



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:46 AM UTC

PDB ID : 8DTY / pdb_00008dty
EMDB ID : EMD-27711
Title : Recombinant mouse RyR2 triple phosphomimetic mutant
S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc under closed-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on : 2022-07-26
Resolution : 3.50 Å (reported)
Based on initial model : 6WOU

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

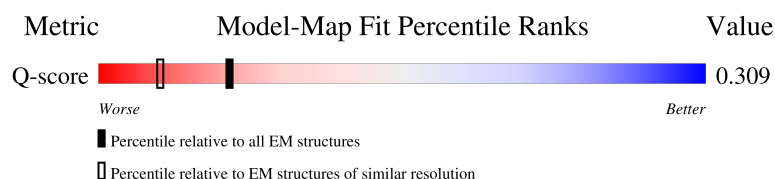
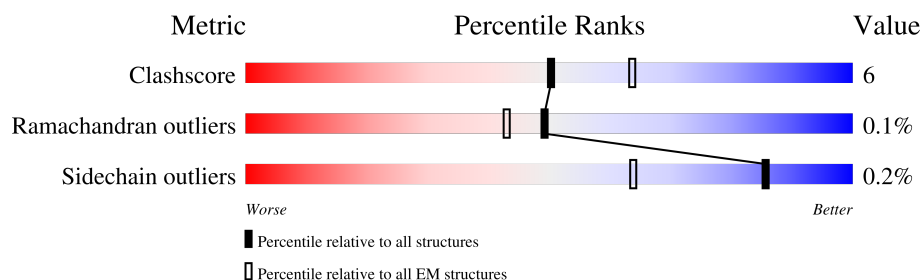
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



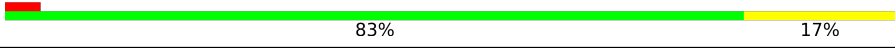
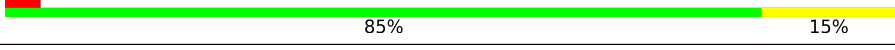
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	4966	19% 69% 11% 19%
1	B	4966	19% 69% 11% 19%
1	C	4966	19% 69% 11% 19%
1	D	4966	19% 69% 11% 19%

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Mol	Chain	Length	Quality of chain
2	E	107	 85%15%
2	F	107	 85%15%
2	G	107	 83%17%
2	H	107	 85%15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 128772 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4004	Total	C	N	O	S	0	0
			31374	19934	5355	5887	198		
1	B	4004	Total	C	N	O	S	0	0
			31374	19934	5355	5887	198		
1	C	4004	Total	C	N	O	S	0	0
			31374	19934	5355	5887	198		
1	D	4004	Total	C	N	O	S	0	0
			31374	19934	5355	5887	198		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ASP	SER	engineered mutation	UNP E9Q401
A	2807	ASP	SER	engineered mutation	UNP E9Q401
A	2813	ASP	SER	engineered mutation	UNP E9Q401
B	2030	ASP	SER	engineered mutation	UNP E9Q401
B	2807	ASP	SER	engineered mutation	UNP E9Q401
B	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2030	ASP	SER	engineered mutation	UNP E9Q401
C	2807	ASP	SER	engineered mutation	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
D	2030	ASP	SER	engineered mutation	UNP E9Q401
D	2807	ASP	SER	engineered mutation	UNP E9Q401
D	2813	ASP	SER	engineered mutation	UNP E9Q401

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

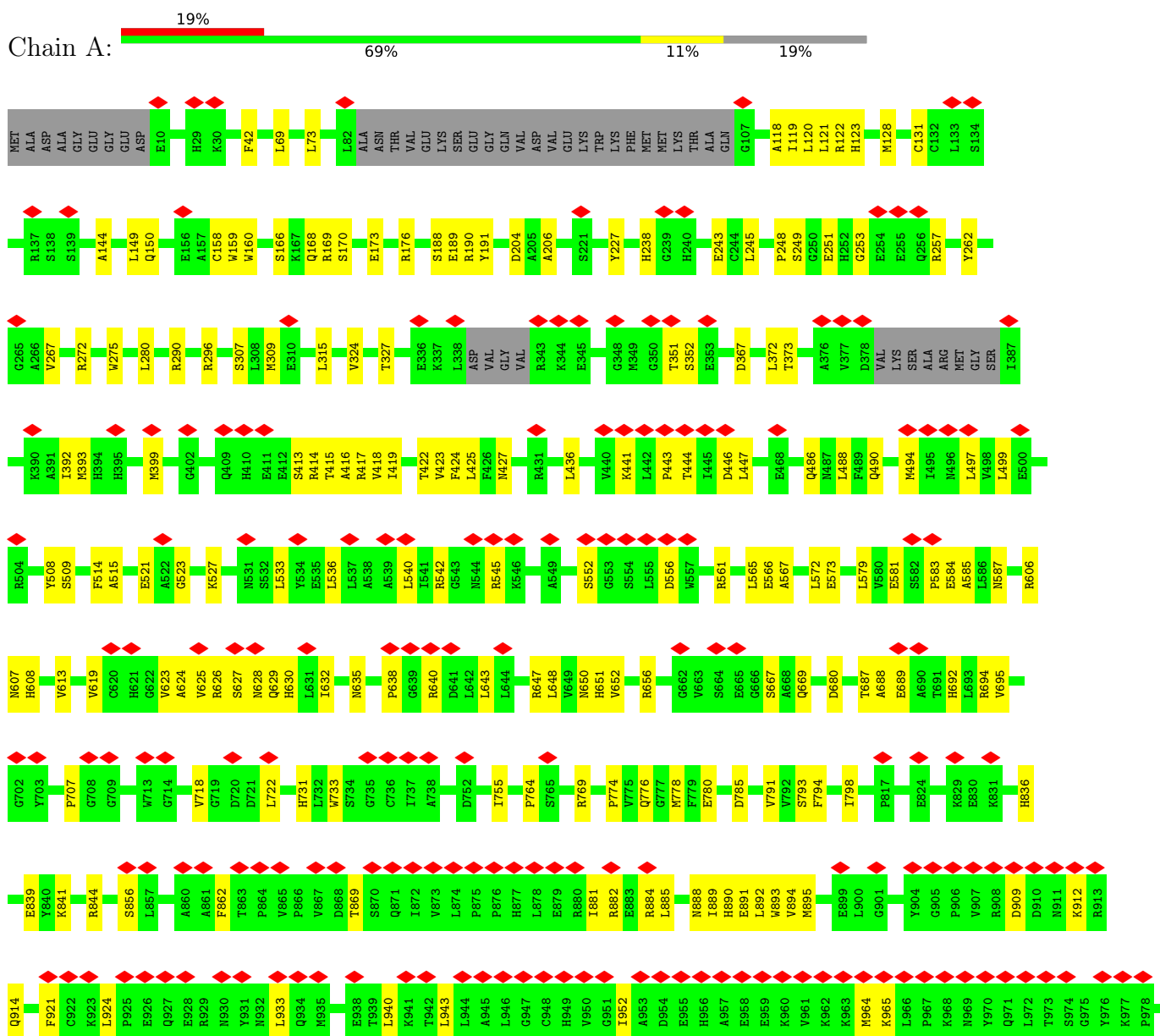
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

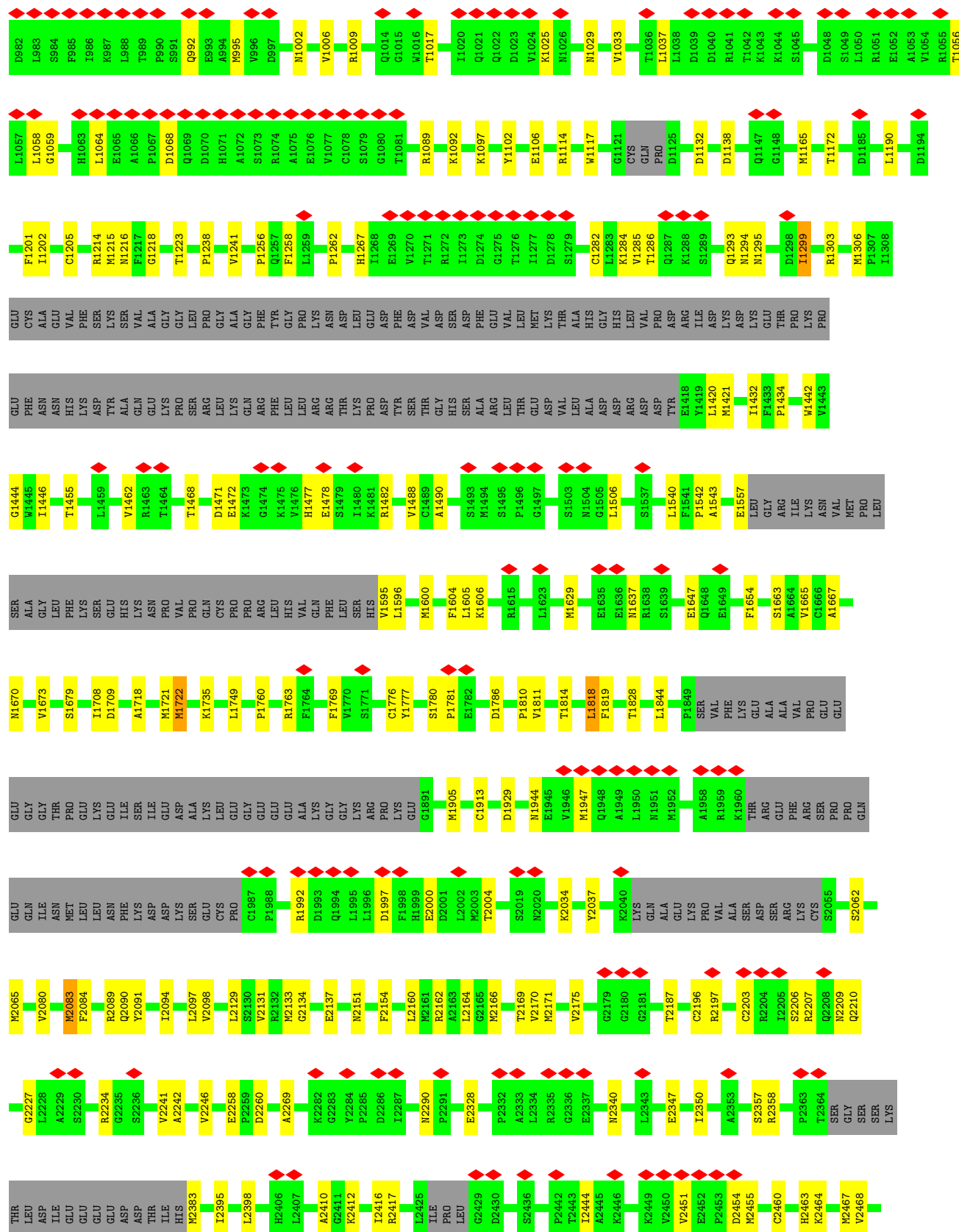
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

3 Residue-property plots

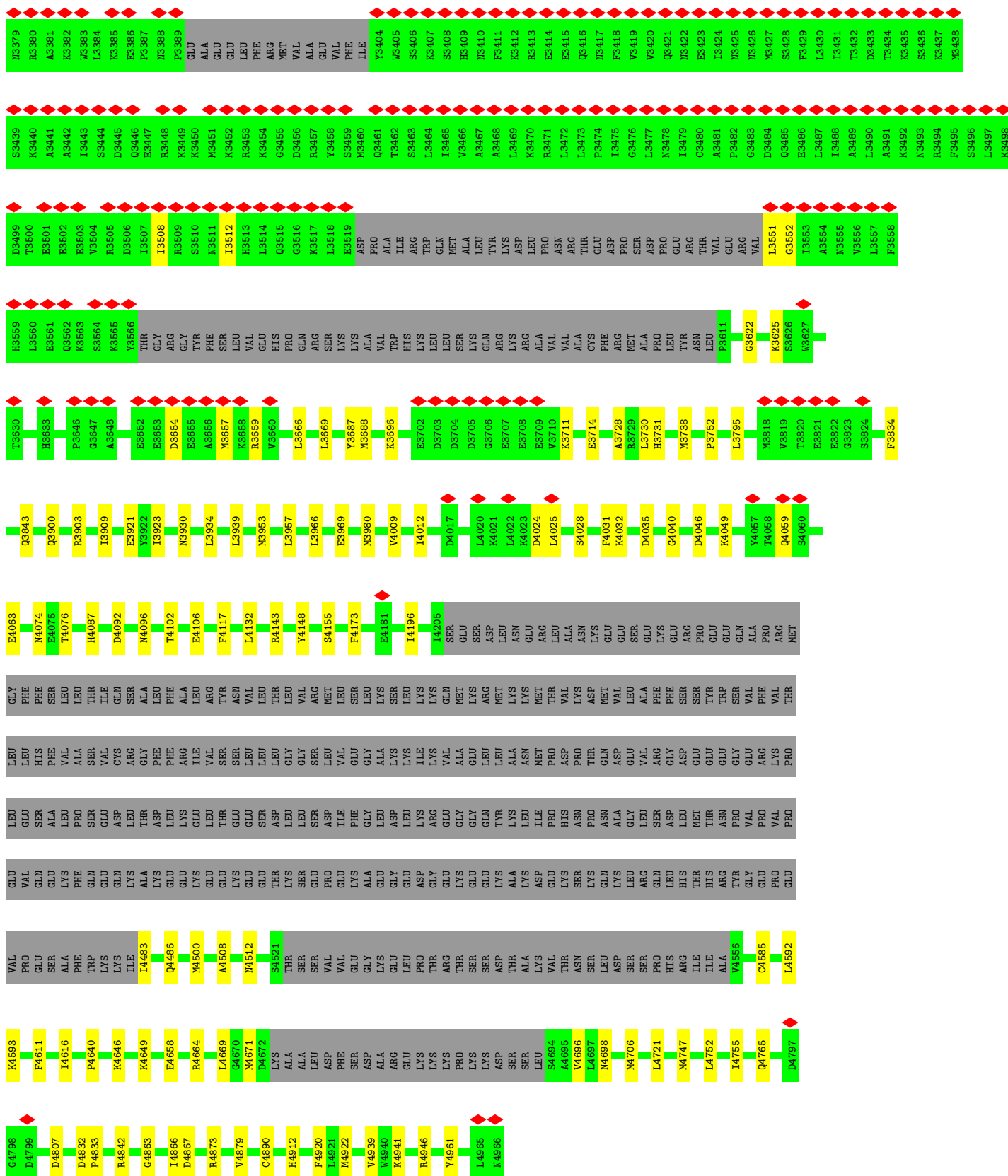
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 2

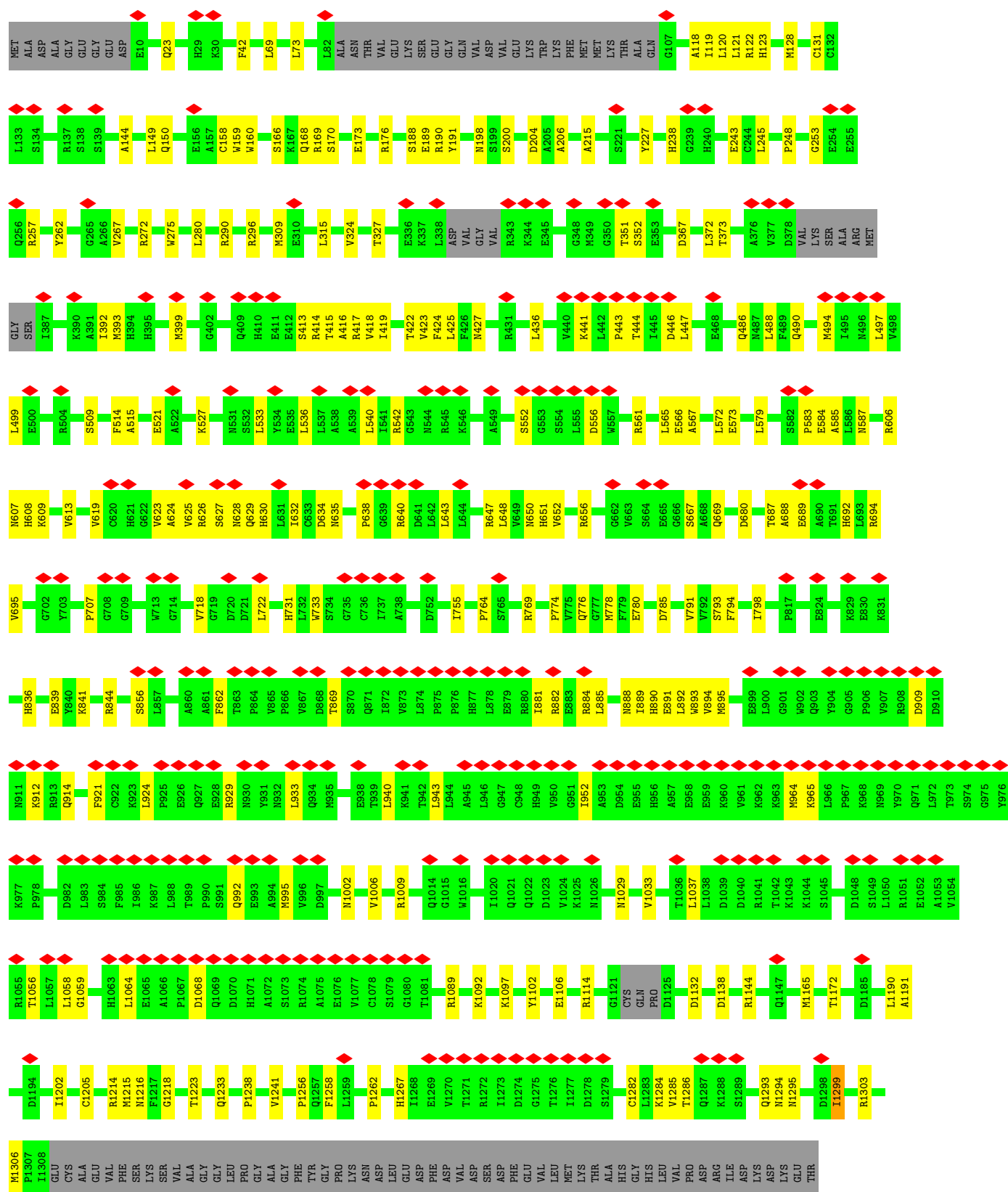








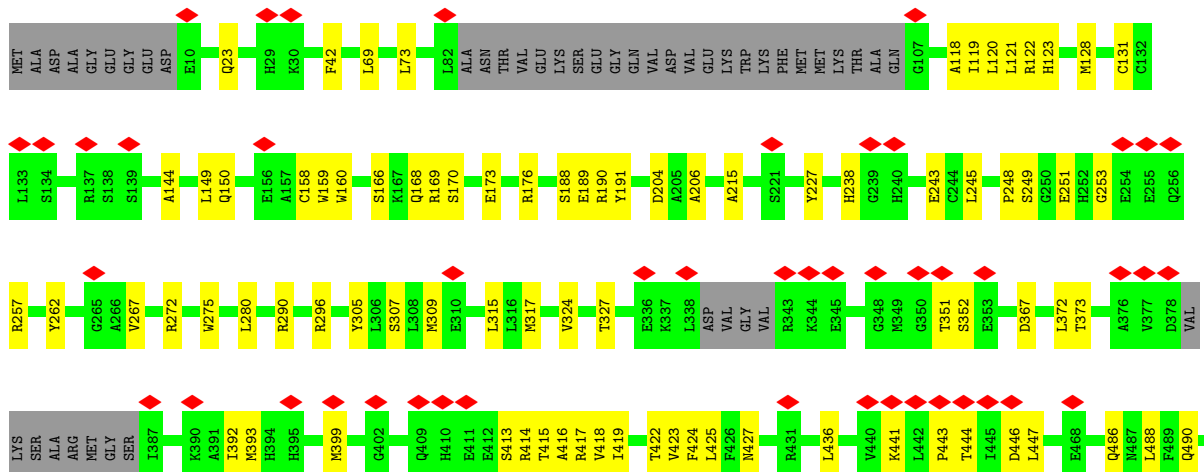
- Molecule 1: Ryanodine receptor 2

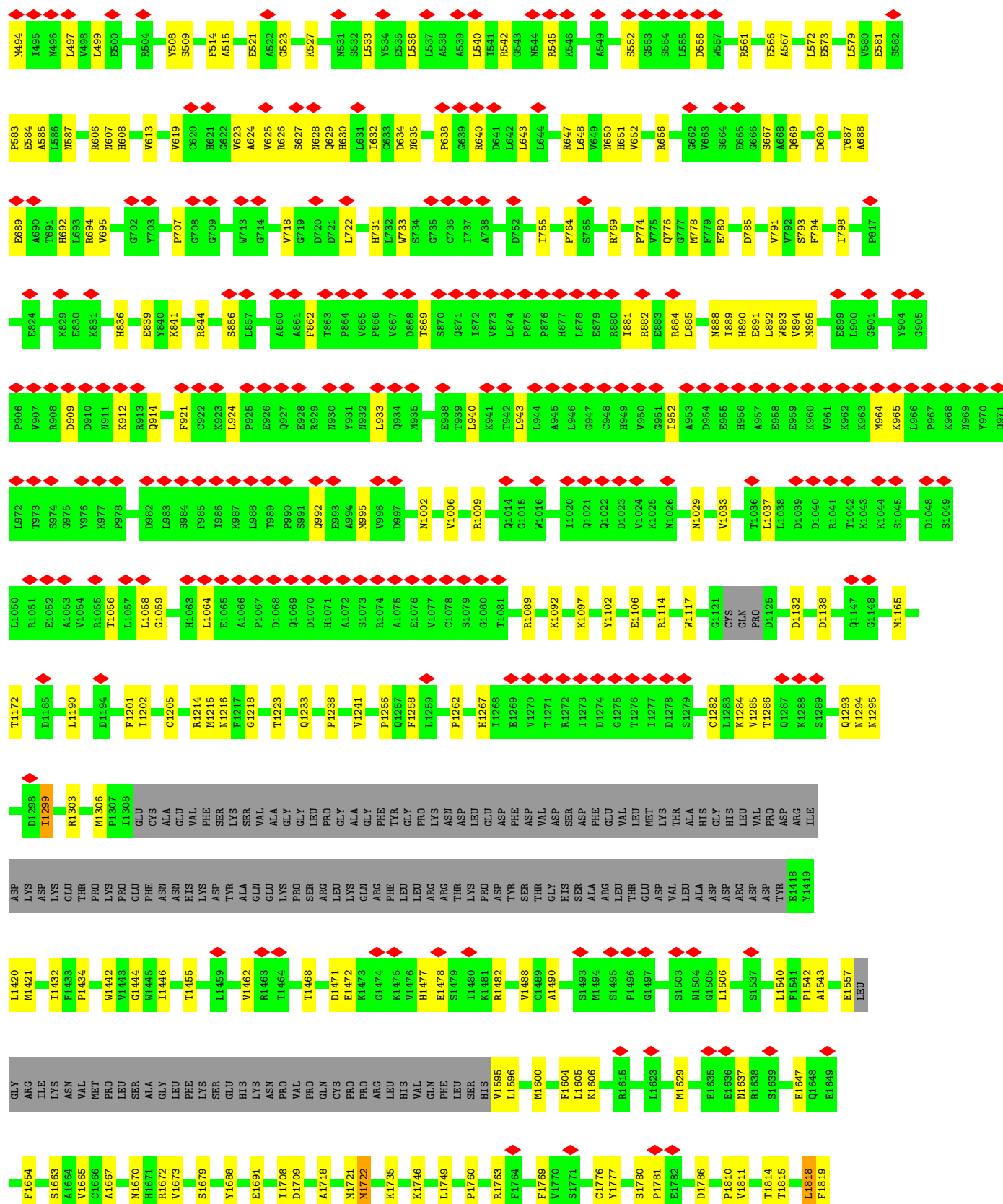


S2708	N2611	LEU	E2452	I2350	C2203	ARG	PRO	GLU	A1664	W1442	PRO
N2709	H2612	LEU	P2453	A2353	R2204	LYS	GLN	GLU	V1665	V1443	LYS
I2710	Y2613	HIS	D2454	R2357	I2205	CYS	GLN	GLU	C1666	G1444	PRO
T2711	E2614	THR	M2455	R2358	S2206	S2062	ILE	THR	N1670	W1445	PHE
I2712	W2617	TVR	C2460	P2363	R2207	M2065	ASN	PRO	H1671	I1446	ASN
P2713	W2617	ARG	P2363	T2364	Q2208	M2065	MET	GLU	H1671	T1455	ASN
E2714	Y2620	LEU	T2364	T2364	N2209	P2077	LEU	GLU	R1672	L1459	HIS
K2715	A2631	SER	H2463	GLY	Q2210	V2080	ASN	LYS	V1673	V1462	LYS
L2716	A2632	GLY	K2464	SER	Q2213	V2080	PHE	ILE	S1679	R1463	TYR
E2717	A2632	SER	M2467	SER	G2227	M2083	LYS	ILE	I1708	T1468	ALA
Y2718	A2632	SER	V2468	SER	I2228	F2084	ASP	GLU	D1709	R1463	GLN
F2719	R2641	LEU	R2473	THR	A2229	M2084	LYS	ASP	R1673	T1464	GLU
I2720	S2640	LYS	E2478	LEU	S2230	Q2089	GLU	ALA	A1718	L1468	LYS
N2721	K2642	GLN	E2478	ASP	R2234	Q2090	CYS	LEU	M1721	T1468	PRO
K2722	L2643	ASP	D2481	GLU	R2235	Y2091	PRO	GLY	M1722	E1471	ARG
Y2723	W2645	SER	L2484	GLU	S2236	I2094	C1987	GLY	K1735	K1473	LYS
A2724	G2645	ILE	L2484	GLU	S2236	V2241	P1988	GLU	P1760	G1474	GLN
E2725	I2647	VAL	E2488	ASP	V2241	V2098	I1991	GLU	R1763	G1474	ARG
H2726	L2651	CYS	L2492	THR	A2242	V2098	I1991	GLY	F1764	E1477	LEU
S2727	S2652	LEU	L2492	THR	V2246	L2129	I1991	GLY	F1764	E1478	ARG
H2728	Q2653	LEU	L2495	HIS	I2256	S2130	D1993	GLY	F1769	S1479	ARG
K2729	Q2654	SER	L2495	HIS	E2257	R2132	Q1994	LYS	V1770	I1480	LYS
K2730	K2655	ILE	A2498	I2395	E2258	M2133	L1996	PRO	S1771	K1481	PRO
W2731	Y2656	CYS	A2499	I2395	E2259	Q2134	D1997	LYS	C1776	R1482	ASP
S2732	Q2657	LEU	S2501	H2406	A2269	E2137	F1998	GLU	Y1777	V1488	TYR
K2733	Q2658	LEU	D2502	L2407	A2269	N2151	H1999	GLU	C1489	C1489	THR
D2734	E2659	ILE	L2502	L2407	A2269	N2151	E2000	GLU	L1596	A1490	GLY
K2735	P2666	CYS	A2505	A2410	K2282	F2154	D2001	GLU	S1780	S1493	SER
L2736	Y2679	LEU	L2506	G2411	G2283	L2160	L2002	GLU	P1781	M1494	HIS
A2737	M2680	LEU	L2506	K2412	Y2284	M2161	M2003	GLU	E1782	M1494	ALA
N2738	E2681	LEU	M2511	I2416	P2285	R2162	T2004	GLU	D1786	S1495	ARG
G2739	Y2684	LEU	L2524	R2417	I2287	A2163	S2019	GLU	P1810	P1496	LEU
W2740	Y2684	LEU	L2527	L2425	N2290	G2165	M2020	GLU	V1811	G1497	GLU
I2741	V2685	ARG	L2527	ILE	P2291	M2166	R2025	GLU	T1814	S1503	ASP
Y2742	S2686	CYS	L2527	PRO	R2296	T2169	L2028	GLU	L1826	N1504	VAL
G2743	M2687	ALA	L2527	LEU	R2296	V2170	A1949	GLU	L1826	G1505	ALA
E2744	M2688	LEU	L2527	LEU	E2328	M2171	K2034	GLU	M1629	L1506	ASP
I2745	E2689	LEU	L2527	D2430	E2328	V2176	Y2037	GLU	E1635	L1519	ARG
Y2746	K2690	LEU	L2527	D2430	P2332	G2179	M1952	GLU	E1636	S1537	ASP
S2747	Q2691	ALA	L2527	S2436	A2333	G2180	A1958	GLU	S1639	T1538	TYR
D2748	M2694	GLY	L2527	S2436	L2334	G2181	R1959	GLU	E1647	Y1419	ASP
S2749	ASP	THR	L2527	P2442	R2335	G2181	K1960	GLU	Q1648	L1420	ASP
S2750	SER	THR	L2527	T2443	G2336	T2187	THR	ALA	E1649	F1541	ASP
K2751	GLU	GLU	L2527	I2444	E2337	T2187	ARG	ALA	F1654	P1542	ASP
I2752	GLY	HIS	L2527	A2445	E2337	C2196	GLU	ALA	E1557	T1432	ASP
Q2753	ASN	ALA	L2527	P2446	E2337	R2197	VAL	ALA	P1434	I1433	ASP
P2754	F2700	LEU	L2527	K2449	L2343	R2197	VAL	ALA	LEU	E1557	LEU
L2755	N2701	ILE	L2527	V2450	L2343	R2197	VAL	ALA	GLY	ARG	GLY
M2756	P2702	ASP	L2527	V2451	E2347	R2197	ASP	ASP	ILE	ILE	ILE
K2757	Q2703	SER	L2527	V2451	E2347	R2197	SER	PRO			
P2758	P2704	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
Y2759	D2705	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
K2760	D2706	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
L2761	L2761	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
L2762	L2762	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
S2763	S2763	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
E2764	E2764	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
K2765	K2765	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
E2766	E2766	LEU	L2527	V2451	E2347	R2197	PRO	PRO			
K2767	K2767	LEU	L2527	V2451	E2347	R2197	PRO	PRO			



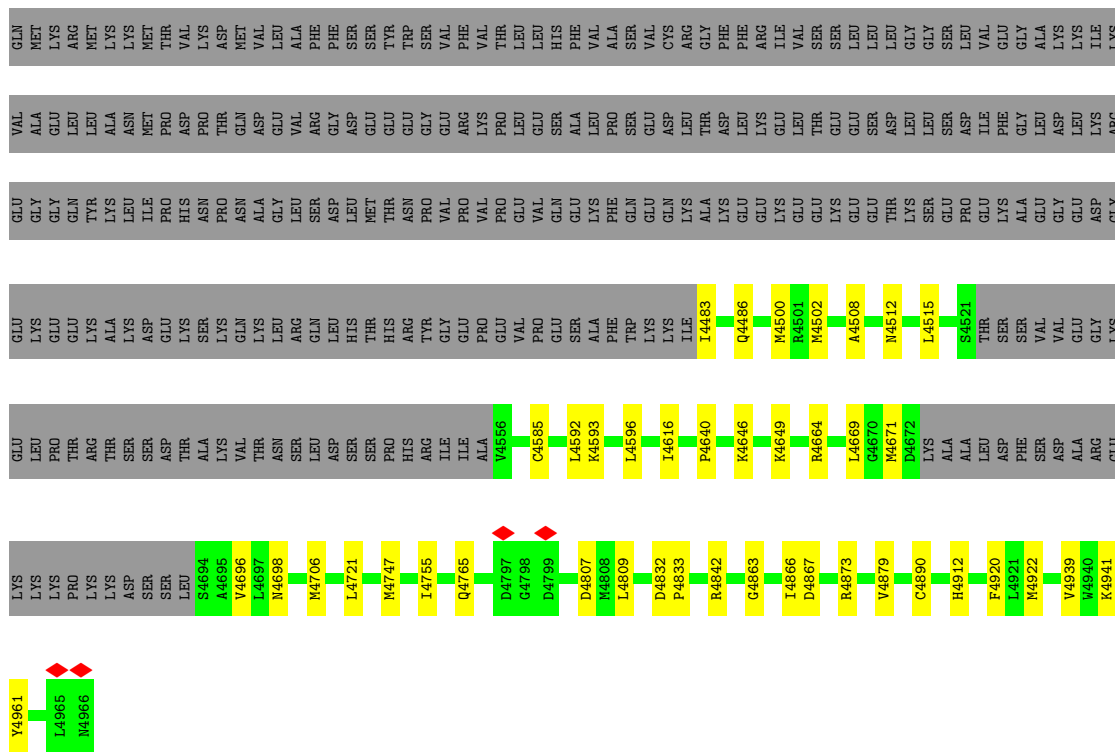
- Molecule 1: Ryanodine receptor 2



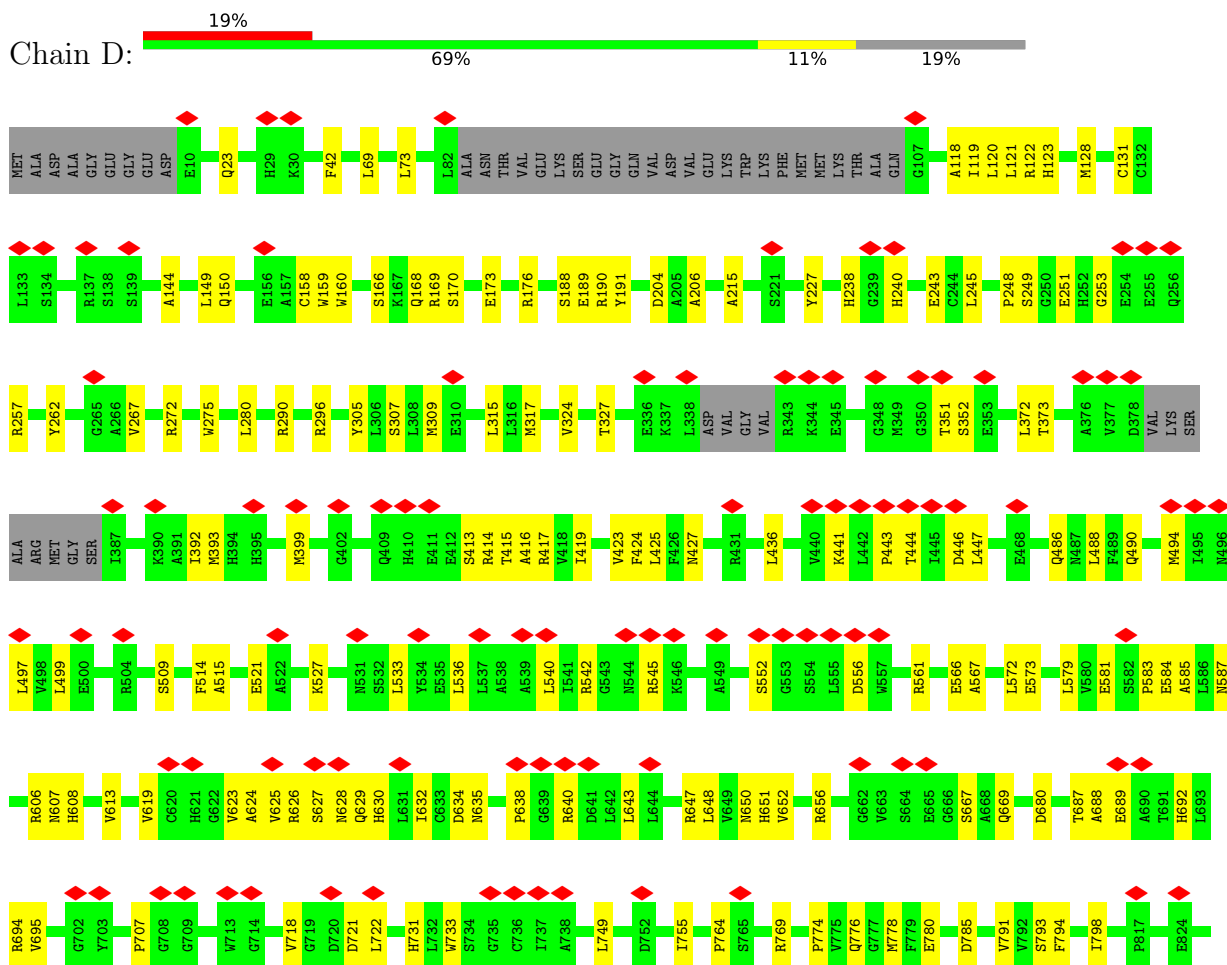








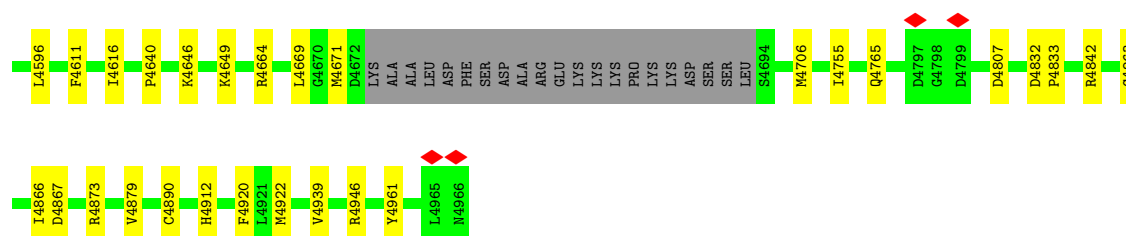
- Molecule 1: Ryanodine receptor 2



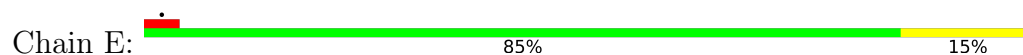
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D909	D910	N911	K912	R913	Q914	F921	C922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	E952	A953	D954	E955	H956	A957	E958	E959	D960	V961	K962	K963	M964	K965	L966	P967	K968	N969	Y970	Q971	L972	T973	S974
G975	Y976	K977	P978	D982	L983	S984	F985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	M995	V996	D997	M1002	V1006	R1009	Q1014	G1015	W1016	T1017	I1020	Q1021	Q1022	D1023	V1024	K1025	M1026	V1033	T1036	L1037	L1038	D1039	D1040	R1041	T1042	K1043	K1044	S1045	D1048	S1049	L1050	R1051	E1052	A1053							
V1054	R1055	T1056	L1057	G1059	H1063	L1064	E1065	A1066	P1067	D1068	Q1069	D1070	H1071	A1072	S1073	R1074	A1075	E1076	V1077	C1078	S1079	G1080	T1081	R1089	K1092	Y1102	E1106	R1114	G1121	CYS	GLN	PRO	D1125	D1138	Q1147	G1148	M1165	T1172	D1185	L1190	D1194	T1202															
C1205	R1214	M1215	N1216	F1217	G1218	T1223	Q1233	P1238	V1241	P1256	Q1257	F1258	L1259	P1262	H1267	E1269	V1270	T1271	I1272	R1273	D1274	G1275	T1276	I1277	D1278	S1279	C1282	L1283	K1284	V1285	T1286	Q1287	K1288	S1289	Q1293	N1294	M1295	D1298	I1299	R1303	M1306	P1307	I1308	GLU	CYS												
ALA	GLU	VAL	PHE	SER	LYS	SER	ALA	GLN	ASN	ALA	GLY	PRO	LEU	PRO	GLY	ALA	GLN	ARG	LEU	LYS	ASP	PHE	TYR	ASP	VAL	ASP	PRO	ASP	ARG	ILE	LYS	LYS	LYS	GLU	THR	GLU	THR	PRO	PRO	LYS	PRO	GLU	PHE														
ASN	ASN	HIS	LYS	ASP	TYR	GLN	GLY	ARG	LEU	LYS	ARG	PHE	LEU	ARG	THR	LYS	PRO	ASP	TYR	SER	GLY	HIS	SER	ALA	ARG	LEU	THR	GLU	ASP	VAL	LEU	ALA	ASP	TYR	E1418	Y1419	L1420	M1421	I1432	F1433	P1434	W1442	V1443	G1444	W1445												
I1446	T1455	L1459	V1462	R1463	T1464	T1468	D1471	E1472	K1473	G1474	K1475	V1476	H1477	S1479	I1480	K1481	R1482	V1488	C1489	A1490	S1493	M1494	S1495	P1496	G1497	S1503	N1504	G1505	L1506	S1537	L1540	F1541	P1542	A1543	E1557	LEU	GLY	ARG	ILE	LYS	ASN	VAL	PRO	PRO	LEU	SER	ALA										
GLY	LEU	PHE	LYS	SER	HIS	LYS	PRO	VAL	PRO	GLN	CYS	PRO	PRO	ARG	LEU	HIS	VAL	GLN	PHE	SER	HIS	V1595	L1596	M1600	F1604	L1605	K1606	R1615	L1623	M1629	E1635	E1636	S1639	E1647	Q1648	E1649	F1654	S1663	A1664	V1665	G1666	A1667	N1670	H1671	R1672												
V1673	S1679	Y1688	E1691	I1708	D1709	A1718	M1721	M1722	K1735	L1749	P1760	R1763	F1764	F1769	V1770	S1771	C1776	S1780	P1781	E1782	D1786	P1810	V1811	T1814	L1818	F1819	T1828	L1844	P1849	SER	VAL	PHE	LYS	GLU	ALA	VAL	PRO																				
GLU	GLU	GLY	THR	PRO	GLU	LYS	ASN	ILE	LYS	SER	ILE	GLU	ASP	ALA	LYS	GLY	GLU	GLU	ALA	LYS	GLY	GLY	ARG	PRO	LYS	GLU	M1946	M1947	Q1948	A1949	L1950	N1951	M1952	A1958	R1959	K1960	THR	ARG	GLU	PHE	ARG	CYS	S2055	S2062													
PRO	GLN	GLN	ASN	MET	LEU	ASP	ASP	LYS	SER	GLU	CYS	PRO	C1987	P1988	R1992	D1993	Q1994	L1995	L1996	D1997	F1998	L2002	S2019	M2020	R2025	K2034	Y2037	K2040	LYS	GLN	ALA	GLU	LYS	VAL	ALA	SER	ASP	SER	ARG	LYS	CYS	S2065	S2062														
M2065	P2077	V2080	M2083	F2084	R2089	Q2090	Y2091	T2094	L2097	V2098	L2129	S2130	V2131	R2132	M2133	G2134	E2137	N2151	F2154	L2160	M2161	A2163	L2164	G2165	M2166	T2169	V2170	M2171	V2175	G2179	G2180	G2181	T2187	C2196	R2197	C2203	R2204	I2205	S2206	R2207	Q2208																



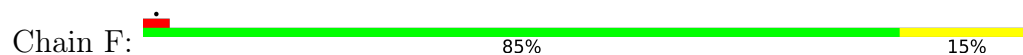




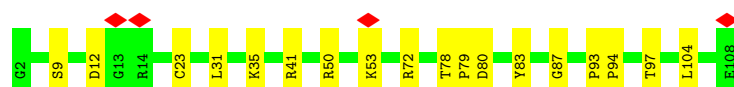
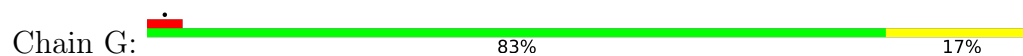
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



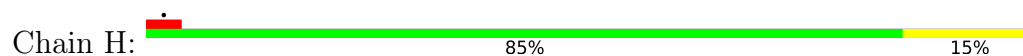
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	406681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.804	Depositor
Minimum map value	-1.458	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	496.80002, 496.80002, 496.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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: 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	0.13	0/32026	0.32	0/43315
1	B	0.13	0/32026	0.32	0/43315
1	C	0.13	0/32026	0.32	0/43315
1	D	0.13	0/32026	0.32	0/43315
2	E	0.13	0/834	0.32	0/1123
2	F	0.13	0/834	0.32	0/1123
2	G	0.13	0/834	0.32	0/1123
2	H	0.13	0/834	0.32	0/1123
All	All	0.13	0/131440	0.32	0/177752

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	31374	0	30394	342	0
1	B	31374	0	30394	351	0
1	C	31374	0	30394	357	0
1	D	31374	0	30394	339	0
2	E	818	0	821	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	0	821	11	0
2	G	818	0	821	12	0
2	H	818	0	821	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	128772	0	124860	1409	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 6.

All (1409) 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:A:1629:MET:SD	1:A:1629:MET:N	2.61	0.73
1:D:1629:MET:SD	1:D:1629:MET:N	2.61	0.73
1:C:1629:MET:SD	1:C:1629:MET:N	2.61	0.72
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.72	0.71
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.73	0.71
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.73	0.70
1:B:1629:MET:SD	1:B:1629:MET:N	2.61	0.70
1:C:69:LEU:HD22	1:C:119:ILE:HD11	1.74	0.70
1:C:1444:GLY:HA3	1:C:1488:VAL:HA	1.72	0.70
1:A:69:LEU:HD22	1:A:119:ILE:HD11	1.74	0.70
1:A:1444:GLY:HA3	1:A:1488:VAL:HA	1.72	0.69
1:B:1444:GLY:HA3	1:B:1488:VAL:HA	1.72	0.69
1:D:69:LEU:HD22	1:D:119:ILE:HD11	1.74	0.69
1:B:69:LEU:HD22	1:B:119:ILE:HD11	1.74	0.69
1:C:296:ARG:HH22	1:C:324:VAL:HG22	1.58	0.69
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.73	0.69
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.73	0.69
1:D:296:ARG:HH22	1:D:324:VAL:HG22	1.58	0.69
1:A:579:LEU:HD12	1:A:583:PRO:HB3	1.75	0.69
1:B:296:ARG:HH22	1:B:324:VAL:HG22	1.58	0.69
1:C:579:LEU:HD12	1:C:583:PRO:HB3	1.75	0.69
1:A:296:ARG:HH22	1:A:324:VAL:HG22	1.58	0.68
1:B:579:LEU:HD12	1:B:583:PRO:HB3	1.75	0.68
1:B:413:SER:OG	1:B:414:ARG:NH1	2.28	0.67
1:A:415:THR:O	1:A:419:ILE:HG12	1.95	0.67
1:D:579:LEU:HD12	1:D:583:PRO:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:SER:OG	1:A:414:ARG:NH1	2.28	0.66
1:D:3688:MET:HE1	1:D:3752:PRO:HB2	1.77	0.66
1:C:413:SER:OG	1:C:414:ARG:NH1	2.28	0.66
1:A:3688:MET:HE1	1:A:3752:PRO:HB2	1.77	0.66
1:D:413:SER:OG	1:D:414:ARG:NH1	2.28	0.66
1:A:4765:GLN:HB3	1:B:4755:ILE:HD11	1.78	0.66
1:C:415:THR:O	1:C:419:ILE:HG12	1.95	0.66
1:D:415:THR:O	1:D:419:ILE:HG12	1.95	0.66
1:D:441:LYS:HG3	1:D:443:PRO:HD2	1.79	0.65
1:B:441:LYS:HG3	1:B:443:PRO:HD2	1.79	0.65
1:C:2084:PHE:HE2	1:C:3666:LEU:HB2	1.61	0.65
1:A:2084:PHE:HE2	1:A:3666:LEU:HB2	1.61	0.65
1:B:2084:PHE:HE2	1:B:3666:LEU:HB2	1.61	0.65
1:D:619:VAL:HA	1:D:624:ALA:HB2	1.78	0.65
1:B:415:THR:O	1:B:419:ILE:HG12	1.95	0.65
1:B:619:VAL:HA	1:B:624:ALA:HB2	1.78	0.65
1:B:3688:MET:HE1	1:B:3752:PRO:HB2	1.77	0.65
1:D:2084:PHE:HE2	1:D:3666:LEU:HB2	1.61	0.64
1:C:3688:MET:HE1	1:C:3752:PRO:HB2	1.77	0.64
1:C:441:LYS:HG3	1:C:443:PRO:HD2	1.79	0.64
1:A:619:VAL:HA	1:A:624:ALA:HB2	1.78	0.64
1:A:778:MET:HE1	1:A:780:GLU:HB2	1.80	0.64
1:A:131:CYS:HA	1:A:160:TRP:HE1	1.62	0.64
1:B:778:MET:HE1	1:B:780:GLU:HB2	1.80	0.64
1:C:619:VAL:HA	1:C:624:ALA:HB2	1.78	0.64
1:A:441:LYS:HG3	1:A:443:PRO:HD2	1.79	0.64
1:B:131:CYS:HA	1:B:160:TRP:HE1	1.62	0.64
1:C:2584:MET:SD	1:C:2584:MET:N	2.71	0.63
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.64	0.63
1:B:2062:SER:OG	1:B:2090:GLN:NE2	2.32	0.63
1:B:2584:MET:SD	1:B:2584:MET:N	2.71	0.63
1:D:778:MET:HE1	1:D:780:GLU:HB2	1.80	0.63
1:D:2062:SER:OG	1:D:2090:GLN:NE2	2.32	0.63
1:A:1303:ARG:HH22	1:A:1540:LEU:HD12	1.64	0.63
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.64	0.63
1:C:2062:SER:OG	1:C:2090:GLN:NE2	2.32	0.63
1:A:2062:SER:OG	1:A:2090:GLN:NE2	2.32	0.63
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.64	0.63
1:C:131:CYS:HA	1:C:160:TRP:HE1	1.62	0.63
1:B:131:CYS:SG	1:B:150:GLN:NE2	2.72	0.62
1:D:131:CYS:HA	1:D:160:TRP:HE1	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.64	0.62
1:B:3233:MET:HG2	1:B:3235:GLU:H	1.64	0.62
1:A:3233:MET:HG2	1:A:3235:GLU:H	1.64	0.62
1:C:131:CYS:SG	1:C:150:GLN:NE2	2.72	0.62
1:C:778:MET:HE1	1:C:780:GLU:HB2	1.80	0.62
1:D:131:CYS:SG	1:D:150:GLN:NE2	2.72	0.62
1:A:131:CYS:SG	1:A:150:GLN:NE2	2.72	0.62
1:B:1303:ARG:HH22	1:B:1540:LEU:HD12	1.64	0.62
1:C:1303:ARG:HH22	1:C:1540:LEU:HD12	1.64	0.62
1:D:3233:MET:HG2	1:D:3235:GLU:H	1.64	0.62
1:B:248:PRO:O	1:B:257:ARG:NH2	2.33	0.61
1:C:722:LEU:O	1:C:1482:ARG:NH1	2.34	0.61
1:C:1033:VAL:HB	1:C:1037:LEU:HB2	1.82	0.61
1:C:3233:MET:HG2	1:C:3235:GLU:H	1.64	0.61
1:D:509:SER:H	1:D:514:PHE:HE2	1.48	0.61
1:D:731:HIS:CE1	1:D:733:TRP:HB3	2.36	0.61
1:D:1303:ARG:HH22	1:D:1540:LEU:HD12	1.64	0.61
1:C:731:HIS:CE1	1:C:733:TRP:HB3	2.36	0.61
1:D:1033:VAL:HB	1:D:1037:LEU:HB2	1.82	0.61
1:D:2584:MET:SD	1:D:2584:MET:N	2.71	0.61
1:B:731:HIS:CE1	1:B:733:TRP:HB3	2.36	0.61
1:A:731:HIS:CE1	1:A:733:TRP:HB3	2.36	0.60
1:A:4755:ILE:HD11	1:C:4765:GLN:HB3	1.83	0.60
1:B:722:LEU:O	1:B:1482:ARG:NH1	2.34	0.60
1:B:1033:VAL:HB	1:B:1037:LEU:HB2	1.82	0.60
1:C:509:SER:H	1:C:514:PHE:HE2	1.48	0.60
1:A:1033:VAL:HB	1:A:1037:LEU:HB2	1.82	0.60
1:C:2716:LEU:HD13	1:C:2720:ILE:HG21	1.84	0.60
1:D:2716:LEU:HD13	1:D:2720:ILE:HG21	1.84	0.60
1:B:4765:GLN:HB3	1:D:4755:ILE:HD11	1.83	0.60
1:D:2690:LYS:HG3	1:D:2691:GLN:HG2	1.84	0.60
1:A:509:SER:H	1:A:514:PHE:HE2	1.48	0.60
1:A:722:LEU:O	1:A:1482:ARG:NH1	2.34	0.60
1:C:1718:ALA:HA	1:C:1721:MET:HE2	1.83	0.60
1:A:2716:LEU:HD13	1:A:2720:ILE:HG21	1.84	0.60
1:B:882:ARG:HH22	1:B:933:LEU:HG	1.67	0.60
1:B:1718:ALA:HA	1:B:1721:MET:HE2	1.83	0.60
1:B:2716:LEU:HD13	1:B:2720:ILE:HG21	1.84	0.60
1:D:722:LEU:O	1:D:1482:ARG:NH1	2.34	0.60
1:B:2690:LYS:HG3	1:B:2691:GLN:HG2	1.84	0.59
2:F:83:TYR:HB2	2:F:87:GLY:HA2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2580:ARG:NH1	1:A:2874:ASP:O	2.35	0.59
1:D:2580:ARG:NH1	1:D:2874:ASP:O	2.35	0.59
1:C:4755:ILE:HD11	1:D:4765:GLN:HB3	1.84	0.59
1:D:882:ARG:HH22	1:D:933:LEU:HG	1.67	0.59
2:E:9:SER:HB2	2:E:72:ARG:H	1.67	0.59
1:A:2580:ARG:NH1	1:A:2581:PRO:O	2.35	0.59
1:C:2580:ARG:NH1	1:C:2874:ASP:O	2.35	0.59
1:A:1718:ALA:HA	1:A:1721:MET:HE2	1.83	0.59
1:A:4671:MET:SD	1:A:4671:MET:N	2.75	0.59
1:B:509:SER:H	1:B:514:PHE:HE2	1.48	0.59
1:C:882:ARG:HH22	1:C:933:LEU:HG	1.67	0.59
1:C:4671:MET:SD	1:C:4671:MET:N	2.75	0.59
1:D:2836:LEU:HD21	1:D:2902:VAL:H	1.68	0.59
1:A:2836:LEU:HD21	1:A:2902:VAL:H	1.68	0.59
1:C:2580:ARG:NH1	1:C:2581:PRO:O	2.35	0.59
1:D:1718:ALA:HA	1:D:1721:MET:HE2	1.83	0.59
1:D:2580:ARG:NH1	1:D:2581:PRO:O	2.35	0.59
2:H:83:TYR:HB2	2:H:87:GLY:HA2	1.85	0.59
1:D:248:PRO:O	1:D:257:ARG:NH2	2.33	0.59
2:E:83:TYR:HB2	2:E:87:GLY:HA2	1.85	0.59
1:B:189:GLU:OE2	1:D:2417:ARG:NH1	2.35	0.59
1:C:2690:LYS:HG3	1:C:2691:GLN:HG2	1.84	0.59
1:D:1432:ILE:HG22	1:D:1506:LEU:HD13	1.84	0.59
1:A:776:GLN:NE2	1:A:1471:ASP:O	2.36	0.58
1:C:776:GLN:NE2	1:C:1471:ASP:O	2.36	0.58
1:C:1432:ILE:HG22	1:C:1506:LEU:HD13	1.84	0.58
1:B:1432:ILE:HG22	1:B:1506:LEU:HD13	1.84	0.58
1:B:2836:LEU:HD21	1:B:2902:VAL:H	1.68	0.58
2:G:83:TYR:HB2	2:G:87:GLY:HA2	1.85	0.58
1:B:2580:ARG:NH1	1:B:2581:PRO:O	2.35	0.58
1:B:2580:ARG:NH1	1:B:2874:ASP:O	2.35	0.58
1:C:607:ASN:O	1:C:608:HIS:ND1	2.36	0.58
1:A:2690:LYS:HG3	1:A:2691:GLN:HG2	1.84	0.58
1:C:267:VAL:HG22	1:C:272:ARG:HD3	1.85	0.58
1:D:607:ASN:O	1:D:608:HIS:ND1	2.36	0.58
1:D:776:GLN:NE2	1:D:1471:ASP:O	2.36	0.58
2:G:9:SER:HB2	2:G:72:ARG:H	1.67	0.58
1:A:2034:LYS:HA	1:A:2037:TYR:HE2	1.69	0.58
1:A:882:ARG:HH22	1:A:933:LEU:HG	1.67	0.58
1:A:1432:ILE:HG22	1:A:1506:LEU:HD13	1.84	0.58
1:C:248:PRO:O	1:C:257:ARG:NH2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:SER:HB2	2:F:72:ARG:H	1.67	0.58
1:A:267:VAL:HG22	1:A:272:ARG:HD3	1.85	0.58
1:D:619:VAL:HG21	1:D:1667:ALA:HB3	1.85	0.58
1:B:776:GLN:NE2	1:B:1471:ASP:O	2.36	0.58
1:D:2034:LYS:HA	1:D:2037:TYR:HE2	1.69	0.58
1:A:248:PRO:O	1:A:257:ARG:NH2	2.33	0.57
1:C:2836:LEU:HD21	1:C:2902:VAL:H	1.68	0.57
1:D:992:GLN:HG3	1:D:1058:LEU:HD11	1.86	0.57
1:B:267:VAL:HG22	1:B:272:ARG:HD3	1.85	0.57
1:C:619:VAL:HG21	1:C:1667:ALA:HB3	1.85	0.57
1:D:2162:ARG:NH1	1:D:2206:SER:OG	2.38	0.57
1:A:189:GLU:OE2	1:B:2417:ARG:NH1	2.38	0.57
1:B:607:ASN:O	1:B:608:HIS:ND1	2.36	0.57
1:B:2034:LYS:HA	1:B:2037:TYR:HE2	1.69	0.57
1:D:3015:ARG:HH22	1:D:3081:HIS:HA	1.69	0.57
1:A:992:GLN:HG3	1:A:1058:LEU:HD11	1.86	0.57
1:D:267:VAL:HG22	1:D:272:ARG:HD3	1.85	0.57
1:B:2498:ALA:HA	1:B:2590:ARG:HH22	1.70	0.57
1:D:4640:PRO:HG2	1:D:4646:LYS:HG3	1.87	0.57
1:B:619:VAL:HG21	1:B:1667:ALA:HB3	1.85	0.57
1:B:4640:PRO:HG2	1:B:4646:LYS:HG3	1.87	0.57
2:H:9:SER:HB2	2:H:72:ARG:H	1.67	0.57
1:B:486:GLN:HB3	1:B:540:LEU:HA	1.86	0.57
1:B:992:GLN:HG3	1:B:1058:LEU:HD11	1.86	0.57
1:A:2584:MET:SD	1:A:2584:MET:N	2.71	0.57
1:C:2417:ARG:NH1	1:D:189:GLU:OE2	2.38	0.57
1:C:2498:ALA:HA	1:C:2590:ARG:HH22	1.70	0.57
1:A:607:ASN:O	1:A:608:HIS:ND1	2.36	0.57
1:A:1256:PRO:HB2	1:A:1596:LEU:HD22	1.87	0.57
1:B:1256:PRO:HB2	1:B:1596:LEU:HD22	1.87	0.56
1:D:4173:PHE:HD1	1:D:4879:VAL:HG21	1.70	0.56
1:A:2162:ARG:NH1	1:A:2206:SER:OG	2.38	0.56
1:B:2162:ARG:NH1	1:B:2206:SER:OG	2.38	0.56
1:C:2034:LYS:HA	1:C:2037:TYR:HE2	1.69	0.56
1:A:486:GLN:HB3	1:A:540:LEU:HA	1.86	0.56
1:A:542:ARG:NH2	1:A:573:GLU:OE1	2.38	0.56
1:A:619:VAL:HG21	1:A:1667:ALA:HB3	1.85	0.56
1:A:1670:ASN:O	1:A:1777:TYR:OH	2.19	0.56
1:C:486:GLN:HB3	1:C:540:LEU:HA	1.86	0.56
1:C:542:ARG:NH2	1:C:573:GLU:OE1	2.38	0.56
1:C:992:GLN:HG3	1:C:1058:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4640:PRO:HG2	1:C:4646:LYS:HG3	1.87	0.56
1:A:3657:MET:HE1	1:A:3659:ARG:HB2	1.88	0.56
1:B:626:ARG:HE	1:B:2131:VAL:HG11	1.71	0.56
1:B:2878:ALA:HA	1:B:2881:LYS:HB2	1.87	0.56
1:A:4173:PHE:HD1	1:A:4879:VAL:HG21	1.70	0.56
1:B:940:LEU:HD23	1:B:943:LEU:HD21	1.88	0.56
1:B:2416:ILE:HD12	1:B:2416:ILE:H	1.71	0.56
1:C:2878:ALA:HA	1:C:2881:LYS:HB2	1.87	0.56
1:C:3015:ARG:HH22	1:C:3081:HIS:HA	1.69	0.56
1:D:542:ARG:NH2	1:D:573:GLU:OE1	2.38	0.56
1:D:626:ARG:HE	1:D:2131:VAL:HG11	1.71	0.56
1:A:2410:ALA:O	1:A:2412:LYS:NZ	2.39	0.56
1:B:3015:ARG:HH22	1:B:3081:HIS:HA	1.69	0.56
1:C:1256:PRO:HB2	1:C:1596:LEU:HD22	1.87	0.56
2:G:79:PRO:HD3	2:G:97:THR:HG22	1.88	0.56
1:A:4640:PRO:HG2	1:A:4646:LYS:HG3	1.87	0.56
1:B:1258:PHE:HB3	1:B:1303:ARG:HD2	1.88	0.56
1:B:2410:ALA:O	1:B:2412:LYS:NZ	2.39	0.56
2:E:79:PRO:HD3	2:E:97:THR:HG22	1.88	0.56
2:F:79:PRO:HD3	2:F:97:THR:HG22	1.88	0.56
1:A:2498:ALA:HA	1:A:2590:ARG:HH22	1.70	0.56
1:B:542:ARG:NH2	1:B:573:GLU:OE1	2.38	0.56
1:C:626:ARG:HE	1:C:2131:VAL:HG11	1.71	0.56
1:C:2416:ILE:HD12	1:C:2416:ILE:H	1.71	0.56
1:C:3934:LEU:HD12	1:C:3939:LEU:HD22	1.88	0.56
1:D:1258:PHE:HB3	1:D:1303:ARG:HD2	1.88	0.56
1:D:3508:ILE:O	1:D:3551:LEU:N	2.39	0.56
1:A:1258:PHE:HB3	1:A:1303:ARG:HD2	1.88	0.56
1:A:2417:ARG:NH1	1:C:189:GLU:OE2	2.38	0.56
1:A:3934:LEU:HD12	1:A:3939:LEU:HD22	1.88	0.56
1:B:1102:TYR:HB2	1:B:1165:MET:HE1	1.88	0.56
1:C:1258:PHE:HB3	1:C:1303:ARG:HD2	1.88	0.56
1:C:3657:MET:HE1	1:C:3659:ARG:HB2	1.88	0.56
1:C:4173:PHE:HD1	1:C:4879:VAL:HG21	1.70	0.56
1:C:4890:CYS:SG	1:C:4912:HIS:HE1	2.22	0.56
1:D:940:LEU:HD23	1:D:943:LEU:HD21	1.88	0.55
1:A:667:SER:O	1:A:669:GLN:NE2	2.40	0.55
1:A:940:LEU:HD23	1:A:943:LEU:HD21	1.88	0.55
1:B:3508:ILE:O	1:B:3551:LEU:N	2.39	0.55
1:C:2162:ARG:NH1	1:C:2206:SER:OG	2.38	0.55
1:C:3508:ILE:O	1:C:3551:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:GLN:HB3	1:D:540:LEU:HA	1.86	0.55
1:D:1256:PRO:HB2	1:D:1596:LEU:HD22	1.87	0.55
2:H:79:PRO:HD3	2:H:97:THR:HG22	1.88	0.55
1:B:166:SER:OG	1:B:168:GLN:OE1	2.19	0.55
1:D:667:SER:O	1:D:669:GLN:NE2	2.40	0.55
1:A:3102:PRO:HG3	1:A:3226:ARG:HD2	1.89	0.55
1:A:3508:ILE:O	1:A:3551:LEU:N	2.39	0.55
1:B:4173:PHE:HD1	1:B:4879:VAL:HG21	1.70	0.55
1:D:794:PHE:HB2	1:D:798:ILE:HG21	1.89	0.55
1:D:2416:ILE:HD12	1:D:2416:ILE:H	1.71	0.55
1:A:2878:ALA:HA	1:A:2881:LYS:HB2	1.87	0.55
1:C:667:SER:O	1:C:669:GLN:NE2	2.40	0.55
1:C:940:LEU:HD23	1:C:943:LEU:HD21	1.88	0.55
1:C:1102:TYR:HB2	1:C:1165:MET:HE1	1.88	0.55
1:C:2410:ALA:O	1:C:2412:LYS:NZ	2.39	0.55
1:C:3200:VAL:HG23	1:C:3213:LEU:HD21	1.89	0.55
1:D:2878:ALA:HA	1:D:2881:LYS:HB2	1.87	0.55
1:D:3200:VAL:HG23	1:D:3213:LEU:HD21	1.89	0.55
1:B:1665:VAL:HG12	1:B:1673:VAL:HG11	1.89	0.55
1:D:2410:ALA:O	1:D:2412:LYS:NZ	2.39	0.55
1:B:3934:LEU:HD12	1:B:3939:LEU:HD22	1.88	0.55
1:A:794:PHE:HB2	1:A:798:ILE:HG21	1.89	0.55
1:B:2134:GLY:H	1:B:2137:GLU:HB2	1.72	0.55
1:B:3622:GLY:HA2	1:B:3625:LYS:HZ2	1.71	0.55
1:D:688:ALA:HA	2:H:41:ARG:HD2	1.89	0.55
1:D:3934:LEU:HD12	1:D:3939:LEU:HD22	1.88	0.55
1:D:4671:MET:SD	1:D:4671:MET:N	2.75	0.55
1:A:166:SER:OG	1:A:168:GLN:OE1	2.19	0.55
1:A:3015:ARG:HH22	1:A:3081:HIS:HA	1.69	0.55
1:C:527:LYS:NZ	1:C:566:GLU:OE1	2.40	0.55
1:C:3909:ILE:HG21	1:C:3969:GLU:HB3	1.89	0.55
1:D:2498:ALA:HA	1:D:2590:ARG:HH22	1.70	0.55
1:D:3622:GLY:HA2	1:D:3625:LYS:HZ2	1.72	0.55
1:C:794:PHE:HB2	1:C:798:ILE:HG21	1.89	0.55
1:C:3102:PRO:HG3	1:C:3226:ARG:HD2	1.89	0.55
1:A:688:ALA:HA	2:E:41:ARG:HD2	1.89	0.54
1:A:2416:ILE:H	1:A:2416:ILE:HD12	1.71	0.54
1:B:667:SER:O	1:B:669:GLN:NE2	2.40	0.54
1:B:794:PHE:HB2	1:B:798:ILE:HG21	1.89	0.54
1:C:688:ALA:HA	2:G:41:ARG:HD2	1.89	0.54
1:C:3622:GLY:HA2	1:C:3625:LYS:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2134:GLY:H	1:A:2137:GLU:HB2	1.72	0.54
1:A:626:ARG:HE	1:A:2131:VAL:HG11	1.71	0.54
1:B:527:LYS:NZ	1:B:566:GLU:OE1	2.40	0.54
1:B:688:ALA:HA	2:F:41:ARG:HD2	1.89	0.54
1:B:1763:ARG:NH1	1:B:1776:CYS:O	2.41	0.54
1:A:1665:VAL:HG12	1:A:1673:VAL:HG11	1.89	0.54
1:B:399:MET:HA	1:B:399:MET:HE2	1.89	0.54
1:C:2134:GLY:H	1:C:2137:GLU:HB2	1.72	0.54
1:D:527:LYS:NZ	1:D:566:GLU:OE1	2.40	0.54
1:D:1102:TYR:HB2	1:D:1165:MET:HE1	1.88	0.54
1:D:3657:MET:HE1	1:D:3659:ARG:HB2	1.88	0.54
1:A:4024:ASP:OD1	1:A:4024:ASP:N	2.41	0.54
1:B:423:VAL:O	1:B:427:ASN:ND2	2.41	0.54
1:B:4671:MET:SD	1:B:4671:MET:N	2.75	0.54
1:C:423:VAL:O	1:C:427:ASN:ND2	2.41	0.54
1:C:1665:VAL:HG12	1:C:1673:VAL:HG11	1.89	0.54
1:B:3102:PRO:HG3	1:B:3226:ARG:HD2	1.89	0.54
1:D:2358:ARG:O	1:D:2383:MET:N	2.41	0.54
1:A:1102:TYR:HB2	1:A:1165:MET:HE1	1.88	0.54
1:C:894:VAL:HG23	1:C:895:MET:HE3	1.90	0.54
1:D:2134:GLY:H	1:D:2137:GLU:HB2	1.72	0.54
1:A:912:LYS:O	1:A:914:GLN:NE2	2.38	0.54
1:B:3657:MET:HE1	1:B:3659:ARG:HB2	1.88	0.54
1:D:423:VAL:O	1:D:427:ASN:ND2	2.41	0.54
1:D:533:LEU:HD23	1:D:536:LEU:HD21	1.90	0.54
1:D:3909:ILE:HG21	1:D:3969:GLU:HB3	1.89	0.54
1:A:2358:ARG:O	1:A:2383:MET:N	2.41	0.54
1:A:399:MET:HE2	1:A:399:MET:HA	1.89	0.54
1:A:894:VAL:HG23	1:A:895:MET:HE3	1.90	0.54
1:A:1763:ARG:NH1	1:A:1776:CYS:O	2.41	0.54
1:B:2358:ARG:O	1:B:2383:MET:N	2.41	0.54
1:D:1763:ARG:NH1	1:D:1776:CYS:O	2.41	0.54
1:D:3102:PRO:HG3	1:D:3226:ARG:HD2	1.89	0.54
1:A:694:ARG:HH22	1:A:733:TRP:CD1	2.26	0.53
1:A:3200:VAL:HG23	1:A:3213:LEU:HD21	1.89	0.53
1:A:3909:ILE:HG21	1:A:3969:GLU:HB3	1.89	0.53
1:B:694:ARG:HH22	1:B:733:TRP:CD1	2.26	0.53
1:C:1763:ARG:NH1	1:C:1776:CYS:O	2.41	0.53
1:D:1665:VAL:HG12	1:D:1673:VAL:HG11	1.89	0.53
1:A:423:VAL:O	1:A:427:ASN:ND2	2.41	0.53
1:B:894:VAL:HG23	1:B:895:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3200:VAL:HG23	1:B:3213:LEU:HD21	1.89	0.53
1:D:4890:CYS:SG	1:D:4912:HIS:HE1	2.22	0.53
1:D:894:VAL:HG23	1:D:895:MET:HE3	1.90	0.53
1:A:4890:CYS:SG	1:A:4912:HIS:HE1	2.22	0.53
1:B:3909:ILE:HG21	1:B:3969:GLU:HB3	1.89	0.53
1:C:2358:ARG:O	1:C:2383:MET:N	2.41	0.53
1:A:280:LEU:HD22	1:A:296:ARG:HH21	1.74	0.53
1:A:552:SER:OG	1:A:584:GLU:OE2	2.25	0.53
1:B:280:LEU:HD22	1:B:296:ARG:HH21	1.74	0.53
1:B:4024:ASP:N	1:B:4024:ASP:OD1	2.41	0.53
1:C:3711:LYS:HD3	1:C:3714:GLU:HB2	1.91	0.53
1:D:170:SER:N	1:D:173:GLU:OE2	2.41	0.53
1:D:2987:ARG:O	1:D:2994:HIS:NE2	2.39	0.53
1:A:3711:LYS:HD3	1:A:3714:GLU:HB2	1.91	0.53
1:C:399:MET:HE2	1:C:399:MET:HA	1.89	0.53
1:C:533:LEU:HD23	1:C:536:LEU:HD21	1.90	0.53
1:C:556:ASP:OD1	1:C:556:ASP:N	2.42	0.53
1:C:694:ARG:HH22	1:C:733:TRP:CD1	2.26	0.53
1:C:4024:ASP:OD1	1:C:4024:ASP:N	2.41	0.53
1:A:1477:HIS:ND1	1:A:1478:GLU:OE1	2.42	0.53
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.41	0.53
1:A:556:ASP:OD1	1:A:556:ASP:N	2.42	0.53
1:C:1670:ASN:O	1:C:1777:TYR:OH	2.19	0.53
1:C:2987:ARG:O	1:C:2994:HIS:NE2	2.39	0.53
1:D:652:VAL:HG11	1:D:692:HIS:HB3	1.91	0.53
1:D:4616:ILE:HB	1:D:4664:ARG:HH12	1.74	0.53
1:A:527:LYS:NZ	1:A:566:GLU:OE1	2.40	0.52
1:B:158:CYS:HG	1:B:159:TRP:CD1	2.27	0.52
1:B:3711:LYS:HD3	1:B:3714:GLU:HB2	1.91	0.52
1:C:280:LEU:HD22	1:C:296:ARG:HH21	1.74	0.52
1:D:399:MET:HE2	1:D:399:MET:HA	1.89	0.52
1:D:3711:LYS:HD3	1:D:3714:GLU:HB2	1.91	0.52
1:A:3622:GLY:HA2	1:A:3625:LYS:HZ2	1.73	0.52
1:B:556:ASP:N	1:B:556:ASP:OD1	2.42	0.52
1:B:2260:ASP:OD1	1:B:2260:ASP:N	2.43	0.52
1:D:280:LEU:HD22	1:D:296:ARG:HH21	1.74	0.52
1:D:1605:LEU:O	1:D:1606:LYS:NZ	2.34	0.52
1:B:4019:PHE:O	1:B:4027:SER:OG	2.21	0.52
1:B:533:LEU:HD23	1:B:536:LEU:HD21	1.90	0.52
1:C:373:THR:OG1	1:C:392:ILE:O	2.28	0.52
1:A:373:THR:OG1	1:A:392:ILE:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1477:HIS:ND1	1:B:1478:GLU:OE1	2.42	0.52
1:C:2395:ILE:HG13	1:C:2467:MET:HE1	1.92	0.52
1:C:4616:ILE:HB	1:C:4664:ARG:HH12	1.74	0.52
1:A:652:VAL:HG11	1:A:692:HIS:HB3	1.91	0.52
1:A:2395:ILE:HG13	1:A:2467:MET:HE1	1.92	0.52
1:D:694:ARG:HH22	1:D:733:TRP:CD1	2.26	0.52
1:D:785:ASP:OD1	1:D:785:ASP:N	2.39	0.52
1:D:1477:HIS:ND1	1:D:1478:GLU:OE1	2.42	0.52
1:C:785:ASP:N	1:C:785:ASP:OD1	2.39	0.52
1:A:533:LEU:HD23	1:A:536:LEU:HD21	1.90	0.52
1:B:441:LYS:O	1:B:444:THR:OG1	2.28	0.52
1:C:169:ARG:HE	1:C:176:ARG:HE	1.57	0.52
1:C:441:LYS:O	1:C:444:THR:OG1	2.28	0.52
1:C:652:VAL:HG11	1:C:692:HIS:HB3	1.91	0.52
1:C:4009:VAL:HG11	1:C:4117:PHE:HE2	1.75	0.52
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.42	0.52
1:A:170:SER:N	1:A:173:GLU:OE2	2.41	0.52
1:B:2464:LYS:O	1:B:2468:VAL:HG13	2.10	0.52
1:D:2395:ILE:HG13	1:D:2467:MET:HE1	1.92	0.52
1:A:4616:ILE:HB	1:A:4664:ARG:HH12	1.74	0.51
1:B:1092:LYS:HD2	1:B:1647:GLU:HG2	1.92	0.51
1:C:166:SER:OG	1:C:168:GLN:OE1	2.19	0.51
1:C:290:ARG:NH1	1:C:351:THR:OG1	2.43	0.51
1:C:552:SER:OG	1:C:584:GLU:OE2	2.25	0.51
1:C:1477:HIS:ND1	1:C:1478:GLU:OE1	2.42	0.51
1:D:169:ARG:HE	1:D:176:ARG:HE	1.57	0.51
1:B:778:MET:O	1:B:1468:THR:OG1	2.28	0.51
1:B:1670:ASN:O	1:B:1777:TYR:OH	2.19	0.51
1:B:2196:CYS:HB2	1:B:2241:VAL:HG13	1.93	0.51
1:B:2395:ILE:HG13	1:B:2467:MET:HE1	1.92	0.51
1:B:2987:ARG:O	1:B:2994:HIS:NE2	2.39	0.51
1:A:1132:ASP:OD1	1:A:1132:ASP:N	2.43	0.51
1:A:2464:LYS:O	1:A:2468:VAL:HG13	2.10	0.51
1:B:4616:ILE:HB	1:B:4664:ARG:HH12	1.74	0.51
1:D:4009:VAL:HG11	1:D:4117:PHE:HE2	1.75	0.51
1:A:2987:ARG:O	1:A:2994:HIS:NE2	2.39	0.51
1:B:169:ARG:HE	1:B:176:ARG:HE	1.57	0.51
1:D:441:LYS:O	1:D:444:THR:OG1	2.28	0.51
1:D:2196:CYS:HB2	1:D:2241:VAL:HG13	1.93	0.51
1:A:2196:CYS:HB2	1:A:2241:VAL:HG13	1.93	0.51
1:A:3900:GLN:OE1	1:A:3903:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1218:GLY:HA3	1:B:1238:PRO:HB3	1.92	0.51
1:C:1092:LYS:HD2	1:C:1647:GLU:HG2	1.92	0.51
1:A:169:ARG:HE	1:A:176:ARG:HE	1.57	0.51
1:B:290:ARG:NH1	1:B:351:THR:OG1	2.43	0.51
1:C:1442:TRP:HD1	1:C:1490:ALA:HA	1.76	0.51
1:C:2196:CYS:HB2	1:C:2241:VAL:HG13	1.93	0.51
1:C:2464:LYS:O	1:C:2468:VAL:HG13	2.10	0.51
1:B:42:PHE:HB3	1:B:425:LEU:HG	1.93	0.51
1:B:1722:MET:HE1	1:B:1760:PRO:HD3	1.93	0.51
1:D:42:PHE:HB3	1:D:425:LEU:HG	1.93	0.51
1:D:158:CYS:HG	1:D:159:TRP:CD1	2.29	0.51
1:D:2464:LYS:O	1:D:2468:VAL:HG13	2.10	0.51
1:A:267:VAL:HG13	1:A:272:ARG:HB2	1.93	0.51
1:A:2234:ARG:NH2	1:A:2290:ASN:O	2.44	0.51
1:B:170:SER:N	1:B:173:GLU:OE2	2.41	0.51
1:C:158:CYS:HG	1:C:159:TRP:CD1	2.29	0.51
1:C:170:SER:N	1:C:173:GLU:OE2	2.41	0.51
1:C:912:LYS:O	1:C:914:GLN:NE2	2.38	0.51
1:C:4046:ASP:HA	1:C:4049:LYS:HG2	1.93	0.51
1:B:4890:CYS:SG	1:B:4912:HIS:HE1	2.22	0.51
1:C:1722:MET:HE1	1:C:1760:PRO:HD3	1.93	0.51
1:D:4046:ASP:HA	1:D:4049:LYS:HG2	1.93	0.51
1:A:158:CYS:HG	1:A:159:TRP:CD1	2.29	0.51
1:A:785:ASP:N	1:A:785:ASP:OD1	2.39	0.51
1:A:1092:LYS:HD2	1:A:1647:GLU:HG2	1.92	0.51
1:C:1218:GLY:HA3	1:C:1238:PRO:HB3	1.92	0.51
1:D:1722:MET:HE1	1:D:1760:PRO:HD3	1.93	0.51
1:D:2234:ARG:NH2	1:D:2290:ASN:O	2.44	0.51
1:D:3322:MET:SD	1:D:3322:MET:N	2.79	0.51
2:G:78:THR:HG22	2:G:80:ASP:H	1.76	0.51
1:A:1722:MET:HE1	1:A:1760:PRO:HD3	1.93	0.50
1:A:2260:ASP:OD1	1:A:2260:ASP:N	2.42	0.50
1:B:1763:ARG:HH12	1:B:1777:TYR:HA	1.77	0.50
1:B:4649:LYS:HE2	1:B:4669:LEU:HD12	1.94	0.50
1:D:778:MET:O	1:D:1468:THR:OG1	2.28	0.50
1:D:1442:TRP:HD1	1:D:1490:ALA:HA	1.76	0.50
1:D:1763:ARG:HH12	1:D:1777:TYR:HA	1.76	0.50
1:A:290:ARG:NH1	1:A:351:THR:OG1	2.43	0.50
1:A:1218:GLY:HA3	1:A:1238:PRO:HB3	1.92	0.50
1:B:965:LYS:NZ	1:B:1059:GLY:O	2.41	0.50
1:B:1442:TRP:HD1	1:B:1490:ALA:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4009:VAL:HG11	1:B:4117:PHE:HE2	1.75	0.50
1:C:267:VAL:HG13	1:C:272:ARG:HB2	1.93	0.50
1:C:2234:ARG:NH2	1:C:2290:ASN:O	2.44	0.50
1:D:4649:LYS:HE2	1:D:4669:LEU:HD12	1.93	0.50
1:A:4009:VAL:HG11	1:A:4117:PHE:HE2	1.75	0.50
1:B:652:VAL:HG11	1:B:692:HIS:HB3	1.91	0.50
1:D:1092:LYS:HD2	1:D:1647:GLU:HG2	1.92	0.50
2:E:78:THR:HG22	2:E:80:ASP:H	1.76	0.50
2:F:78:THR:HG22	2:F:80:ASP:H	1.76	0.50
2:G:50:ARG:HH21	2:G:53:LYS:HE3	1.77	0.50
1:B:1132:ASP:OD1	1:B:1132:ASP:N	2.43	0.50
1:D:1218:GLY:HA3	1:D:1238:PRO:HB3	1.92	0.50
1:D:4024:ASP:N	1:D:4024:ASP:OD1	2.41	0.50
2:H:78:THR:HG22	2:H:80:ASP:H	1.76	0.50
1:A:638:PRO:O	1:A:640:ARG:NH1	2.45	0.50
1:A:778:MET:O	1:A:1468:THR:OG1	2.28	0.50
1:B:2234:ARG:NH2	1:B:2290:ASN:O	2.44	0.50
1:C:4035:ASP:OD1	1:C:4035:ASP:N	2.45	0.50
1:D:373:THR:OG1	1:D:392:ILE:O	2.28	0.50
2:H:50:ARG:HH21	2:H:53:LYS:HE3	1.77	0.50
1:A:42:PHE:HB3	1:A:425:LEU:HG	1.93	0.50
1:A:2581:PRO:HB2	1:A:2584:MET:HE1	1.94	0.50
1:A:4873:ARG:NE	1:C:4867:ASP:OD1	2.38	0.50
1:B:892:LEU:HD21	1:B:1056:THR:HG21	1.94	0.50
1:B:3900:GLN:OE1	1:B:3903:ARG:NH1	2.41	0.50
1:C:42:PHE:HB3	1:C:425:LEU:HG	1.93	0.50
1:C:778:MET:O	1:C:1468:THR:OG1	2.28	0.50
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.41	0.50
1:B:638:PRO:O	1:B:640:ARG:NH1	2.45	0.50
1:C:4649:LYS:HE2	1:C:4669:LEU:HD12	1.94	0.50
1:D:625:VAL:HG12	1:D:627:SER:H	1.76	0.50
1:A:1763:ARG:HH12	1:A:1777:TYR:HA	1.77	0.50
1:A:892:LEU:HD21	1:A:1056:THR:HG21	1.94	0.50
1:A:4046:ASP:HA	1:A:4049:LYS:HG2	1.93	0.50
1:B:4046:ASP:HA	1:B:4049:LYS:HG2	1.93	0.50
1:D:909:ASP:OD1	1:D:909:ASP:N	2.44	0.50
1:D:4143:ARG:NE	1:D:4961:TYR:OH	2.43	0.50
1:A:2587:LEU:HD23	1:A:2591:LEU:HD23	1.93	0.49
1:A:4649:LYS:HE2	1:A:4669:LEU:HD12	1.94	0.49
1:B:625:VAL:HG12	1:B:627:SER:H	1.76	0.49
1:C:625:VAL:HG12	1:C:627:SER:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:PRO:O	1:C:640:ARG:NH1	2.45	0.49
1:C:2260:ASP:N	1:C:2260:ASP:OD1	2.42	0.49
1:B:2581:PRO:HB2	1:B:2584:MET:HE1	1.94	0.49
1:B:2587:LEU:HD23	1:B:2591:LEU:HD23	1.93	0.49
1:D:638:PRO:O	1:D:640:ARG:NH1	2.45	0.49
1:B:191:TYR:N	1:B:206:ALA:O	2.42	0.49
1:B:4035:ASP:OD1	1:B:4035:ASP:N	2.45	0.49
1:C:2587:LEU:HD23	1:C:2591:LEU:HD23	1.93	0.49
1:D:2094:ILE:O	1:D:2098:VAL:HG12	2.13	0.49
1:D:3900:GLN:OE1	1:D:3903:ARG:NH1	2.41	0.49
2:F:50:ARG:HH21	2:F:53:LYS:HE3	1.77	0.49
1:A:2816:ALA:N	1:A:2820:TYR:O	2.46	0.49
1:A:4143:ARG:NE	1:A:4961:TYR:OH	2.43	0.49
1:B:267:VAL:HG13	1:B:272:ARG:HB2	1.93	0.49
1:C:964:MET:O	1:C:964:MET:HE2	2.13	0.49
1:C:1763:ARG:HH12	1:C:1777:TYR:HA	1.77	0.49
1:D:267:VAL:HG13	1:D:272:ARG:HB2	1.93	0.49
1:D:764:PRO:HB2	1:D:780:GLU:HG3	1.94	0.49
1:D:912:LYS:O	1:D:914:GLN:NE2	2.38	0.49
1:D:2581:PRO:HB2	1:D:2584:MET:HE1	1.94	0.49
1:D:4035:ASP:N	1:D:4035:ASP:OD1	2.45	0.49
1:A:441:LYS:O	1:A:444:THR:OG1	2.28	0.49
1:A:964:MET:HE2	1:A:964:MET:O	2.13	0.49
1:A:1442:TRP:HD1	1:A:1490:ALA:HA	1.76	0.49
1:B:1811:VAL:H	1:B:1818:LEU:HD22	1.77	0.49
1:D:1267:HIS:CD2	1:D:1293:GLN:HB2	2.47	0.49
1:B:1267:HIS:CD2	1:B:1293:GLN:HB2	2.47	0.49
1:B:4102:THR:HG21	1:B:4132:LEU:HD21	1.95	0.49
1:C:1267:HIS:CD2	1:C:1293:GLN:HB2	2.47	0.49
1:C:2094:ILE:O	1:C:2098:VAL:HG12	2.13	0.49
1:C:3322:MET:SD	1:C:3322:MET:N	2.79	0.49
1:D:4102:THR:HG21	1:D:4132:LEU:HD21	1.95	0.49
1:A:625:VAL:HG12	1:A:627:SER:H	1.76	0.49
1:A:3320:PRO:HA	1:A:3323:GLU:HB3	1.95	0.49
1:B:128:MET:HB3	1:B:149:LEU:HD22	1.95	0.49
1:D:290:ARG:NH1	1:D:351:THR:OG1	2.43	0.49
1:D:625:VAL:O	1:D:629:GLN:HB3	2.12	0.49
1:D:2160:LEU:O	1:D:2164:LEU:HB2	2.12	0.49
1:D:3320:PRO:HA	1:D:3323:GLU:HB3	1.95	0.49
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.41	0.49
2:E:50:ARG:HH21	2:E:53:LYS:HE3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2094:ILE:O	1:B:2098:VAL:HG12	2.13	0.49
1:C:625:VAL:O	1:C:629:GLN:HB3	2.12	0.49
1:C:2581:PRO:HB2	1:C:2584:MET:HE1	1.94	0.49
1:C:3320:PRO:HA	1:C:3323:GLU:HB3	1.95	0.49
1:D:2587:LEU:HD23	1:D:2591:LEU:HD23	1.93	0.49
1:D:2816:ALA:N	1:D:2820:TYR:O	2.46	0.49
1:A:1267:HIS:CD2	1:A:1293:GLN:HB2	2.47	0.49
1:B:764:PRO:HB2	1:B:780:GLU:HG3	1.94	0.49
1:D:892:LEU:HD21	1:D:1056:THR:HG21	1.94	0.49
1:A:2357:SER:OG	1:A:2358:ARG:N	2.46	0.48
1:B:964:MET:HE2	1:B:964:MET:O	2.13	0.48
1:B:3320:PRO:HA	1:B:3323:GLU:HB3	1.95	0.48
1:A:128:MET:HB3	1:A:149:LEU:HD22	1.95	0.48
1:A:624:ALA:HB3	1:A:2131:VAL:HG23	1.95	0.48
1:A:2094:ILE:O	1:A:2098:VAL:HG12	2.13	0.48
1:C:892:LEU:HD21	1:C:1056:THR:HG21	1.94	0.48
1:D:964:MET:HE2	1:D:964:MET:O	2.13	0.48
1:D:1811:VAL:H	1:D:1818:LEU:HD22	1.77	0.48
1:D:2227:GLY:HA2	1:D:2234:ARG:HA	1.94	0.48
1:D:2795:ASP:OD1	1:D:2795:ASP:N	2.47	0.48
1:A:2160:LEU:O	1:A:2164:LEU:HB2	2.12	0.48
1:B:144:ALA:HB1	1:B:204:ASP:HB3	1.96	0.48
1:B:625:VAL:O	1:B:629:GLN:HB3	2.12	0.48
1:B:640:ARG:HA	1:B:643:LEU:HG	1.95	0.48
1:C:144:ALA:HB1	1:C:204:ASP:HB3	1.95	0.48
1:C:689:GLU:OE1	2:G:41:ARG:NH2	2.37	0.48
1:A:3687:TYR:HE1	1:A:3738:MET:HE3	1.78	0.48
1:B:2357:SER:OG	1:B:2358:ARG:N	2.46	0.48
1:C:2816:ALA:N	1:C:2820:TYR:O	2.46	0.48
1:C:3262:MET:SD	1:C:3262:MET:N	2.79	0.48
1:D:640:ARG:HA	1:D:643:LEU:HG	1.95	0.48
1:D:1172:THR:HB	1:D:1190:LEU:HD22	1.96	0.48
1:A:144:ALA:HB1	1:A:204:ASP:HB3	1.95	0.48
1:A:764:PRO:HB2	1:A:780:GLU:HG3	1.94	0.48
1:A:2227:GLY:HA2	1:A:2234:ARG:HA	1.95	0.48
1:A:4035:ASP:N	1:A:4035:ASP:OD1	2.45	0.48
1:B:2160:LEU:O	1:B:2164:LEU:HB2	2.12	0.48
1:B:2227:GLY:HA2	1:B:2234:ARG:HA	1.95	0.48
1:B:2816:ALA:N	1:B:2820:TYR:O	2.46	0.48
1:C:909:ASP:N	1:C:909:ASP:OD1	2.44	0.48
1:C:1947:MET:SD	1:C:1947:MET:N	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:N	1:D:556:ASP:OD1	2.42	0.48
1:A:625:VAL:O	1:A:629:GLN:HB3	2.12	0.48
1:B:2795:ASP:OD1	1:B:2795:ASP:N	2.46	0.48
1:C:624:ALA:HB3	1:C:2131:VAL:HG23	1.95	0.48
1:D:144:ALA:HB1	1:D:204:ASP:HB3	1.96	0.48
1:D:166:SER:OG	1:D:168:GLN:OE1	2.19	0.48
1:D:2187:THR:O	1:D:2187:THR:OG1	2.31	0.48
1:D:2604:MET:HE2	1:D:2604:MET:N	2.29	0.48
1:B:785:ASP:OD1	1:B:785:ASP:N	2.39	0.48
1:B:1172:THR:HB	1:B:1190:LEU:HD22	1.96	0.48
1:C:764:PRO:HB2	1:C:780:GLU:HG3	1.94	0.48
1:C:1172:THR:HB	1:C:1190:LEU:HD22	1.96	0.48
1:C:2160:LEU:O	1:C:2164:LEU:HB2	2.12	0.48
1:C:2848:HIS:CE1	1:C:2873:TYR:HH	2.31	0.48
1:C:3687:TYR:HE1	1:C:3738:MET:HE3	1.78	0.48
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.46	0.48
1:A:1172:THR:HB	1:A:1190:LEU:HD22	1.96	0.48
1:A:1811:VAL:H	1:A:1818:LEU:HD22	1.77	0.48
1:B:909:ASP:OD1	1:B:909:ASP:N	2.44	0.48
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.41	0.48
1:C:2604:MET:N	1:C:2604:MET:HE2	2.29	0.48
1:C:4102:THR:HG21	1:C:4132:LEU:HD21	1.95	0.48
1:C:4143:ARG:NE	1:C:4961:TYR:OH	2.43	0.48
1:D:128:MET:HB3	1:D:149:LEU:HD22	1.95	0.48
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.96	0.48
1:B:373:THR:OG1	1:B:392:ILE:O	2.28	0.48
1:B:836:HIS:ND1	1:B:839:GLU:HG3	2.29	0.48
1:B:4092:ASP:O	1:B:4096:ASN:ND2	2.47	0.48
1:C:128:MET:HB3	1:C:149:LEU:HD22	1.95	0.48
1:C:776:GLN:HE21	1:C:1472:GLU:HB2	1.79	0.48
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.96	0.48
2:E:31:LEU:N	2:E:35:LYS:O	2.47	0.48
1:A:2187:THR:O	1:A:2187:THR:OG1	2.31	0.48
1:C:836:HIS:ND1	1:C:839:GLU:HG3	2.29	0.48
1:C:4092:ASP:O	1:C:4096:ASN:ND2	2.47	0.48
1:D:624:ALA:HB3	1:D:2131:VAL:HG23	1.95	0.48
1:D:776:GLN:HE21	1:D:1472:GLU:HB2	1.79	0.48
1:D:3687:TYR:HE1	1:D:3738:MET:HE3	1.78	0.48
1:D:4592:LEU:HD23	1:D:4593:LYS:HG3	1.96	0.48
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.46	0.48
2:F:31:LEU:N	2:F:35:LYS:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4092:ASP:O	1:A:4096:ASN:ND2	2.47	0.47
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.46	0.47
1:B:3687:TYR:HE1	1:B:3738:MET:HE3	1.78	0.47
1:C:1811:VAL:H	1:C:1818:LEU:HD22	1.77	0.47
1:D:836:HIS:ND1	1:D:839:GLU:HG3	2.29	0.47
1:B:606:ARG:HH12	1:B:1654:PHE:HB3	1.79	0.47
1:B:2084:PHE:HD2	1:B:3666:LEU:HD13	1.80	0.47
2:H:31:LEU:N	2:H:35:LYS:O	2.47	0.47
1:A:446:ASP:N	1:A:446:ASP:OD1	2.48	0.47
1:A:1605:LEU:O	1:A:1606:LYS:NZ	2.34	0.47
1:A:4102:THR:HG21	1:A:4132:LEU:HD21	1.95	0.47
1:A:4592:LEU:HD23	1:A:4593:LYS:HG3	1.96	0.47
1:B:309:MET:HG3	1:B:315:LEU:HD23	1.97	0.47
1:C:2227:GLY:HA2	1:C:2234:ARG:HA	1.95	0.47
1:D:2357:SER:OG	1:D:2358:ARG:N	2.46	0.47
1:A:309:MET:HG3	1:A:315:LEU:HD23	1.97	0.47
1:A:2787:ARG:NH2	1:A:2904:ARG:O	2.48	0.47
1:B:912:LYS:O	1:B:914:GLN:NE2	2.38	0.47
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.96	0.47
1:C:1735:LYS:NZ	1:C:1929:ASP:OD2	2.41	0.47
1:C:4592:LEU:HD23	1:C:4593:LYS:HG3	1.96	0.47
1:A:606:ARG:HH12	1:A:1654:PHE:HB3	1.79	0.47
1:B:884:ARG:O	1:B:888:ASN:ND2	2.48	0.47
1:C:3458:TYR:O	1:C:3462:THR:OG1	2.25	0.47
1:D:689:GLU:OE1	2:H:41:ARG:NH2	2.37	0.47
1:D:769:ARG:HA	1:D:774:PRO:HA	1.96	0.47
1:D:4019:PHE:O	1:D:4027:SER:OG	2.21	0.47
1:A:769:ARG:HA	1:A:774:PRO:HA	1.96	0.47
1:A:909:ASP:N	1:A:909:ASP:OD1	2.44	0.47
1:B:446:ASP:OD1	1:B:446:ASP:N	2.48	0.47
1:B:776:GLN:HE21	1:B:1472:GLU:HB2	1.79	0.47
1:B:4592:LEU:HD23	1:B:4593:LYS:HG3	1.96	0.47
1:C:2495:LEU:HD22	1:C:2871:VAL:HG21	1.96	0.47
1:A:776:GLN:HE21	1:A:1472:GLU:HB2	1.79	0.47
1:A:836:HIS:ND1	1:A:839:GLU:HG3	2.29	0.47
1:A:1947:MET:SD	1:A:1947:MET:N	2.86	0.47
1:A:2084:PHE:HD2	1:A:3666:LEU:HD13	1.79	0.47
1:A:2495:LEU:HD22	1:A:2871:VAL:HG21	1.96	0.47
1:A:2604:MET:N	1:A:2604:MET:HE2	2.29	0.47
1:A:3262:MET:SD	1:A:3262:MET:N	2.79	0.47
1:B:2511:MET:HE2	1:B:2511:MET:HB2	1.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:MET:HG3	1:C:315:LEU:HD23	1.97	0.47
1:C:606:ARG:HH12	1:C:1654:PHE:HB3	1.79	0.47
1:C:656:ARG:HB3	1:C:791:VAL:HG12	1.97	0.47
1:C:2460:CYS:HB3	1:C:2463:HIS:CE1	2.50	0.47
1:D:446:ASP:OD1	1:D:446:ASP:N	2.48	0.47
1:D:884:ARG:O	1:D:888:ASN:ND2	2.48	0.47
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.96	0.47
1:D:4092:ASP:O	1:D:4096:ASN:ND2	2.47	0.47
1:A:561:ARG:NH2	1:A:567:ALA:O	2.48	0.47
1:A:2460:CYS:HB3	1:A:2463:HIS:CE1	2.50	0.47
1:C:640:ARG:HA	1:C:643:LEU:HG	1.95	0.47
1:C:2787:ARG:NH2	1:C:2904:ARG:O	2.48	0.47
2:G:31:LEU:N	2:G:35:LYS:O	2.47	0.47
1:B:624:ALA:HB3	1:B:2131:VAL:HG23	1.95	0.47
1:B:632:ILE:HA	1:B:635:ASN:HB2	1.97	0.47
1:B:2495:LEU:HD22	1:B:2871:VAL:HG21	1.96	0.47
1:C:446:ASP:OD1	1:C:446:ASP:N	2.48	0.47
1:D:191:TYR:N	1:D:206:ALA:O	2.42	0.47
1:A:243:GLU:HG3	1:A:262:TYR:HD2	1.80	0.47
1:A:640:ARG:HA	1:A:643:LEU:HG	1.95	0.47
1:A:4025:LEU:HD22	1:A:4087:HIS:HA	1.97	0.47
1:B:561:ARG:NH2	1:B:567:ALA:O	2.48	0.47
1:B:587:ASN:HA	1:B:628:ASN:HB2	1.97	0.47
1:B:1006:VAL:HA	1:B:1009:ARG:HG2	1.97	0.47
1:B:1947:MET:SD	1:B:1947:MET:N	2.86	0.47
1:C:191:TYR:N	1:C:206:ALA:O	2.42	0.47
1:C:2258:GLU:N	1:C:2258:GLU:OE2	2.48	0.47
1:D:1947:MET:SD	1:D:1947:MET:N	2.86	0.47
1:D:2084:PHE:HD2	1:D:3666:LEU:HD13	1.79	0.47
1:D:3045:MET:HE1	1:D:3093:ILE:HG21	1.97	0.47
1:A:632:ILE:HA	1:A:635:ASN:HB2	1.98	0.46
1:A:656:ARG:HB3	1:A:791:VAL:HG12	1.97	0.46
1:A:884:ARG:O	1:A:888:ASN:ND2	2.48	0.46
1:B:656:ARG:HB3	1:B:791:VAL:HG12	1.97	0.46
1:B:2258:GLU:OE2	1:B:2258:GLU:N	2.48	0.46
1:B:2460:CYS:HB3	1:B:2463:HIS:CE1	2.50	0.46
1:B:2604:MET:HE2	1:B:2604:MET:N	2.29	0.46
1:C:243:GLU:HG3	1:C:262:TYR:HD2	1.80	0.46
1:C:1097:LYS:HA	1:C:1097:LYS:HD3	1.74	0.46
1:C:2795:ASP:OD1	1:C:2795:ASP:N	2.46	0.46
1:D:2876:LEU:HD22	1:D:2880:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4025:LEU:HD22	1:D:4087:HIS:HA	1.97	0.46
1:A:191:TYR:N	1:A:206:ALA:O	2.42	0.46
1:A:587:ASN:HA	1:A:628:ASN:HB2	1.97	0.46
1:B:552:SER:OG	1:B:584:GLU:OE2	2.25	0.46
1:B:885:LEU:O	1:B:889:ILE:HG12	2.16	0.46
1:B:2787:ARG:NH2	1:B:2904:ARG:O	2.48	0.46
1:B:2876:LEU:HD22	1:B:2880:GLU:HG3	1.97	0.46
1:B:3458:TYR:O	1:B:3462:THR:OG1	2.25	0.46
1:C:3225:ILE:O	1:C:3269:SER:OG	2.33	0.46
1:D:656:ARG:HB3	1:D:791:VAL:HG12	1.97	0.46
1:D:2460:CYS:HB3	1:D:2463:HIS:CE1	2.50	0.46
1:A:2795:ASP:OD1	1:A:2795:ASP:N	2.47	0.46
1:A:4483:ILE:HG22	1:A:4486:GLN:H	1.81	0.46
1:C:884:ARG:O	1:C:888:ASN:ND2	2.48	0.46
1:C:3045:MET:HE1	1:C:3093:ILE:HG21	1.97	0.46
1:D:869:THR:OG1	1:D:1002:ASN:OD1	2.29	0.46
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.48	0.46
1:A:2258:GLU:N	1:A:2258:GLU:OE2	2.48	0.46
1:B:3225:ILE:O	1:B:3269:SER:OG	2.33	0.46
1:C:1679:SER:HB2	1:C:1769:PHE:CZ	2.51	0.46
1:C:1810:PRO:HG2	1:C:1814:THR:HA	1.97	0.46
1:C:4025:LEU:HD22	1:C:4087:HIS:HA	1.97	0.46
1:D:2258:GLU:OE2	1:D:2258:GLU:N	2.48	0.46
1:D:2495:LEU:HD22	1:D:2871:VAL:HG21	1.96	0.46
1:A:1810:PRO:HG2	1:A:1814:THR:HA	1.97	0.46
1:A:4074:ASN:HB3	1:A:4076:THR:HG22	1.98	0.46
1:B:769:ARG:HA	1:B:774:PRO:HA	1.96	0.46
1:B:1810:PRO:HG2	1:B:1814:THR:HA	1.97	0.46
1:B:4025:LEU:HD22	1:B:4087:HIS:HA	1.97	0.46
1:C:416:ALA:HA	1:C:419:ILE:HD11	1.98	0.46
1:C:632:ILE:HA	1:C:635:ASN:HB2	1.97	0.46
1:C:869:THR:OG1	1:C:1002:ASN:OD1	2.29	0.46
1:C:2876:LEU:HD22	1:C:2880:GLU:HG3	1.97	0.46
1:D:2848:HIS:CG	1:D:2873:TYR:HH	2.32	0.46
1:D:3225:ILE:O	1:D:3269:SER:OG	2.33	0.46
1:A:1679:SER:HB2	1:A:1769:PHE:CZ	2.51	0.46
1:B:4143:ARG:NE	1:B:4961:TYR:OH	2.43	0.46
1:C:882:ARG:NH2	1:C:933:LEU:O	2.49	0.46
1:D:309:MET:HG3	1:D:315:LEU:HD23	1.97	0.46
1:D:372:LEU:HD22	1:D:393:MET:HE1	1.97	0.46
1:D:490:GLN:HG3	1:D:494:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ARG:HH12	1:D:1654:PHE:HB3	1.79	0.46
1:D:965:LYS:NZ	1:D:1059:GLY:O	2.41	0.46
1:A:372:LEU:HD22	1:A:393:MET:HE1	1.97	0.46
1:A:882:ARG:NH2	1:A:933:LEU:O	2.49	0.46
1:B:4059:GLN:NE2	1:B:4063:GLU:OE1	2.49	0.46
1:B:4863:GLY:HA2	1:D:4866:ILE:HD13	1.98	0.46
1:C:587:ASN:HA	1:C:628:ASN:HB2	1.97	0.46
1:C:4074:ASN:HB3	1:C:4076:THR:HG22	1.98	0.46
1:C:4483:ILE:HG22	1:C:4486:GLN:H	1.81	0.46
1:D:561:ARG:NH2	1:D:567:ALA:O	2.48	0.46
1:D:2787:ARG:NH2	1:D:2904:ARG:O	2.48	0.46
1:A:2876:LEU:HD22	1:A:2880:GLU:HG3	1.97	0.46
1:A:3225:ILE:O	1:A:3269:SER:OG	2.33	0.46
1:A:4832:ASP:OD1	1:A:4832:ASP:N	2.49	0.46
1:B:1097:LYS:HA	1:B:1097:LYS:HD3	1.74	0.46
1:B:3512:ILE:H	1:B:3552:GLY:HA2	1.81	0.46
1:C:561:ARG:NH2	1:C:567:ALA:O	2.48	0.46
1:C:4019:PHE:O	1:C:4027:SER:OG	2.21	0.46
1:D:632:ILE:HA	1:D:635:ASN:HB2	1.97	0.46
1:D:885:LEU:O	1:D:889:ILE:HG12	2.16	0.46
1:D:4074:ASN:HB3	1:D:4076:THR:HG22	1.98	0.46
1:B:695:VAL:HG21	1:B:755:ILE:HG21	1.98	0.46
1:B:2166:MET:HE2	1:B:2166:MET:HB3	1.83	0.46
1:B:2473:ARG:HA	1:B:2473:ARG:HD2	1.76	0.46
1:B:4074:ASN:HB3	1:B:4076:THR:HG22	1.98	0.46
1:C:418:VAL:O	1:C:422:THR:OG1	2.32	0.46
1:D:1679:SER:HB2	1:D:1769:PHE:CZ	2.51	0.46
1:A:416:ALA:HA	1:A:419:ILE:HD11	1.98	0.46
1:A:680:ASP:OD2	1:A:680:ASP:N	2.49	0.46
1:A:695:VAL:HG21	1:A:755:ILE:HG21	1.98	0.46
1:A:1735:LYS:NZ	1:A:1929:ASP:OD2	2.41	0.46
1:A:4059:GLN:NE2	1:A:4063:GLU:OE1	2.49	0.46
1:C:2694:MET:O	1:C:3051:SER:OG	2.34	0.46
1:D:882:ARG:NH2	1:D:933:LEU:O	2.49	0.46
1:A:367:ASP:OD1	1:A:367:ASP:N	2.48	0.45
1:A:718:VAL:HG23	1:A:793:SER:HB3	1.98	0.45
1:A:2242:ALA:O	1:A:2246:VAL:HG22	2.17	0.45
1:B:372:LEU:HD22	1:B:393:MET:HE1	1.97	0.45
1:B:3045:MET:HE1	1:B:3093:ILE:HG21	1.97	0.45
1:B:4009:VAL:HA	1:B:4012:ILE:HG12	1.98	0.45
1:B:4046:ASP:OD1	1:B:4046:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4483:ILE:HG22	1:B:4486:GLN:H	1.81	0.45
1:C:718:VAL:HG23	1:C:793:SER:HB3	1.98	0.45
1:C:4941:LYS:HB3	1:C:4941:LYS:HE2	1.80	0.45
1:B:367:ASP:OD1	1:B:367:ASP:N	2.48	0.45
1:B:1679:SER:HB2	1:B:1769:PHE:CZ	2.51	0.45
1:B:2242:ALA:O	1:B:2246:VAL:HG22	2.17	0.45
1:C:372:LEU:HD22	1:C:393:MET:HE1	1.97	0.45
1:C:841:LYS:HG2	1:C:844:ARG:HE	1.81	0.45
1:C:885:LEU:O	1:C:889:ILE:HG12	2.16	0.45
1:D:1006:VAL:HA	1:D:1009:ARG:HG2	1.97	0.45
1:D:2473:ARG:HD2	1:D:2473:ARG:HA	1.76	0.45
1:A:3322:MET:SD	1:A:3322:MET:N	2.79	0.45
1:A:4046:ASP:N	1:A:4046:ASP:OD1	2.48	0.45
1:B:912:LYS:HB3	1:B:914:GLN:HG2	1.99	0.45
1:C:490:GLN:HG3	1:C:494:MET:SD	2.56	0.45
1:D:587:ASN:HA	1:D:628:ASN:HB2	1.97	0.45
1:D:1810:PRO:HG2	1:D:1814:THR:HA	1.97	0.45
1:A:885:LEU:O	1:A:889:ILE:HG12	2.16	0.45
1:A:4009:VAL:HA	1:A:4012:ILE:HG12	1.98	0.45
1:B:490:GLN:HG3	1:B:494:MET:SD	2.56	0.45
1:C:1006:VAL:HA	1:C:1009:ARG:HG2	1.97	0.45
1:C:2242:ALA:O	1:C:2246:VAL:HG22	2.17	0.45
1:C:3512:ILE:H	1:C:3552:GLY:HA2	1.81	0.45
1:D:243:GLU:HG3	1:D:262:TYR:HD2	1.80	0.45
1:D:416:ALA:HA	1:D:419:ILE:HD11	1.98	0.45
1:D:841:LYS:HG2	1:D:844:ARG:HE	1.81	0.45
1:A:1006:VAL:HA	1:A:1009:ARG:HG2	1.97	0.45
1:B:1605:LEU:O	1:B:1606:LYS:NZ	2.34	0.45
1:C:680:ASP:OD2	1:C:680:ASP:N	2.49	0.45
1:C:769:ARG:HA	1:C:774:PRO:HA	1.96	0.45
1:C:965:LYS:NZ	1:C:1059:GLY:O	2.41	0.45
1:C:2084:PHE:HD2	1:C:3666:LEU:HD13	1.79	0.45
1:C:2654:LYS:HE2	1:C:2656:TYR:HD2	1.82	0.45
1:C:4873:ARG:NE	1:D:4867:ASP:OD1	2.38	0.45
1:D:3512:ILE:H	1:D:3552:GLY:HA2	1.81	0.45
1:A:552:SER:HB2	1:A:585:ALA:HB2	1.99	0.45
1:B:243:GLU:HG3	1:B:262:TYR:HD2	1.80	0.45
1:B:2171:MET:O	1:B:2175:VAL:HG23	2.17	0.45
1:B:3984:MET:HE2	1:B:3984:MET:HB2	1.80	0.45
1:C:3900:GLN:OE1	1:C:3903:ARG:NH1	2.41	0.45
1:C:4059:GLN:NE2	1:C:4063:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4721:LEU:HD23	1:C:4721:LEU:HA	1.84	0.45
1:D:680:ASP:OD2	1:D:680:ASP:N	2.49	0.45
1:D:2694:MET:O	1:D:3051:SER:OG	2.35	0.45
1:A:3512:ILE:H	1:A:3552:GLY:HA2	1.81	0.45
1:B:882:ARG:NH2	1:B:933:LEU:O	2.49	0.45
1:B:1905:MET:HA	1:B:1905:MET:HE3	1.98	0.45
1:C:695:VAL:HG21	1:C:755:ILE:HG21	1.98	0.45
1:D:2129:LEU:HD22	1:D:2169:THR:HG23	1.98	0.45
1:D:4059:GLN:NE2	1:D:4063:GLU:OE1	2.49	0.45
1:D:4483:ILE:HG22	1:D:4486:GLN:H	1.81	0.45
1:A:490:GLN:HG3	1:A:494:MET:SD	2.56	0.45
1:A:890:HIS:HA	1:A:893:TRP:CD1	2.52	0.45
1:A:1905:MET:HE3	1:A:1905:MET:HA	1.98	0.45
1:A:2171:MET:O	1:A:2175:VAL:HG23	2.17	0.45
1:A:2848:HIS:ND1	1:A:2873:TYR:OH	2.40	0.45
1:B:552:SER:HB2	1:B:585:ALA:HB2	1.99	0.45
1:D:2713:PRO:HD2	1:D:2782:LEU:HD13	1.99	0.45
1:D:4596:LEU:HD12	1:D:4596:LEU:HA	1.78	0.45
1:A:841:LYS:HG2	1:A:844:ARG:HE	1.81	0.45
1:A:965:LYS:NZ	1:A:1059:GLY:O	2.41	0.45
1:A:2347:GLU:HA	1:A:2350:ILE:HG12	1.99	0.45
1:A:3045:MET:HE1	1:A:3093:ILE:HG21	1.97	0.45
1:D:552:SER:OG	1:D:584:GLU:OE2	2.25	0.45
1:D:2654:LYS:HE2	1:D:2656:TYR:HD2	1.82	0.45
1:D:3291:GLU:OE1	1:D:3301:PHE:N	2.50	0.45
1:D:4009:VAL:HA	1:D:4012:ILE:HG12	1.98	0.45
1:A:2455:MET:HE3	1:A:2455:MET:HA	1.99	0.45
1:B:890:HIS:HA	1:B:893:TRP:CD1	2.52	0.45
1:B:2296:ARG:HA	1:B:2296:ARG:HD3	1.87	0.45
1:C:651:HIS:CE1	1:C:1605:LEU:HD11	2.52	0.45
1:C:2166:MET:O	1:C:2170:VAL:HG23	2.17	0.45
1:C:2455:MET:HE3	1:C:2455:MET:HA	1.99	0.45
1:D:120:LEU:HB2	1:D:159:TRP:CZ3	2.52	0.45
1:D:912:LYS:HB3	1:D:914:GLN:HG2	1.99	0.45
1:D:1670:ASN:O	1:D:1777:TYR:OH	2.19	0.45
1:D:1905:MET:HE3	1:D:1905:MET:HA	1.98	0.45
1:D:2583:MET:SD	1:D:2583:MET:N	2.90	0.45
1:B:416:ALA:HA	1:B:419:ILE:HD11	1.98	0.44
1:B:1106:GLU:HB2	1:B:1214:ARG:HB3	2.00	0.44
1:B:2065:MET:HE2	1:B:2065:MET:HB2	1.84	0.44
1:B:2347:GLU:HA	1:B:2350:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2583:MET:SD	1:B:2583:MET:N	2.90	0.44
1:C:1905:MET:HE3	1:C:1905:MET:HA	1.98	0.44
1:C:3291:GLU:OE1	1:C:3301:PHE:N	2.50	0.44
1:C:3984:MET:HE2	1:C:3984:MET:HB2	1.80	0.44
1:D:1106:GLU:HB2	1:D:1214:ARG:HB3	2.00	0.44
1:D:2347:GLU:HA	1:D:2350:ILE:HG12	1.99	0.44
1:D:2642:LYS:HG2	1:D:2645:TRP:HE3	1.82	0.44
1:D:3939:LEU:HD21	1:D:3980:MET:HE1	1.99	0.44
1:A:2000:GLU:O	1:A:2004:THR:OG1	2.32	0.44
1:A:2583:MET:SD	1:A:2583:MET:N	2.90	0.44
1:B:120:LEU:HB2	1:B:159:TRP:CZ3	2.52	0.44
1:B:651:HIS:CE1	1:B:1605:LEU:HD11	2.52	0.44
1:B:2129:LEU:HD22	1:B:2169:THR:HG23	1.98	0.44
1:B:2187:THR:O	1:B:2187:THR:OG1	2.31	0.44
1:B:2654:LYS:HE2	1:B:2656:TYR:HD2	1.82	0.44
1:C:120:LEU:HB2	1:C:159:TRP:CZ3	2.52	0.44
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.87	0.44
1:C:890:HIS:HA	1:C:893:TRP:CD1	2.52	0.44
1:D:651:HIS:CE1	1:D:1605:LEU:HD11	2.52	0.44
1:D:695:VAL:HG21	1:D:755:ILE:HG21	1.98	0.44
1:A:120:LEU:HB2	1:A:159:TRP:CZ3	2.52	0.44
1:A:651:HIS:CE1	1:A:1605:LEU:HD11	2.52	0.44
1:A:2694:MET:O	1:A:3051:SER:OG	2.34	0.44
1:B:73:LEU:O	1:B:118:ALA:N	2.51	0.44
1:B:680:ASP:OD2	1:B:680:ASP:N	2.49	0.44
1:B:3939:LEU:HD21	1:B:3980:MET:HE1	2.00	0.44
1:C:2357:SER:OG	1:C:2358:ARG:N	2.46	0.44
1:C:3939:LEU:HD21	1:C:3980:MET:HE1	2.00	0.44
1:D:296:ARG:NH1	1:D:327:THR:OG1	2.51	0.44
1:D:650:ASN:ND2	1:D:687:THR:OG1	2.43	0.44
1:D:2242:ALA:O	1:D:2246:VAL:HG22	2.17	0.44
1:D:2502:ASP:N	1:D:2502:ASP:OD1	2.50	0.44
1:A:3939:LEU:HD21	1:A:3980:MET:HE1	2.00	0.44
1:B:841:LYS:HG2	1:B:844:ARG:HE	1.81	0.44
1:B:995:MET:HE3	1:B:1064:LEU:HD21	1.99	0.44
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.46	0.44
1:C:2129:LEU:HD22	1:C:2169:THR:HG23	1.98	0.44
1:C:2347:GLU:HA	1:C:2350:ILE:HG12	1.99	0.44
1:D:890:HIS:HA	1:D:893:TRP:CD1	2.52	0.44
1:A:249:SER:OG	1:A:251:GLU:OE1	2.27	0.44
1:A:2129:LEU:HD22	1:A:2169:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2654:LYS:HE2	1:A:2656:TYR:HD2	1.82	0.44
1:A:3291:GLU:OE1	1:A:3301:PHE:N	2.50	0.44
1:B:3291:GLU:OE1	1:B:3301:PHE:N	2.50	0.44
1:C:419:ILE:HG21	1:C:488:LEU:HD22	1.99	0.44
1:C:579:LEU:HG	1:C:623:VAL:HG23	1.99	0.44
1:C:1420:LEU:HG	1:C:1421:MET:HG3	2.00	0.44
1:C:2171:MET:O	1:C:2175:VAL:HG23	2.17	0.44
1:C:2583:MET:SD	1:C:2583:MET:N	2.90	0.44
1:A:419:ILE:HG21	1:A:488:LEU:HD22	1.99	0.44
1:A:912:LYS:HB3	1:A:914:GLN:HG2	1.99	0.44
1:B:579:LEU:HG	1:B:623:VAL:HG23	1.99	0.44
1:B:2166:MET:O	1:B:2170:VAL:HG23	2.17	0.44
1:B:3923:ILE:HG22	1:B:3930:ASN:HB3	2.00	0.44
1:C:249:SER:OG	1:C:251:GLU:OE1	2.27	0.44
1:C:912:LYS:HB3	1:C:914:GLN:HG2	1.99	0.44
1:C:2593:PHE:HD2	1:C:2595:VAL:HG23	1.83	0.44
1:C:4009:VAL:HA	1:C:4012:ILE:HG12	1.98	0.44
2:H:23:CYS:HB3	2:H:104:LEU:HD11	2.00	0.44
1:A:1420:LEU:HG	1:A:1421:MET:HG3	2.00	0.44
1:A:2713:PRO:HD2	1:A:2782:LEU:HD13	1.99	0.44
1:A:4941:LYS:HB3	1:A:4941:LYS:HE2	1.80	0.44
1:B:650:ASN:ND2	1:B:687:THR:OG1	2.43	0.44
1:B:718:VAL:HG23	1:B:793:SER:HB3	1.98	0.44
1:B:2694:MET:O	1:B:3051:SER:OG	2.34	0.44
1:C:296:ARG:NH1	1:C:327:THR:OG1	2.51	0.44
1:C:552:SER:HB2	1:C:585:ALA:HB2	1.99	0.44
1:C:2642:LYS:HG2	1:C:2645:TRP:HE3	1.83	0.44
1:D:718:VAL:HG23	1:D:793:SER:HB3	1.98	0.44
1:D:1663:SER:OG	1:D:1709:ASP:OD2	2.31	0.44
1:D:2171:MET:O	1:D:2175:VAL:HG23	2.17	0.44
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.87	0.44
1:A:3058:ALA:O	1:A:3062:ASN:HB2	2.18	0.44
1:B:2025:ARG:HA	1:B:2025:ARG:HD2	1.85	0.44
1:C:921:PHE:HA	1:C:924:LEU:HD12	2.00	0.44
1:C:1786:ASP:OD1	1:C:1786:ASP:N	2.51	0.44
1:C:4028:SER:HB2	1:C:4032:LYS:HE2	2.00	0.44
1:C:4046:ASP:N	1:C:4046:ASP:OD1	2.48	0.44
1:D:424:PHE:HA	1:D:427:ASN:HD21	1.83	0.44
1:D:2593:PHE:HD2	1:D:2595:VAL:HG23	1.83	0.44
1:D:3923:ILE:HG22	1:D:3930:ASN:HB3	2.00	0.44
1:A:579:LEU:HG	1:A:623:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:GLU:HB2	1:A:1214:ARG:HB3	2.00	0.44
1:B:2455:MET:HE3	1:B:2455:MET:HA	1.99	0.44
1:D:552:SER:HB2	1:D:585:ALA:HB2	1.99	0.44
1:D:995:MET:HE3	1:D:1064:LEU:HD21	2.00	0.44
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.53	0.44
1:A:418:VAL:O	1:A:422:THR:OG1	2.32	0.43
1:A:3953:MET:HE2	1:A:3953:MET:HA	2.00	0.43
1:B:921:PHE:HA	1:B:924:LEU:HD12	2.00	0.43
1:B:2213:MET:HE2	1:B:2213:MET:HB3	1.94	0.43
1:B:4500:MET:HG3	1:B:4585:CYS:SG	2.58	0.43
1:B:4867:ASP:OD1	1:D:4873:ARG:NE	2.38	0.43
1:C:1132:ASP:OD1	1:C:1132:ASP:N	2.43	0.43
1:C:2000:GLU:O	1:C:2004:THR:OG1	2.32	0.43
1:C:4500:MET:HG3	1:C:4585:CYS:SG	2.58	0.43
1:D:2025:ARG:HA	1:D:2025:ARG:HD2	1.85	0.43
1:D:4832:ASP:OD1	1:D:4832:ASP:N	2.49	0.43
1:A:995:MET:HE3	1:A:1064:LEU:HD21	1.99	0.43
1:A:1992:ARG:HD2	1:A:1997:ASP:HA	2.00	0.43
1:B:296:ARG:NH1	1:B:327:THR:OG1	2.51	0.43
1:B:1735:LYS:NZ	1:B:1929:ASP:OD2	2.41	0.43
1:B:2209:ASN:OD1	1:B:2210:GLN:N	2.52	0.43
1:B:2642:LYS:HG2	1:B:2645:TRP:HE3	1.83	0.43
1:B:2713:PRO:HD2	1:B:2782:LEU:HD13	1.99	0.43
1:C:995:MET:HE3	1:C:1064:LEU:HD21	1.99	0.43
1:C:1106:GLU:HB2	1:C:1214:ARG:HB3	2.00	0.43
1:C:2713:PRO:HD2	1:C:2782:LEU:HD13	1.99	0.43
1:D:73:LEU:O	1:D:118:ALA:N	2.51	0.43
1:D:121:LEU:HD12	1:D:121:LEU:HA	1.87	0.43
2:F:23:CYS:HB3	2:F:104:LEU:HD11	2.00	0.43
1:A:245:LEU:HB2	1:A:275:TRP:HH2	1.84	0.43
1:A:424:PHE:HA	1:A:427:ASN:HD21	1.83	0.43
1:A:2166:MET:O	1:A:2170:VAL:HG23	2.17	0.43
1:A:4500:MET:HG3	1:A:4585:CYS:SG	2.58	0.43
1:B:419:ILE:HG21	1:B:488:LEU:HD22	1.99	0.43
1:B:1064:LEU:HD12	1:B:1064:LEU:HA	1.89	0.43
1:B:1282:CYS:O	1:B:1284:LYS:N	2.50	0.43
1:B:1786:ASP:N	1:B:1786:ASP:OD1	2.51	0.43
1:B:2196:CYS:SG	1:B:2197:ARG:N	2.92	0.43
1:B:2502:ASP:N	1:B:2502:ASP:OD1	2.50	0.43
1:C:515:ALA:HB1	1:C:521:GLU:HA	2.01	0.43
1:D:1735:LYS:NZ	1:D:1929:ASP:OD2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4833:PRO:HG3	1:D:4842:ARG:HG2	2.00	0.43
2:G:23:CYS:HB3	2:G:104:LEU:HD11	2.00	0.43
1:A:296:ARG:NH1	1:A:327:THR:OG1	2.51	0.43
1:A:2771:ARG:HE	1:A:2775:LYS:HD2	1.83	0.43
1:A:4833:PRO:HG3	1:A:4842:ARG:HG2	2.00	0.43
1:B:1663:SER:OG	1:B:1709:ASP:OD2	2.31	0.43
1:B:1993:ASP:OD1	1:B:1993:ASP:N	2.51	0.43
1:B:2256:LEU:HD23	1:B:2256:LEU:HA	1.90	0.43
1:C:1992:ARG:HD2	1:C:1997:ASP:HA	2.00	0.43
1:C:2502:ASP:OD1	1:C:2502:ASP:N	2.50	0.43
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.53	0.43
1:C:3923:ILE:HG22	1:C:3930:ASN:HB3	2.00	0.43
1:C:3953:MET:HE2	1:C:3953:MET:HA	2.00	0.43
1:D:1600:MET:HE2	1:D:1600:MET:HB3	1.90	0.43
1:D:4500:MET:HG3	1:D:4585:CYS:SG	2.58	0.43
1:A:2593:PHE:HD2	1:A:2595:VAL:HG23	1.83	0.43
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.53	0.43
1:B:2000:GLU:O	1:B:2004:THR:OG1	2.32	0.43
1:B:3654:ASP:OD1	1:B:3654:ASP:N	2.52	0.43
1:B:4833:PRO:HG3	1:B:4842:ARG:HG2	2.00	0.43
1:C:245:LEU:HB2	1:C:275:TRP:HH2	1.84	0.43
1:C:1446:ILE:HG21	1:C:1543:ALA:HB3	2.00	0.43
1:C:4833:PRO:HG3	1:C:4842:ARG:HG2	2.00	0.43
1:D:515:ALA:HB1	1:D:521:GLU:HA	2.01	0.43
1:D:1282:CYS:O	1:D:1284:LYS:N	2.50	0.43
1:D:2166:MET:O	1:D:2170:VAL:HG23	2.17	0.43
1:D:4028:SER:HB2	1:D:4032:LYS:HE2	2.00	0.43
1:A:921:PHE:HA	1:A:924:LEU:HD12	2.00	0.43
1:A:1663:SER:OG	1:A:1709:ASP:OD2	2.31	0.43
1:A:2196:CYS:SG	1:A:2197:ARG:N	2.92	0.43
1:B:2593:PHE:HD2	1:B:2595:VAL:HG23	1.83	0.43
1:B:2771:ARG:HE	1:B:2775:LYS:HD2	1.83	0.43
1:C:4747:MET:HE3	1:C:4747:MET:HB3	1.84	0.43
1:D:245:LEU:HB2	1:D:275:TRP:HH2	1.84	0.43
1:D:419:ILE:HG21	1:D:488:LEU:HD22	1.99	0.43
1:D:579:LEU:HG	1:D:623:VAL:HG23	1.99	0.43
1:D:891:GLU:O	1:D:895:MET:HG2	2.19	0.43
1:D:921:PHE:HA	1:D:924:LEU:HD12	2.00	0.43
1:D:2455:MET:HE3	1:D:2455:MET:HA	1.99	0.43
1:A:436:LEU:HD12	1:A:447:LEU:HD13	2.01	0.43
1:A:1446:ILE:HG21	1:A:1543:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:ASP:OD1	1:A:1786:ASP:N	2.51	0.43
1:A:2642:LYS:HG2	1:A:2645:TRP:CE3	2.54	0.43
1:B:418:VAL:O	1:B:422:THR:OG1	2.32	0.43
1:B:1299:ILE:HG21	1:B:1455:THR:HA	2.00	0.43
1:B:2642:LYS:HG2	1:B:2645:TRP:CE3	2.54	0.43
1:B:3058:ALA:O	1:B:3062:ASN:HB2	2.18	0.43
1:B:4502:MET:HE3	1:B:4502:MET:HB3	1.89	0.43
1:C:2588:LEU:HA	1:C:2591:LEU:HG	2.00	0.43
1:C:2771:ARG:HE	1:C:2775:LYS:HD2	1.83	0.43
1:C:3058:ALA:O	1:C:3062:ASN:HB2	2.18	0.43
1:C:4196:ILE:HG12	1:C:4922:MET:HB2	2.01	0.43
1:C:4809:LEU:HD12	1:C:4809:LEU:HA	1.85	0.43
1:C:4832:ASP:OD1	1:C:4832:ASP:N	2.49	0.43
1:D:1420:LEU:HG	1:D:1421:MET:HG3	2.00	0.43
1:D:2642:LYS:HG2	1:D:2645:TRP:CE3	2.54	0.43
1:D:3058:ALA:O	1:D:3062:ASN:HB2	2.18	0.43
1:A:869:THR:OG1	1:A:1002:ASN:OD1	2.29	0.43
1:A:2398:LEU:HD23	1:A:2398:LEU:HA	1.82	0.43
1:A:2588:LEU:HA	1:A:2591:LEU:HG	2.00	0.43
1:A:3923:ILE:HG22	1:A:3930:ASN:HB3	2.00	0.43
1:B:2034:LYS:HA	1:B:2037:TYR:CE2	2.53	0.43
1:D:2593:PHE:CD2	1:D:2595:VAL:HG23	2.54	0.43
1:D:3984:MET:HE2	1:D:3984:MET:HB2	1.79	0.43
1:A:2642:LYS:HG2	1:A:2645:TRP:HE3	1.83	0.43
1:B:227:TYR:CD2	1:B:352:SER:HB2	2.54	0.43
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.59	0.43
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.53	0.43
1:B:4028:SER:HB2	1:B:4032:LYS:HE2	2.00	0.43
1:C:707:PRO:HD3	1:C:1604:PHE:CE1	2.54	0.43
1:C:1064:LEU:HD12	1:C:1064:LEU:HA	1.89	0.43
1:C:2196:CYS:SG	1:C:2197:ARG:N	2.92	0.43
1:C:2473:ARG:HA	1:C:2473:ARG:HD2	1.76	0.43
1:C:4031:PHE:HZ	1:C:4040:GLY:HA2	1.84	0.43
1:D:1064:LEU:HD12	1:D:1064:LEU:HA	1.89	0.43
1:D:2771:ARG:HE	1:D:2775:LYS:HD2	1.83	0.43
1:D:4077:LEU:HD23	1:D:4077:LEU:HA	1.87	0.43
1:A:1029:ASN:OD1	1:A:1029:ASN:N	2.52	0.43
1:A:2065:MET:SD	1:A:2083:MET:HG3	2.59	0.43
1:A:2097:LEU:HD12	1:A:2097:LEU:HA	1.89	0.43
1:A:2269:ALA:HA	1:A:2328:GLU:HB2	2.01	0.43
1:A:4196:ILE:HG12	1:A:4922:MET:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:GLU:O	1:B:895:MET:HG2	2.19	0.43
1:B:929:ARG:HA	1:B:929:ARG:HD2	1.93	0.43
1:B:1420:LEU:HG	1:B:1421:MET:HG3	2.00	0.43
1:B:1432:ILE:HG23	1:B:1434:PRO:HD3	2.01	0.43
1:C:647:ARG:HE	1:C:648:LEU:H	1.67	0.43
1:C:1432:ILE:HG23	1:C:1434:PRO:HD3	2.01	0.43
1:D:894:VAL:HG23	1:D:895:MET:CE	2.49	0.43
1:A:515:ALA:HB1	1:A:521:GLU:HA	2.01	0.42
1:A:647:ARG:HE	1:A:648:LEU:H	1.66	0.42
1:A:1299:ILE:HG21	1:A:1455:THR:HA	2.00	0.42
1:A:2593:PHE:CD2	1:A:2595:VAL:HG23	2.54	0.42
1:B:869:THR:OG1	1:B:1002:ASN:OD1	2.29	0.42
1:B:2593:PHE:CD2	1:B:2595:VAL:HG23	2.54	0.42
1:C:367:ASP:OD1	1:C:367:ASP:N	2.48	0.42
1:D:1294:ASN:OD1	1:D:1295:ASN:ND2	2.51	0.42
2:E:23:CYS:HB3	2:E:104:LEU:HD11	2.00	0.42
1:A:4752:LEU:HD12	1:A:4752:LEU:HA	1.86	0.42
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.85	0.42
1:B:2588:LEU:HA	1:B:2591:LEU:HG	2.00	0.42
1:B:4832:ASP:N	1:B:4832:ASP:OD1	2.49	0.42
1:C:122:ARG:HG2	1:C:123:HIS:H	1.84	0.42
1:C:1216:ASN:HD21	1:C:1223:THR:HG22	1.84	0.42
1:C:1605:LEU:O	1:C:1606:LYS:NZ	2.34	0.42
1:C:1944:ASN:OD1	1:C:1944:ASN:N	2.52	0.42
1:C:2385:ASN:O	1:C:2389:THR:OG1	2.32	0.42
1:D:436:LEU:HD12	1:D:447:LEU:HD13	2.01	0.42
1:D:707:PRO:HD3	1:D:1604:PHE:CE1	2.54	0.42
1:D:1786:ASP:N	1:D:1786:ASP:OD1	2.51	0.42
1:D:3262:MET:SD	1:D:3262:MET:N	2.79	0.42
1:D:3953:MET:HE2	1:D:3953:MET:HA	2.00	0.42
1:A:891:GLU:O	1:A:895:MET:HG2	2.19	0.42
1:A:1306:MET:HE2	1:A:1542:PRO:HD3	2.01	0.42
1:A:1606:LYS:HA	1:A:1606:LYS:HD3	1.87	0.42
1:B:565:LEU:HA	1:B:565:LEU:HD23	1.81	0.42
1:B:1216:ASN:HD21	1:B:1223:THR:HG22	1.84	0.42
1:B:1992:ARG:HD2	1:B:1997:ASP:HA	2.00	0.42
1:B:3953:MET:HA	1:B:3953:MET:HE2	2.00	0.42
1:C:424:PHE:HA	1:C:427:ASN:HD21	1.83	0.42
1:C:1029:ASN:OD1	1:C:1029:ASN:N	2.52	0.42
1:C:1282:CYS:O	1:C:1284:LYS:N	2.50	0.42
1:C:1600:MET:HE2	1:C:1600:MET:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:CD2	1:D:352:SER:HB2	2.54	0.42
1:D:1446:ILE:HG21	1:D:1543:ALA:HB3	2.00	0.42
1:D:4196:ILE:HG12	1:D:4922:MET:HB2	2.01	0.42
2:H:12:ASP:OD1	2:H:12:ASP:N	2.52	0.42
1:A:626:ARG:HG2	1:A:630:HIS:CE1	2.55	0.42
1:A:707:PRO:HD3	1:A:1604:PHE:CE1	2.54	0.42
1:A:3015:ARG:NH2	1:A:3080:THR:O	2.53	0.42
1:A:3711:LYS:HB2	1:A:3711:LYS:HE2	1.81	0.42
1:A:4028:SER:HB2	1:A:4032:LYS:HE2	2.00	0.42
1:A:4863:GLY:HA2	1:B:4866:ILE:HD13	2.02	0.42
1:B:626:ARG:HG2	1:B:630:HIS:CE1	2.55	0.42
1:B:647:ARG:HE	1:B:648:LEU:H	1.66	0.42
1:B:1306:MET:HE2	1:B:1542:PRO:HD3	2.01	0.42
1:C:650:ASN:ND2	1:C:687:THR:OG1	2.43	0.42
1:C:891:GLU:O	1:C:895:MET:HG2	2.19	0.42
1:C:2025:ARG:HD2	1:C:2025:ARG:HA	1.85	0.42
1:D:626:ARG:HG2	1:D:630:HIS:CE1	2.55	0.42
1:D:1992:ARG:HD2	1:D:1997:ASP:HA	2.00	0.42
1:D:2588:LEU:HA	1:D:2591:LEU:HG	2.00	0.42
1:A:3215:THR:HA	1:A:3218:ILE:HD12	2.02	0.42
1:C:626:ARG:HG2	1:C:630:HIS:CE1	2.55	0.42
1:C:1205:CYS:HB2	1:C:1215:MET:HE2	2.02	0.42
1:D:497:LEU:O	1:D:499:LEU:N	2.52	0.42
1:D:1299:ILE:HG21	1:D:1455:THR:HA	2.00	0.42
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.84	0.42
1:A:253:GLY:HA2	1:A:257:ARG:HB2	2.02	0.42
1:A:1286:THR:HB	1:A:1557:GLU:HA	2.02	0.42
1:A:1944:ASN:OD1	1:A:1944:ASN:N	2.52	0.42
1:A:2209:ASN:OD1	1:A:2210:GLN:N	2.51	0.42
1:A:4721:LEU:HD23	1:A:4721:LEU:HA	1.84	0.42
1:B:424:PHE:HA	1:B:427:ASN:HD21	1.83	0.42
1:B:515:ALA:HB1	1:B:521:GLU:HA	2.01	0.42
1:B:4196:ILE:HG12	1:B:4922:MET:HB2	2.01	0.42
1:C:1306:MET:HE2	1:C:1542:PRO:HD3	2.01	0.42
1:C:1600:MET:H	1:C:1600:MET:HG2	1.58	0.42
1:C:2269:ALA:HA	1:C:2328:GLU:HB2	2.01	0.42
1:C:2398:LEU:HD23	1:C:2398:LEU:HA	1.82	0.42
1:C:3680:LYS:HA	1:C:3680:LYS:HD2	1.92	0.42
1:C:4077:LEU:HD23	1:C:4077:LEU:HA	1.87	0.42
1:D:253:GLY:HA2	1:D:257:ARG:HB2	2.02	0.42
1:D:1987:CYS:HA	1:D:1988:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2065:MET:SD	1:D:2083:MET:HG3	2.59	0.42
1:D:2196:CYS:SG	1:D:2197:ARG:N	2.92	0.42
1:D:2209:ASN:OD1	1:D:2210:GLN:N	2.52	0.42
1:D:3000:LYS:HD2	1:D:3000:LYS:HA	1.92	0.42
1:D:3792:LEU:HD23	1:D:3792:LEU:HA	1.87	0.42
1:B:436:LEU:HD12	1:B:447:LEU:HD13	2.01	0.42
1:B:1286:THR:HB	1:B:1557:GLU:HA	2.02	0.42
1:B:3696:LYS:HA	1:B:3696:LYS:HD3	1.85	0.42
1:C:227:TYR:CD2	1:C:352:SER:HB2	2.54	0.42
1:C:253:GLY:HA2	1:C:257:ARG:HB2	2.02	0.42
1:C:572:LEU:HB2	1:C:613:VAL:HG22	2.02	0.42
1:C:2642:LYS:HG2	1:C:2645:TRP:CE3	2.54	0.42
1:C:2848:HIS:ND1	1:C:2873:TYR:OH	2.40	0.42
1:C:3981:LEU:HD23	1:C:3981:LEU:HA	1.91	0.42
1:D:1944:ASN:OD1	1:D:1944:ASN:N	2.52	0.42
1:A:3233:MET:SD	1:A:3233:MET:N	2.92	0.42
1:B:245:LEU:HB2	1:B:275:TRP:HH2	1.84	0.42
1:B:707:PRO:HD3	1:B:1604:PHE:CE1	2.54	0.42
1:B:881:ILE:HG21	1:B:952:ILE:HD11	2.02	0.42
1:B:894:VAL:HG23	1:B:895:MET:CE	2.49	0.42
1:B:1446:ILE:HG21	1:B:1543:ALA:HB3	2.00	0.42
1:C:1663:SER:OG	1:C:1709:ASP:OD2	2.31	0.42
1:C:2065:MET:SD	1:C:2083:MET:HG3	2.59	0.42
1:A:856:SER:HB2	1:A:862:PHE:CE1	2.55	0.42
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.48	0.42
1:A:1205:CYS:HB2	1:A:1215:MET:HE2	2.02	0.42
1:A:1432:ILE:HG23	1:A:1434:PRO:HD3	2.01	0.42
1:A:1600:MET:H	1:A:1600:MET:HG2	1.58	0.42
1:A:3696:LYS:HD3	1:A:3696:LYS:HA	1.85	0.42
1:C:1294:ASN:OD1	1:C:1295:ASN:ND2	2.51	0.42
1:C:1299:ILE:HG21	1:C:1455:THR:HA	2.00	0.42
1:D:856:SER:HB2	1:D:862:PHE:CE1	2.55	0.42
1:D:1432:ILE:HG23	1:D:1434:PRO:HD3	2.01	0.42
1:D:3254:GLU:OE1	1:D:3256:HIS:NE2	2.53	0.42
1:D:3795:LEU:HD22	1:D:3834:PHE:HZ	1.85	0.42
1:A:607:ASN:OD1	1:A:607:ASN:N	2.53	0.42
1:A:1097:LYS:HA	1:A:1097:LYS:HD3	1.74	0.42
1:A:1294:ASN:OD1	1:A:1295:ASN:ND2	2.51	0.42
1:A:3654:ASP:OD1	1:A:3654:ASP:N	2.52	0.42
1:B:121:LEU:HD12	1:B:121:LEU:HA	1.87	0.42
1:B:2133:MET:SD	1:B:2133:MET:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:894:VAL:HG23	1:C:895:MET:CE	2.49	0.42
1:C:1606:LYS:HD3	1:C:1606:LYS:HA	1.87	0.42
1:C:2593:PHE:CD2	1:C:2595:VAL:HG23	2.54	0.42
1:D:1089:ARG:HG2	1:D:1202:ILE:HD12	2.02	0.42
1:D:1216:ASN:HD21	1:D:1223:THR:HG22	1.84	0.42
1:D:2133:MET:SD	1:D:2133:MET:N	2.93	0.42
1:D:2269:ALA:HA	1:D:2328:GLU:HB2	2.01	0.42
2:E:12:ASP:OD1	2:E:12:ASP:N	2.52	0.42
1:A:227:TYR:CD2	1:A:352:SER:HB2	2.54	0.41
1:A:1216:ASN:HD21	1:A:1223:THR:HG22	1.84	0.41
1:A:2502:ASP:OD1	1:A:2502:ASP:N	2.50	0.41
1:A:4031:PHE:HZ	1:A:4040:GLY:HA2	1.84	0.41
1:A:4867:ASP:OD1	1:B:4873:ARG:NE	2.40	0.41
1:B:23:GLN:HE22	1:B:215:ALA:HB2	1.85	0.41
1:B:1068:ASP:OD1	1:B:1068:ASP:N	2.48	0.41
1:B:4106:GLU:OE1	1:B:4148:TYR:OH	2.37	0.41
1:C:73:LEU:O	1:C:118:ALA:N	2.51	0.41
1:C:1286:THR:HB	1:C:1557:GLU:HA	2.02	0.41
1:C:3015:ARG:NH2	1:C:3080:THR:O	2.53	0.41
1:C:3215:THR:HA	1:C:3218:ILE:HD12	2.02	0.41
1:C:3711:LYS:HE2	1:C:3711:LYS:HB2	1.81	0.41
1:D:122:ARG:HG2	1:D:123:HIS:H	1.84	0.41
1:D:607:ASN:OD1	1:D:607:ASN:N	2.53	0.41
1:D:1780:SER:HB2	1:D:1781:PRO:HD3	2.02	0.41
1:D:3015:ARG:NH2	1:D:3080:THR:O	2.53	0.41
1:D:3967:LEU:HD12	1:D:3967:LEU:HA	1.89	0.41
2:G:50:ARG:HE	2:G:50:ARG:HB3	1.74	0.41
1:A:650:ASN:ND2	1:A:687:THR:OG1	2.43	0.41
1:A:1282:CYS:O	1:A:1284:LYS:N	2.50	0.41
1:A:2151:ASN:OD1	1:A:2154:PHE:N	2.53	0.41
1:A:2848:HIS:CE1	1:A:2873:TYR:HH	2.31	0.41
1:B:238:HIS:ND1	1:B:243:GLU:HB3	2.36	0.41
1:B:2848:HIS:CE1	1:B:2873:TYR:HH	2.34	0.41
1:B:3015:ARG:NH2	1:B:3080:THR:O	2.53	0.41
1:B:3795:LEU:HD22	1:B:3834:PHE:HZ	1.85	0.41
1:B:4752:LEU:HD12	1:B:4752:LEU:HA	1.86	0.41
1:C:2607:LYS:HE3	1:C:2641:ARG:HH22	1.85	0.41
1:D:1306:MET:HE2	1:D:1542:PRO:HD3	2.01	0.41
2:H:50:ARG:HE	2:H:50:ARG:HB3	1.74	0.41
1:A:497:LEU:O	1:A:499:LEU:N	2.52	0.41
1:A:689:GLU:OE1	2:E:41:ARG:NH2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2759:TYR:HA	1:A:2762:LEU:HD12	2.02	0.41
1:B:414:ARG:O	1:B:417:ARG:HG3	2.20	0.41
1:B:689:GLU:OE1	2:F:41:ARG:NH2	2.37	0.41
1:D:572:LEU:HB2	1:D:613:VAL:HG22	2.02	0.41
1:D:2398:LEU:HD23	1:D:2398:LEU:HA	1.82	0.41
1:D:3344:ARG:O	1:D:3366:TYR:OH	2.26	0.41
1:A:1114:ARG:NH1	1:A:1138:ASP:HB3	2.36	0.41
1:A:1780:SER:HB2	1:A:1781:PRO:HD3	2.02	0.41
1:A:2133:MET:SD	1:A:2133:MET:N	2.93	0.41
1:B:1944:ASN:OD1	1:B:1944:ASN:N	2.52	0.41
1:B:2269:ALA:HA	1:B:2328:GLU:HB2	2.01	0.41
1:B:3711:LYS:HB2	1:B:3711:LYS:HE2	1.81	0.41
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.85	0.41
1:C:1089:ARG:HG2	1:C:1202:ILE:HD12	2.02	0.41
1:C:2133:MET:SD	1:C:2133:MET:N	2.93	0.41
1:A:73:LEU:O	1:A:118:ALA:N	2.51	0.41
1:A:238:HIS:ND1	1:A:243:GLU:HB3	2.36	0.41
1:A:1238:PRO:HB2	1:A:1241:VAL:HB	2.03	0.41
1:A:1637:ASN:OD1	1:A:1637:ASN:N	2.53	0.41
1:A:3730:LEU:HD23	1:A:3730:LEU:HA	1.84	0.41
1:A:4866:ILE:HD13	1:C:4863:GLY:HA2	2.02	0.41
1:B:122:ARG:HG2	1:B:123:HIS:H	1.85	0.41
1:B:1780:SER:HB2	1:B:1781:PRO:HD3	2.02	0.41
1:B:2028:LEU:HD12	1:B:2028:LEU:HA	1.91	0.41
1:B:3254:GLU:OE1	1:B:3256:HIS:NE2	2.53	0.41
1:C:23:GLN:HE22	1:C:215:ALA:HB2	1.86	0.41
1:C:238:HIS:ND1	1:C:243:GLU:HB3	2.36	0.41
1:C:1746:LYS:HD3	1:C:1746:LYS:HA	1.94	0.41
1:C:2209:ASN:OD1	1:C:2210:GLN:N	2.52	0.41
1:C:2296:ARG:HA	1:C:2296:ARG:HD3	1.87	0.41
1:D:414:ARG:O	1:D:417:ARG:HG3	2.20	0.41
1:D:881:ILE:HG21	1:D:952:ILE:HD11	2.02	0.41
1:D:2065:MET:HE2	1:D:2065:MET:HB2	1.84	0.41
1:D:2151:ASN:OD1	1:D:2154:PHE:N	2.53	0.41
1:A:307:SER:HB3	1:A:327:THR:HG22	2.03	0.41
1:A:3254:GLU:OE1	1:A:3256:HIS:NE2	2.53	0.41
1:A:4611:PHE:HE2	1:A:4946:ARG:HD3	1.85	0.41
1:B:253:GLY:HA2	1:B:257:ARG:HB2	2.02	0.41
1:B:572:LEU:HB2	1:B:613:VAL:HG22	2.02	0.41
1:B:856:SER:HB2	1:B:862:PHE:CE1	2.55	0.41
1:B:1262:PRO:HG3	1:B:1595:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1539:LYS:HE2	1:B:1539:LYS:HB2	1.90	0.41
1:B:1913:CYS:HB3	1:B:2089:ARG:HH12	1.85	0.41
1:B:2077:PRO:HA	1:B:2080:VAL:HG12	2.03	0.41
1:B:3322:MET:SD	1:B:3322:MET:N	2.79	0.41
1:B:4611:PHE:HE2	1:B:4946:ARG:HD3	1.85	0.41
1:C:305:TYR:O	1:C:317:MET:N	2.54	0.41
1:C:307:SER:HB3	1:C:327:THR:HG22	2.03	0.41
1:C:436:LEU:HD12	1:C:447:LEU:HD13	2.01	0.41
1:C:1238:PRO:HB2	1:C:1241:VAL:HB	2.03	0.41
1:D:305:TYR:O	1:D:317:MET:N	2.54	0.41
1:D:3458:TYR:O	1:D:3462:THR:OG1	2.25	0.41
1:D:4173:PHE:CD1	1:D:4879:VAL:HG21	2.54	0.41
1:B:1294:ASN:OD1	1:B:1295:ASN:ND2	2.51	0.41
1:B:1626:LEU:HD23	1:B:1626:LEU:HA	1.91	0.41
1:C:2759:TYR:HA	1:C:2762:LEU:HD12	2.03	0.41
1:D:647:ARG:HE	1:D:648:LEU:H	1.66	0.41
1:D:1286:THR:HB	1:D:1557:GLU:HA	2.02	0.41
1:D:3215:THR:HA	1:D:3218:ILE:HD12	2.02	0.41
1:A:122:ARG:HG2	1:A:123:HIS:H	1.85	0.41
1:A:414:ARG:O	1:A:417:ARG:HG3	2.20	0.41
1:A:565:LEU:HD23	1:A:565:LEU:HA	1.81	0.41
1:A:881:ILE:HG21	1:A:952:ILE:HD11	2.02	0.41
1:A:1089:ARG:HG2	1:A:1202:ILE:HD12	2.02	0.41
1:A:1262:PRO:HG3	1:A:1595:VAL:HG12	2.03	0.41
1:A:2203:CYS:O	1:A:2207:ARG:NE	2.54	0.41
1:A:3957:LEU:HD11	1:A:3966:LEU:HD23	2.03	0.41
1:B:198:ASN:OD1	1:B:200:SER:OG	2.32	0.41
1:B:634:ASP:HB3	1:B:1672:ARG:HH21	1.86	0.41
1:B:1205:CYS:HB2	1:B:1215:MET:HE2	2.02	0.41
1:B:2151:ASN:OD1	1:B:2154:PHE:N	2.54	0.41
1:B:3262:MET:SD	1:B:3262:MET:N	2.79	0.41
1:B:3957:LEU:HD11	1:B:3966:LEU:HD23	2.03	0.41
1:B:4031:PHE:HZ	1:B:4040:GLY:HA2	1.84	0.41
1:C:545:ARG:HG2	1:C:581:GLU:HG2	2.03	0.41
1:C:607:ASN:OD1	1:C:607:ASN:N	2.53	0.41
1:C:856:SER:HB2	1:C:862:PHE:CE1	2.55	0.41
1:C:1114:ARG:NH1	1:C:1138:ASP:HB3	2.36	0.41
1:C:1262:PRO:HG3	1:C:1595:VAL:HG12	2.03	0.41
1:C:1637:ASN:N	1:C:1637:ASN:OD1	2.53	0.41
1:C:1913:CYS:HB3	1:C:2089:ARG:HH12	1.85	0.41
1:C:2213:MET:HE2	1:C:2213:MET:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3957:LEU:HD11	1:C:3966:LEU:HD23	2.03	0.41
1:C:4696:VAL:HG12	1:C:4698:ASN:HB2	2.03	0.41
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.84	0.41
1:D:2077:PRO:HA	1:D:2080:VAL:HG12	2.03	0.41
2:F:12:ASP:OD1	2:F:12:ASP:N	2.52	0.41
2:G:12:ASP:N	2:G:12:ASP:OD1	2.52	0.41
1:A:894:VAL:HG23	1:A:895:MET:CE	2.49	0.41
1:A:2511:MET:HE2	1:A:2511:MET:HB2	1.85	0.41
1:B:2607:LYS:HE3	1:B:2641:ARG:HH22	1.85	0.41
1:B:4078:ASP:OD1	1:B:4078:ASP:N	2.53	0.41
1:B:4766:LEU:HD23	1:B:4766:LEU:HA	1.90	0.41
1:C:1688:TYR:HA	1:C:1691:GLU:HG2	2.02	0.41
1:C:1814:THR:OG1	1:C:1815:THR:N	2.54	0.41
1:C:3795:LEU:HD22	1:C:3834:PHE:HZ	1.85	0.41
1:C:4502:MET:HE3	1:C:4502:MET:HB3	1.89	0.41
1:C:4515:LEU:HD12	1:C:4515:LEU:HA	1.88	0.41
1:D:238:HIS:ND1	1:D:243:GLU:HB3	2.36	0.41
1:D:4031:PHE:HZ	1:D:4040:GLY:HA2	1.84	0.41
1:D:4611:PHE:HE2	1:D:4946:ARG:HD3	1.85	0.41
1:A:1117:TRP:HB3	1:A:1201:PHE:HB3	2.03	0.41
1:A:2607:LYS:HE3	1:A:2641:ARG:HH22	1.86	0.41
1:B:609:LYS:HD2	1:B:609:LYS:HA	1.91	0.41
1:B:2203:CYS:O	1:B:2207:ARG:NE	2.54	0.41
1:B:4941:LYS:HB3	1:B:4941:LYS:HE2	1.80	0.41
1:C:2065:MET:HE2	1:C:2065:MET:HB2	1.84	0.41
1:C:2203:CYS:O	1:C:2207:ARG:NE	2.54	0.41
1:C:2347:GLU:OE1	1:C:2347:GLU:N	2.54	0.41
1:C:3254:GLU:OE1	1:C:3256:HIS:NE2	2.53	0.41
1:C:4078:ASP:N	1:C:4078:ASP:OD1	2.54	0.41
1:C:4596:LEU:HA	1:C:4596:LEU:HD12	1.78	0.41
1:C:4866:ILE:HD13	1:D:4863:GLY:HA2	2.02	0.41
1:D:307:SER:HB3	1:D:327:THR:HG22	2.03	0.41
1:D:721:ASP:OD1	1:D:721:ASP:N	2.50	0.41
1:D:889:ILE:HB	1:D:893:TRP:CZ2	2.56	0.41
1:D:1205:CYS:HB2	1:D:1215:MET:HE2	2.02	0.41
1:D:1913:CYS:HB3	1:D:2089:ARG:HH12	1.85	0.41
1:D:2203:CYS:O	1:D:2207:ARG:NE	2.54	0.41
1:D:4155:SER:OG	1:D:4922:MET:HE1	2.21	0.41
1:A:545:ARG:HG2	1:A:581:GLU:HG2	2.03	0.40
1:A:2895:LEU:HD12	1:A:2895:LEU:HA	1.96	0.40
1:A:4106:GLU:OE1	1:A:4148:TYR:OH	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4155:SER:OG	1:A:4922:MET:HE1	2.21	0.40
1:B:198:ASN:OD1	1:B:198:ASN:N	2.54	0.40
1:B:889:ILE:HB	1:B:893:TRP:CZ2	2.56	0.40
1:B:1029:ASN:OD1	1:B:1029:ASN:N	2.52	0.40
1:B:1519:LEU:HD12	1:B:1519:LEU:HA	1.90	0.40
1:C:414:ARG:O	1:C:417:ARG:HG3	2.20	0.40
1:C:1749:LEU:HD12	1:C:1844:LEU:HG	2.03	0.40
1:D:545:ARG:HG2	1:D:581:GLU:HG2	2.03	0.40
1:D:1233:GLN:H	1:D:1233:GLN:CD	2.29	0.40
1:D:1262:PRO:HG3	1:D:1595:VAL:HG12	2.03	0.40
1:D:3957:LEU:HD11	1:D:3966:LEU:HD23	2.03	0.40
1:D:4502:MET:HE3	1:D:4502:MET:HB3	1.89	0.40
2:G:93:PRO:HA	2:G:94:PRO:HD3	1.97	0.40
1:A:508:TYR:CZ	1:A:523:GLY:HA3	2.57	0.40
1:A:889:ILE:HB	1:A:893:TRP:CZ2	2.56	0.40
1:A:1749:LEU:HD12	1:A:1844:LEU:HG	2.03	0.40
1:A:1913:CYS:HB3	1:A:2089:ARG:HH12	1.85	0.40
1:A:2473:ARG:HD2	1:A:2473:ARG:HA	1.76	0.40
1:A:3795:LEU:HD22	1:A:3834:PHE:HZ	1.85	0.40
1:A:4696:VAL:HG12	1:A:4698:ASN:HB2	2.03	0.40
1:B:168:GLN:HE21	1:D:240:HIS:HB2	1.87	0.40
1:B:497:LEU:O	1:B:499:LEU:N	2.52	0.40
1:B:607:ASN:OD1	1:B:607:ASN:N	2.53	0.40
1:B:1089:ARG:HG2	1:B:1202:ILE:HD12	2.02	0.40
1:B:1238:PRO:HB2	1:B:1241:VAL:HB	2.03	0.40
1:C:885:LEU:HA	1:C:888:ASN:HD21	1.86	0.40
1:C:889:ILE:HB	1:C:893:TRP:CZ2	2.56	0.40
1:C:1233:GLN:H	1:C:1233:GLN:CD	2.30	0.40
1:C:2028:LEU:HD12	1:C:2028:LEU:HA	1.91	0.40
1:D:23:GLN:HE22	1:D:215:ALA:HB2	1.86	0.40
1:D:249:SER:OG	1:D:251:GLU:OE1	2.27	0.40
1:D:962:LYS:HD3	1:D:962:LYS:HA	1.88	0.40
1:D:1114:ARG:NH1	1:D:1138:ASP:HB3	2.36	0.40
1:D:1688:TYR:HA	1:D:1691:GLU:HG2	2.02	0.40
1:A:572:LEU:HB2	1:A:613:VAL:HG22	2.02	0.40
1:A:2080:VAL:HG13	1:A:3669:LEU:HD22	2.04	0.40
1:A:3006:LEU:HD13	1:A:3044:VAL:HG21	2.03	0.40
1:B:2501:LEU:HD22	1:B:2589:ARG:HG2	2.03	0.40
1:B:3000:LYS:HD2	1:B:3000:LYS:HA	1.92	0.40
1:B:3083:ARG:HD3	1:B:3189:ARG:NH1	2.37	0.40
1:C:497:LEU:O	1:C:499:LEU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:ILE:HG21	1:C:952:ILE:HD11	2.02	0.40
1:C:1780:SER:HB2	1:C:1781:PRO:HD3	2.02	0.40
1:C:2151:ASN:OD1	1:C:2154:PHE:N	2.53	0.40
1:C:3967:LEU:HD12	1:C:3967:LEU:HA	1.89	0.40
1:B:885:LEU:HA	1:B:888:ASN:HD21	1.86	0.40
1:B:3006:LEU:HD13	1:B:3044:VAL:HG21	2.03	0.40
1:C:634:ASP:HB3	1:C:1672:ARG:HH21	1.86	0.40
1:C:2077:PRO:HA	1:C:2080:VAL:HG12	2.03	0.40
1:C:2187:THR:O	1:C:2187:THR:OG1	2.31	0.40
1:C:3083:ARG:HD3	1:C:3189:ARG:NH1	2.37	0.40
1:D:634:ASP:HB3	1:D:1672:ARG:HH21	1.86	0.40
1:D:749:LEU:HD22	1:D:755:ILE:HD11	2.02	0.40
1:D:1749:LEU:HD12	1:D:1844:LEU:HG	2.03	0.40
1:D:2227:GLY:O	1:D:2237:THR:OG1	2.30	0.40
1:D:2759:TYR:HA	1:D:2762:LEU:HD12	2.02	0.40
2:E:50:ARG:HE	2:E:50:ARG:HB3	1.74	0.40
1:A:1017:THR:HA	1:A:1025:LYS:HD3	2.04	0.40
1:A:2395:ILE:HD13	1:A:2395:ILE:HA	1.94	0.40
1:A:4658:GLU:H	1:A:4658:GLU:HG3	1.74	0.40
1:B:1114:ARG:NH1	1:B:1138:ASP:HB3	2.36	0.40
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.55	0.40
1:B:1233:GLN:CD	1:B:1233:GLN:H	2.29	0.40
1:C:508:TYR:CZ	1:C:523:GLY:HA3	2.57	0.40
1:C:1117:TRP:HB3	1:C:1201:PHE:HB3	2.03	0.40
1:C:3000:LYS:HD2	1:C:3000:LYS:HA	1.92	0.40
1:D:1017:THR:HA	1:D:1025:LYS:HD3	2.04	0.40
1:D:1238:PRO:HB2	1:D:1241:VAL:HB	2.03	0.40
1:D:2097:LEU:HD12	1:D:2097:LEU:HA	1.89	0.40
1:D:2895:LEU:HD12	1:D:2895:LEU:HA	1.96	0.40
2:F:50:ARG:HE	2:F:50:ARG:HB3	1.74	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	3952/4966 (80%)	3722 (94%)	224 (6%)	6 (0%)	43	74
1	B	3952/4966 (80%)	3724 (94%)	222 (6%)	6 (0%)	43	74
1	C	3952/4966 (80%)	3725 (94%)	221 (6%)	6 (0%)	43	74
1	D	3952/4966 (80%)	3722 (94%)	224 (6%)	6 (0%)	43	74
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	16228/20292 (80%)	15285 (94%)	919 (6%)	24 (0%)	49	79

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1299	ILE
1	B	1299	ILE
1	C	1299	ILE
1	D	1299	ILE
1	A	1462	VAL
1	A	2451	VAL
1	B	1462	VAL
1	B	2451	VAL
1	C	1462	VAL
1	C	2451	VAL
1	D	1462	VAL
1	D	2451	VAL
1	A	2444	ILE
1	B	2444	ILE
1	C	2444	ILE
1	D	2444	ILE
1	A	2454	ASP
1	B	2454	ASP
1	C	2454	ASP
1	D	2454	ASP
1	A	1285	VAL
1	B	1285	VAL
1	C	1285	VAL
1	D	1285	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	3331/4355 (76%)	3323 (100%)	8 (0%)	87	85
1	B	3331/4355 (76%)	3323 (100%)	8 (0%)	87	85
1	C	3331/4355 (76%)	3324 (100%)	7 (0%)	87	85
1	D	3331/4355 (76%)	3323 (100%)	8 (0%)	87	85
2	E	88/88 (100%)	88 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	G	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
All	All	13676/17772 (77%)	13645 (100%)	31 (0%)	85	85

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1722	MET
1	A	1818	LEU
1	A	1819	PHE
1	A	2083	MET
1	A	2091	TYR
1	A	2340	ASN
1	A	4706	MET
1	A	4747	MET
1	B	1722	MET
1	B	1818	LEU
1	B	1819	PHE
1	B	2091	TYR
1	B	2340	ASN
1	B	2405	MET
1	B	4706	MET
1	B	4747	MET
1	C	1722	MET
1	C	1818	LEU
1	C	1819	PHE

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Mol	Chain	Res	Type
1	C	2083	MET
1	C	2091	TYR
1	C	2340	ASN
1	C	4706	MET
1	D	1722	MET
1	D	1818	LEU
1	D	1819	PHE
1	D	2083	MET
1	D	2091	TYR
1	D	2340	ASN
1	D	2405	MET
1	D	4706	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	394	HIS
1	A	476	GLN
1	A	490	GLN
1	A	496	ASN
1	A	658	ASN
1	A	745	ASN
1	A	771	ASN
1	A	776	GLN
1	A	783	ASN
1	A	915	HIS
1	A	932	ASN
1	A	1021	GLN
1	A	1146	HIS
1	A	1151	HIS
1	A	1157	GLN
1	A	1216	ASN
1	A	1293	GLN
1	A	1440	ASN
1	A	1502	ASN
1	A	1504	ASN
1	A	1621	GLN
1	A	1627	GLN
1	A	1685	GLN
1	A	1845	GLN
1	A	2070	GLN

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Mol	Chain	Res	Type
1	A	2088	HIS
1	A	2108	ASN
1	A	2216	HIS
1	A	2340	ASN
1	A	2480	GLN
1	A	2628	ASN
1	A	2703	GLN
1	A	2738	ASN
1	A	2753	GLN
1	A	2801	ASN
1	A	3016	HIS
1	A	3094	ASN
1	A	3303	GLN
1	A	3317	HIS
1	A	3421	GLN
1	A	3422	ASN
1	A	3617	ASN
1	A	3855	ASN
1	A	3868	ASN
1	A	3963	GLN
1	A	4129	GLN
1	A	4637	GLN
1	B	33	GLN
1	B	394	HIS
1	B	427	ASN
1	B	476	GLN
1	B	490	GLN
1	B	496	ASN
1	B	544	ASN
1	B	658	ASN
1	B	745	ASN
1	B	771	ASN
1	B	776	GLN
1	B	783	ASN
1	B	871	GLN
1	B	932	ASN
1	B	1021	GLN
1	B	1146	HIS
1	B	1151	HIS
1	B	1157	GLN
1	B	1216	ASN
1	B	1293	GLN

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Mol	Chain	Res	Type
1	B	1440	ASN
1	B	1502	ASN
1	B	1504	ASN
1	B	1621	GLN
1	B	1685	GLN
1	B	1845	GLN
1	B	2070	GLN
1	B	2088	HIS
1	B	2108	ASN
1	B	2216	HIS
1	B	2340	ASN
1	B	2628	ASN
1	B	2703	GLN
1	B	2738	ASN
1	B	2753	GLN
1	B	2801	ASN
1	B	3016	HIS
1	B	3094	ASN
1	B	3303	GLN
1	B	3317	HIS
1	B	3421	GLN
1	B	3422	ASN
1	B	3617	ASN
1	B	3849	HIS
1	B	3855	ASN
1	B	3868	ASN
1	B	4129	GLN
1	B	4637	GLN
1	C	33	GLN
1	C	394	HIS
1	C	427	ASN
1	C	476	GLN
1	C	490	GLN
1	C	496	ASN
1	C	544	ASN
1	C	658	ASN
1	C	745	ASN
1	C	771	ASN
1	C	776	GLN
1	C	783	ASN
1	C	871	GLN
1	C	932	ASN

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Mol	Chain	Res	Type
1	C	1021	GLN
1	C	1146	HIS
1	C	1151	HIS
1	C	1157	GLN
1	C	1216	ASN
1	C	1293	GLN
1	C	1440	ASN
1	C	1504	ASN
1	C	1621	GLN
1	C	1685	GLN
1	C	1845	GLN
1	C	2070	GLN
1	C	2088	HIS
1	C	2108	ASN
1	C	2216	HIS
1	C	2340	ASN
1	C	2628	ASN
1	C	2703	GLN
1	C	2738	ASN
1	C	2753	GLN
1	C	2801	ASN
1	C	3016	HIS
1	C	3094	ASN
1	C	3303	GLN
1	C	3317	HIS
1	C	3421	GLN
1	C	3422	ASN
1	C	3617	ASN
1	C	3849	HIS
1	C	3855	ASN
1	C	3868	ASN
1	C	4129	GLN
1	C	4628	GLN
1	C	4637	GLN
1	C	4966	ASN
1	D	33	GLN
1	D	394	HIS
1	D	476	GLN
1	D	490	GLN
1	D	496	ASN
1	D	658	ASN
1	D	745	ASN

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Mol	Chain	Res	Type
1	D	771	ASN
1	D	776	GLN
1	D	783	ASN
1	D	871	GLN
1	D	888	ASN
1	D	915	HIS
1	D	932	ASN
1	D	1021	GLN
1	D	1146	HIS
1	D	1151	HIS
1	D	1157	GLN
1	D	1216	ASN
1	D	1293	GLN
1	D	1440	ASN
1	D	1504	ASN
1	D	1621	GLN
1	D	1685	GLN
1	D	1836	HIS
1	D	1845	GLN
1	D	2070	GLN
1	D	2088	HIS
1	D	2108	ASN
1	D	2216	HIS
1	D	2340	ASN
1	D	2480	GLN
1	D	2628	ASN
1	D	2703	GLN
1	D	2738	ASN
1	D	2753	GLN
1	D	2801	ASN
1	D	3016	HIS
1	D	3094	ASN
1	D	3303	GLN
1	D	3317	HIS
1	D	3421	GLN
1	D	3422	ASN
1	D	3617	ASN
1	D	3849	HIS
1	D	3855	ASN
1	D	3868	ASN
1	D	4129	GLN
1	D	4637	GLN

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Mol	Chain	Res	Type
1	D	4960	GLN
1	D	4966	ASN
2	E	26	HIS
2	E	32	GLN
2	F	26	HIS
2	F	44	ASN
2	G	26	HIS
2	G	44	ASN
2	H	26	HIS
2	H	32	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

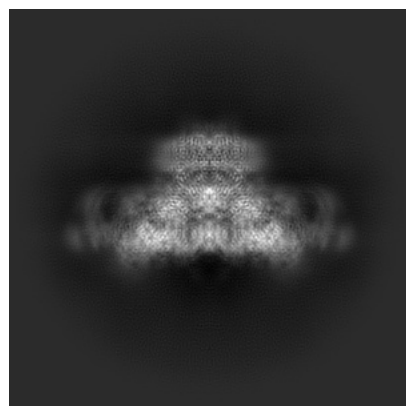
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27711. These allow visual inspection of the internal detail of the map and identification of artifacts.

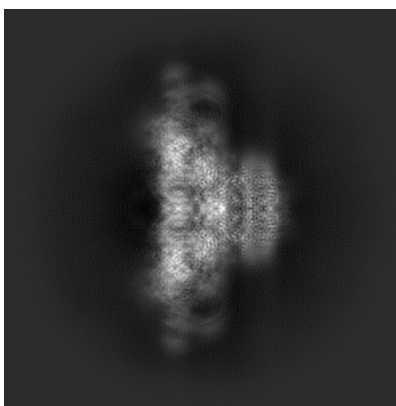
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

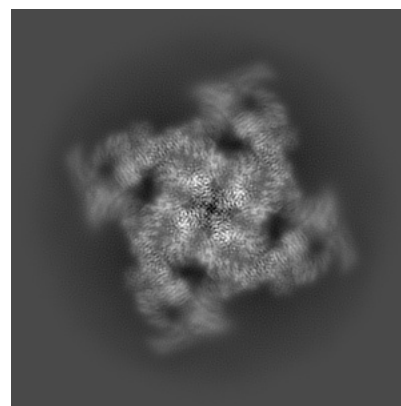
6.1.1 Primary map



X

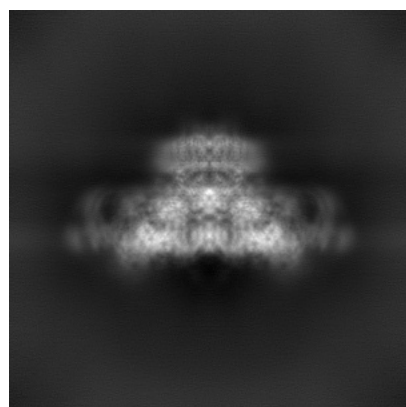


Y

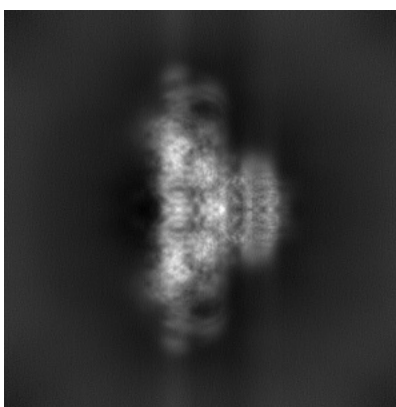


Z

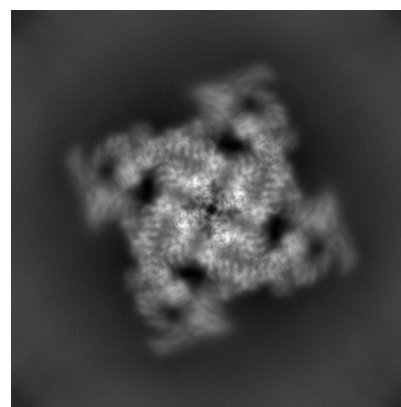
6.1.2 Raw map



X



Y

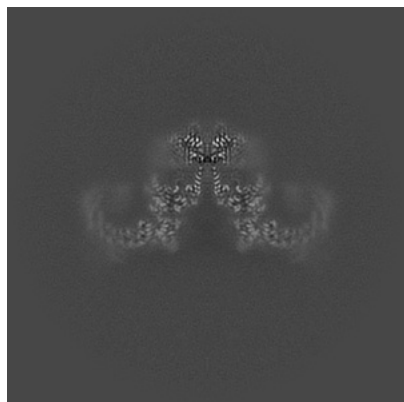


Z

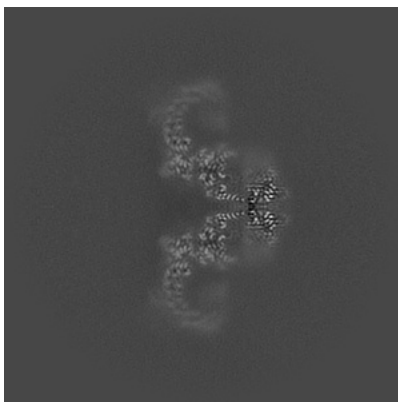
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

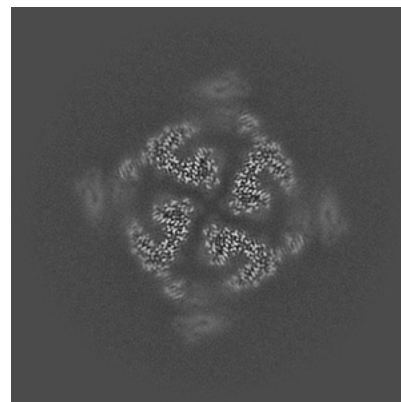
6.2.1 Primary map



X Index: 230

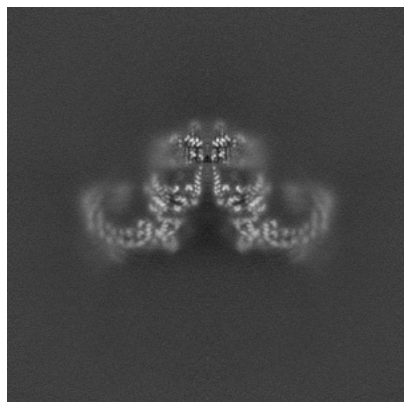


Y Index: 230

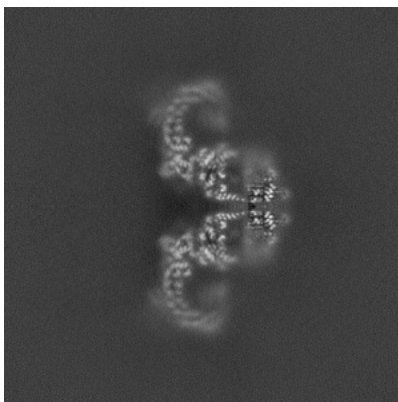


Z Index: 230

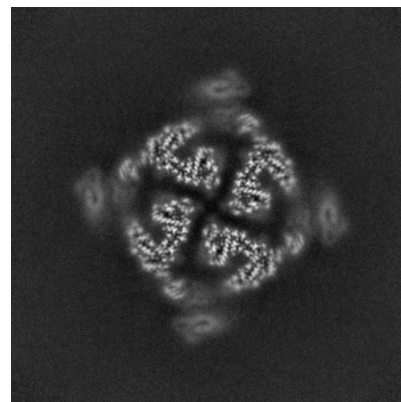
6.2.2 Raw map



X Index: 230



Y Index: 230

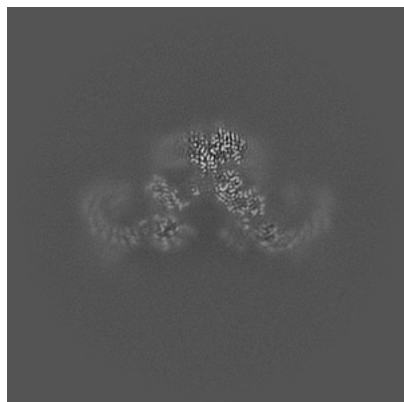


Z Index: 230

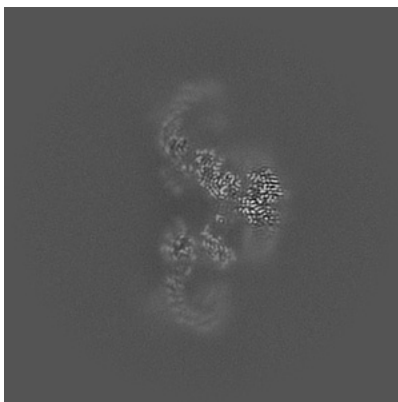
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

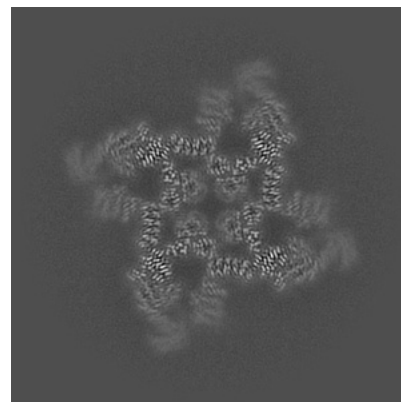
6.3.1 Primary map



X Index: 224

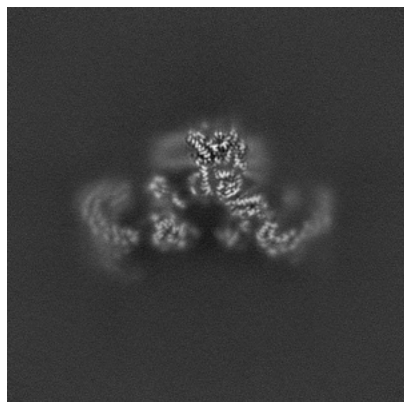


Y Index: 236

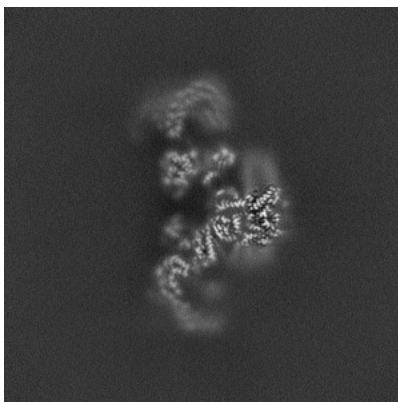


Z Index: 201

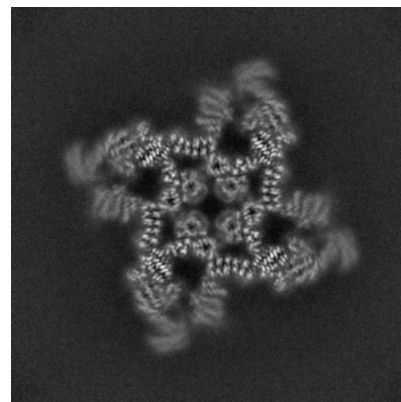
6.3.2 Raw map



X Index: 221



Y Index: 221

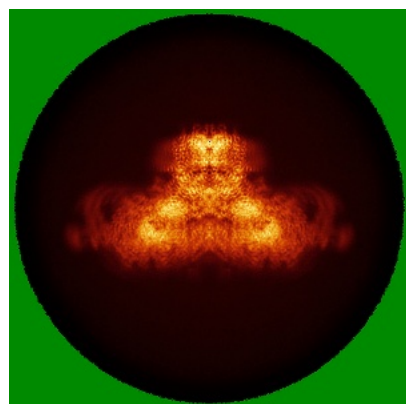


Z Index: 201

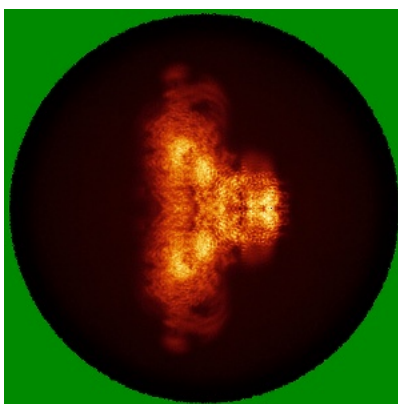
The images above show the largest variance slices of the map in three orthogonal directions.

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

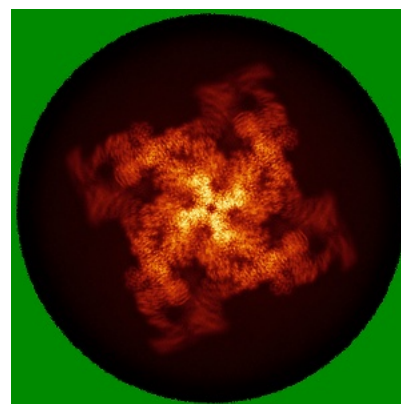
6.4.1 Primary map



X

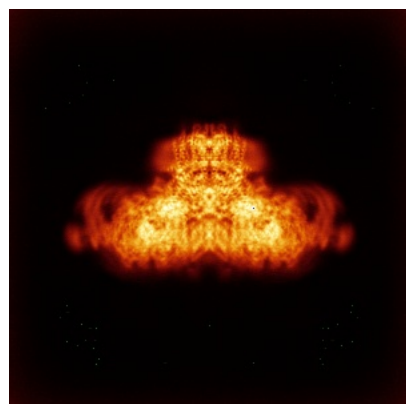


Y

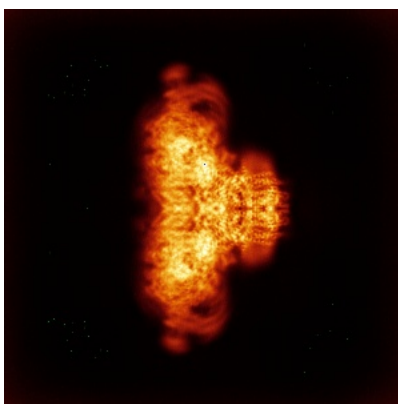


Z

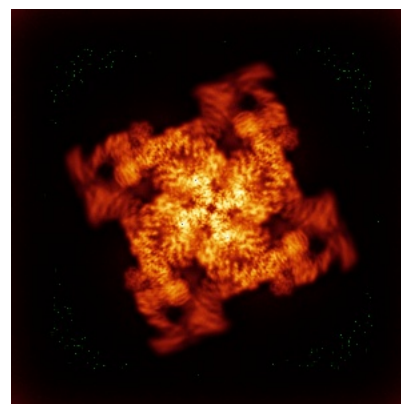
6.4.2 Raw map



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 0.24. 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.

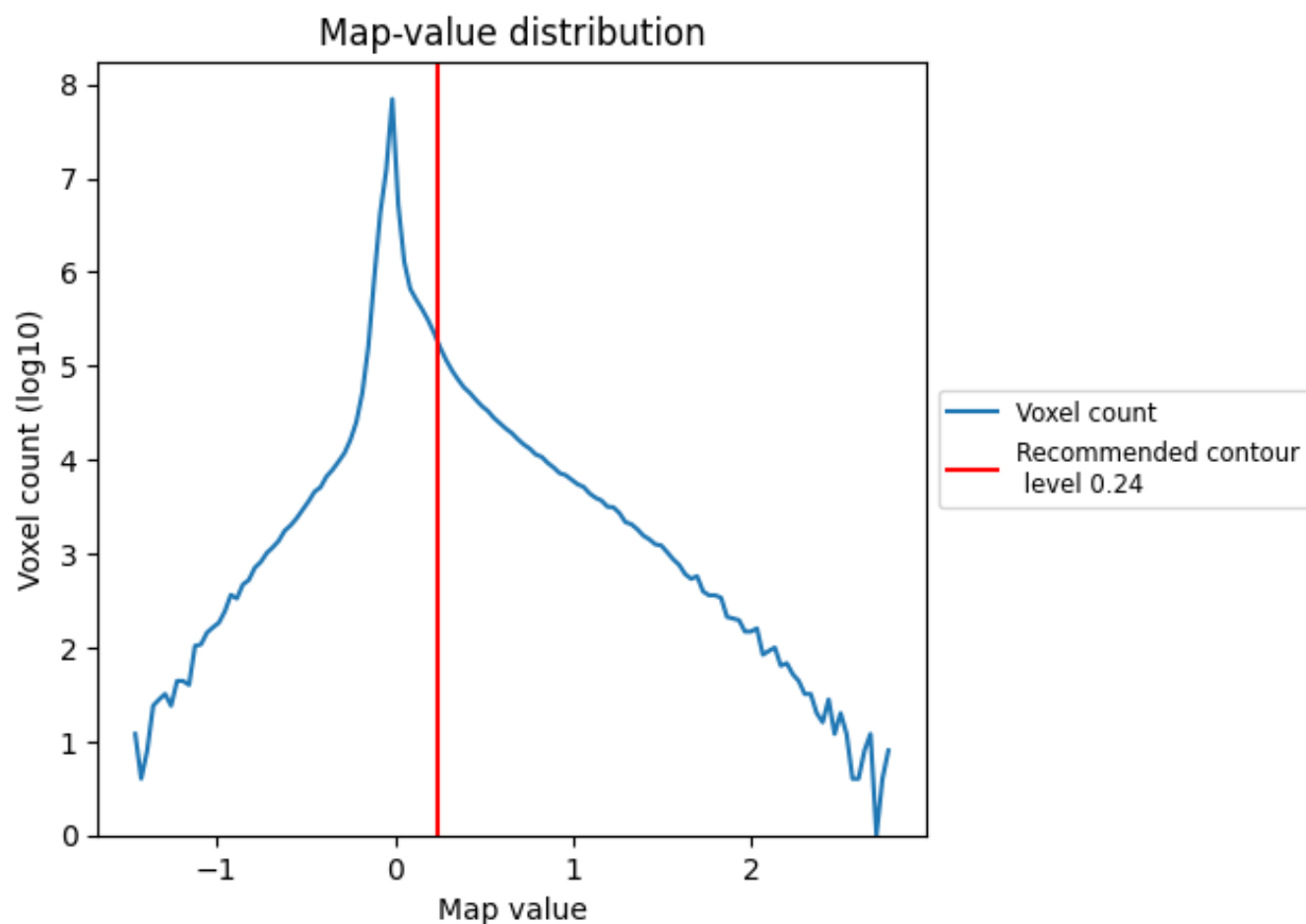
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

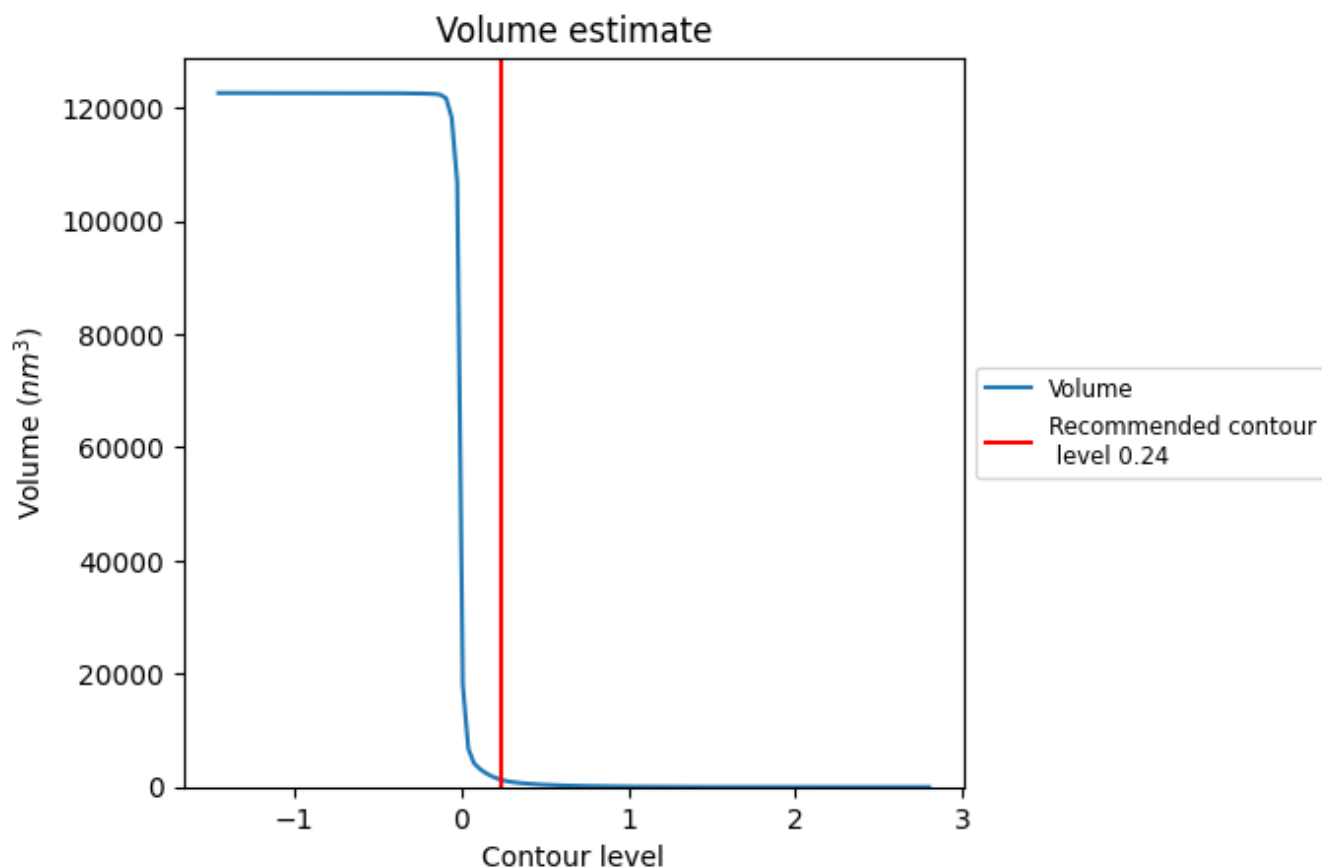
This section contains the results of statistical analysis of the map.

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.

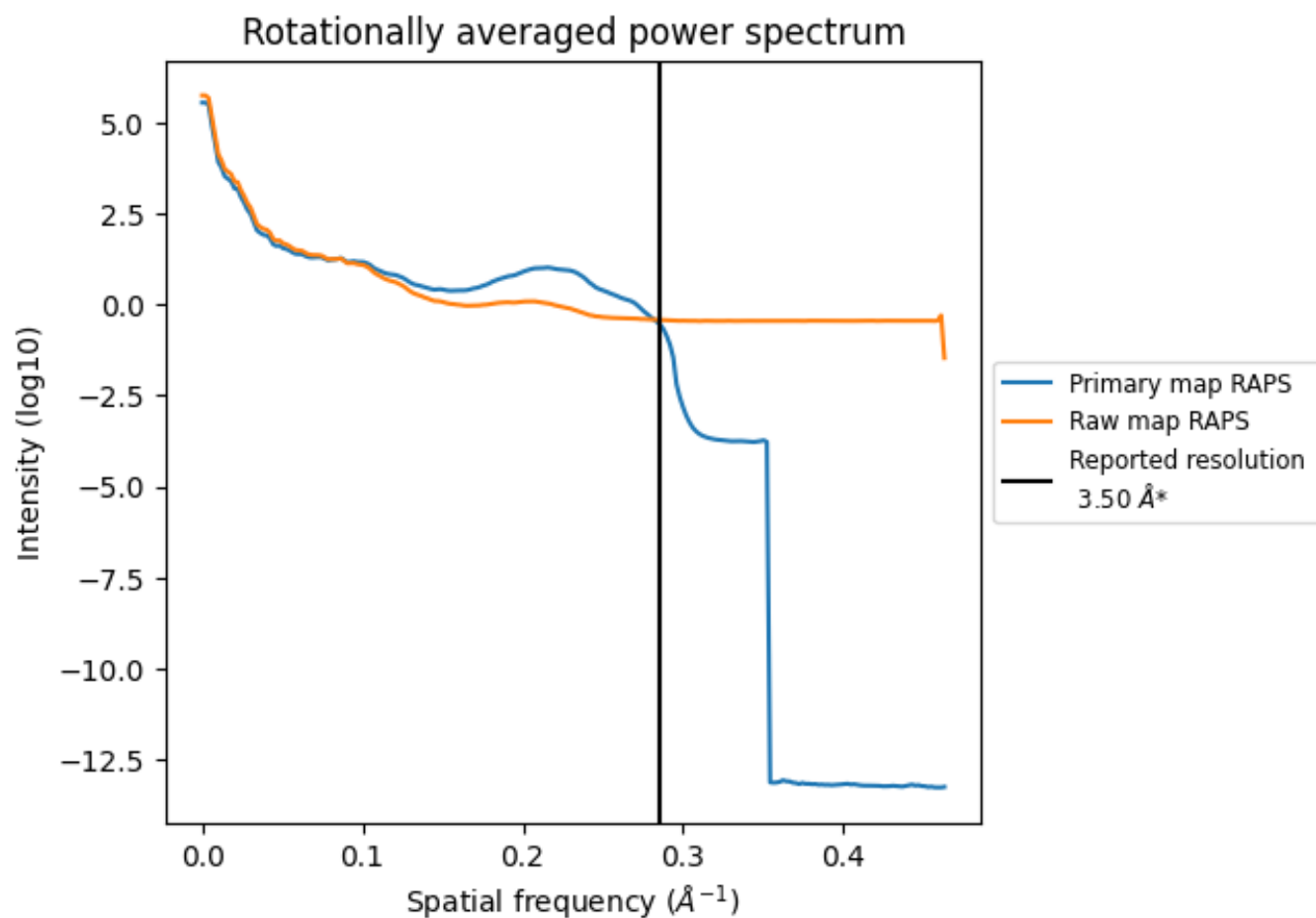
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1250 nm³; this corresponds to an approximate mass of 1129 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 ⓘ

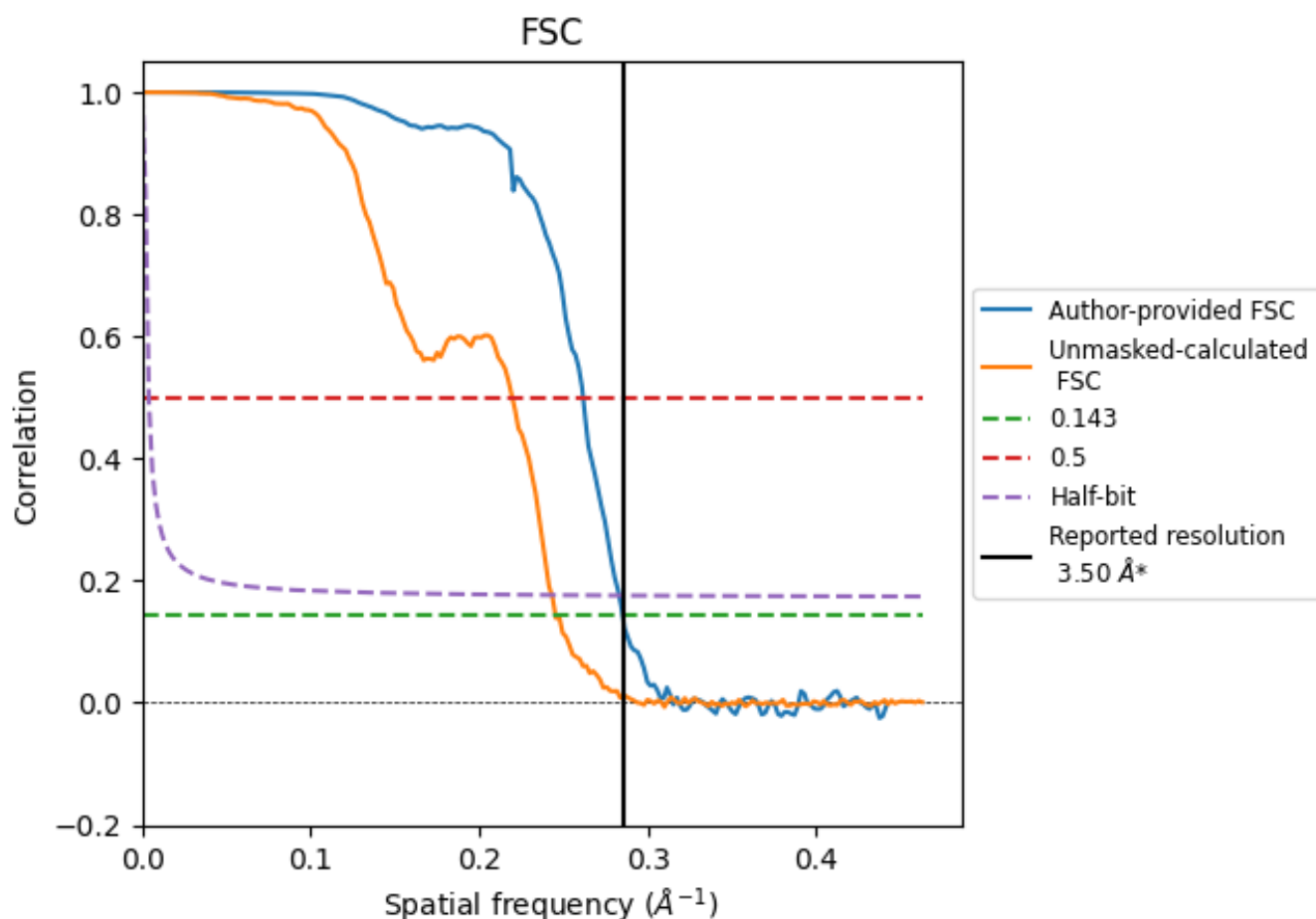


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

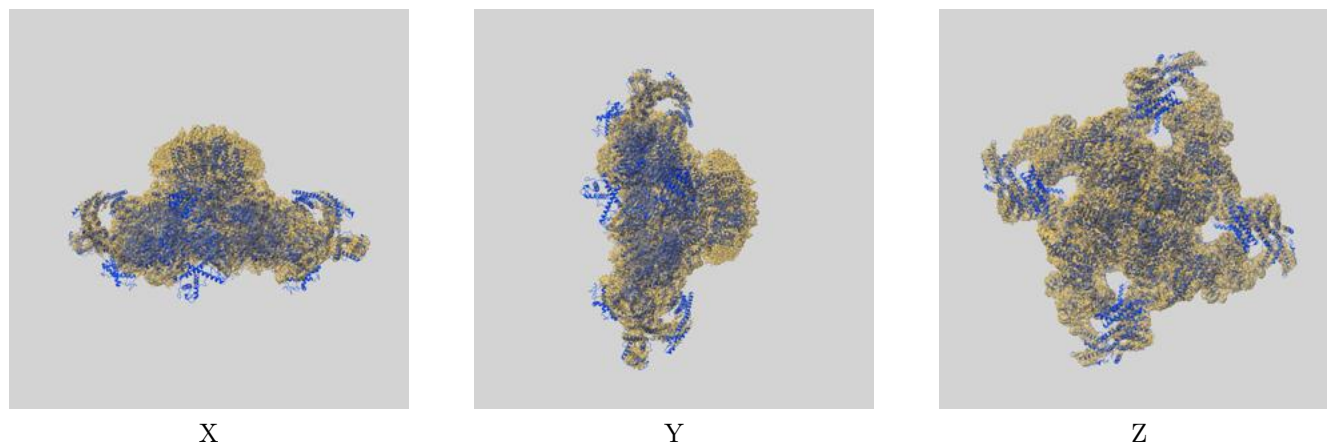
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.82	3.53
Unmasked-calculated*	4.08	4.55	4.11

*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 4.08 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

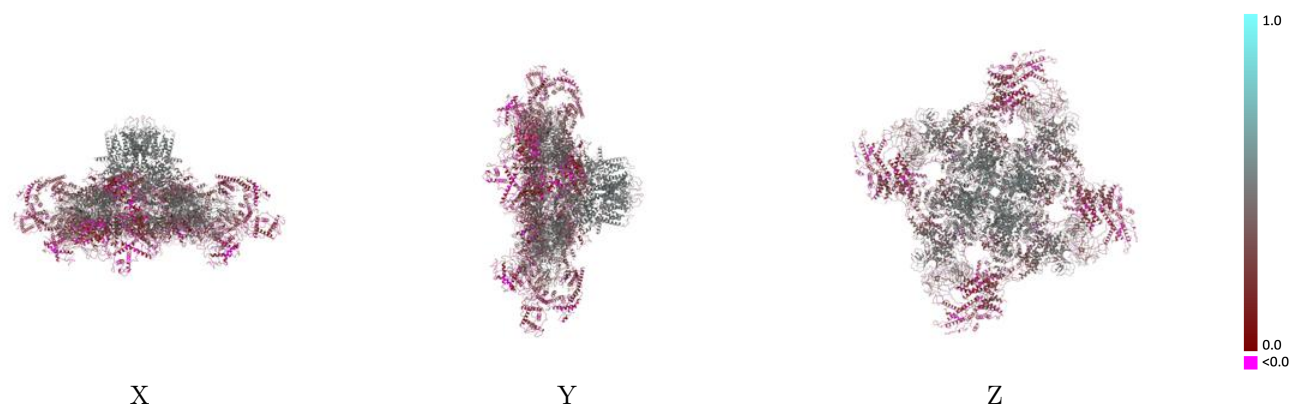
This section contains information regarding the fit between EMDB map EMD-27711 and PDB model 8DTY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



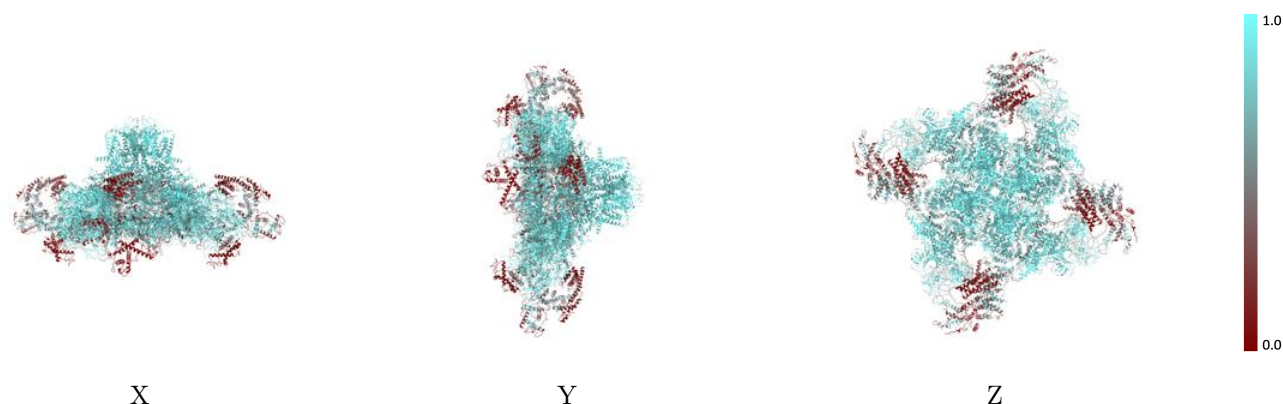
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



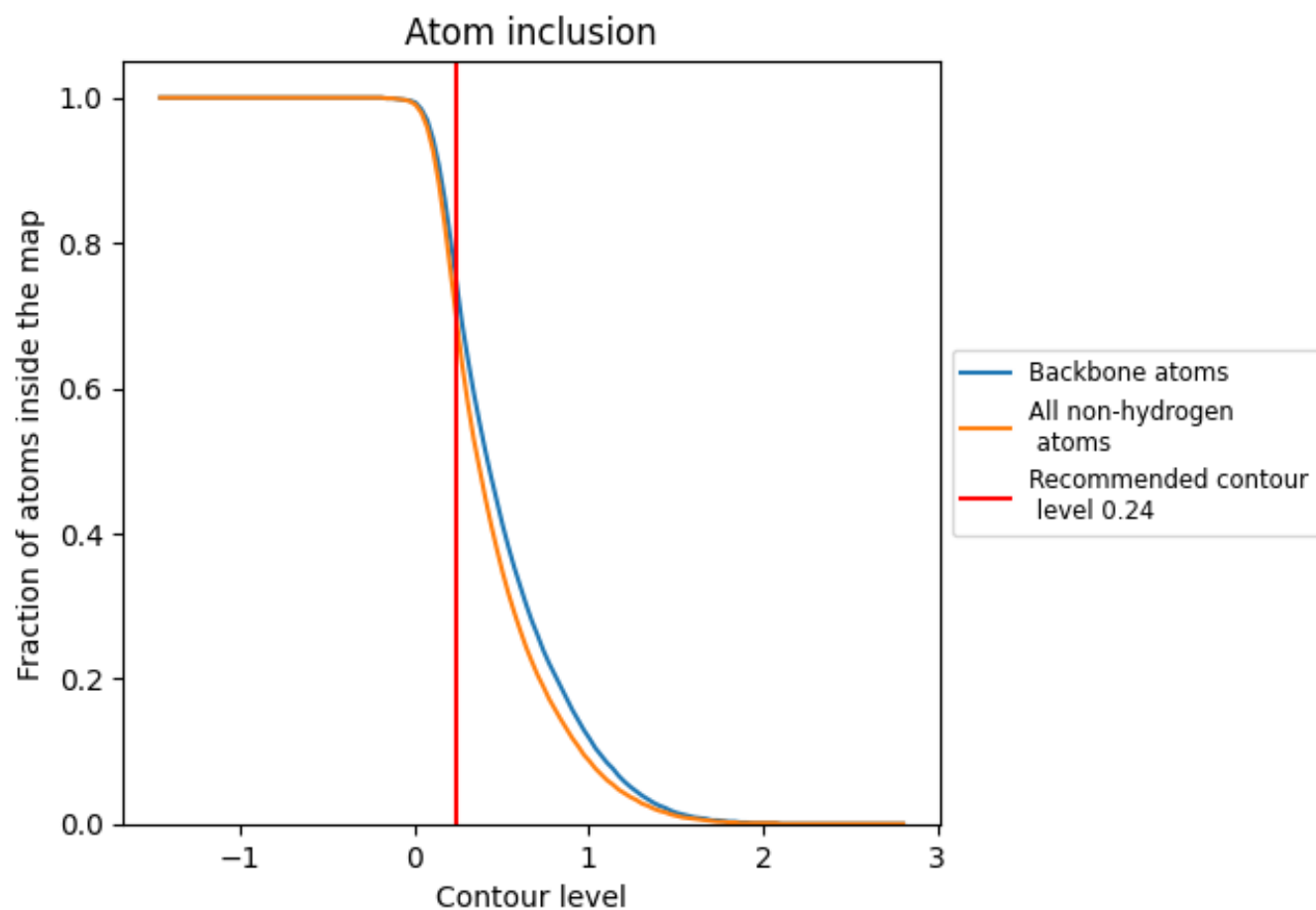
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.3090
A	0.6930	0.3070
B	0.6930	0.3070
C	0.6930	0.3070
D	0.6930	0.3070
E	0.8570	0.3930
F	0.8590	0.3950
G	0.8570	0.3930
H	0.8570	0.3960

1.0

0.0

<0.0