:4901:ILE:CD1	1:C:4913:ARG:HH22	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:CD2	1:D:178:ARG:HG3	2.44	0.47
1:D:158:SER:N	1:D:161:GLU:OE2	2.43	0.47
1:D:1148:VAL:HG21	1:D:1212:ARG:HG3	1.96	0.47
1:D:1226:PHE:O	1:D:1827:ARG:NH1	2.39	0.47
1:D:1491:ASN:HA	1:D:1540:PHE:CD2	2.50	0.47
1:D:2292:GLU:O	1:D:2295:LEU:N	2.47	0.47
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.14	0.47
1:D:4206:GLU:HA	1:D:4211:LYS:NZ	2.30	0.47
1:A:1283:LEU:HD23	1:A:1284:VAL:N	2.30	0.47
1:A:3572:GLN:NE2	1:D:1228:ILE:O	2.48	0.47
1:B:3927:GLN:HB3	1:B:3992:PHE:CE2	2.50	0.47
1:C:923:GLN:O	1:C:927:GLU:HG2	2.15	0.47
1:C:1228:ILE:O	1:D:3572:GLN:NE2	2.48	0.47
1:C:1243:PRO:HB2	1:C:1600:LEU:HD12	1.96	0.47
1:C:3667:HIS:ND1	1:C:3667:HIS:O	2.48	0.47
1:C:4799:SER:CA	1:C:4812:HIS:HE1	2.27	0.47
1:D:1283:LEU:HD23	1:D:1284:VAL:N	2.30	0.47
1:D:3396:ASP:O	1:D:3400:VAL:HG23	2.14	0.47
1:D:3842:LEU:HD21	1:D:3954:ALA:HB2	1.95	0.47
1:A:244:LEU:HB3	1:A:246:TYR:CE1	2.50	0.47
1:A:711:LEU:HA	1:A:1532:ASN:HD21	1.80	0.47
1:B:293:LEU:HD23	1:B:311:ALA:HB1	1.96	0.47
1:B:663:TYR:CE1	1:B:745:SER:HB2	2.50	0.47
1:B:1107:PRO:HA	1:B:1189:LEU:HD12	1.95	0.47
1:B:3184:GLU:OE1	1:B:3184:GLU:N	2.45	0.47
1:B:3830:GLN:HA	1:B:3833:GLN:HG2	1.97	0.47
1:C:131:LEU:CD2	1:C:178:ARG:HG3	2.44	0.47
1:C:1252:HIS:ND1	1:C:1255:TYR:HB2	2.29	0.47
1:D:345:LEU:HD23	1:D:389:PHE:HB3	1.96	0.47
1:D:489:ASN:O	1:D:493:ARG:HG2	2.14	0.47
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.15	0.47
1:D:2191:PHE:CD1	1:D:2198:MET:HG3	2.50	0.47
1:A:468:LEU:O	1:A:472:ARG:HG2	2.15	0.47
1:A:1243:PRO:HB2	1:A:1600:LEU:HD12	1.96	0.47
1:A:1592:PRO:HD2	1:A:1595:LEU:HD23	1.97	0.47
1:A:2191:PHE:CD1	1:A:2198:MET:HG3	2.50	0.47
1:A:2340:PHE:HD1	1:A:2435:ARG:HG2	1.80	0.47
1:A:4206:GLU:HA	1:A:4211:LYS:NZ	2.30	0.47
1:B:244:LEU:HB3	1:B:246:TYR:CE1	2.50	0.47
1:B:2339:VAL:O	1:B:2345:SER:OG	2.20	0.47
1:C:591:ASP:O	1:C:1594:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1087:ARG:NH1	1:C:1154:ASP:OD2	2.48	0.47
1:C:1283:LEU:HD23	1:C:1284:VAL:N	2.30	0.47
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.15	0.47
1:C:2245:GLN:O	1:C:2248:ARG:HG2	2.15	0.47
1:C:3927:GLN:HB3	1:C:3992:PHE:CE2	2.50	0.47
1:C:4886:HIS:CD2	1:C:4897:ILE:HG21	2.50	0.47
1:C:4983:HIS:CD2	1:C:5027:CYS:HG	2.32	0.47
1:D:2245:GLN:O	1:D:2248:ARG:HG2	2.15	0.47
1:D:3927:GLN:HB3	1:D:3992:PHE:CE2	2.50	0.47
1:D:4799:SER:CA	1:D:4812:HIS:HE1	2.27	0.47
1:A:103:TYR:CE1	1:A:163:VAL:HG22	2.49	0.46
1:A:663:TYR:CE1	1:A:745:SER:HB2	2.50	0.46
1:A:1819:VAL:HG22	1:A:1926:LEU:HD13	1.98	0.46
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.26	0.46
1:B:923:GLN:O	1:B:927:GLU:HG2	2.15	0.46
1:B:4206:GLU:HA	1:B:4211:LYS:NZ	2.30	0.46
1:C:131:LEU:HD21	1:C:178:ARG:HG3	1.98	0.46
1:C:468:LEU:O	1:C:472:ARG:HG2	2.15	0.46
1:C:4064:MET:HE1	1:C:4110:PHE:CD2	2.50	0.46
1:C:4805:ASN:O	1:C:4807:PHE:HB2	2.15	0.46
1:A:110:ARG:NH1	1:A:117:TYR:OH	2.48	0.46
1:A:317:ARG:NH2	1:A:321:GLU:O	2.47	0.46
1:A:1087:ARG:NH1	1:A:1154:ASP:OD2	2.48	0.46
1:A:1100:MET:HE3	1:A:1198:GLN:HB3	1.96	0.46
1:A:1127:HIS:HB3	1:A:1128:ARG:NH2	2.31	0.46
1:B:158:SER:N	1:B:161:GLU:OE2	2.43	0.46
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.15	0.46
1:B:4805:ASN:O	1:B:4807:PHE:HB2	2.15	0.46
1:C:289:ARG:HB2	1:C:301:VAL:HG12	1.96	0.46
1:C:4181:ILE:HG12	1:C:4193:ILE:HB	1.97	0.46
1:D:131:LEU:HD21	1:D:178:ARG:HG3	1.98	0.46
1:D:649:PHE:HA	1:D:778:PHE:CE1	2.50	0.46
1:D:1965:TYR:CE2	1:D:1969:LEU:HD12	2.49	0.46
1:D:3569:LEU:O	1:D:3569:LEU:HD12	2.15	0.46
1:D:3667:HIS:ND1	1:D:3667:HIS:O	2.48	0.46
1:D:4064:MET:HE1	1:D:4110:PHE:CD2	2.50	0.46
1:D:4239:GLU:OE1	1:D:4679:ARG:NH2	2.45	0.46
1:A:971:ASP:OD1	1:A:971:ASP:N	2.44	0.46
1:B:110:ARG:NH1	1:B:117:TYR:OH	2.48	0.46
1:B:468:LEU:O	1:B:472:ARG:HG2	2.15	0.46
1:B:649:PHE:HA	1:B:778:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1601:MET:HE3	1:B:1602:PRO:HD2	1.96	0.46
1:C:3213:TYR:O	1:C:3294:PRO:HG2	2.16	0.46
1:C:3569:LEU:HD12	1:C:3569:LEU:O	2.15	0.46
1:C:4901:ILE:HD12	1:C:4913:ARG:NH2	2.23	0.46
1:D:629:ARG:HB3	1:D:634:GLN:CD	2.35	0.46
1:A:629:ARG:HB3	1:A:634:GLN:CD	2.35	0.46
1:A:774:ASP:OD1	1:A:774:ASP:N	2.41	0.46
1:A:3525:CYS:O	1:A:3528:THR:HG22	2.16	0.46
1:A:3667:HIS:ND1	1:A:3667:HIS:O	2.48	0.46
1:B:289:ARG:HB2	1:B:301:VAL:HG12	1.96	0.46
1:B:1207:ASP:OD2	1:B:1209:SER:OG	2.19	0.46
1:B:1430:THR:N	1:B:1451:GLY:O	2.49	0.46
1:B:4807:PHE:O	1:B:4808:PHE:C	2.54	0.46
1:C:2191:PHE:CD1	1:C:2198:MET:HG3	2.50	0.46
1:C:3525:CYS:O	1:C:3528:THR:HG22	2.16	0.46
1:D:1127:HIS:HB3	1:D:1128:ARG:NH2	2.31	0.46
1:A:131:LEU:HD21	1:A:178:ARG:HG3	1.98	0.46
1:A:4901:ILE:CD1	1:A:4913:ARG:HH22	2.24	0.46
1:B:1819:VAL:HG22	1:B:1926:LEU:HD13	1.98	0.46
1:B:2191:PHE:CD1	1:B:2198:MET:HG3	2.50	0.46
1:B:2340:PHE:HD1	1:B:2435:ARG:HG2	1.80	0.46
1:B:2613:TYR:C	1:B:2616:PRO:HD2	2.36	0.46
1:B:3525:CYS:O	1:B:3528:THR:HG22	2.16	0.46
1:C:2340:PHE:HD1	1:C:2435:ARG:HG2	1.80	0.46
1:D:663:TYR:CE1	1:D:745:SER:HB2	2.50	0.46
1:D:923:GLN:O	1:D:927:GLU:HG2	2.15	0.46
1:D:1252:HIS:ND1	1:D:1255:TYR:HB2	2.29	0.46
1:D:3213:TYR:O	1:D:3294:PRO:HG2	2.16	0.46
1:D:5035:GLN:O	1:D:5036:LEU:HD22	2.16	0.46
1:B:629:ARG:HB3	1:B:634:GLN:CD	2.35	0.46
1:B:2245:GLN:O	1:B:2248:ARG:HG2	2.15	0.46
1:B:3667:HIS:ND1	1:B:3667:HIS:O	2.48	0.46
1:D:1087:ARG:NH1	1:D:1154:ASP:OD2	2.48	0.46
1:D:3525:CYS:O	1:D:3528:THR:HG22	2.16	0.46
1:A:635:THR:HG22	1:A:636:ASN:N	2.29	0.46
1:A:1805:GLU:OE1	1:A:1808:ARG:NH2	2.49	0.46
1:A:1965:TYR:CE2	1:A:1969:LEU:HD12	2.49	0.46
1:B:131:LEU:HD21	1:B:178:ARG:HG3	1.98	0.46
1:D:1819:VAL:HG22	1:D:1926:LEU:HD13	1.98	0.46
1:A:4805:ASN:O	1:A:4807:PHE:HB2	2.15	0.46
1:B:649:PHE:HB2	1:B:776:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:PHE:HZ	1:B:791:PHE:CD1	2.34	0.46
1:B:748:LEU:HD13	1:B:755:ILE:HG13	1.98	0.46
1:C:1430:THR:N	1:C:1451:GLY:O	2.49	0.46
1:C:1491:ASN:HA	1:C:1540:PHE:CD2	2.50	0.46
1:C:2613:TYR:C	1:C:2616:PRO:HD2	2.36	0.46
1:C:3717:ASP:OD1	1:C:3717:ASP:N	2.45	0.46
1:D:317:ARG:NH2	1:D:321:GLU:O	2.47	0.46
1:D:1430:THR:N	1:D:1451:GLY:O	2.49	0.46
1:D:1450:VAL:HG22	1:D:1452:TRP:HE3	1.79	0.46
1:D:1457:TYR:O	1:D:1496:TRP:HB2	2.16	0.46
1:D:2311:PRO:HA	1:D:2314:LEU:HB3	1.98	0.46
1:A:1716:ILE:CD1	1:A:1843:LYS:HG2	2.46	0.46
1:A:2996:LYS:HE3	1:A:2996:LYS:HB2	1.79	0.46
1:B:1096:THR:OG1	1:B:1198:GLN:OE1	2.25	0.46
1:B:4983:HIS:CD2	1:B:5027:CYS:HG	2.31	0.46
1:C:711:LEU:HA	1:C:1532:ASN:HD21	1.80	0.46
1:C:748:LEU:HD13	1:C:755:ILE:HG13	1.98	0.46
1:C:1459:GLN:H	1:C:1496:TRP:HA	1.81	0.46
1:C:1475:THR:OG1	1:C:1482:ASN:O	2.32	0.46
1:C:3184:GLU:OE1	1:C:3184:GLU:N	2.45	0.46
1:D:649:PHE:HB2	1:D:776:LEU:HD23	1.97	0.46
1:D:4807:PHE:O	1:D:4808:PHE:C	2.54	0.46
1:A:664:PHE:HZ	1:A:791:PHE:CD1	2.34	0.46
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.51	0.46
1:A:2245:GLN:O	1:A:2248:ARG:HG2	2.15	0.46
1:B:1716:ILE:CD1	1:B:1843:LYS:HG2	2.46	0.46
1:B:3213:TYR:O	1:B:3294:PRO:HG2	2.16	0.46
1:B:3569:LEU:HD12	1:B:3569:LEU:O	2.15	0.46
1:B:4181:ILE:HG12	1:B:4193:ILE:HB	1.97	0.46
1:B:4886:HIS:CD2	1:B:4897:ILE:HG21	2.50	0.46
1:B:4897:ILE:HD11	1:B:4916:PHE:HE2	1.78	0.46
1:C:4991:PHE:HE2	1:C:5010:VAL:HG11	1.81	0.46
1:C:5035:GLN:O	1:C:5036:LEU:HD22	2.16	0.46
1:D:1096:THR:OG1	1:D:1198:GLN:OE1	2.25	0.46
1:D:3986:TRP:HA	1:D:3989:VAL:HG12	1.98	0.46
1:D:4679:ARG:HH21	1:D:5017:ARG:NH2	2.14	0.46
1:D:4898:GLY:HA2	1:D:4901:ILE:HD13	1.98	0.46
1:A:46:LEU:HD11	1:A:134:ASP:OD2	2.15	0.45
1:A:793:LEU:HD23	1:A:793:LEU:H	1.81	0.45
1:A:1228:ILE:O	1:B:3572:GLN:NE2	2.48	0.45
1:A:1491:ASN:HA	1:A:1540:PHE:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2311:PRO:HA	1:A:2314:LEU:HB3	1.98	0.45
1:A:2613:TYR:C	1:A:2616:PRO:HD2	2.36	0.45
1:A:3213:TYR:O	1:A:3294:PRO:HG2	2.16	0.45
1:B:1087:ARG:NH1	1:B:1154:ASP:OD2	2.48	0.45
1:B:1127:HIS:HB3	1:B:1128:ARG:NH2	2.31	0.45
1:B:1727:ARG:O	1:B:1731:LEU:HG	2.16	0.45
1:B:1965:TYR:CE2	1:B:1969:LEU:HD12	2.49	0.45
1:B:2112:GLN:O	1:B:2113:SER:OG	2.29	0.45
1:B:4209:GLN:CD	1:B:4209:GLN:H	2.19	0.45
1:B:4807:PHE:O	1:B:4809:PHE:N	2.50	0.45
1:B:4807:PHE:C	1:B:4809:PHE:N	2.68	0.45
1:C:649:PHE:HB2	1:C:776:LEU:HD23	1.97	0.45
1:C:4873:ASP:OD1	1:C:4873:ASP:N	2.40	0.45
1:D:963:ASN:OD1	1:D:964:GLY:N	2.50	0.45
1:D:2613:TYR:C	1:D:2616:PRO:HD2	2.36	0.45
1:D:3878:ASP:N	1:D:3878:ASP:OD1	2.49	0.45
1:A:1229:ASN:OD1	1:B:3572:GLN:NE2	2.49	0.45
1:A:1430:THR:N	1:A:1451:GLY:O	2.49	0.45
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.15	0.45
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.51	0.45
1:B:2311:PRO:HA	1:B:2314:LEU:HB3	1.98	0.45
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.26	0.45
1:C:793:LEU:HD23	1:C:793:LEU:H	1.81	0.45
1:C:1819:VAL:HG22	1:C:1926:LEU:HD13	1.98	0.45
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.26	0.45
1:C:4209:GLN:H	1:C:4209:GLN:CD	2.19	0.45
1:C:4679:ARG:HH21	1:C:5017:ARG:NH2	2.14	0.45
1:C:4898:GLY:HA2	1:C:4901:ILE:HD13	1.98	0.45
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.51	0.45
1:D:1805:GLU:OE1	1:D:1808:ARG:NH2	2.49	0.45
1:D:4209:GLN:H	1:D:4209:GLN:CD	2.19	0.45
1:D:4817:ALA:C	1:D:4819:GLY:N	2.65	0.45
1:A:4209:GLN:H	1:A:4209:GLN:CD	2.19	0.45
1:A:4898:GLY:HA2	1:A:4901:ILE:HD13	1.98	0.45
1:B:1491:ASN:HA	1:B:1540:PHE:CD2	2.50	0.45
1:B:4799:SER:HB2	1:B:4812:HIS:HE1	1.82	0.45
1:C:110:ARG:NH1	1:C:117:TYR:OH	2.48	0.45
1:C:158:SER:N	1:C:161:GLU:OE2	2.43	0.45
1:C:1127:HIS:HB3	1:C:1128:ARG:NH2	2.31	0.45
1:C:1229:ASN:OD1	1:D:3572:GLN:NE2	2.49	0.45
1:D:46:LEU:HD11	1:D:134:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3779:VAL:O	1:D:3783:ILE:HG12	2.17	0.45
1:D:4901:ILE:HD12	1:D:4913:ARG:NH2	2.23	0.45
1:A:649:PHE:HA	1:A:778:PHE:CE1	2.50	0.45
1:A:923:GLN:O	1:A:927:GLU:HG2	2.15	0.45
1:A:1089:TYR:CD1	1:A:1152:MET:HG2	2.51	0.45
1:A:2584:HIS:CG	1:A:2585:THR:H	2.34	0.45
1:A:3569:LEU:O	1:A:3569:LEU:HD12	2.15	0.45
1:A:4799:SER:HB2	1:A:4812:HIS:HE1	1.82	0.45
1:B:919:ASN:OD1	1:B:920:TYR:N	2.50	0.45
1:B:2584:HIS:CG	1:B:2585:THR:H	2.34	0.45
1:C:3779:VAL:O	1:C:3783:ILE:HG12	2.17	0.45
1:C:4807:PHE:O	1:C:4809:PHE:N	2.50	0.45
1:D:919:ASN:OD1	1:D:920:TYR:N	2.50	0.45
1:D:1459:GLN:H	1:D:1496:TRP:HA	1.81	0.45
1:D:1835:GLU:C	1:D:1837:GLN:N	2.68	0.45
1:D:4181:ILE:HG12	1:D:4193:ILE:HB	1.97	0.45
1:D:4807:PHE:O	1:D:4809:PHE:N	2.50	0.45
1:D:4886:HIS:CD2	1:D:4897:ILE:HG21	2.50	0.45
1:A:649:PHE:HB2	1:A:776:LEU:HD23	1.97	0.45
1:A:1457:TYR:O	1:A:1496:TRP:HB2	2.16	0.45
1:A:3793:MET:O	1:A:3797:THR:HG23	2.17	0.45
1:A:4679:ARG:HH21	1:A:5017:ARG:NH2	2.14	0.45
1:A:4886:HIS:CD2	1:A:4897:ILE:HG21	2.50	0.45
1:B:1089:TYR:CD1	1:B:1152:MET:HG2	2.51	0.45
1:B:1478:ASP:OD1	1:B:1479:GLU:N	2.49	0.45
1:B:1805:GLU:OE1	1:B:1808:ARG:NH2	2.49	0.45
1:B:3986:TRP:HA	1:B:3989:VAL:HG12	1.98	0.45
1:C:664:PHE:HZ	1:C:791:PHE:CD1	2.34	0.45
1:C:1805:GLU:OE1	1:C:1808:ARG:NH2	2.49	0.45
1:C:3986:TRP:HA	1:C:3989:VAL:HG12	1.98	0.45
1:D:915:GLU:O	1:D:918:ARG:HG2	2.17	0.45
1:D:3793:MET:O	1:D:3797:THR:HG23	2.17	0.45
1:D:4808:PHE:C	1:D:4810:ALA:N	2.68	0.45
1:A:2579:VAL:O	1:A:2591:ARG:NH1	2.39	0.45
1:A:4799:SER:HA	1:A:4812:HIS:HE1	1.82	0.45
1:A:4807:PHE:O	1:A:4809:PHE:N	2.50	0.45
1:A:5035:GLN:O	1:A:5036:LEU:HD22	2.16	0.45
1:B:2094:LEU:O	1:B:2098:VAL:HG12	2.17	0.45
1:B:4991:PHE:HE2	1:B:5010:VAL:HG11	1.81	0.45
1:C:1478:ASP:OD1	1:C:1479:GLU:N	2.49	0.45
1:C:1965:TYR:CE2	1:C:1969:LEU:HD12	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2584:HIS:CG	1:C:2585:THR:H	2.34	0.45
1:C:2995:ILE:HD12	1:C:2997:PHE:HB2	1.99	0.45
1:D:1478:ASP:OD1	1:D:1479:GLU:N	2.49	0.45
1:D:1716:ILE:CD1	1:D:1843:LYS:HG2	2.46	0.45
1:D:2149:VAL:O	1:D:2153:MET:HG2	2.17	0.45
1:D:2584:HIS:CG	1:D:2585:THR:H	2.34	0.45
1:D:2995:ILE:HD12	1:D:2997:PHE:HB2	1.99	0.45
1:A:915:GLU:O	1:A:918:ARG:HG2	2.17	0.45
1:A:963:ASN:OD1	1:A:964:GLY:N	2.50	0.45
1:A:1727:ARG:O	1:A:1731:LEU:HG	2.16	0.45
1:A:3805:LEU:HB3	1:A:3812:VAL:HG21	1.98	0.45
1:A:3986:TRP:HA	1:A:3989:VAL:HG12	1.98	0.45
1:A:4807:PHE:O	1:A:4808:PHE:C	2.54	0.45
1:B:793:LEU:H	1:B:793:LEU:HD23	1.81	0.45
1:B:963:ASN:OD1	1:B:964:GLY:N	2.50	0.45
1:B:4898:GLY:HA2	1:B:4901:ILE:HD13	1.98	0.45
1:C:963:ASN:OD1	1:C:964:GLY:N	2.50	0.45
1:C:1457:TYR:O	1:C:1496:TRP:HB2	2.16	0.45
1:C:4779:LYS:O	1:C:4783:ILE:HG12	2.17	0.45
1:C:4807:PHE:C	1:C:4809:PHE:N	2.68	0.45
1:D:1089:TYR:HD1	1:D:1152:MET:HG2	1.82	0.45
1:D:2579:VAL:O	1:D:2591:ARG:NH1	2.39	0.45
1:D:3805:LEU:HB3	1:D:3812:VAL:HG21	1.98	0.45
1:A:3572:GLN:NE2	1:D:1229:ASN:OD1	2.49	0.45
1:B:1229:ASN:OD1	1:C:3572:GLN:NE2	2.49	0.45
1:B:1453:VAL:HG23	1:B:1454:THR:N	2.32	0.45
1:B:2995:ILE:HD12	1:B:2997:PHE:HB2	1.99	0.45
1:C:1276:THR:OG1	1:C:1466:LEU:HD13	2.17	0.45
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.17	0.45
1:D:2138:LEU:HD23	1:D:2138:LEU:HA	1.82	0.45
1:D:4939:ALA:O	1:D:4942:GLU:HB2	2.17	0.45
1:A:873:LYS:O	1:A:877:ASN:ND2	2.44	0.45
1:A:919:ASN:OD1	1:A:920:TYR:N	2.50	0.45
1:B:915:GLU:O	1:B:918:ARG:HG2	2.17	0.45
1:B:1862:ILE:HA	1:B:1865:MET:HG3	1.99	0.45
1:B:3779:VAL:O	1:B:3783:ILE:HG12	2.17	0.45
1:C:3793:MET:O	1:C:3797:THR:HG23	2.17	0.45
1:D:413:GLN:OE1	1:D:437:PRO:HG2	2.17	0.45
1:A:551:LEU:HG	1:A:553:ARG:HH12	1.82	0.45
1:A:3773:ARG:HD3	1:A:3815:LYS:HZ3	1.82	0.45
1:A:4658:ILE:HD13	1:A:4792:LEU:HB3	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1859:VAL:HA	1:B:1862:ILE:HG12	1.99	0.45
1:C:49:LEU:HD11	1:C:191:VAL:HB	1.99	0.45
1:C:919:ASN:OD1	1:C:920:TYR:N	2.50	0.45
1:C:2308:GLN:O	1:C:2323:TRP:HA	2.17	0.45
1:C:4865:LYS:H	1:C:4873:ASP:HB2	1.82	0.45
1:D:1089:TYR:CD1	1:D:1152:MET:HG2	2.51	0.45
1:D:2167:ILE:HG13	1:D:2168:VAL:N	2.32	0.45
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.81	0.45
1:A:748:LEU:HD13	1:A:755:ILE:HG13	1.98	0.44
1:A:1601:MET:HE3	1:A:1602:PRO:HD2	1.97	0.44
1:A:1843:LYS:HE2	1:A:1843:LYS:HB2	1.74	0.44
1:A:2149:VAL:O	1:A:2153:MET:HG2	2.17	0.44
1:A:2995:ILE:HD12	1:A:2997:PHE:HB2	1.99	0.44
1:B:632:LEU:HD23	1:B:1666:THR:HG23	1.99	0.44
1:B:3805:LEU:HB3	1:B:3812:VAL:HG21	1.98	0.44
1:B:4939:ALA:O	1:B:4942:GLU:HB2	2.17	0.44
1:C:915:GLU:O	1:C:918:ARG:HG2	2.17	0.44
1:C:1089:TYR:HD1	1:C:1152:MET:HG2	1.82	0.44
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.51	0.44
1:C:2167:ILE:HG13	1:C:2168:VAL:N	2.32	0.44
1:C:3805:LEU:HB3	1:C:3812:VAL:HG21	1.98	0.44
1:C:3878:ASP:N	1:C:3878:ASP:OD1	2.49	0.44
1:C:4696:ASP:OD1	1:C:4696:ASP:N	2.46	0.44
1:C:4939:ALA:O	1:C:4942:GLU:HB2	2.17	0.44
1:C:5027:CYS:O	1:C:5029:ARG:N	2.50	0.44
1:D:664:PHE:HZ	1:D:791:PHE:CD1	2.34	0.44
1:D:2142:TYR:CG	1:D:2197:LEU:HD13	2.52	0.44
1:D:4799:SER:HB2	1:D:4812:HIS:HE1	1.82	0.44
1:A:2142:TYR:CG	1:A:2197:LEU:HD13	2.52	0.44
1:A:4181:ILE:HG12	1:A:4193:ILE:HB	1.97	0.44
1:B:551:LEU:HG	1:B:553:ARG:HH12	1.82	0.44
1:B:1459:GLN:H	1:B:1496:TRP:HA	1.81	0.44
1:B:1849:LEU:HD12	1:B:1849:LEU:HA	1.82	0.44
1:B:2242:ILE:HG23	1:B:2242:ILE:O	2.18	0.44
1:B:4679:ARG:HH21	1:B:5017:ARG:NH2	2.14	0.44
1:B:4901:ILE:CD1	1:B:4913:ARG:HH22	2.24	0.44
1:C:1206:GLN:HA	1:C:1227:ALA:O	2.18	0.44
1:C:1727:ARG:O	1:C:1731:LEU:HG	2.16	0.44
1:D:134:ASP:OD1	1:D:134:ASP:N	2.50	0.44
1:D:632:LEU:HD23	1:D:1666:THR:HG23	1.99	0.44
1:D:793:LEU:HD23	1:D:793:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1206:GLN:HA	1:D:1227:ALA:O	2.18	0.44
1:D:1466:LEU:HD23	1:D:1466:LEU:HA	1.74	0.44
1:D:1862:ILE:HA	1:D:1865:MET:HG3	1.99	0.44
1:D:2242:ILE:HG23	1:D:2242:ILE:O	2.18	0.44
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.17	0.44
1:A:3779:VAL:O	1:A:3783:ILE:HG12	2.17	0.44
1:B:49:LEU:HD11	1:B:191:VAL:HB	1.99	0.44
1:B:520:ASN:O	1:B:524:GLU:HG3	2.18	0.44
1:B:1206:GLN:HA	1:B:1227:ALA:O	2.18	0.44
1:B:2167:ILE:HG13	1:B:2168:VAL:N	2.32	0.44
1:B:2667:THR:HA	1:B:2671:GLU:HB2	2.00	0.44
1:C:794:GLY:N	1:C:798:GLY:HA3	2.32	0.44
1:C:1862:ILE:HA	1:C:1865:MET:HG3	1.99	0.44
1:C:2149:VAL:O	1:C:2153:MET:HG2	2.17	0.44
1:C:2311:PRO:HA	1:C:2314:LEU:HB3	1.98	0.44
1:C:4799:SER:HA	1:C:4812:HIS:HE1	1.82	0.44
1:C:4799:SER:HB2	1:C:4812:HIS:HE1	1.82	0.44
1:C:4816:ILE:HG22	1:C:4817:ALA:N	2.32	0.44
1:D:748:LEU:HD13	1:D:755:ILE:HG13	1.98	0.44
1:D:1727:ARG:O	1:D:1731:LEU:HG	2.16	0.44
1:D:2667:THR:HA	1:D:2671:GLU:HB2	2.00	0.44
1:D:4807:PHE:O	1:D:4810:ALA:N	2.51	0.44
1:A:1276:THR:CA	1:A:1466:LEU:HD22	2.45	0.44
1:A:1283:LEU:HD13	1:A:1506:GLN:OE1	2.18	0.44
1:A:2667:THR:HA	1:A:2671:GLU:HB2	2.00	0.44
1:B:101:LEU:HD11	1:B:107:ILE:HD12	1.99	0.44
1:B:273:HIS:NE2	1:B:337:PRO:HA	2.33	0.44
1:B:3793:MET:O	1:B:3797:THR:HG23	2.17	0.44
1:B:4658:ILE:HD13	1:B:4792:LEU:HB3	2.00	0.44
1:B:4983:HIS:NE2	1:B:5027:CYS:SG	2.82	0.44
1:C:101:LEU:HD11	1:C:107:ILE:HD12	1.99	0.44
1:C:1283:LEU:HD13	1:C:1506:GLN:OE1	2.18	0.44
1:C:2112:GLN:O	1:C:2113:SER:OG	2.29	0.44
1:C:4808:PHE:O	1:C:4810:ALA:N	2.51	0.44
1:D:101:LEU:HD11	1:D:107:ILE:HD12	1.99	0.44
1:D:5027:CYS:O	1:D:5029:ARG:N	2.50	0.44
1:A:413:GLN:OE1	1:A:437:PRO:HG2	2.17	0.44
1:A:1276:THR:OG1	1:A:1466:LEU:HD13	2.17	0.44
1:A:1475:THR:OG1	1:A:1482:ASN:O	2.32	0.44
1:A:1830:VAL:C	1:A:1832:GLY:N	2.71	0.44
1:A:4991:PHE:HE2	1:A:5010:VAL:HG11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1811:ALA:HA	1:B:1814:MET:HE2	2.00	0.44
1:B:1830:VAL:C	1:B:1832:GLY:N	2.71	0.44
1:B:2440:MET:N	1:B:2440:MET:SD	2.91	0.44
1:B:4865:LYS:H	1:B:4873:ASP:HB2	1.82	0.44
1:B:5035:GLN:O	1:B:5036:LEU:HD22	2.16	0.44
1:C:413:GLN:OE1	1:C:437:PRO:HG2	2.17	0.44
1:C:1540:PHE:CE1	1:C:1552:VAL:HG11	2.51	0.44
1:C:4206:GLU:HA	1:C:4211:LYS:HZ2	1.82	0.44
1:C:4763:GLY:O	1:C:4766:THR:OG1	2.26	0.44
1:D:551:LEU:HG	1:D:553:ARG:HH12	1.82	0.44
1:D:650:VAL:O	1:D:777:PHE:N	2.46	0.44
1:D:1078:GLU:HB3	1:D:1237:TRP:CD1	2.53	0.44
1:D:3292:PRO:O	1:D:3294:PRO:HD3	2.18	0.44
1:D:3773:ARG:HD3	1:D:3815:LYS:HZ3	1.82	0.44
1:D:4799:SER:HA	1:D:4812:HIS:HE1	1.82	0.44
1:D:4865:LYS:H	1:D:4873:ASP:HB2	1.82	0.44
1:A:2308:GLN:O	1:A:2323:TRP:HA	2.17	0.44
1:A:3827:GLY:HA2	1:A:3830:GLN:HG2	2.00	0.44
1:B:413:GLN:OE1	1:B:437:PRO:HG2	2.17	0.44
1:B:1283:LEU:HD13	1:B:1506:GLN:OE1	2.18	0.44
1:B:3773:ARG:HD3	1:B:3815:LYS:HZ3	1.83	0.44
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.83	0.44
1:C:632:LEU:HD23	1:C:1666:THR:HG23	1.99	0.44
1:C:3292:PRO:O	1:C:3294:PRO:HD3	2.18	0.44
1:D:1859:VAL:HA	1:D:1862:ILE:HG12	1.99	0.44
1:A:1089:TYR:HD1	1:A:1152:MET:HG2	1.82	0.44
1:A:1459:GLN:H	1:A:1496:TRP:HA	1.81	0.44
1:A:3966:THR:HG22	1:A:4026:MET:HA	2.00	0.44
1:A:4206:GLU:HA	1:A:4211:LYS:HZ2	1.82	0.44
1:A:4808:PHE:O	1:A:4810:ALA:N	2.51	0.44
1:B:1457:TYR:O	1:B:1496:TRP:HB2	2.16	0.44
1:B:2308:GLN:O	1:B:2323:TRP:HA	2.17	0.44
1:B:4779:LYS:O	1:B:4783:ILE:HG12	2.17	0.44
1:B:4807:PHE:O	1:B:4810:ALA:N	2.51	0.44
1:C:1716:ILE:CD1	1:C:1843:LYS:HG2	2.46	0.44
1:C:2242:ILE:HG23	1:C:2242:ILE:O	2.18	0.44
1:C:2667:THR:HA	1:C:2671:GLU:HB2	2.00	0.44
1:C:4658:ILE:HD13	1:C:4792:LEU:HB3	2.00	0.44
1:D:273:HIS:NE2	1:D:337:PRO:HA	2.33	0.44
1:D:1172:ASP:OD1	1:D:1172:ASP:N	2.51	0.44
1:D:1453:VAL:HG23	1:D:1454:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.17	0.44
1:D:2308:GLN:O	1:D:2323:TRP:HA	2.17	0.44
1:D:2380:ILE:O	1:D:2384:ILE:HG12	2.18	0.44
1:D:3827:GLY:HA2	1:D:3830:GLN:HG2	2.00	0.44
1:A:134:ASP:OD1	1:A:134:ASP:N	2.50	0.44
1:A:1466:LEU:HD23	1:A:1466:LEU:HA	1.74	0.44
1:B:714:TYR:HB3	1:B:768:PHE:CE2	2.53	0.44
1:C:1089:TYR:CD1	1:C:1152:MET:HG2	2.51	0.44
1:C:2440:MET:SD	1:C:2440:MET:N	2.91	0.44
1:D:215:THR:OG1	1:D:271:GLY:O	2.30	0.44
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	2.00	0.44
1:D:1283:LEU:HD13	1:D:1506:GLN:OE1	2.18	0.44
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.83	0.44
1:D:4779:LYS:O	1:D:4783:ILE:HG12	2.17	0.44
1:A:520:ASN:O	1:A:524:GLU:HG3	2.18	0.44
1:A:714:TYR:HB3	1:A:768:PHE:CE2	2.53	0.44
1:A:2357:LEU:HB3	1:A:2364:PHE:CZ	2.53	0.44
1:B:721:LEU:HD22	1:B:768:PHE:CZ	2.53	0.44
1:B:1078:GLU:HB3	1:B:1237:TRP:CD1	2.53	0.44
1:B:1246:GLU:OE2	1:B:1601:MET:HG3	2.18	0.44
1:B:1276:THR:OG1	1:B:1466:LEU:HD13	2.17	0.44
1:B:1276:THR:CA	1:B:1466:LEU:HD22	2.45	0.44
1:B:4808:PHE:O	1:B:4810:ALA:N	2.51	0.44
1:C:273:HIS:NE2	1:C:337:PRO:HA	2.33	0.44
1:C:1846:SER:O	1:C:1847:THR:C	2.54	0.44
1:D:1246:GLU:OE2	1:D:1601:MET:HG3	2.18	0.44
1:D:3215:ALA:O	1:D:3218:VAL:HG12	2.18	0.44
1:D:3966:THR:HG22	1:D:4026:MET:HA	2.00	0.44
1:A:1862:ILE:HA	1:A:1865:MET:HG3	1.99	0.43
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.83	0.43
1:A:4779:LYS:O	1:A:4783:ILE:HG12	2.17	0.43
1:A:4816:ILE:HG22	1:A:4817:ALA:N	2.32	0.43
1:A:4939:ALA:O	1:A:4942:GLU:HB2	2.17	0.43
1:B:101:LEU:HD12	1:B:150:MET:HE1	2.00	0.43
1:B:3966:THR:HG22	1:B:4026:MET:HA	2.00	0.43
1:B:5027:CYS:O	1:B:5029:ARG:N	2.50	0.43
1:C:134:ASP:OD1	1:C:134:ASP:N	2.50	0.43
1:C:551:LEU:HG	1:C:553:ARG:HH12	1.82	0.43
1:C:4807:PHE:O	1:C:4808:PHE:C	2.54	0.43
1:D:2202:GLY:HA2	1:D:2204:HIS:CE1	2.53	0.43
1:D:4658:ILE:HD13	1:D:4792:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD11	1:A:191:VAL:HB	1.99	0.43
1:A:3292:PRO:O	1:A:3294:PRO:HD3	2.18	0.43
1:B:134:ASP:N	1:B:134:ASP:OD1	2.50	0.43
1:B:1540:PHE:CE1	1:B:1552:VAL:HG11	2.51	0.43
1:B:2142:TYR:CG	1:B:2197:LEU:HD13	2.52	0.43
1:B:2159:LEU:HD22	1:B:2201:LEU:HD23	2.00	0.43
1:B:4799:SER:HA	1:B:4812:HIS:HE1	1.82	0.43
1:C:2142:TYR:CG	1:C:2197:LEU:HD13	2.52	0.43
1:C:4807:PHE:O	1:C:4810:ALA:N	2.51	0.43
1:D:520:ASN:O	1:D:524:GLU:HG3	2.18	0.43
1:D:2357:LEU:HB3	1:D:2364:PHE:CZ	2.53	0.43
1:D:3725:TYR:HA	1:D:3728:ILE:HG12	2.00	0.43
1:D:4807:PHE:C	1:D:4809:PHE:N	2.68	0.43
1:A:1859:VAL:HA	1:A:1862:ILE:HG12	1.99	0.43
1:A:2202:GLY:HA2	1:A:2204:HIS:CE1	2.53	0.43
1:A:2242:ILE:HG23	1:A:2242:ILE:O	2.18	0.43
1:B:3292:PRO:O	1:B:3294:PRO:HD3	2.18	0.43
1:B:4816:ILE:HG22	1:B:4817:ALA:N	2.32	0.43
1:C:1271:ARG:NH2	1:C:1470:ARG:O	2.45	0.43
1:C:4772:ASP:N	1:C:4772:ASP:OD1	2.51	0.43
1:D:721:LEU:HD22	1:D:768:PHE:CZ	2.53	0.43
1:D:1276:THR:OG1	1:D:1466:LEU:HD13	2.17	0.43
1:A:1078:GLU:HB3	1:A:1237:TRP:CD1	2.53	0.43
1:A:1221:GLU:OE2	1:A:1221:GLU:N	2.52	0.43
1:A:2159:LEU:HD22	1:A:2201:LEU:HD23	2.00	0.43
1:A:2380:ILE:O	1:A:2384:ILE:HG12	2.18	0.43
1:A:2440:MET:N	1:A:2440:MET:SD	2.91	0.43
1:A:3215:ALA:O	1:A:3218:VAL:HG12	2.18	0.43
1:A:3878:ASP:N	1:A:3878:ASP:OD1	2.49	0.43
1:B:1089:TYR:HD1	1:B:1152:MET:HG2	1.82	0.43
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	2.00	0.43
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.17	0.43
1:B:4989:MET:O	1:B:4993:MET:HG3	2.19	0.43
1:C:3966:THR:HG22	1:C:4026:MET:HA	2.00	0.43
1:D:223:PHE:HD1	1:D:230:CYS:HB3	1.84	0.43
1:D:2438:PRO:HB3	1:D:2453:ILE:HB	2.00	0.43
1:D:4089:SER:OG	1:D:4090:LYS:N	2.52	0.43
1:D:4808:PHE:O	1:D:4810:ALA:N	2.51	0.43
1:A:721:LEU:HD22	1:A:768:PHE:CZ	2.53	0.43
1:A:794:GLY:N	1:A:798:GLY:HA3	2.32	0.43
1:A:2204:HIS:O	1:A:2208:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3725:TYR:HA	1:A:3728:ILE:HG12	2.00	0.43
1:B:3827:GLY:HA2	1:B:3830:GLN:HG2	2.00	0.43
1:B:3934:TYR:CE2	1:B:3994:HIS:HE1	2.36	0.43
1:C:1859:VAL:HA	1:C:1862:ILE:HG12	1.99	0.43
1:C:2159:LEU:HD22	1:C:2201:LEU:HD23	2.00	0.43
1:C:3934:TYR:CE2	1:C:3994:HIS:HE1	2.36	0.43
1:C:4717:ASP:OD2	1:C:4723:LYS:NZ	2.50	0.43
1:C:4983:HIS:NE2	1:C:5027:CYS:SG	2.82	0.43
1:D:714:TYR:HB3	1:D:768:PHE:CE2	2.53	0.43
1:D:2204:HIS:O	1:D:2208:MET:HG3	2.19	0.43
1:D:2440:MET:N	1:D:2440:MET:SD	2.91	0.43
1:A:273:HIS:NE2	1:A:337:PRO:HA	2.33	0.43
1:A:1206:GLN:HA	1:A:1227:ALA:O	2.18	0.43
1:A:2271:THR:CG2	1:A:2272:PRO:HD2	2.49	0.43
1:A:4865:LYS:H	1:A:4873:ASP:HB2	1.82	0.43
1:A:5027:CYS:O	1:A:5029:ARG:N	2.50	0.43
1:B:2204:HIS:O	1:B:2208:MET:HG3	2.19	0.43
1:B:2357:LEU:HB3	1:B:2364:PHE:CZ	2.53	0.43
1:B:2380:ILE:O	1:B:2384:ILE:HG12	2.18	0.43
1:C:1830:VAL:C	1:C:1832:GLY:H	2.15	0.43
1:C:4989:MET:O	1:C:4993:MET:HG3	2.19	0.43
1:D:49:LEU:HD11	1:D:191:VAL:HB	1.99	0.43
1:D:1483:VAL:HB	1:D:1575:LEU:HD22	2.00	0.43
1:D:1846:SER:O	1:D:1847:THR:C	2.54	0.43
1:D:4816:ILE:HG22	1:D:4817:ALA:N	2.32	0.43
1:D:4989:MET:O	1:D:4993:MET:HG3	2.19	0.43
1:A:632:LEU:HD23	1:A:1666:THR:HG23	1.99	0.43
1:A:1246:GLU:OE2	1:A:1601:MET:HG3	2.18	0.43
1:A:1607:ARG:NH1	1:A:1610:ASN:OD1	2.52	0.43
1:A:4807:PHE:O	1:A:4810:ALA:N	2.51	0.43
1:B:1607:ARG:NH1	1:B:1610:ASN:OD1	2.52	0.43
1:B:3891:LEU:HD23	1:B:3891:LEU:HA	1.89	0.43
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	2.00	0.43
1:C:1607:ARG:NH1	1:C:1610:ASN:OD1	2.52	0.43
1:C:1653:LEU:HD13	1:C:1660:GLN:HA	2.00	0.43
1:C:1811:ALA:HA	1:C:1814:MET:HE2	2.01	0.43
1:C:3215:ALA:O	1:C:3218:VAL:HG12	2.18	0.43
1:C:3603:LEU:HA	1:C:3607:GLU:OE2	2.19	0.43
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.83	0.43
1:A:223:PHE:HD1	1:A:230:CYS:HB3	1.84	0.43
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3603:LEU:HA	1:A:3607:GLU:OE2	2.19	0.43
1:A:4075:GLU:OE1	1:D:4736:ARG:NH2	2.52	0.43
1:A:4736:ARG:NH2	1:B:4075:GLU:OE1	2.52	0.43
1:B:2271:THR:CG2	1:B:2272:PRO:HD2	2.49	0.43
1:B:2342:ASN:N	1:B:2342:ASN:OD1	2.51	0.43
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.26	0.43
1:C:714:TYR:HB3	1:C:768:PHE:CE2	2.53	0.43
1:C:4736:ARG:NH2	1:D:4075:GLU:OE1	2.52	0.43
1:D:2271:THR:CG2	1:D:2272:PRO:HD2	2.49	0.43
1:D:2339:VAL:O	1:D:2345:SER:OG	2.20	0.43
1:D:4772:ASP:OD1	1:D:4772:ASP:N	2.51	0.43
1:A:101:LEU:HD11	1:A:107:ILE:HD12	1.99	0.43
1:A:645:ARG:HD2	1:A:778:PHE:HD2	1.83	0.43
1:B:635:THR:HG21	1:B:1637:MET:CG	2.49	0.43
1:B:1087:ARG:HG3	1:B:1223:PHE:HA	2.01	0.43
1:B:2202:GLY:HA2	1:B:2204:HIS:CE1	2.53	0.43
1:B:3215:ALA:O	1:B:3218:VAL:HG12	2.18	0.43
1:B:3878:ASP:OD1	1:B:3878:ASP:N	2.49	0.43
1:C:520:ASN:O	1:C:524:GLU:HG3	2.18	0.43
1:C:1246:GLU:OE2	1:C:1601:MET:HG3	2.18	0.43
1:C:2204:HIS:O	1:C:2208:MET:HG3	2.19	0.43
1:C:2210:VAL:O	1:C:2214:VAL:HG13	2.19	0.43
1:C:3827:GLY:HA2	1:C:3830:GLN:HG2	2.00	0.43
1:D:1811:ALA:HA	1:D:1814:MET:HE2	2.00	0.43
1:D:3934:TYR:CE2	1:D:3994:HIS:HE1	2.36	0.43
1:A:1286:MET:N	1:A:1286:MET:SD	2.92	0.43
1:A:3577:ARG:NH2	1:D:1208:VAL:HG23	2.34	0.43
1:C:874:LEU:O	1:C:878:ILE:HG12	2.19	0.43
1:C:1078:GLU:HB3	1:C:1237:TRP:CD1	2.53	0.43
1:C:1096:THR:OG1	1:C:1198:GLN:OE1	2.25	0.43
1:C:1172:ASP:OD1	1:C:1172:ASP:N	2.51	0.43
1:C:1468:LYS:HE2	1:C:1468:LYS:HB3	1.90	0.43
1:C:2357:LEU:HB3	1:C:2364:PHE:CZ	2.53	0.43
1:D:1115:LEU:HD23	1:D:1123:VAL:HG21	2.01	0.43
1:D:3049:LEU:HD12	1:D:3051:ARG:NE	2.34	0.43
1:A:1087:ARG:HG3	1:A:1223:PHE:HA	2.01	0.42
1:A:2296:GLU:HA	1:A:2299:VAL:HG22	2.01	0.42
1:A:2438:PRO:HD3	1:A:2457:LEU:HD22	2.01	0.42
1:A:3934:TYR:CE2	1:A:3994:HIS:HE1	2.36	0.42
1:B:102:LEU:HB2	1:B:105:HIS:HD2	1.83	0.42
1:B:210:GLU:HG3	1:B:337:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HD23	1:B:494:LEU:O	2.19	0.42
1:B:2296:GLU:HA	1:B:2299:VAL:HG22	2.01	0.42
1:B:3049:LEU:HD12	1:B:3051:ARG:NE	2.34	0.42
1:B:3603:LEU:HA	1:B:3607:GLU:OE2	2.19	0.42
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.36	0.42
1:C:223:PHE:HD1	1:C:230:CYS:HB3	1.84	0.42
1:C:2271:THR:CG2	1:C:2272:PRO:HD2	2.49	0.42
1:C:2296:GLU:HA	1:C:2299:VAL:HG22	2.01	0.42
1:C:2342:ASN:OD1	1:C:2342:ASN:N	2.51	0.42
1:D:794:GLY:N	1:D:798:GLY:HA3	2.32	0.42
1:D:873:LYS:O	1:D:877:ASN:ND2	2.44	0.42
1:D:1087:ARG:HG3	1:D:1223:PHE:HA	2.01	0.42
1:D:2112:GLN:O	1:D:2113:SER:OG	2.29	0.42
1:A:148:TRP:CZ3	1:A:173:SER:HB2	2.54	0.42
1:A:650:VAL:O	1:A:777:PHE:N	2.46	0.42
1:A:688:LEU:H	1:A:688:LEU:HD23	1.85	0.42
1:A:1653:LEU:HD13	1:A:1660:GLN:HA	2.00	0.42
1:A:2238:TYR:O	1:A:2242:ILE:HG22	2.20	0.42
1:A:4799:SER:HB2	1:A:4812:HIS:CE1	2.54	0.42
1:B:874:LEU:O	1:B:878:ILE:HG12	2.19	0.42
1:B:4799:SER:HB2	1:B:4812:HIS:CE1	2.54	0.42
1:C:350:HIS:CD2	1:C:352:ALA:H	2.34	0.42
1:C:721:LEU:HD22	1:C:768:PHE:CZ	2.53	0.42
1:C:2438:PRO:HB3	1:C:2453:ILE:HB	2.00	0.42
1:C:4185:GLY:HA3	1:C:5009:TYR:CE2	2.54	0.42
1:D:210:GLU:HG3	1:D:337:PRO:HB3	2.01	0.42
1:D:2159:LEU:HD22	1:D:2201:LEU:HD23	2.00	0.42
1:D:2296:GLU:HA	1:D:2299:VAL:HG22	2.01	0.42
1:D:2438:PRO:HD3	1:D:2457:LEU:HD22	2.01	0.42
1:D:4799:SER:HB2	1:D:4812:HIS:CE1	2.54	0.42
1:A:2167:ILE:HG13	1:A:2168:VAL:N	2.32	0.42
1:A:2438:PRO:HB3	1:A:2453:ILE:HB	2.00	0.42
1:B:551:LEU:O	1:B:553:ARG:NH2	2.52	0.42
1:B:1286:MET:N	1:B:1286:MET:SD	2.92	0.42
1:B:2210:VAL:O	1:B:2214:VAL:HG13	2.19	0.42
1:C:210:GLU:HG3	1:C:337:PRO:HB3	2.01	0.42
1:C:926:GLY:O	1:C:929:LEU:HG	2.19	0.42
1:C:1286:MET:SD	1:C:1286:MET:N	2.92	0.42
1:C:2202:GLY:HA2	1:C:2204:HIS:CE1	2.53	0.42
1:C:2380:ILE:O	1:C:2384:ILE:HG12	2.18	0.42
1:C:2438:PRO:HD3	1:C:2457:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1653:LEU:HD13	1:D:1660:GLN:HA	2.00	0.42
1:D:2646:ASN:O	1:D:2688:HIS:NE2	2.47	0.42
1:A:210:GLU:HG3	1:A:337:PRO:HB3	2.01	0.42
1:A:551:LEU:O	1:A:553:ARG:NH2	2.52	0.42
1:A:874:LEU:O	1:A:878:ILE:HG12	2.19	0.42
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.37	0.42
1:A:2342:ASN:OD1	1:A:2342:ASN:N	2.51	0.42
1:A:3572:GLN:NE2	1:D:1228:ILE:HG13	2.33	0.42
1:A:4089:SER:OG	1:A:4090:LYS:N	2.52	0.42
1:B:1208:VAL:HG23	1:C:3577:ARG:NH2	2.34	0.42
1:B:1221:GLU:OE2	1:B:1221:GLU:N	2.52	0.42
1:C:293:LEU:H	1:C:311:ALA:HB1	1.85	0.42
1:C:494:LEU:O	1:C:494:LEU:HD23	2.19	0.42
1:C:1453:VAL:HG23	1:C:1454:THR:N	2.32	0.42
1:C:1815:LEU:HD23	1:C:1815:LEU:HA	1.86	0.42
1:D:350:HIS:CD2	1:D:352:ALA:H	2.34	0.42
1:D:2210:VAL:O	1:D:2214:VAL:HG13	2.19	0.42
1:A:340:LYS:HB2	1:A:343:GLU:HB3	2.02	0.42
1:A:635:THR:HG21	1:A:1637:MET:CG	2.49	0.42
1:A:3049:LEU:HD12	1:A:3051:ARG:NE	2.34	0.42
1:A:4989:MET:O	1:A:4993:MET:HG3	2.19	0.42
1:B:223:PHE:HD1	1:B:230:CYS:HB3	1.84	0.42
1:B:293:LEU:H	1:B:311:ALA:HB1	1.85	0.42
1:B:650:VAL:O	1:B:777:PHE:N	2.46	0.42
1:B:794:GLY:N	1:B:798:GLY:HA3	2.32	0.42
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.37	0.42
1:B:3946:GLN:OE1	1:B:3949:ARG:NH1	2.53	0.42
1:B:4772:ASP:N	1:B:4772:ASP:OD1	2.51	0.42
1:B:4923:PHE:O	1:B:4928:LEU:HD23	2.20	0.42
1:C:615:ARG:NE	1:C:2168:VAL:HG21	2.35	0.42
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.36	0.42
1:D:874:LEU:O	1:D:878:ILE:HG12	2.19	0.42
1:D:960:MET:HE1	1:D:967:PRO:HD2	2.01	0.42
1:D:1607:ARG:NH1	1:D:1610:ASN:OD1	2.52	0.42
1:D:3946:GLN:OE1	1:D:3949:ARG:NH1	2.53	0.42
1:A:615:ARG:NE	1:A:2168:VAL:HG21	2.35	0.42
1:A:1208:VAL:HG23	1:B:3577:ARG:NH2	2.34	0.42
1:A:1483:VAL:HB	1:A:1575:LEU:HD22	2.00	0.42
1:A:1815:LEU:HD23	1:A:1815:LEU:HA	1.86	0.42
1:A:4923:PHE:O	1:A:4928:LEU:HD23	2.20	0.42
1:B:1483:VAL:HB	1:B:1575:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2438:PRO:HD3	1:B:2457:LEU:HD22	2.01	0.42
1:B:4717:ASP:OD2	1:B:4723:LYS:NZ	2.50	0.42
1:C:1208:VAL:HG23	1:D:3577:ARG:NH2	2.34	0.42
1:C:1221:GLU:OE2	1:C:1221:GLU:N	2.52	0.42
1:C:1483:VAL:HB	1:C:1575:LEU:HD22	2.00	0.42
1:C:1830:VAL:C	1:C:1832:GLY:N	2.71	0.42
1:C:2238:TYR:O	1:C:2242:ILE:HG22	2.20	0.42
1:C:3725:TYR:HA	1:C:3728:ILE:HG12	2.00	0.42
1:C:4089:SER:OG	1:C:4090:LYS:N	2.52	0.42
1:C:4650:HIS:HE2	1:C:4812:HIS:CE1	2.38	0.42
1:C:4811:ALA:C	1:C:4813:LEU:H	2.23	0.42
1:D:340:LYS:HB2	1:D:343:GLU:HB3	2.02	0.42
1:D:721:LEU:N	1:D:728:ARG:O	2.53	0.42
1:D:926:GLY:O	1:D:929:LEU:HG	2.19	0.42
1:D:1286:MET:N	1:D:1286:MET:SD	2.92	0.42
1:D:2248:ARG:HA	1:D:2251:PHE:HB3	2.01	0.42
1:D:4911:LEU:HA	1:D:4914:VAL:HG12	2.02	0.42
1:A:721:LEU:N	1:A:728:ARG:O	2.53	0.42
1:A:926:GLY:O	1:A:929:LEU:HG	2.19	0.42
1:A:1674:CYS:SG	1:A:1718:ILE:HD13	2.60	0.42
1:B:615:ARG:NE	1:B:2168:VAL:HG21	2.35	0.42
1:B:636:ASN:N	1:B:636:ASN:OD1	2.53	0.42
1:B:1053:ILE:HD12	1:B:1053:ILE:HA	1.92	0.42
1:B:1653:LEU:HD13	1:B:1660:GLN:HA	2.00	0.42
1:B:2438:PRO:HB3	1:B:2453:ILE:HB	2.00	0.42
1:B:4185:GLY:HA3	1:B:5009:TYR:CE2	2.54	0.42
1:C:102:LEU:HB2	1:C:105:HIS:HD2	1.83	0.42
1:C:1100:MET:HE3	1:C:1198:GLN:HB3	2.00	0.42
1:C:3049:LEU:HD12	1:C:3051:ARG:NE	2.34	0.42
1:D:3603:LEU:HA	1:D:3607:GLU:OE2	2.19	0.42
1:A:1115:LEU:HD23	1:A:1123:VAL:HG21	2.01	0.42
1:A:2112:GLN:O	1:A:2113:SER:OG	2.29	0.42
1:B:175:SER:C	1:C:2452:ARG:HH22	2.23	0.42
1:B:1271:ARG:NH2	1:B:1470:ARG:O	2.45	0.42
1:C:1269:CYS:SG	1:C:1270:LEU:N	2.93	0.42
1:C:1457:TYR:OH	1:C:1643:GLU:O	2.32	0.42
1:C:4242:ILE:HG13	1:C:4989:MET:CE	2.50	0.42
1:D:1269:CYS:SG	1:D:1270:LEU:N	2.93	0.42
1:D:1276:THR:CA	1:D:1466:LEU:HD22	2.45	0.42
1:D:2342:ASN:OD1	1:D:2342:ASN:N	2.51	0.42
1:A:293:LEU:H	1:A:311:ALA:HB1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2210:VAL:O	1:A:2214:VAL:HG13	2.19	0.42
1:A:4650:HIS:HE2	1:A:4812:HIS:CE1	2.38	0.42
1:A:4888:TYR:CD1	1:D:4914:VAL:HG23	2.55	0.42
1:A:4914:VAL:HG23	1:B:4888:TYR:CD1	2.55	0.42
1:B:148:TRP:CZ3	1:B:173:SER:HB2	2.54	0.42
1:B:571:SER:O	1:B:574:VAL:HG12	2.20	0.42
1:B:2331:TYR:O	1:B:2332:LEU:HB2	2.20	0.42
1:B:3725:TYR:HA	1:B:3728:ILE:HG12	2.00	0.42
1:B:4811:ALA:C	1:B:4813:LEU:H	2.23	0.42
1:C:340:LYS:HB2	1:C:343:GLU:HB3	2.02	0.42
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.37	0.42
1:C:1674:CYS:SG	1:C:1718:ILE:HD13	2.60	0.42
1:C:2138:LEU:HD23	1:C:2138:LEU:HA	1.82	0.42
1:C:2248:ARG:HA	1:C:2251:PHE:HB3	2.01	0.42
1:C:3218:VAL:HG22	1:C:3219:TYR:H	1.85	0.42
1:C:3927:GLN:NE2	1:C:3928:GLU:HG3	2.35	0.42
1:D:102:LEU:HB2	1:D:105:HIS:HD2	1.83	0.42
1:D:2238:TYR:O	1:D:2242:ILE:HG22	2.20	0.42
1:D:3144:PHE:O	1:D:3147:ILE:HG22	2.20	0.42
1:D:3927:GLN:NE2	1:D:3928:GLU:HG3	2.35	0.42
1:D:4185:GLY:HA3	1:D:5009:TYR:CE2	2.54	0.42
1:D:4923:PHE:O	1:D:4928:LEU:HD23	2.20	0.42
1:A:2418:LEU:O	1:A:2422:ILE:HG12	2.20	0.42
1:B:1829:PRO:C	1:B:1830:VAL:O	2.56	0.42
1:B:1846:SER:O	1:B:1847:THR:C	2.54	0.42
1:B:3218:VAL:HG22	1:B:3219:TYR:H	1.85	0.42
1:B:4736:ARG:NH2	1:C:4075:GLU:OE1	2.52	0.42
1:C:721:LEU:N	1:C:728:ARG:O	2.53	0.42
1:C:1829:PRO:C	1:C:1830:VAL:O	2.56	0.42
1:C:3946:GLN:OE1	1:C:3949:ARG:NH1	2.53	0.42
1:D:215:THR:OG1	1:D:272:SER:O	2.38	0.42
1:D:545:ASP:HA	1:D:548:VAL:HG12	2.02	0.42
1:D:636:ASN:N	1:D:636:ASN:OD1	2.53	0.42
1:D:1843:LYS:HE2	1:D:1843:LYS:HB2	1.74	0.42
1:D:4811:ALA:C	1:D:4813:LEU:H	2.23	0.42
1:A:545:ASP:HA	1:A:548:VAL:HG12	2.02	0.41
1:A:3218:VAL:HG22	1:A:3219:TYR:H	1.85	0.41
1:A:4185:GLY:HA3	1:A:5009:TYR:CE2	2.54	0.41
1:B:215:THR:OG1	1:B:272:SER:O	2.38	0.41
1:B:688:LEU:HD23	1:B:688:LEU:H	1.85	0.41
1:B:721:LEU:N	1:B:728:ARG:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:926:GLY:O	1:B:929:LEU:HG	2.19	0.41
1:B:1728:ARG:HA	1:B:1731:LEU:CD1	2.50	0.41
1:B:2248:ARG:HA	1:B:2251:PHE:HB3	2.01	0.41
1:B:4860:ARG:CZ	1:C:4582:VAL:HG11	2.50	0.41
1:B:4914:VAL:HG23	1:C:4888:TYR:CD1	2.55	0.41
1:C:636:ASN:N	1:C:636:ASN:OD1	2.53	0.41
1:C:2331:TYR:O	1:C:2332:LEU:HB2	2.20	0.41
1:C:4799:SER:HB2	1:C:4812:HIS:CE1	2.54	0.41
1:C:4860:ARG:CZ	1:D:4582:VAL:HG11	2.50	0.41
1:D:29:LEU:H	1:D:29:LEU:HD23	1.85	0.41
1:D:494:LEU:O	1:D:494:LEU:HD23	2.19	0.41
1:D:645:ARG:HD2	1:D:778:PHE:HD2	1.83	0.41
1:D:719:LEU:O	1:D:720:HIS:CG	2.73	0.41
1:D:2331:TYR:O	1:D:2332:LEU:HB2	2.20	0.41
1:D:3752:SER:HB3	1:D:3755:GLU:HB2	2.02	0.41
1:D:4650:HIS:HE2	1:D:4812:HIS:CE1	2.38	0.41
1:D:4824:ARG:HA	1:D:4824:ARG:HD2	1.88	0.41
1:A:636:ASN:N	1:A:636:ASN:OD1	2.53	0.41
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.93	0.41
1:A:3144:PHE:O	1:A:3147:ILE:HG22	2.20	0.41
1:A:4911:LEU:HA	1:A:4914:VAL:HG12	2.02	0.41
1:B:340:LYS:HB2	1:B:343:GLU:HB3	2.02	0.41
1:B:579:GLN:H	1:B:582:HIS:CD2	2.38	0.41
1:B:1726:SER:O	1:B:1730:MET:HG2	2.20	0.41
1:B:2418:LEU:O	1:B:2422:ILE:HG12	2.20	0.41
1:B:2583:LEU:H	1:B:2583:LEU:HD23	1.85	0.41
1:B:3752:SER:HB3	1:B:3755:GLU:HB2	2.02	0.41
1:C:215:THR:OG1	1:C:272:SER:O	2.38	0.41
1:C:1087:ARG:HG3	1:C:1223:PHE:HA	2.01	0.41
1:C:3844:LEU:HD22	1:C:3933:PHE:CZ	2.56	0.41
1:C:4911:LEU:HA	1:C:4914:VAL:HG12	2.02	0.41
1:D:148:TRP:CZ3	1:D:173:SER:HB2	2.54	0.41
1:D:551:LEU:O	1:D:553:ARG:NH2	2.52	0.41
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	2.03	0.41
1:D:3218:VAL:HG22	1:D:3219:TYR:H	1.85	0.41
1:A:1053:ILE:HD12	1:A:1053:ILE:HA	1.92	0.41
1:A:1478:ASP:OD1	1:A:1479:GLU:N	2.49	0.41
1:A:1851:MET:HE2	1:A:1851:MET:HB2	1.87	0.41
1:A:3946:GLN:OE1	1:A:3949:ARG:NH1	2.53	0.41
1:A:4052:SER:O	1:A:4056:GLU:HG3	2.21	0.41
1:B:1269:CYS:SG	1:B:1270:LEU:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4052:SER:O	1:B:4056:GLU:HG3	2.21	0.41
1:B:4078:GLN:O	1:B:4081:VAL:HG22	2.21	0.41
1:C:148:TRP:CZ3	1:C:173:SER:HB2	2.54	0.41
1:C:719:LEU:O	1:C:720:HIS:CG	2.73	0.41
1:C:2155:LEU:HD21	1:C:2198:MET:SD	2.60	0.41
1:D:310:LYS:O	1:D:350:HIS:NE2	2.47	0.41
1:D:579:GLN:H	1:D:582:HIS:CD2	2.38	0.41
1:D:1674:CYS:SG	1:D:1718:ILE:HD13	2.60	0.41
1:D:2155:LEU:HD21	1:D:2198:MET:SD	2.60	0.41
1:D:3844:LEU:HD22	1:D:3933:PHE:CZ	2.56	0.41
1:D:5035:GLN:HG3	1:D:5036:LEU:HD23	2.02	0.41
1:A:873:LYS:NZ	1:A:947:GLU:OE1	2.34	0.41
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	2.03	0.41
1:A:1540:PHE:CE1	1:A:1552:VAL:HG11	2.51	0.41
1:A:2552:ARG:NH1	1:A:2556:LEU:HD23	2.36	0.41
1:A:2583:LEU:H	1:A:2583:LEU:HD23	1.85	0.41
1:A:3752:SER:HB3	1:A:3755:GLU:HB2	2.02	0.41
1:A:4582:VAL:HG11	1:D:4860:ARG:CZ	2.50	0.41
1:B:645:ARG:HD2	1:B:778:PHE:HD2	1.83	0.41
1:B:1489:CYS:SG	1:B:1490:SER:N	2.94	0.41
1:B:2238:TYR:O	1:B:2242:ILE:HG22	2.20	0.41
1:B:3717:ASP:OD1	1:B:3717:ASP:N	2.45	0.41
1:B:4650:HIS:HE2	1:B:4812:HIS:CE1	2.38	0.41
1:C:1726:SER:O	1:C:1730:MET:HG2	2.20	0.41
1:C:5035:GLN:HG3	1:C:5036:LEU:HD23	2.02	0.41
1:A:102:LEU:HB2	1:A:105:HIS:HD2	1.83	0.41
1:A:215:THR:OG1	1:A:272:SER:O	2.38	0.41
1:A:494:LEU:O	1:A:494:LEU:HD23	2.19	0.41
1:A:579:GLN:H	1:A:582:HIS:CD2	2.38	0.41
1:A:1457:TYR:OH	1:A:1643:GLU:O	2.32	0.41
1:A:4078:GLN:O	1:A:4081:VAL:HG22	2.21	0.41
1:B:29:LEU:H	1:B:29:LEU:HD23	1.85	0.41
1:B:1115:LEU:HD23	1:B:1123:VAL:HG21	2.01	0.41
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	2.03	0.41
1:B:1773:PRO:HA	1:B:1774:PRO:HD3	1.97	0.41
1:B:2155:LEU:HD21	1:B:2198:MET:SD	2.60	0.41
1:C:1276:THR:CA	1:C:1466:LEU:HD22	2.45	0.41
1:C:2583:LEU:HD23	1:C:2583:LEU:H	1.85	0.41
1:C:3317:GLY:O	1:C:3320:LEU:HG	2.21	0.41
1:D:571:SER:O	1:D:574:VAL:HG12	2.20	0.41
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1489:CYS:SG	1:D:1490:SER:N	2.94	0.41
1:D:1815:LEU:HD23	1:D:1815:LEU:HA	1.86	0.41
1:A:516:LYS:O	1:A:520:ASN:ND2	2.34	0.41
1:A:1811:ALA:HA	1:A:1814:MET:HE2	2.02	0.41
1:A:1851:MET:HE3	1:A:1851:MET:HB3	1.66	0.41
1:A:3927:GLN:NE2	1:A:3928:GLU:HG3	2.35	0.41
1:A:4650:HIS:NE2	1:A:4812:HIS:ND1	2.68	0.41
1:A:4811:ALA:C	1:A:4813:LEU:H	2.23	0.41
1:B:565:TYR:CE1	1:B:569:ILE:HD11	2.56	0.41
1:B:1100:MET:O	1:B:1125:ASN:ND2	2.47	0.41
1:B:1172:ASP:OD1	1:B:1172:ASP:N	2.51	0.41
1:B:2996:LYS:HE3	1:B:2996:LYS:HB2	1.79	0.41
1:B:3144:PHE:O	1:B:3147:ILE:HG22	2.20	0.41
1:B:3186:LEU:HG	1:B:3188:PRO:HD3	2.03	0.41
1:B:3844:LEU:HD22	1:B:3933:PHE:CZ	2.56	0.41
1:B:4206:GLU:HA	1:B:4211:LYS:HZ2	1.85	0.41
1:C:103:TYR:CD1	1:C:163:VAL:HG22	2.56	0.41
1:C:551:LEU:O	1:C:553:ARG:NH2	2.52	0.41
1:C:720:HIS:HB3	1:C:722:TRP:CD1	2.56	0.41
1:C:1851:MET:HE3	1:C:1851:MET:HB3	1.73	0.41
1:C:3186:LEU:HG	1:C:3188:PRO:HD3	2.03	0.41
1:C:4914:VAL:HG23	1:D:4888:TYR:CD1	2.55	0.41
1:C:4923:PHE:O	1:C:4928:LEU:HD23	2.20	0.41
1:D:615:ARG:NE	1:D:2168:VAL:HG21	2.35	0.41
1:D:720:HIS:HB3	1:D:722:TRP:CD1	2.56	0.41
1:D:2583:LEU:HD23	1:D:2583:LEU:H	1.85	0.41
1:D:3317:GLY:O	1:D:3320:LEU:HG	2.21	0.41
1:A:103:TYR:CD1	1:A:163:VAL:HG22	2.56	0.41
1:A:565:TYR:CE1	1:A:569:ILE:HD11	2.56	0.41
1:A:719:LEU:O	1:A:720:HIS:CG	2.73	0.41
1:A:978:THR:HG23	1:A:981:GLN:H	1.86	0.41
1:A:1489:CYS:SG	1:A:1490:SER:N	2.94	0.41
1:B:103:TYR:CD1	1:B:163:VAL:HG22	2.56	0.41
1:B:215:THR:OG1	1:B:271:GLY:O	2.30	0.41
1:B:668:VAL:HG11	1:B:682:LEU:HD21	2.03	0.41
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	2.02	0.41
1:B:1495:VAL:HB	1:B:1537:ASN:HA	2.03	0.41
1:B:1674:CYS:SG	1:B:1718:ILE:HD13	2.60	0.41
1:B:4089:SER:OG	1:B:4090:LYS:N	2.52	0.41
1:B:4792:LEU:HD23	1:B:4792:LEU:HA	1.92	0.41
1:C:29:LEU:HD23	1:C:29:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:VAL:HG11	1:C:682:LEU:HD21	2.03	0.41
1:C:2418:LEU:O	1:C:2422:ILE:HG12	2.20	0.41
1:C:3658:LYS:HD2	1:C:3661:TRP:CZ2	2.56	0.41
1:C:4918:ILE:HD11	1:D:4888:TYR:HA	2.03	0.41
1:D:668:VAL:HG11	1:D:682:LEU:HD21	2.03	0.41
1:A:720:HIS:HB3	1:A:722:TRP:CD1	2.56	0.41
1:A:998:ARG:NH1	1:A:1003:GLN:HG2	2.36	0.41
1:A:2155:LEU:HD21	1:A:2198:MET:SD	2.60	0.41
1:A:4772:ASP:OD1	1:A:4772:ASP:N	2.51	0.41
1:A:5035:GLN:HG3	1:A:5036:LEU:HD23	2.02	0.41
1:B:998:ARG:NH1	1:B:1003:GLN:HG2	2.36	0.41
1:B:3658:LYS:HD2	1:B:3661:TRP:CZ2	2.56	0.41
1:C:175:SER:C	1:D:2452:ARG:HH22	2.23	0.41
1:C:223:PHE:CD1	1:C:230:CYS:HB3	2.56	0.41
1:C:688:LEU:HD23	1:C:688:LEU:H	1.85	0.41
1:C:873:LYS:O	1:C:877:ASN:ND2	2.44	0.41
1:C:2552:ARG:HB3	1:C:2552:ARG:CZ	2.51	0.41
1:C:2552:ARG:NH1	1:C:2556:LEU:HD23	2.36	0.41
1:C:3752:SER:HB3	1:C:3755:GLU:HB2	2.02	0.41
1:D:223:PHE:CD1	1:D:230:CYS:HB3	2.56	0.41
1:D:688:LEU:H	1:D:688:LEU:HD23	1.85	0.41
1:D:1053:ILE:HD12	1:D:1053:ILE:HA	1.92	0.41
1:D:3658:LYS:HD2	1:D:3661:TRP:CZ2	2.56	0.41
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.21	0.41
1:A:960:MET:HE1	1:A:967:PRO:HD2	2.03	0.41
1:A:1271:ARG:NH2	1:A:1470:ARG:O	2.45	0.41
1:A:1495:VAL:HB	1:A:1537:ASN:HA	2.03	0.41
1:A:1726:SER:O	1:A:1730:MET:HG2	2.20	0.41
1:A:2646:ASN:O	1:A:2688:HIS:NE2	2.47	0.41
1:A:3658:LYS:HD2	1:A:3661:TRP:CZ2	2.56	0.41
1:A:4650:HIS:CD2	1:A:4809:PHE:HE1	2.39	0.41
1:A:4973:HIS:CE1	1:D:4227:GLU:HB2	2.56	0.41
1:B:1471:ALA:O	1:B:1472:VAL:C	2.60	0.41
1:B:2128:TYR:CE2	1:B:3673:MET:HG3	2.56	0.41
1:B:2956:ALA:HB3	1:B:3030:HIS:ND1	2.36	0.41
1:B:3049:LEU:HD12	1:B:3051:ARG:HE	1.86	0.41
1:B:3771:HIS:HA	1:B:3773:ARG:NH2	2.36	0.41
1:B:4832:HIS:NE2	1:B:4942:GLU:HG3	2.36	0.41
1:B:4968:PHE:O	1:B:4974:GLY:HA3	2.21	0.41
1:C:571:SER:O	1:C:574:VAL:HG12	2.20	0.41
1:C:579:GLN:H	1:C:582:HIS:CD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1228:ILE:HG13	1:D:3572:GLN:NE2	2.33	0.41
1:C:1489:CYS:SG	1:C:1490:SER:N	2.94	0.41
1:C:1687:SER:HB3	1:C:1782:PHE:CZ	2.56	0.41
1:C:1694:LEU:HD23	1:C:1715:LEU:HB2	2.03	0.41
1:C:3049:LEU:HD12	1:C:3051:ARG:HE	1.86	0.41
1:C:3426:GLU:N	1:C:3427:PRO:HD2	2.36	0.41
1:C:3771:HIS:HA	1:C:3773:ARG:NH2	2.36	0.41
1:C:4052:SER:O	1:C:4056:GLU:HG3	2.21	0.41
1:C:4650:HIS:CD2	1:C:4809:PHE:HE1	2.39	0.41
1:C:4650:HIS:NE2	1:C:4812:HIS:ND1	2.68	0.41
1:C:4666:VAL:HA	1:C:4669:VAL:HG22	2.03	0.41
1:C:4792:LEU:HD23	1:C:4792:LEU:HA	1.92	0.41
1:C:4826:ILE:O	1:C:4829:SER:OG	2.33	0.41
1:D:293:LEU:H	1:D:311:ALA:HB1	1.85	0.41
1:D:1100:MET:HE3	1:D:1198:GLN:HB3	2.01	0.41
1:D:2418:LEU:O	1:D:2422:ILE:HG12	2.20	0.41
1:D:2552:ARG:CZ	1:D:2552:ARG:HB3	2.51	0.41
1:D:4078:GLN:O	1:D:4081:VAL:HG22	2.21	0.41
1:D:4717:ASP:OD2	1:D:4723:LYS:NZ	2.50	0.41
1:A:175:SER:C	1:B:2452:ARG:HH22	2.23	0.41
1:A:571:SER:O	1:A:574:VAL:HG12	2.20	0.41
1:A:635:THR:HG22	1:A:1637:MET:HG3	2.03	0.41
1:A:1830:VAL:HB	1:A:1837:GLN:HG3	2.03	0.41
1:A:2128:TYR:CE2	1:A:3673:MET:HG3	2.56	0.41
1:A:2276:ALA:O	1:A:2279:SER:OG	2.30	0.41
1:A:2331:TYR:O	1:A:2332:LEU:HB2	2.20	0.41
1:A:2956:ALA:HB3	1:A:3030:HIS:ND1	2.36	0.41
1:A:3426:GLU:N	1:A:3427:PRO:HD2	2.36	0.41
1:B:516:LYS:O	1:B:520:ASN:ND2	2.34	0.41
1:B:719:LEU:O	1:B:720:HIS:CG	2.73	0.41
1:B:873:LYS:O	1:B:877:ASN:ND2	2.44	0.41
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	2.03	0.41
1:C:1467:SER:HB2	1:C:1468:LYS:H	1.50	0.41
1:C:4227:GLU:HB2	1:D:4973:HIS:CE1	2.56	0.41
1:D:697:GLY:O	1:D:704:GLY:N	2.54	0.41
1:D:878:ILE:O	1:D:881:LEU:HB2	2.21	0.41
1:A:223:PHE:CD1	1:A:230:CYS:HB3	2.56	0.40
1:A:4666:VAL:HA	1:A:4669:VAL:HG22	2.03	0.40
1:B:1457:TYR:OH	1:B:1643:GLU:O	2.32	0.40
1:B:1634:LEU:HD12	1:B:1634:LEU:HA	1.93	0.40
1:B:1687:SER:HB3	1:B:1782:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4666:VAL:HA	1:B:4669:VAL:HG22	2.03	0.40
1:B:5035:GLN:HG3	1:B:5036:LEU:HD23	2.02	0.40
1:C:2277:ALA:HA	1:C:2280:VAL:HG12	2.03	0.40
1:C:3144:PHE:O	1:C:3147:ILE:HG22	2.20	0.40
1:C:4832:HIS:NE2	1:C:4942:GLU:HG3	2.36	0.40
1:D:565:TYR:CE1	1:D:569:ILE:HD11	2.56	0.40
1:D:992:GLY:HA2	1:D:995:VAL:HG22	2.03	0.40
1:D:998:ARG:NH1	1:D:1003:GLN:HG2	2.36	0.40
1:D:1009:ALA:HA	1:D:1020:ARG:HD3	2.03	0.40
1:D:1694:LEU:HD23	1:D:1715:LEU:HB2	2.03	0.40
1:D:1726:SER:O	1:D:1730:MET:HG2	2.20	0.40
1:D:1830:VAL:HB	1:D:1837:GLN:HG3	2.03	0.40
1:D:2552:ARG:NH1	1:D:2556:LEU:HD23	2.36	0.40
1:D:3771:HIS:HA	1:D:3773:ARG:NH2	2.36	0.40
1:A:881:LEU:HD23	1:A:881:LEU:HA	1.92	0.40
1:A:1009:ALA:HA	1:A:1020:ARG:HD3	2.03	0.40
1:A:1269:CYS:SG	1:A:1270:LEU:N	2.93	0.40
1:A:1471:ALA:O	1:A:1472:VAL:C	2.60	0.40
1:A:4832:HIS:NE2	1:A:4942:GLU:HG3	2.36	0.40
1:A:4860:ARG:CZ	1:B:4582:VAL:HG11	2.50	0.40
1:A:4888:TYR:HA	1:D:4918:ILE:HD11	2.03	0.40
1:A:4983:HIS:NE2	1:A:5027:CYS:SG	2.82	0.40
1:B:545:ASP:HA	1:B:548:VAL:HG12	2.02	0.40
1:B:575:LEU:HD22	1:B:606:LEU:HD12	2.04	0.40
1:B:720:HIS:HB3	1:B:722:TRP:CD1	2.56	0.40
1:B:1286:MET:HB2	1:B:1600:LEU:HD22	2.03	0.40
1:B:1762:LEU:O	1:B:1765:VAL:HG22	2.22	0.40
1:B:3927:GLN:NE2	1:B:3928:GLU:HG3	2.35	0.40
1:B:4075:GLU:HA	1:B:4078:GLN:CB	2.51	0.40
1:B:4650:HIS:NE2	1:B:4812:HIS:ND1	2.68	0.40
1:C:635:THR:HG21	1:C:1637:MET:CG	2.49	0.40
1:C:650:VAL:O	1:C:777:PHE:N	2.46	0.40
1:C:1115:LEU:HD23	1:C:1123:VAL:HG21	2.01	0.40
1:C:1286:MET:HB2	1:C:1600:LEU:HD22	2.03	0.40
1:C:2956:ALA:HB3	1:C:3030:HIS:ND1	2.36	0.40
1:D:1687:SER:HB3	1:D:1782:PHE:CZ	2.56	0.40
1:D:2277:ALA:HA	1:D:2280:VAL:HG12	2.03	0.40
1:D:3426:GLU:N	1:D:3427:PRO:HD2	2.36	0.40
1:D:4000:MET:CE	1:D:4058:ILE:HG12	2.51	0.40
1:D:4052:SER:O	1:D:4056:GLU:HG3	2.21	0.40
1:D:4650:HIS:CD2	1:D:4809:PHE:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.36	0.40
1:A:29:LEU:HD23	1:A:29:LEU:H	1.85	0.40
1:A:1172:ASP:OD1	1:A:1172:ASP:N	2.51	0.40
1:A:1687:SER:HB3	1:A:1782:PHE:CZ	2.56	0.40
1:A:2211:MET:O	1:A:2214:VAL:HG22	2.22	0.40
1:A:3049:LEU:HD12	1:A:3051:ARG:HE	1.86	0.40
1:A:3157:ILE:HA	1:A:3160:ASP:OD1	2.22	0.40
1:A:3771:HIS:HA	1:A:3773:ARG:NH2	2.36	0.40
1:B:350:HIS:CD2	1:B:352:ALA:H	2.34	0.40
1:B:697:GLY:O	1:B:704:GLY:N	2.54	0.40
1:B:998:ARG:NH2	1:B:1004:GLY:HA2	2.37	0.40
1:B:2552:ARG:NH1	1:B:2556:LEU:HD23	2.36	0.40
1:B:4911:LEU:HA	1:B:4914:VAL:HG12	2.02	0.40
1:C:565:TYR:CE1	1:C:569:ILE:HD11	2.56	0.40
1:C:2155:LEU:HD12	1:C:2185:ILE:HG22	2.03	0.40
1:C:3941:ASP:OD1	1:C:3941:ASP:N	2.45	0.40
1:D:978:THR:HG23	1:D:981:GLN:H	1.86	0.40
1:D:1221:GLU:OE2	1:D:1221:GLU:N	2.52	0.40
1:D:3891:LEU:HD22	1:D:3899:PHE:CE2	2.57	0.40
1:A:1728:ARG:HA	1:A:1731:LEU:CD1	2.50	0.40
1:A:1762:LEU:O	1:A:1765:VAL:HG22	2.22	0.40
1:A:2248:ARG:HA	1:A:2251:PHE:HB3	2.01	0.40
1:A:3518:LEU:HB2	1:A:3519:PRO:HD3	2.04	0.40
1:A:3844:LEU:HD22	1:A:3933:PHE:CZ	2.56	0.40
1:B:1009:ALA:HA	1:B:1020:ARG:HD3	2.03	0.40
1:B:1845:VAL:HG13	1:B:1846:SER:N	2.37	0.40
1:B:2211:MET:O	1:B:2214:VAL:HG22	2.22	0.40
1:C:878:ILE:O	1:C:881:LEU:HB2	2.21	0.40
1:C:1851:MET:HE2	1:C:1851:MET:HB2	1.79	0.40
1:C:4078:GLN:O	1:C:4081:VAL:HG22	2.21	0.40
1:D:575:LEU:HD22	1:D:606:LEU:HD12	2.04	0.40
1:D:1269:CYS:HG	1:D:1471:ALA:HB1	1.86	0.40
1:D:4787:ASN:OD1	1:D:4787:ASN:N	2.55	0.40
1:D:4832:HIS:NE2	1:D:4942:GLU:HG3	2.36	0.40
1:A:1829:PRO:C	1:A:1830:VAL:O	2.56	0.40
1:A:4000:MET:CE	1:A:4058:ILE:HG12	2.51	0.40
1:A:4696:ASP:OD1	1:A:4696:ASP:N	2.46	0.40
1:B:292:ALA:HA	1:B:311:ALA:O	2.22	0.40
1:B:2336:ARG:O	1:B:2340:PHE:CB	2.66	0.40
1:B:3518:LEU:HB2	1:B:3519:PRO:HD3	2.04	0.40
1:B:4650:HIS:CD2	1:B:4809:PHE:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ILE:HG13	1:C:416:LYS:N	2.37	0.40
1:C:575:LEU:HD22	1:C:606:LEU:HD12	2.04	0.40
1:C:2211:MET:O	1:C:2214:VAL:HG22	2.22	0.40
1:C:4000:MET:CE	1:C:4058:ILE:HG12	2.51	0.40
1:D:2128:TYR:CE2	1:D:3673:MET:HG3	2.56	0.40
1:D:2155:LEU:HD12	1:D:2185:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	B	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	C	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	D	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
All	All	15624/20148 (78%)	14052 (90%)	1504 (10%)	68 (0%)	32	60

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1469	VAL
1	A	1470	ARG
1	A	1472	VAL
1	A	1836	PHE
1	B	1469	VAL
1	B	1470	ARG
1	B	1472	VAL
1	B	1836	PHE
1	C	1469	VAL

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Mol	Chain	Res	Type
1	C	1470	ARG
1	C	1472	VAL
1	C	1836	PHE
1	D	1469	VAL
1	D	1470	ARG
1	D	1472	VAL
1	D	1836	PHE
1	A	1467	SER
1	A	1471	ALA
1	A	1831	GLY
1	A	4806	ASN
1	A	4807	PHE
1	A	4812	HIS
1	A	4815	ASP
1	A	4818	MET
1	B	1467	SER
1	B	1471	ALA
1	B	1831	GLY
1	B	4806	ASN
1	B	4807	PHE
1	B	4812	HIS
1	B	4815	ASP
1	B	4818	MET
1	C	1467	SER
1	C	1471	ALA
1	C	1831	GLY
1	C	4806	ASN
1	C	4807	PHE
1	C	4812	HIS
1	C	4815	ASP
1	C	4818	MET
1	D	1467	SER
1	D	1471	ALA
1	D	1831	GLY
1	D	4806	ASN
1	D	4807	PHE
1	D	4812	HIS
1	D	4815	ASP
1	D	4818	MET
1	A	4805	ASN
1	A	4809	PHE
1	B	4805	ASN

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Mol	Chain	Res	Type
1	B	4809	PHE
1	C	4805	ASN
1	C	4809	PHE
1	D	4805	ASN
1	D	4809	PHE
1	A	4819	GLY
1	B	4819	GLY
1	C	4819	GLY
1	D	4819	GLY
1	A	1466	LEU
1	B	1466	LEU
1	C	1466	LEU
1	D	1466	LEU
1	A	1830	VAL
1	B	1830	VAL
1	C	1830	VAL
1	D	1830	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	B	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	C	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	D	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
All	All	11540/17104 (68%)	11460 (99%)	80 (1%)	80	88

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	GLU
1	A	426	ARG
1	A	921	ASN
1	A	976	ARG

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Mol	Chain	Res	Type
1	A	1467	SER
1	A	1468	LYS
1	A	1469	VAL
1	A	1473	THR
1	A	1797	ARG
1	A	1838	PHE
1	A	1841	VAL
1	A	1843	LYS
1	A	1846	SER
1	A	3773	ARG
1	A	4804	TYR
1	A	4806	ASN
1	A	4807	PHE
1	A	4813	LEU
1	A	4816	ILE
1	A	4818	MET
1	B	338	GLU
1	B	426	ARG
1	B	921	ASN
1	B	976	ARG
1	B	1467	SER
1	B	1468	LYS
1	B	1469	VAL
1	B	1473	THR
1	B	1797	ARG
1	B	1838	PHE
1	B	1841	VAL
1	B	1843	LYS
1	B	1846	SER
1	B	3773	ARG
1	B	4804	TYR
1	B	4806	ASN
1	B	4807	PHE
1	B	4813	LEU
1	B	4816	ILE
1	B	4818	MET
1	C	338	GLU
1	C	426	ARG
1	C	921	ASN
1	C	976	ARG
1	C	1467	SER
1	C	1468	LYS

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Mol	Chain	Res	Type
1	C	1469	VAL
1	C	1473	THR
1	C	1797	ARG
1	C	1838	PHE
1	C	1841	VAL
1	C	1843	LYS
1	C	1846	SER
1	C	3773	ARG
1	C	4804	TYR
1	C	4806	ASN
1	C	4807	PHE
1	C	4813	LEU
1	C	4816	ILE
1	C	4818	MET
1	D	338	GLU
1	D	426	ARG
1	D	921	ASN
1	D	976	ARG
1	D	1467	SER
1	D	1468	LYS
1	D	1469	VAL
1	D	1473	THR
1	D	1797	ARG
1	D	1838	PHE
1	D	1841	VAL
1	D	1843	LYS
1	D	1846	SER
1	D	3773	ARG
1	D	4804	TYR
1	D	4806	ASN
1	D	4807	PHE
1	D	4813	LEU
1	D	4816	ILE
1	D	4818	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	HIS
1	A	582	HIS
1	A	1505	GLN
1	A	1563	GLN

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Mol	Chain	Res	Type
1	A	2127	GLN
1	A	2184	ASN
1	A	2551	ASN
1	A	3430	ASN
1	A	3572	GLN
1	A	3643	ASN
1	A	3809	ASN
1	A	3994	HIS
1	A	3998	HIS
1	A	4094	GLN
1	A	4201	ASN
1	A	4754	ASN
1	B	273	HIS
1	B	582	HIS
1	B	1505	GLN
1	B	2127	GLN
1	B	2184	ASN
1	B	2551	ASN
1	B	3572	GLN
1	B	3643	ASN
1	B	3809	ASN
1	B	3994	HIS
1	B	3998	HIS
1	B	4094	GLN
1	B	4201	ASN
1	B	4754	ASN
1	C	582	HIS
1	C	1505	GLN
1	C	2127	GLN
1	C	2184	ASN
1	C	2551	ASN
1	C	3572	GLN
1	C	3643	ASN
1	C	3809	ASN
1	C	3994	HIS
1	C	3998	HIS
1	C	4094	GLN
1	C	4201	ASN
1	C	4754	ASN
1	D	582	HIS
1	D	1505	GLN
1	D	1563	GLN

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Mol	Chain	Res	Type
1	D	2127	GLN
1	D	2184	ASN
1	D	2551	ASN
1	D	3430	ASN
1	D	3572	GLN
1	D	3643	ASN
1	D	3809	ASN
1	D	3994	HIS
1	D	3998	HIS
1	D	4094	GLN
1	D	4201	ASN
1	D	4754	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

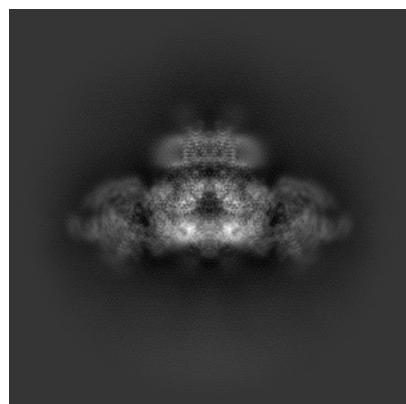
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38043. These allow visual inspection of the internal detail of the map and identification of artifacts.

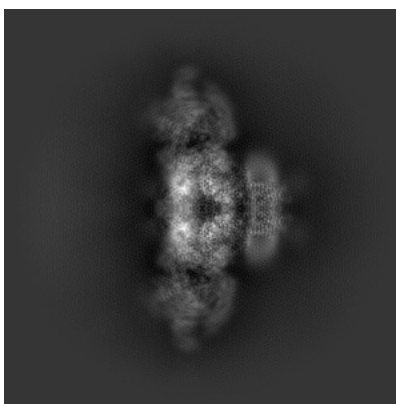
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

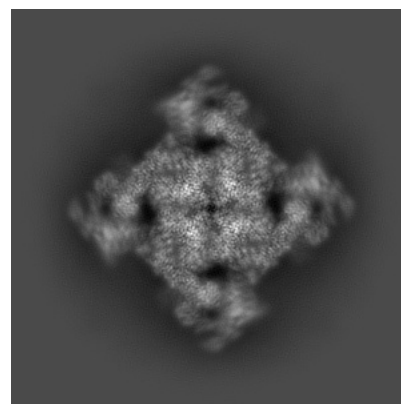
#### 6.1.1 Primary map



X

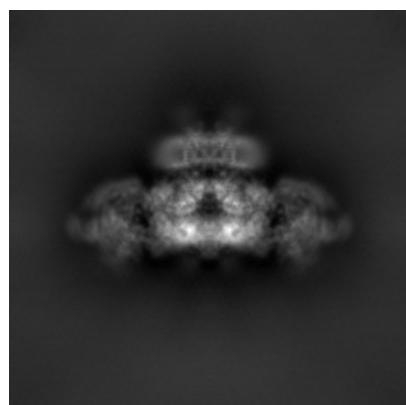


Y

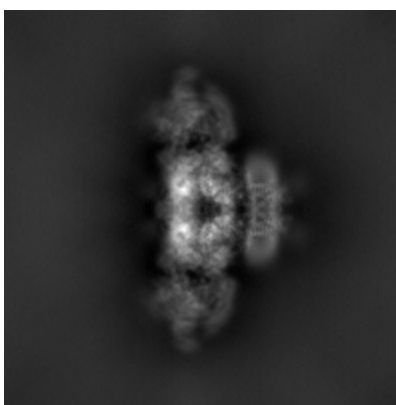


Z

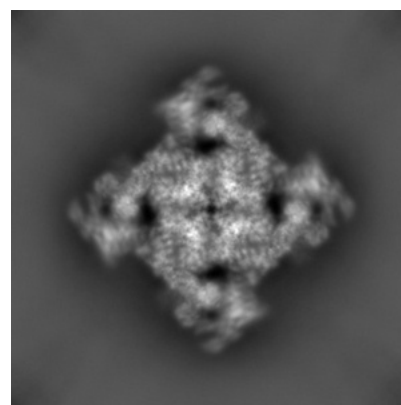
#### 6.1.2 Raw map



X



Y

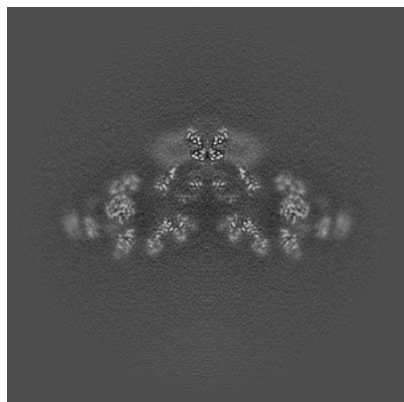


Z

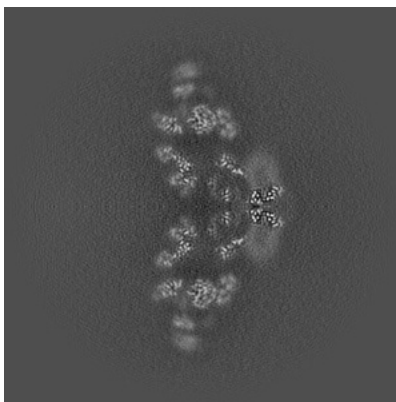
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

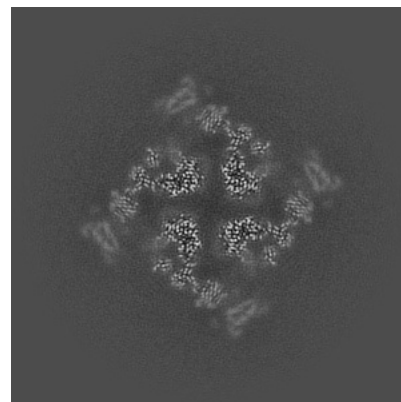
### 6.2.1 Primary map



X Index: 240

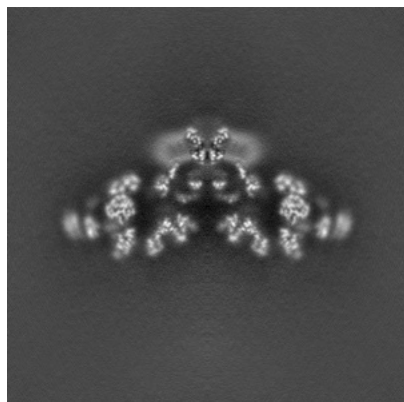


Y Index: 240

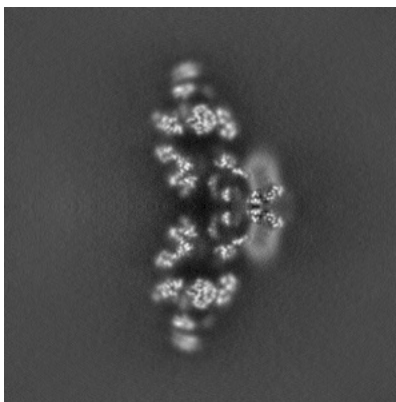


Z Index: 240

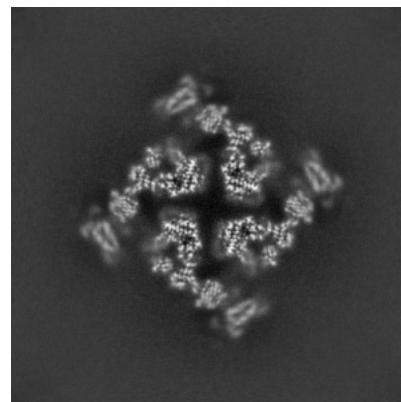
### 6.2.2 Raw map



X Index: 240



Y Index: 240

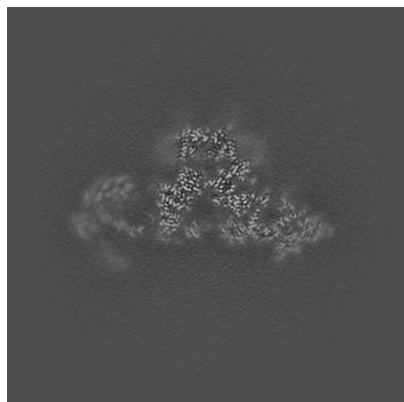


Z Index: 240

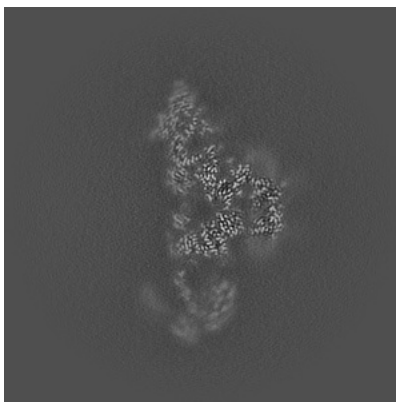
The images above show central slices of the map in three orthogonal directions.

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

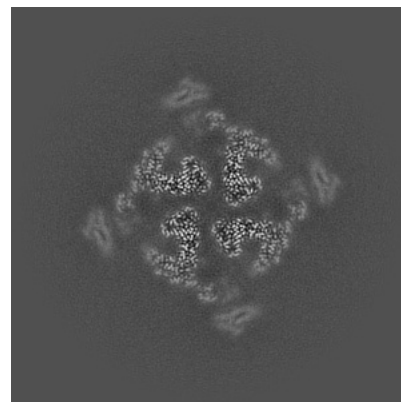
### 6.3.1 Primary map



X Index: 259

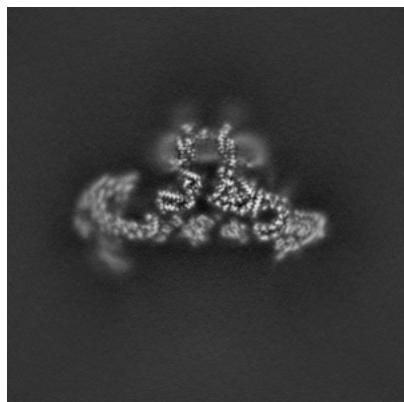


Y Index: 221

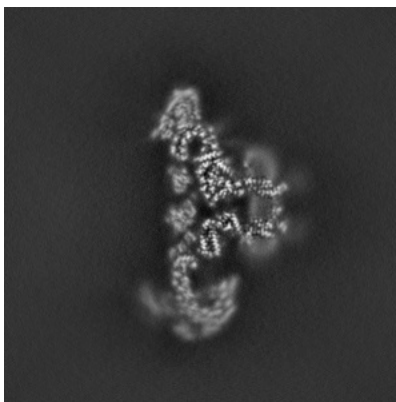


Z Index: 248

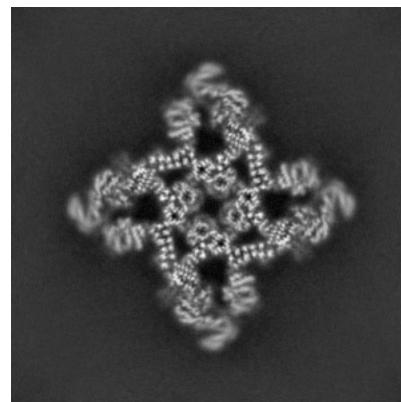
### 6.3.2 Raw map



X Index: 265



Y Index: 215

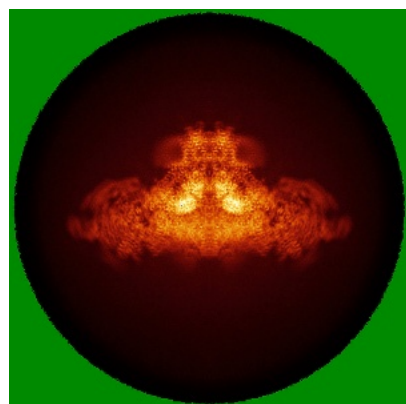


Z Index: 218

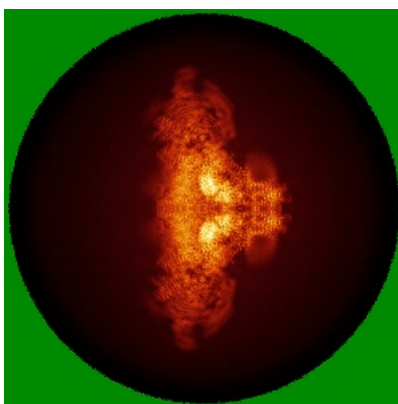
The images above show the largest variance slices of the map in three orthogonal directions.

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

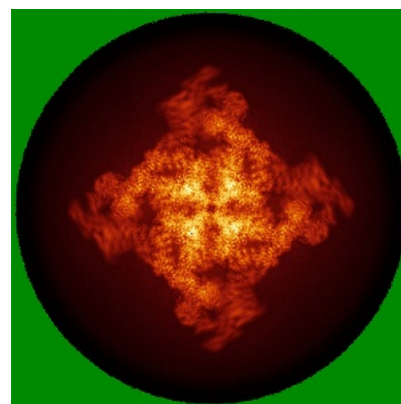
### 6.4.1 Primary map



X

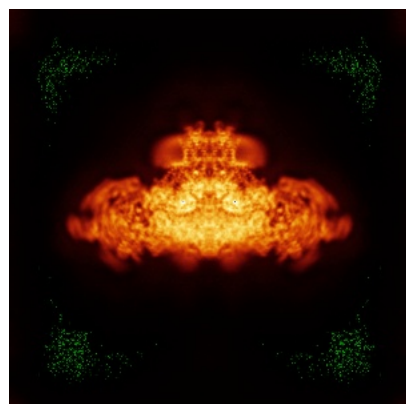


Y

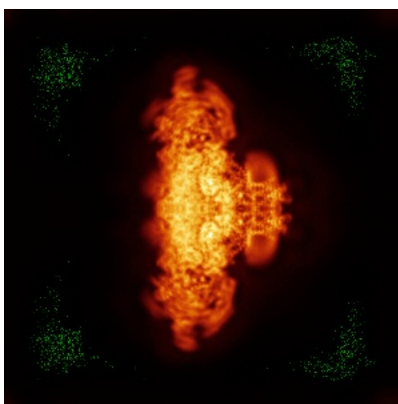


Z

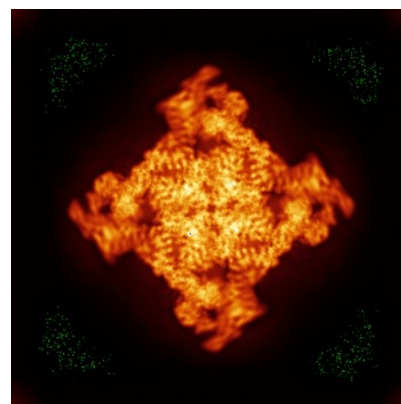
### 6.4.2 Raw map



X



Y



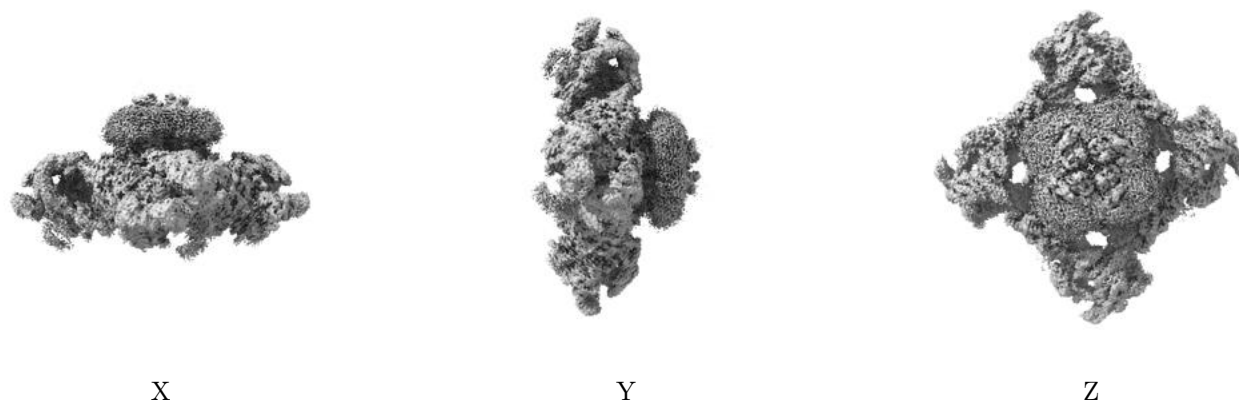
Z

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.



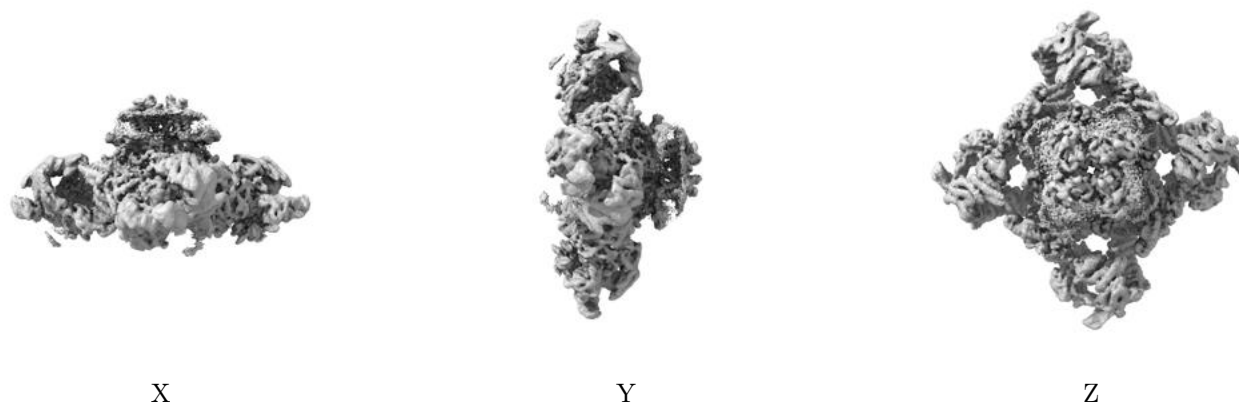
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.466. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

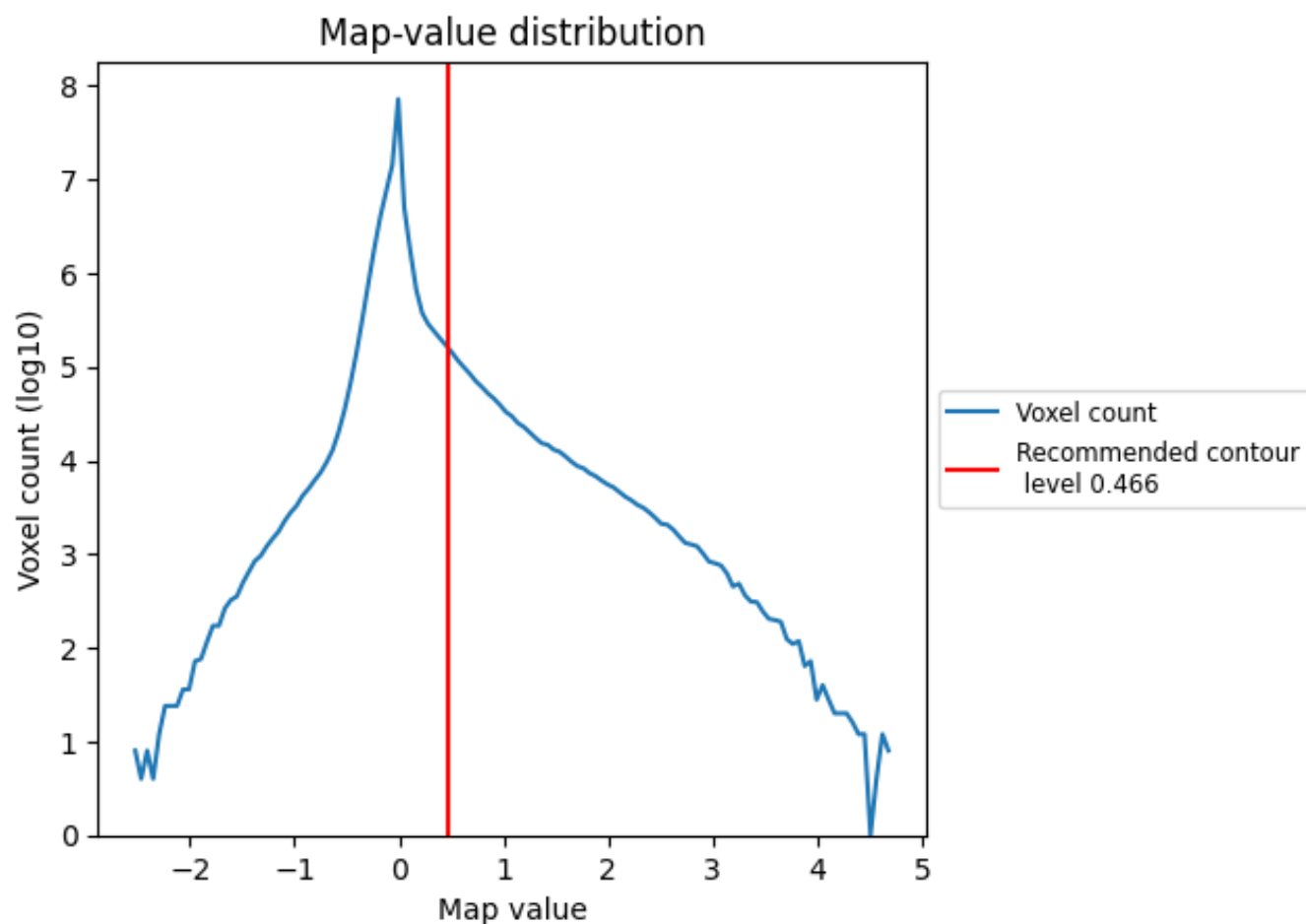
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

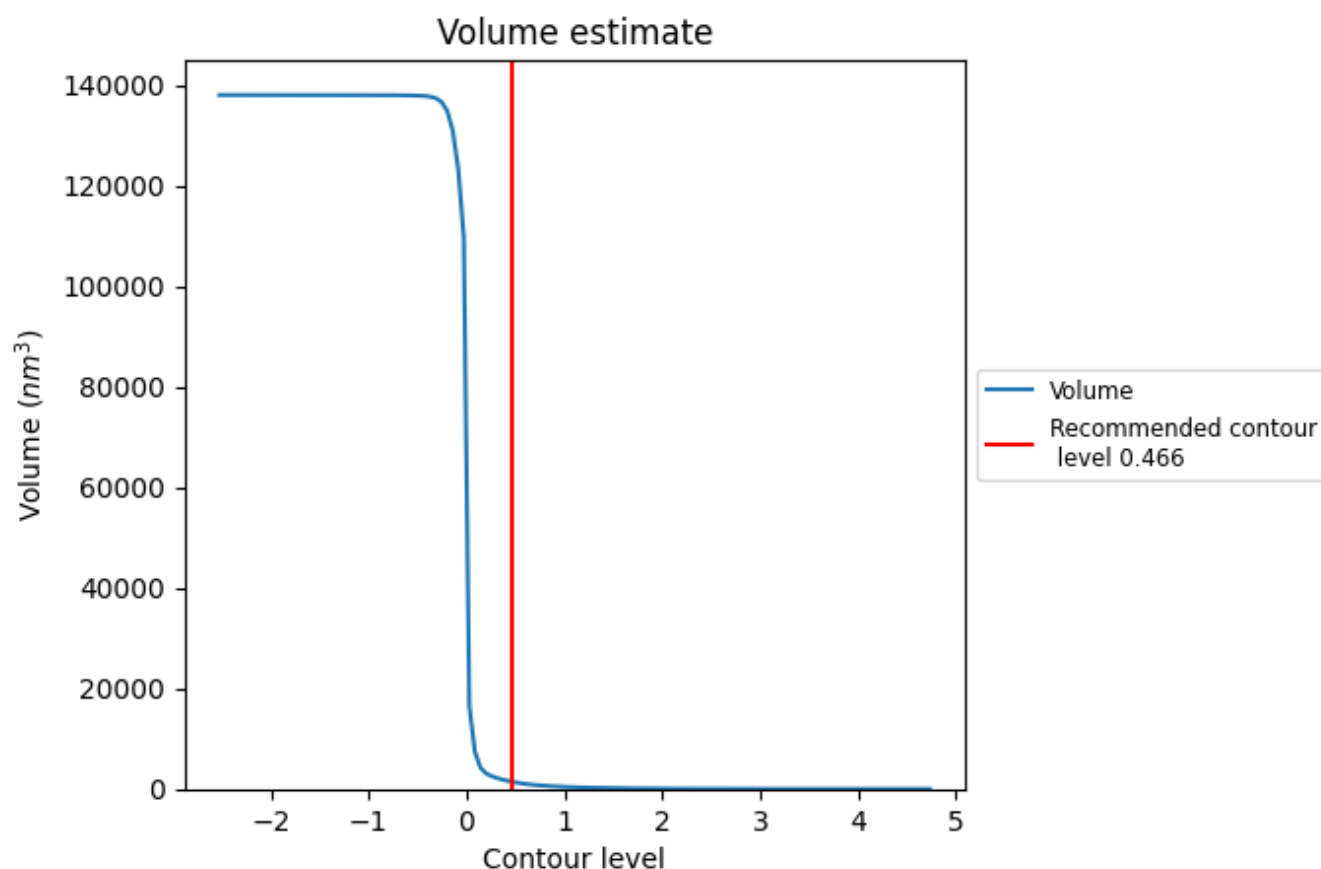
This section contains the results of statistical analysis of the map.

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



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

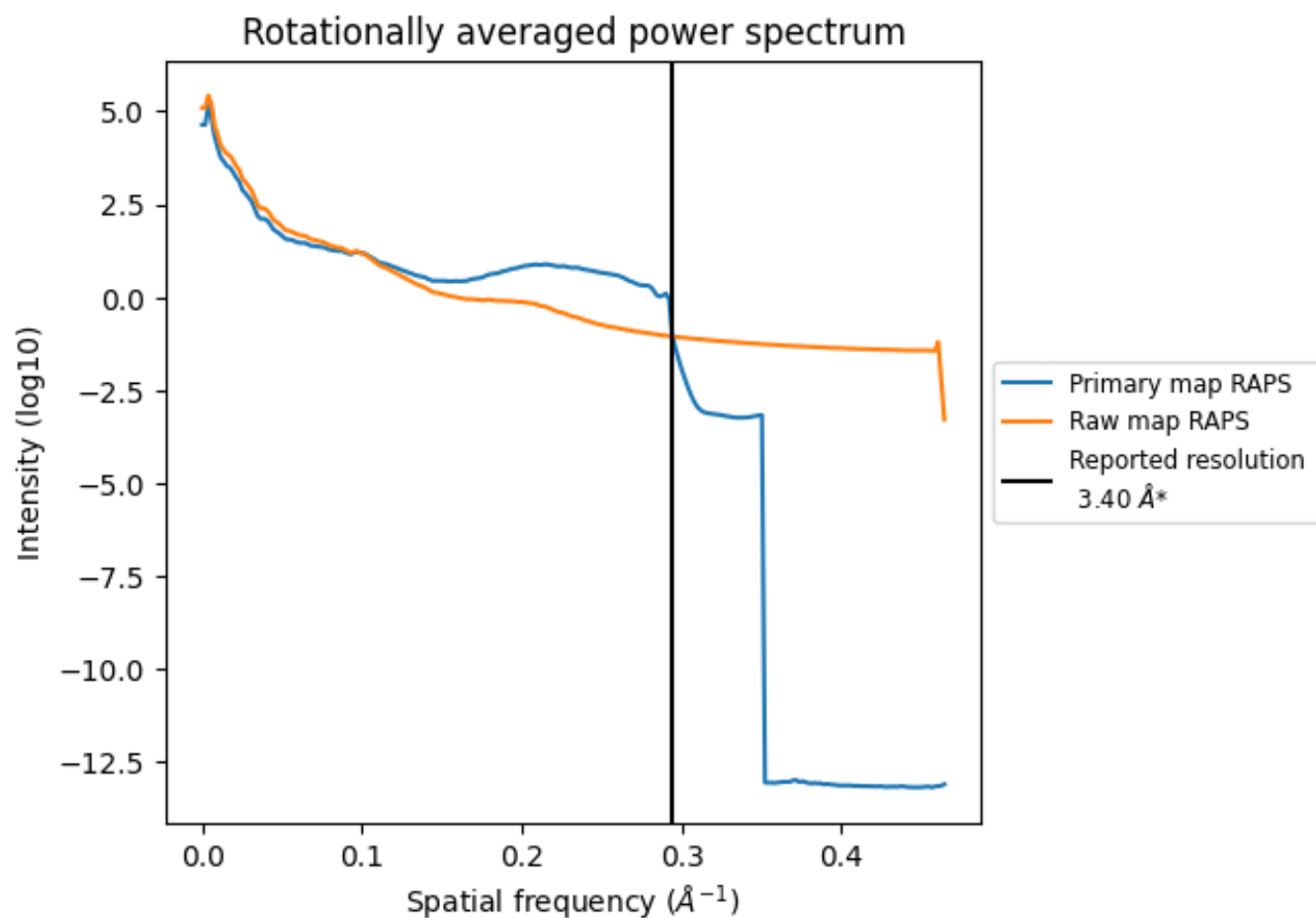
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1425  $\text{nm}^3$ ; this corresponds to an approximate mass of 1287 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 ⓘ

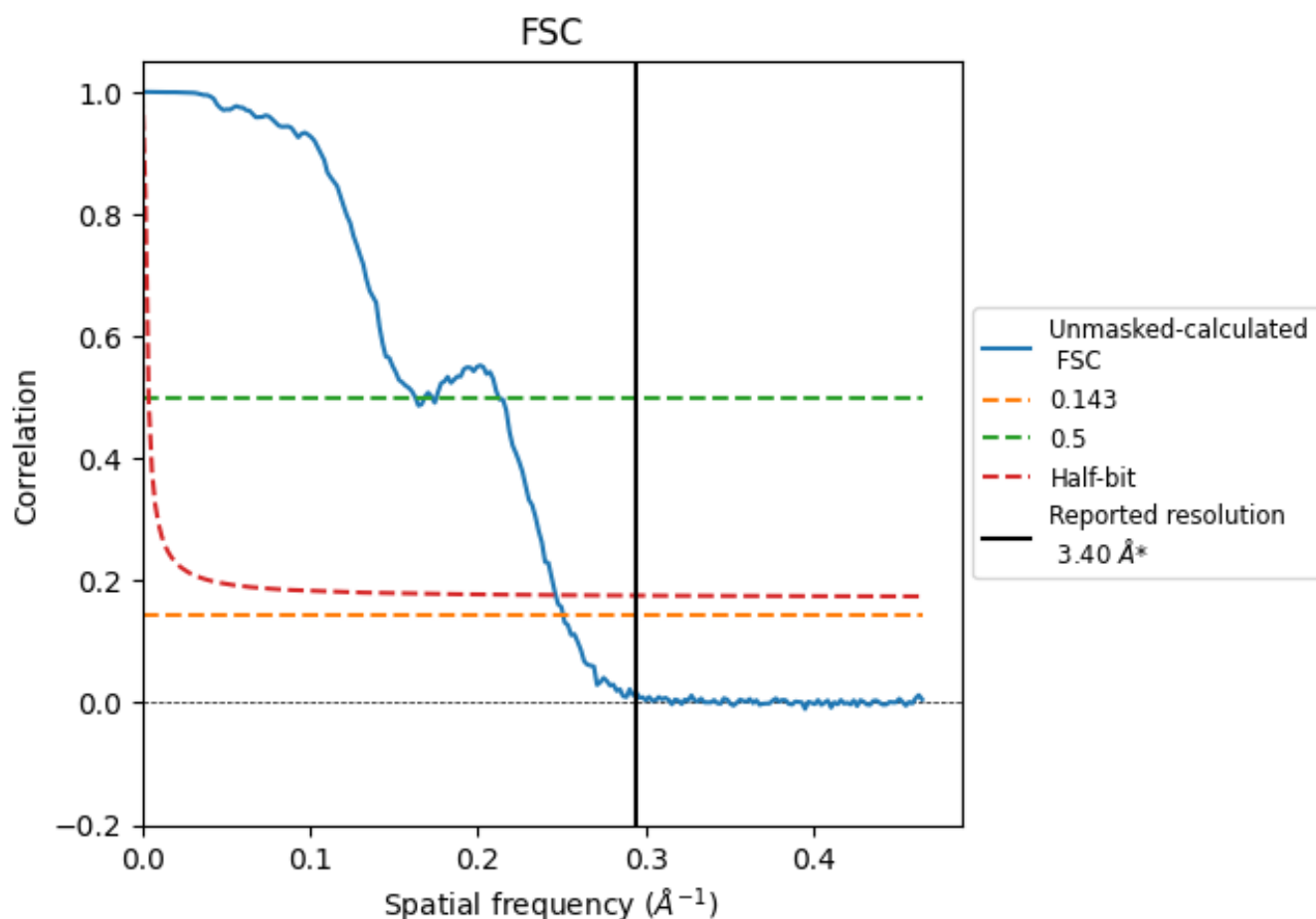


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

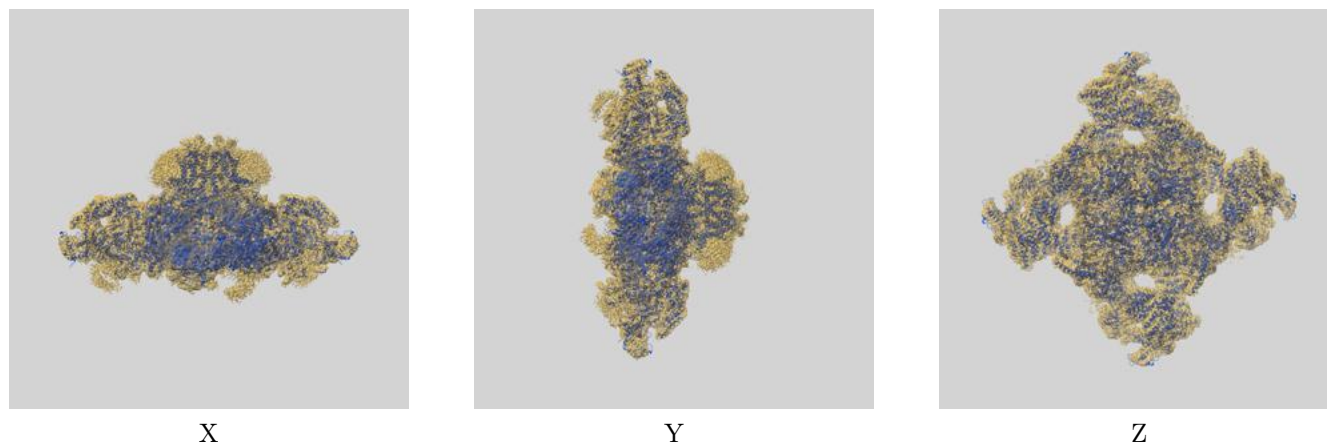
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	6.15	4.06

\*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 3.99 differs from the reported value 3.4 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-38043 and PDB model 8X49. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

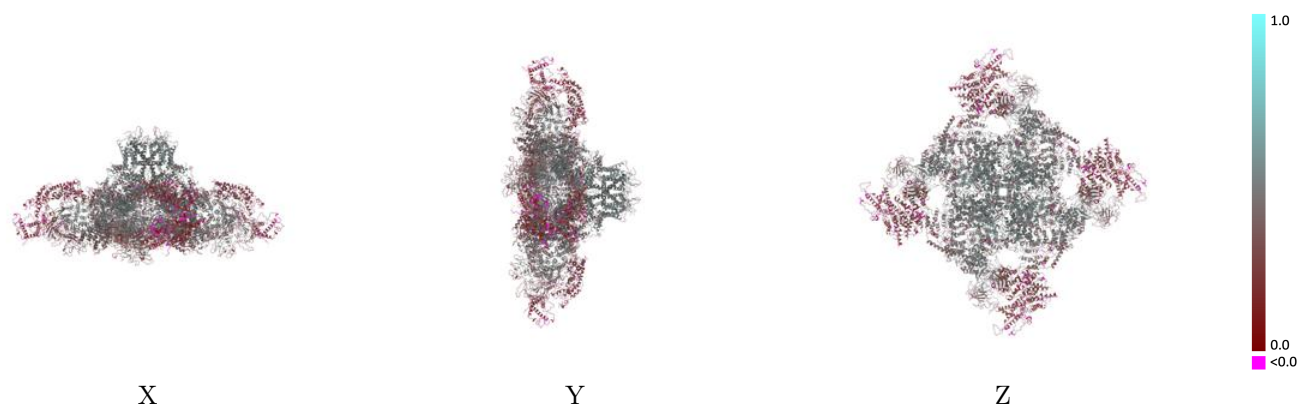
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.466 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.

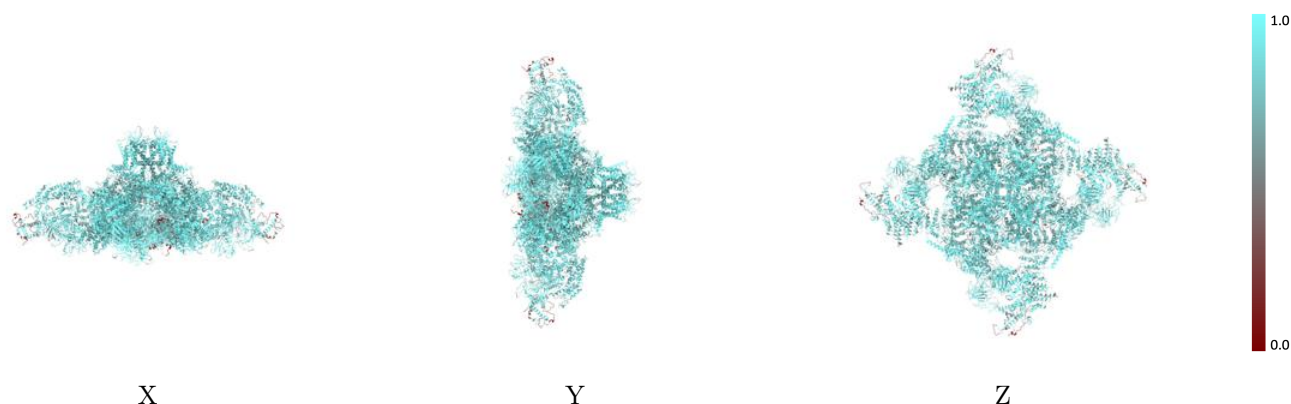


## 9.2 Q-score mapped to coordinate model [i](#)



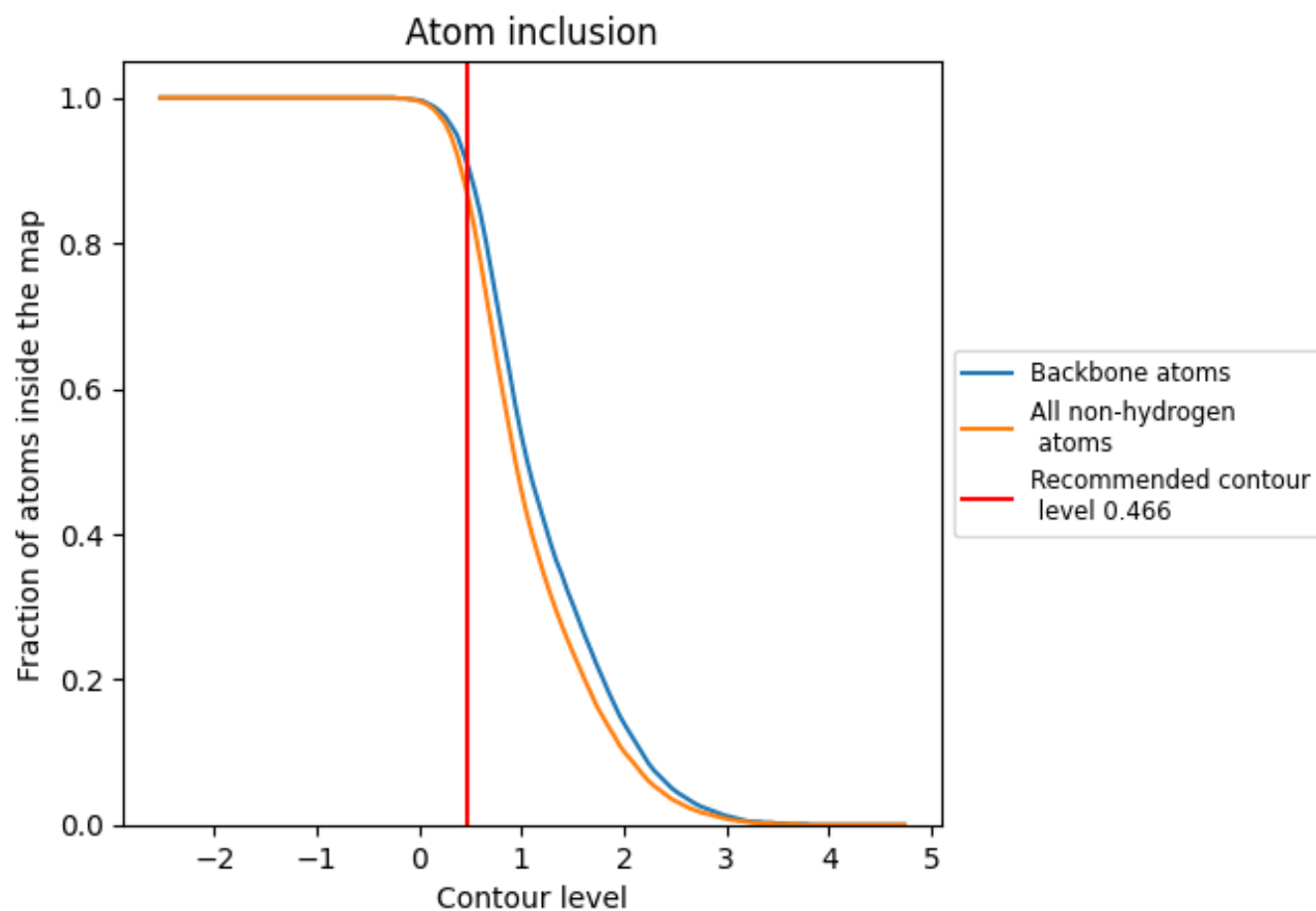
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.466).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.466) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8710	<div></div> 0.3900
A	<div></div> 0.8710	<div></div> 0.3900
B	<div></div> 0.8710	<div></div> 0.3900
C	<div></div> 0.8710	<div></div> 0.3900
D	<div></div> 0.8710	<div></div> 0.3900

