



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:36 AM UTC

PDB ID : 6JI0 / pdb_00006ji0
EMDB ID : EMD-9831
Title : Structure of RyR2 (F/A/C/Ca²⁺ dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-19
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

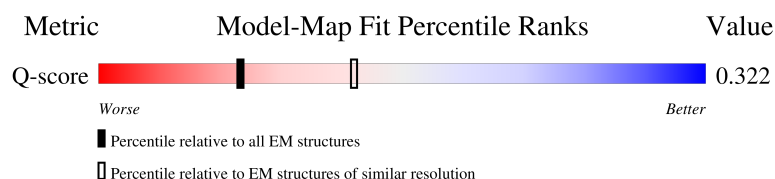
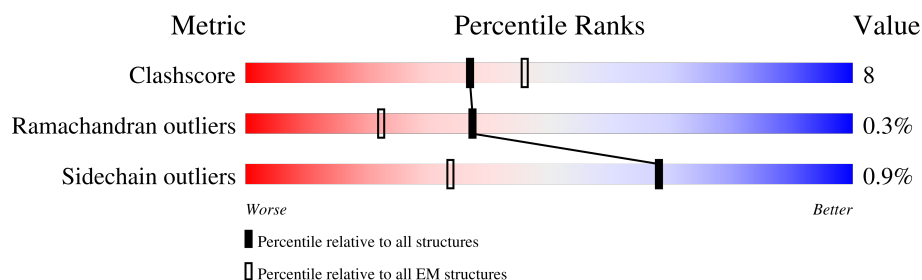
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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.



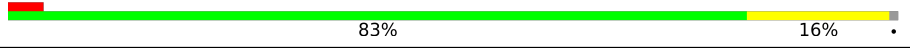
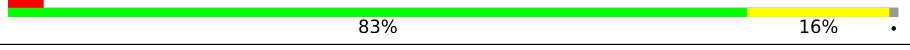
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	4968	
1	C	4968	
1	E	4968	
1	G	4968	

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Mol	Chain	Length	Quality of chain
2	B	108	 81% 19%
2	D	108	 82% 17%
2	F	108	 83% 16%
2	H	108	 83% 16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CFF	A	5103	-	X	-	-
6	CFF	C	5103	-	X	-	-
6	CFF	E	5103	-	X	-	-
6	CFF	G	5103	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 109772 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	C	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	E	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		
1	G	3476	Total	C	N	O	S	0	0
			26577	16924	4546	4949	158		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	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	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

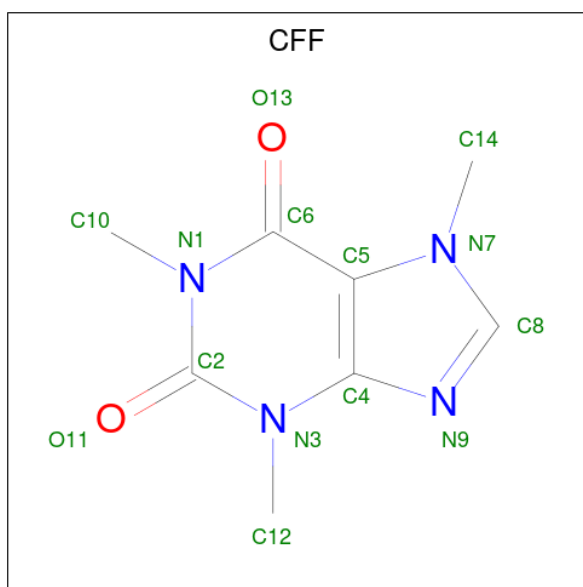


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	E	1	Total	Ca	0
			1	1	
5	G	1	Total	Ca	0
			1	1	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).

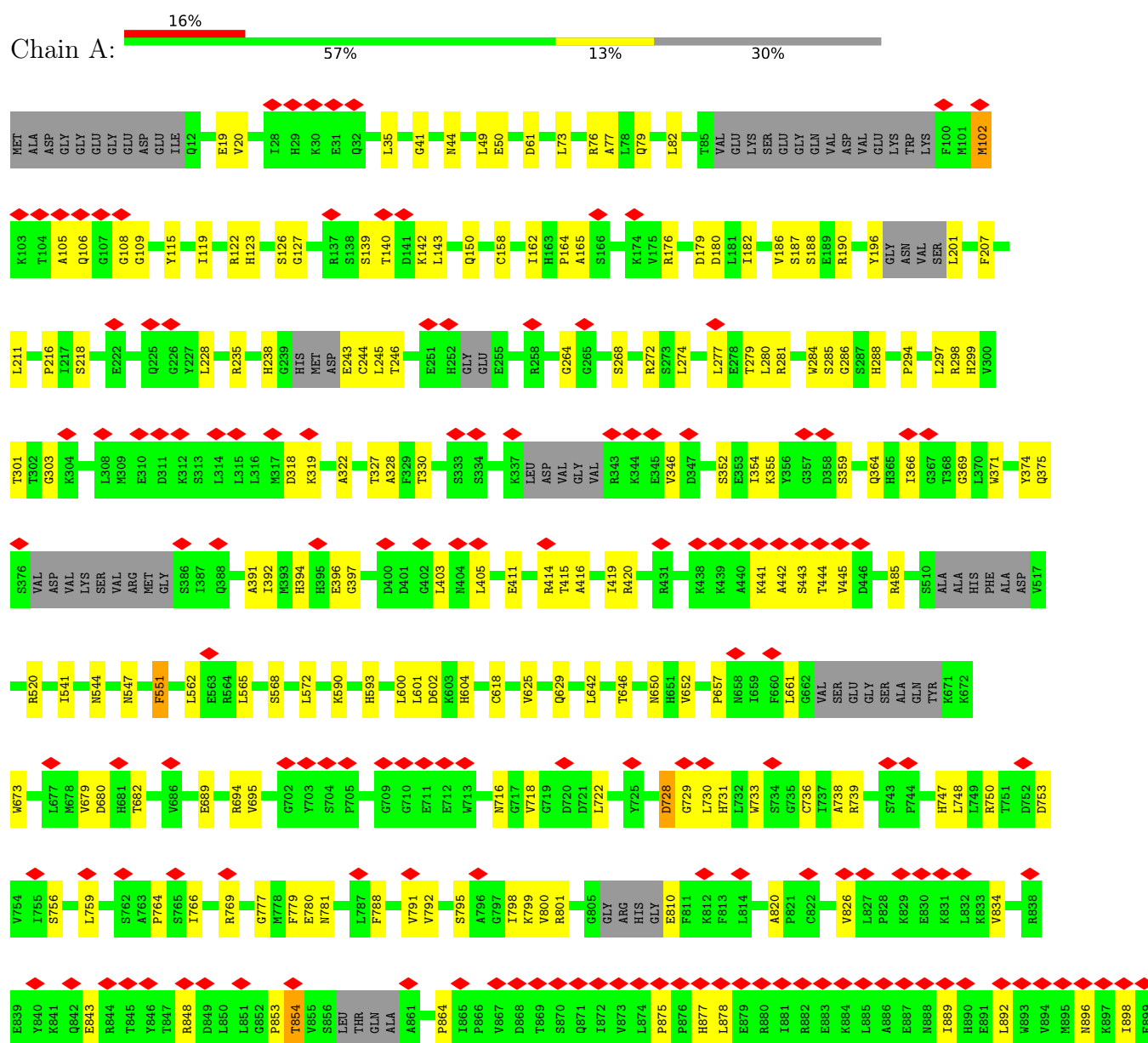


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

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: RyR2



L900	G901	W902	Q903	Y904	G905	P906	V907	R908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	GLU
LYS	VAL	LYS	MET	LYS	LEU	PRO	ASN	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	N981	D982	L983	S984	F985	I986	K987	L988	T989	P990	S991	Q992	E993	M1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ARG	ALA	R1013	G1014	GLY	TRP	THR	THR	TYR	GLY	ILE	GLN	GLN	ASP	VAL	LYS	ASN	R1027
P1030	V1033	P1034	Y1035	A1036	L1037	L1038	D1039	R1040	T1041	T1042	K1043	K1044	S1045	N1046	K1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	R1055	T1056	L1057	L1058	G1059	Y1060	G1061	Y1062	N1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ARG	ALA	GLU	VAL	CYS	THR	GLY	THR	GLY	ILE	GLN	GLN	ASP	VAL	LYS	ASN	R1027
A1098	G1099	E1106	A1107	V1108	T1109	A1110	R1114	G1115	W1117	S1118	R1119	C1122	D1125	G1126	E1127	L1128	G1129	S1130	A1136	F1137	Q1143	H1151	Y1152	G1153	Q1157	C1164	M1165	V1166	T1169	M1173	T1176	T1181	L1182	L1183	D1184	D1185	S1186	G1187	S1188	E1189	L1190	D1196																
D1199	P1203	V1204	C1205	L1207	G1208	V1209	A1210	Q1211	V1212	G1213	R1214	F1217	G1218	S1222	Y1226	I1229	Q1233	Y1236	F1239	A1240	T1243	N1244	R1245	D1246	M1249	W1250	L1251	S1252	K1253	R1254	P1255	Q1257	F1258	V1261	H1267	R1272	L1273	D1274	GLY	THR	ILE	ASP	SER	SER														
PRO	CYS	LEU	LYS	V1285	S1292	Q1293	M1294	S1295	A1296	T1297	D1298	I1299	M1300	F1301	L1304	S1305	M1306	P1307	I1308	E1309	C1310	ALA	GLU	VAL	PHE	SER	GLY	THR	ALA	GLY	ILE	PRO	GLY	ALA	SER	ASP	ASN	LEU	LEU	GLY	THR	ASP	ALA	SER	ASP	ALA	SER	ASP	THR	GLU	VAL	LEU						
MET	LYS	THR	ALA	GLY	HIS	LEU	VAL	ASP	ARG	VAL	ASP	LYS	GLN	THR	ALA	THR	LYS	PRO	GLU	PHE	GLN	GLY	THR	LYS	PRO	ALA	GLY	ARG	LEU	LEU	ARG	THR	ARG	THR	THR	HIS	ALA	SER	ALA	SER	ASP	ALA	SER	ASP	ALA	SER	ASP	THR	GLU	VAL	LEU							
GLU	ASP	VAL	LEU	ALA	ASP	ASP	ASP	TYR	ASP	LEU	MET	THR	SER	T1425	R1431	I1432	F1433	P1434	GLY	GLN	GLU	PRO	ALA	N1440	V1443	G1444	W1445	H1451	D1454	L1459	ASP	ARG	VAL	ARG	THR	V1465	T1466	T1467	T1468	L1469	G1470	D1471	E1472	K1473	G1474	K1475	V1476	H1477	E1478	S1479								
I1480	K1481	R1482	S1483	M1484	CYS	Y1486	M1487	V1488	C1489	A1490	GLY	GLU	SER	MET	SER	PRO	GLY	GLN	GLY	ARG	ASN	N1503	G1504	L1505	E1506	C1509	V1510	V1511	ASP	ALA	ALA	SER	G1516	L1517	L1518	T1519	F1520	K1525	D1526	L1527	S1528	T1529	Y1530	Q1531	V1532	V1533	L1539	V1543	A1547	M1551	E1556							
LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	LEU	SER	A1568	G1569	H1575	K1576	V1579	R1585	L1586	H1587	V1588	Q1589	F1590	V1594	L1595	W1596	S1597	M1598	M1599	P1600	N1601	Q1602	K1605	V1606	D1607	S1609	R1610	I1611	S1612	E1613	R1614	Q1615	G1616	W1617	L1618	V1619	Q1620	C1621	L1622	E1623	Q1626	S1629	L1630							
H1631	I1632	P1633	E1634	R1637	D1640	I1641	L1642	E1643	L1644	T1645	L1651	R1671	S1678	E1682	P1683	Q1684	L1685	T1689	E1690	P1695	Y1703	R1718	L1738	F1739	P1740	D1741	GLU	ASN	LYS	LYS	HIS	G1747	I1751	G1752	L1753	S1756	L1757	R1758	F1768	I1771	M1772	M1773	Y1776															
Q1777	D1785	K1788	A1789	K1790	R1807	D1808	P1809	V1810	P1820	I1830	H1835	K1840	Q1844	L1845	I1846	E1847	P1848	S1849	VAL	PHE	LYS	GLU	ALA	ALA	GLY	PRO	ALA	ALA	GLU	GLU	GLU	ALA	SER	ASP	THR	LYS	GLU	LYS	GLY	PRO	CYS	ALA	SER	GLU	ASP	GLN	ILE	ASN	MET	LEU	LEU	ASN	ALA	PHE	LYS			
GLU	SER	GLY	GLY	LYS	ARG	PRO	LYS	GLU	L1893	R1920	H1921	R1922	F1929	L1937	Q1938	R1942	V1948	MET	GLN	ALA	LEU	ASN	NET	SER	ALA	ALA	ALA	LEU	THR	ALA	ARG	LYS	THR	LYS	GLU	PHE	ARG	PRO	PRO	GLN	GLU	GLN	ILE	ASN	MET	LEU	LEU	ASN	ALA	PHE	LYS							

L2984	S2985	S2988	R2989	P2990	L2991	G2994	G2995	H2996	A2997	S2998	N2999	K3000	E3001	K3002	E3003	K3004	K3005	THR	SER	LEU	F3009	C3010	K3011	L3012	G3013	V3014	L3015	V3016	K3017	H3018	K3019	L3020	S3021	L3022	F3023	G3024	H3025	A3027	T3028	SER	ILE	VAL	ASN	CYS	L3034	H3035	L3036	L3037	T3040	L3041	D3042	A3043	R3044	PHE	V3046																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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E1478	S1479	I1480	K1481	R1482	S1483	M1484	CYS	Y1486	M1487	V1488	C1489	A1490	GLY	GLU	SER	GLY	GLN	GLY	PRO	PRO	GLY	GLY	ARG	ASN	ASN	H1503	G1504	L1505	E1506	C1509	V1510	V1511	ASP	N1601	ALA	ALA	SER	G1516	T1519	F1520	K1525	D1526	L1527	S1528	T1529	V1530	Y1531	Q1532	V1533	L1539	V1543	A1547	M1551						
E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	LEU	SER	A1568	G1569	H1575	K1576	V1579	R1585	L1586	H1587	Q1588	Q1589	F1590	V1594	L1595	H1596	S1597	R1598	M1599	P1600	Q1602	K1605	V1606	D1607	S1608	S1609	R1610	I1611	E1613	R1614	Q1615	G1616	W1617	L1618	V1619	Q1620	C1621	E1623	Q1626	S1629										
L1630	H1631	I1632	P1633	E1634	R1637	D1640	I1641	L1642	E1643	L1644	L1651	R1671	S1678	E1682	Q1683	L1685	I1689	E1690	Y1703	D1704	L1705	R1718	L1738	F1739	P1740	D1741	GLU	ASN	LYS	LYS	HIS	G1747	I1751	G1752	L1753	S1756	L1757	R1758	F1768	I1771	M1772	M1773	Y1776																
Q1777	D1785	K1788	A1789	K1790	R1807	D1808	L1809	V1810	P1820	I1830	M1831	H1835	K1840	Q1844	L1845	I1846	E1847	P1848	S1849	VAL	PHE	LYS	GLU	ALA	GLY	PRO	GLU	GLU	GLU	ASP	THR	GLU	LYS	GLU	PRO	CYS	ALA	SER	GLU	GLN	ASN	ARG	LEU	GLU	GLY	PRO	ALA	GLU											
GLU	GLU	SER	LYS	GLY	GLY	LYS	ARG	PRO	PRO	GLN	LYS	L1894	L1905	R1920	H1921	R1922	F1929	Q1938	R1942	V1948	MET	GLN	ALA	LEU	ASN	NET	SER	ALA	ALA	LYS	THR	LYS	GLN	PHE	ARG	SER	PRO	PRO	GLN	GLU	ILE	ASN	MET	LEU	ASN	PHE	LYS												
ASP	ASP	LYS	SER	CYS	GLY	PRO	CYS	PRO	PRO	GLU	ILE	R1984	H2007	I2010	E2011	L2012	D2013	GLU	ASP	GLY	SER	ASP	GLY	ASN	S2022	T2025	I2026	R2027	G2028	R2029	L2030	Y2039	LEU	LYS	LYS	LYS	GLN	ALA	GLU	LYS	LEU	VAL	GLU	SER	ASP	LYS	SER	T2058	Q2072										
V2075	I2076	E2077	L2081	V2082	R2083	Y2093	D2116	T2117	I2118	L2124	I2127	V2133	M2143	K2154	N2161	R2164	V2177	G2181	GLY	GLY	GLU	ILE	SER	LYS	GLU	THR	F2190	K2191	K2192	M2193	N2196	L2201	D2217	Y2221	S2226	L2230	A2231	S2232	P2233	R2236																			
L2241	G2274	LEU	GLN	SER	CYS	VAL	LEU	SER	LYS	GLY	TYR	PRO	ASP	ILE	GLY	TRP	P2293	D2301	R2304	F2308	S2313	V2314	E2315	L2324	L2325	I2326	R2327	R2328	PRO	GLU	CYS	PHE	GLY	PRO	LEU	ARG	GLY	GLU	GLY	ASN	G2343	L2344	L2345	W2348	E2349														
I2354	ALA	GLU	ASP	PRO	SER	ARG	ASP	GLY	PRO	SER	THR	SER	GLY	LYS	TYR	SER	SER	SER	SER	GLY	ASN	MET	PRO	ASP	THR	GLU	GLY	GLU	GLU	ASP	THR	ILE	HIS	MET	G2386	A2404	PRO	GLU	MET	HIS	ILE	ILE	ALA	ALA	LYS	GLY	E2416	R2419	I2420	R2421	S2422	R2425	SER	LEU	ILE	PRO	LEU	G2431	
V2434	G2435	V2436	I2437	S2438	I2439	G2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	GLY	MET	SER	ALA	GLY	F2461	C2462	P2463	D2464	H2465	K2466	R2475	V2476	GLY	ILE	GLU	V2481	L2485	L2486	H2487	L2488	L2489	VAL	G2492	F2493	D2496	A2500	L2503	ASP	THR	ALA								
ALA	LEU	SER	ALA	T2511	R2519	C2522	P2527	L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	F2536	A2537	G2538	T2539	E2540	L2549	V2553	TYR	ARG	LEU	SER	K2558	Q2566	R2567	L2574	L2575	S2576	ILE	CYS	GLY	GLN	LEU	R2582	P2583	S2584	M2585	M2586	Q2587	H2588	L2589	L2590	L2593	D2596	V2597	P2598									
N2601	H2601	GLU	ALA	K2605	L2608	K2609	L2610	L2611	T2612	MET	M2613	H2614	Y2621	Y2622	C2623	L2624	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	H2640	L2641	K2644	L2645	F2646	F2650	D2651	A2652	L2653	SER	GLN	LYS	LYS	Y2658	E2659	F2663	K2664	L2665	C2669	D2670	K2671	A2672	V2673	A2674								
P2678	P2679	ASP	TYR	MET	GLU	GLU	ASN	TYR	VAL	SER	MET	MET	GLU	LYS	GLN	SER	SER	SER	MET	ASP	SER	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	P2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719	Y2720	F2721	I2722	N2723	K2724	Y2725	K2726	E2727	H2728	S2729	D2730	H2731	K2732	A2733	N2734	A2735	D2736



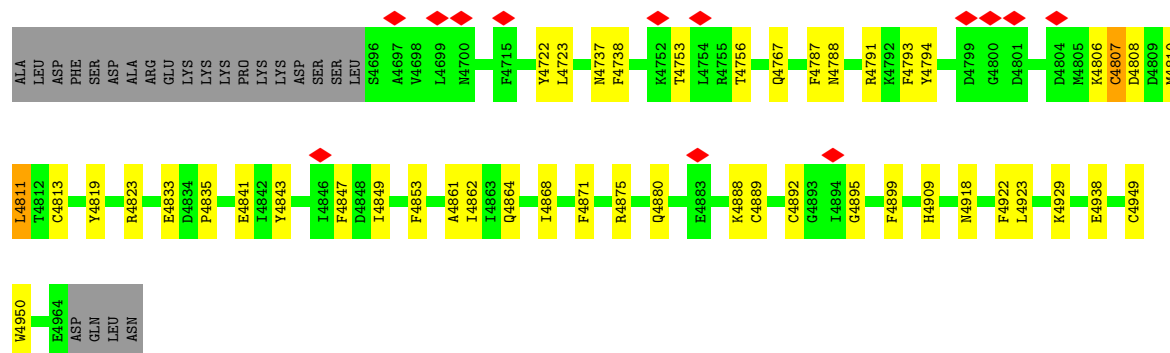




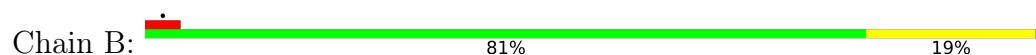


TYR	THR	GLN	MET	PRO	PRO	HIS	VAL	MET	VAL	VAL	LEU	PRO	MET	THR	GLY	ASP	ASP	ASN	GLY	VAL	VAL	GLU	PRO	ASP	MET	SER	SER	ALA	GLY	F2461	H2465	K2466	R2475	V2476	V2477	GLY	ILE	GLU	V2481	L2485	L2486	H2487	L2488	L2489	GLU	VAL	G2492	F2493	D2496	A2500	L2503	ASP	THR	ALA	ALA	LEU	SER	SER	ALA	T2511	C2522
P2527	L2528	L2529	THR	ARG	CYS	ALA	PRO	LEU	F2536	A2537	G2538	T2539	E2540	H2541	L2549	V2553	TYR	ARG	LEU	SER	K2558	Q2566	R2567	L2574	L2575	S2576	ILE	CYS	GLY	GLN	LEU	R2582	P2583	S2584	M2585	M2586	Q2587	H2588	L2589	L2590	L2593	D2596	V2597	P2598	N2601	GLU	HIS	ALA	K2605	L2608	K2609										
L2610	L2611	T2612	N2613	H2614	Y2621	T2622	C2623	L2624	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	H2640	L2641	K2644	L2645	F2646	F2650	D2651	A2652	L2653	SER	GLN	LYS	Y2658	E2659	F2663	K2664	L2665	C2669	L2670	S2671	A2672	V2673	A2674	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN											
TYR	VAL	SER	MET	GLN	GLY	LYS	GLN	SER	SER	MET	ASP	SER	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719	Y2720	P2721	I2722	N2723	K2724	Y2725	A2726	E2727	H2728	S2729	H2730	D2731	K2732	N2733	S2734	N2735	D2736	K2737	L2738	A2739	N2740	G2741	N2742	I2743	Y2744	G2745		
E2746	I2747	Y2748	S2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	K2758	P2759	P2760	Y2761	K2762	L2763	L2764	S2765	E2766	K2767	E2768	K2769	I2770	E2771	Y2772	R2773	W2774	P2775	I2776	K2777	E2778	L2780	K2781	T2782	M2783	L2784	A2785	W2786	G2787	W2788	R2789	I2790	E2791	R2792	T2793	L2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR			
ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	T2822	S2823	P2824	R2825	A2826	T2827	D2828	M2829	S2830	T2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840	M2841	A2842	E2843	M2844	W2845	E2846	N2848	Y2849	H2850	W2851	T2852	W2853	A2854	K2855	K2856	T2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865				
G2866	G2867	N2868	H2869	P2870	L2871	L2872	P2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	Q2897	L2898	N2899	L2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	ASP	THR	PRO	SER	ILE	GLU	ARG	PHE	ALA	TYR	SER			
PHE	LEU	GLN	GLN	LEU	ILE	ARG	TYR	VAL	VAL	GLU	ALA	HIS	GLN	TYR	ILE	GLU	PHE	ASP	GLY	GLY	ARG	SER	SER	LYS	GLY	GLU	HIS	PRO	TYR	GLU	GLN	ILE	LYS	PHE	ALA	LYS	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	ASN	HIS	ARG	LEU	Y2982	F2983	L2984	S2985									
S2988	R2989	P2990	L2991	G2994	G2995	H2996	A2997	S2998	N2999	K3000	E3001	K3002	E3003	M3004	V3005	THR	SER	LEU	F3009	C3010	K3011	L3012	V3014	L3015	L3016	K3017	H3018	R3019	F3081	L3141	G3142	THR	THR	ARG	ASN	GLN	PRO	LYS	GLY	VAL	THR	SER	ILE	VAL	ASN	CYS	L3034	H3035	I3036	L3037	T3040	L3041	D3042	A3043	R3044	T3045	V3046	M3047	K3048		
T3049	G3050	L3051	E3052	S3053	K3055	SER	ALA	ALA	LEU	ARG	ALA	F3061	L3062	D3063	N3064	A3065	A3066	E3067	D3068	L3069	E3070	K3071	T3072	K3073	E3074	N3075	L3076	K3077	Q3078	G3079	Q3080	F3081	L3141	G3142	HIS	THR	ARG	ASN	GLN	PRO	LYS	GLY	VAL	THR	SER	ILE	VAL	ASN	CYS	L3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	
L3109	F3110	E3111	H3112	L3113	G3114	Q3115	H3116	Q3117	F3118	GLY	GLU	ASP	LEU	ILE	L3124	E3125	D3126	V3127	Q3128	V3129	S3130	C3131	R3132	A3133	L3134	L3135	L3136	S3137	L3138	Y3139	A3140	L3141	G3142	THR	THR	ARG	ASN	GLN	PRO	ILE	TYR	V3149	E3150	R3151	Q3152	R3153	S3154	A3155	L3156	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO
VAL	A3170	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	THR	LYS	SER	SER	GLY	PRO	ARG	GLU	ASN	ALA	ALA	GLY	ASN	ARG	GLY	ALA	PRO	TYR	THR	GLY	LEU	LEU	GLY	ASN	GLU	ILE	GLU	ILE	LYS	ILE	ASP	LEU	ALA	GLU	SER	GLY	ILE	ARG					
TYR	THR	GLN	MET	PRO	PRO	HIS	VAL	MET	VAL	VAL	LEU	PRO	MET	THR	GLY	ASP	ASP	ASN	GLY	VAL	VAL	GLU	PRO	ASP	ASN	GLY	ALA	ALA	GLY	ASN	ARG	GLY	ALA	PRO	TYR	THR	GLY	LEU	LEU	GLY	ASN	GLU	ILE	GLU	ILE	LYS	ILE	ASP	LEU	ALA	GLU	SER	GLY	ILE	ARG						

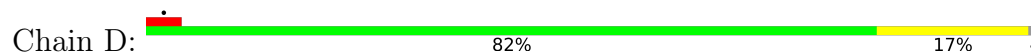




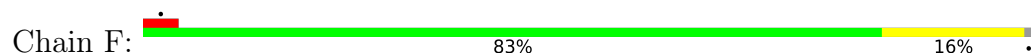
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



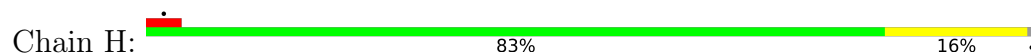
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- 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	78841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/27073	0.65	16/36605 (0.0%)
1	C	0.32	0/27073	0.65	16/36605 (0.0%)
1	E	0.32	0/27073	0.65	16/36605 (0.0%)
1	G	0.32	0/27073	0.65	16/36605 (0.0%)
2	B	0.25	0/835	0.51	0/1123
2	D	0.25	0/835	0.51	0/1123
2	F	0.25	0/835	0.51	0/1123
2	H	0.25	0/835	0.51	0/1123
All	All	0.32	0/111632	0.65	64/150912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	C	0	25
1	E	0	25
1	G	0	25
All	All	0	100

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	CA-C-N	7.16	134.58	121.70
1	A	139	SER	C-N-CA	7.16	134.58	121.70
1	C	139	SER	CA-C-N	7.16	134.58	121.70
1	C	139	SER	C-N-CA	7.16	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	139	SER	CA-C-N	7.16	134.58	121.70
1	E	139	SER	C-N-CA	7.16	134.58	121.70
1	G	139	SER	CA-C-N	7.16	134.58	121.70
1	G	139	SER	C-N-CA	7.16	134.58	121.70
1	A	2133	VAL	CA-C-N	6.72	133.79	121.70
1	A	2133	VAL	C-N-CA	6.72	133.79	121.70
1	C	2133	VAL	CA-C-N	6.72	133.79	121.70
1	C	2133	VAL	C-N-CA	6.72	133.79	121.70
1	G	2133	VAL	CA-C-N	6.72	133.79	121.70
1	G	2133	VAL	C-N-CA	6.72	133.79	121.70
1	E	2133	VAL	CA-C-N	6.70	133.76	121.70
1	E	2133	VAL	C-N-CA	6.70	133.76	121.70
1	A	140	THR	CA-C-N	5.74	132.04	121.70
1	A	140	THR	C-N-CA	5.74	132.04	121.70
1	C	140	THR	CA-C-N	5.74	132.04	121.70
1	C	140	THR	C-N-CA	5.74	132.04	121.70
1	E	140	THR	CA-C-N	5.74	132.04	121.70
1	E	140	THR	C-N-CA	5.74	132.04	121.70
1	G	140	THR	CA-C-N	5.73	132.01	121.70
1	G	140	THR	C-N-CA	5.73	132.01	121.70
1	C	1772	ASN	N-CA-C	5.65	118.09	111.02
1	A	1772	ASN	N-CA-C	5.65	118.09	111.02
1	E	1772	ASN	N-CA-C	5.65	118.09	111.02
1	G	1772	ASN	N-CA-C	5.65	118.09	111.02
1	C	442	ALA	N-CA-C	5.55	126.53	111.00
1	G	442	ALA	N-CA-C	5.55	126.53	111.00
1	E	442	ALA	N-CA-C	5.54	126.51	111.00
1	A	826	VAL	CA-C-N	5.54	130.31	121.62
1	A	826	VAL	C-N-CA	5.54	130.31	121.62
1	C	826	VAL	CA-C-N	5.54	130.31	121.62
1	C	826	VAL	C-N-CA	5.54	130.31	121.62
1	E	826	VAL	CA-C-N	5.54	130.31	121.62
1	E	826	VAL	C-N-CA	5.54	130.31	121.62
1	A	442	ALA	N-CA-C	5.53	126.47	111.00
1	G	826	VAL	CA-C-N	5.52	130.29	121.62
1	G	826	VAL	C-N-CA	5.52	130.29	121.62
1	A	1471	ASP	CA-C-N	5.39	131.84	121.54
1	A	1471	ASP	C-N-CA	5.39	131.84	121.54
1	C	1471	ASP	CA-C-N	5.39	131.83	121.54
1	C	1471	ASP	C-N-CA	5.39	131.83	121.54
1	E	1471	ASP	CA-C-N	5.39	131.83	121.54
1	E	1471	ASP	C-N-CA	5.39	131.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1471	ASP	CA-C-N	5.39	131.83	121.54
1	G	1471	ASP	C-N-CA	5.39	131.83	121.54
1	E	4164	PRO	CA-C-N	5.30	131.67	121.54
1	E	4164	PRO	C-N-CA	5.30	131.67	121.54
1	C	4164	PRO	CA-C-N	5.30	131.66	121.54
1	C	4164	PRO	C-N-CA	5.30	131.66	121.54
1	G	4164	PRO	CA-C-N	5.30	131.66	121.54
1	G	4164	PRO	C-N-CA	5.30	131.66	121.54
1	A	4164	PRO	CA-C-N	5.28	131.62	121.54
1	A	4164	PRO	C-N-CA	5.28	131.62	121.54
1	A	441	LYS	CA-C-N	5.13	130.94	121.70
1	A	441	LYS	C-N-CA	5.13	130.94	121.70
1	C	441	LYS	CA-C-N	5.12	130.92	121.70
1	C	441	LYS	C-N-CA	5.12	130.92	121.70
1	E	441	LYS	CA-C-N	5.12	130.92	121.70
1	E	441	LYS	C-N-CA	5.12	130.92	121.70
1	G	441	LYS	CA-C-N	5.11	130.89	121.70
1	G	441	LYS	C-N-CA	5.11	130.89	121.70

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Peptide
1	A	142	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1602	GLN	Peptide
1	A	1757	LEU	Peptide
1	A	1777	GLN	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2232	SER	Peptide
1	A	2462	CYS	Peptide
1	A	2874	PRO	Peptide
1	A	3634	GLU	Peptide
1	A	4007	SER	Peptide
1	A	4072	GLU	Peptide
1	A	4074	ASP	Peptide
1	A	4130	PHE	Peptide
1	A	4131	GLN	Peptide
1	A	4594	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	4880	GLN	Peptide
1	A	520	ARG	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	854	THR	Peptide
1	C	105	ALA	Peptide
1	C	142	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1602	GLN	Peptide
1	C	1757	LEU	Peptide
1	C	1777	GLN	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2232	SER	Peptide
1	C	2462	CYS	Peptide
1	C	2874	PRO	Peptide
1	C	3634	GLU	Peptide
1	C	4007	SER	Peptide
1	C	4072	GLU	Peptide
1	C	4074	ASP	Peptide
1	C	4130	PHE	Peptide
1	C	4131	GLN	Peptide
1	C	4594	LEU	Peptide
1	C	4880	GLN	Peptide
1	C	520	ARG	Peptide
1	C	728	ASP	Peptide
1	C	729	GLY	Peptide
1	C	739	ARG	Peptide
1	C	854	THR	Peptide
1	E	105	ALA	Peptide
1	E	142	LYS	Peptide
1	E	1579	VAL	Peptide
1	E	1602	GLN	Peptide
1	E	1757	LEU	Peptide
1	E	1777	GLN	Peptide
1	E	1835	HIS	Peptide
1	E	1847	GLU	Peptide
1	E	2075	VAL	Peptide
1	E	2232	SER	Peptide
1	E	2462	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	2874	PRO	Peptide
1	E	3634	GLU	Peptide
1	E	4007	SER	Peptide
1	E	4072	GLU	Peptide
1	E	4074	ASP	Peptide
1	E	4130	PHE	Peptide
1	E	4131	GLN	Peptide
1	E	4594	LEU	Peptide
1	E	4880	GLN	Peptide
1	E	520	ARG	Peptide
1	E	728	ASP	Peptide
1	E	729	GLY	Peptide
1	E	739	ARG	Peptide
1	E	854	THR	Peptide
1	G	105	ALA	Peptide
1	G	142	LYS	Peptide
1	G	1579	VAL	Peptide
1	G	1602	GLN	Peptide
1	G	1757	LEU	Peptide
1	G	1777	GLN	Peptide
1	G	1835	HIS	Peptide
1	G	1847	GLU	Peptide
1	G	2075	VAL	Peptide
1	G	2232	SER	Peptide
1	G	2462	CYS	Peptide
1	G	2874	PRO	Peptide
1	G	3634	GLU	Peptide
1	G	4007	SER	Peptide
1	G	4072	GLU	Peptide
1	G	4074	ASP	Peptide
1	G	4130	PHE	Peptide
1	G	4131	GLN	Peptide
1	G	4594	LEU	Peptide
1	G	4880	GLN	Peptide
1	G	520	ARG	Peptide
1	G	728	ASP	Peptide
1	G	729	GLY	Peptide
1	G	739	ARG	Peptide
1	G	854	THR	Peptide

5.2 Too-close contacts ⓘ

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	26577	0	25112	456	0
1	C	26577	0	25112	439	0
1	E	26577	0	25113	439	0
1	G	26577	0	25113	431	0
2	B	819	0	824	12	0
2	D	819	0	824	11	0
2	F	819	0	824	12	0
2	H	819	0	824	10	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	31	0	12	2	0
4	C	31	0	12	1	0
4	E	31	0	12	1	0
4	G	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	14	0	10	0	0
6	C	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
All	All	109772	0	103834	1614	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 8.

All (1614) 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:E:4853:PHE:CZ	1:G:4823:ARG:HA	1.53	1.43
1:A:4823:ARG:HA	1:G:4853:PHE:CZ	1.54	1.42
1:C:4853:PHE:CZ	1:E:4823:ARG:HA	1.54	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4853:PHE:CZ	1:C:4823:ARG:HA	1.54	1.40
1:A:4794:TYR:HD2	1:A:4807:CYS:CB	1.46	1.27
1:A:4811:LEU:HD11	1:C:4520:PHE:CE1	1.74	1.20
1:A:4520:PHE:HE1	1:G:4811:LEU:HD11	1.03	1.19
1:E:4811:LEU:HD11	1:G:4520:PHE:HE1	1.05	1.19
1:E:4849:ILE:HD11	1:G:4819:TYR:HA	1.25	1.18
1:A:4794:TYR:CD2	1:A:4807:CYS:HB2	1.77	1.18
1:A:4849:ILE:HD11	1:C:4819:TYR:HA	1.26	1.17
1:C:4849:ILE:HD11	1:E:4819:TYR:HA	1.26	1.13
1:A:4819:TYR:HA	1:G:4849:ILE:HD11	1.27	1.11
1:G:4892:CYS:SG	1:G:4909:HIS:CE1	2.44	1.11
1:C:4892:CYS:SG	1:C:4909:HIS:CE1	2.44	1.10
1:E:187:SER:O	1:G:2419:ARG:HD2	1.52	1.10
1:A:187:SER:O	1:C:2419:ARG:HD2	1.52	1.10
1:C:4811:LEU:HD11	1:E:4520:PHE:HE1	1.03	1.09
1:E:4892:CYS:SG	1:E:4909:HIS:CE1	2.44	1.09
1:A:2419:ARG:HD2	1:G:187:SER:O	1.52	1.09
1:A:4892:CYS:SG	1:A:4909:HIS:CE1	2.44	1.09
1:A:4811:LEU:HD11	1:C:4520:PHE:HE1	1.03	1.09
1:A:4520:PHE:CE1	1:G:4811:LEU:HD11	1.88	1.09
1:C:187:SER:O	1:E:2419:ARG:HD2	1.53	1.08
1:C:4811:LEU:HD11	1:E:4520:PHE:CE1	1.88	1.08
1:A:4794:TYR:CD2	1:A:4807:CYS:CB	2.36	1.08
1:E:4811:LEU:HD11	1:G:4520:PHE:CE1	1.90	1.07
1:E:4853:PHE:CZ	1:G:4823:ARG:CA	2.38	1.06
1:E:207:PHE:CE2	1:G:2326:ILE:HG23	1.91	1.06
1:A:4853:PHE:CZ	1:C:4823:ARG:CA	2.40	1.05
1:A:2326:ILE:HG23	1:G:207:PHE:CE2	1.92	1.04
1:C:207:PHE:CE2	1:E:2326:ILE:HG23	1.92	1.04
1:A:207:PHE:CE2	1:C:2326:ILE:HG23	1.91	1.04
1:C:4853:PHE:CZ	1:E:4823:ARG:CA	2.40	1.04
1:E:4861:ALA:CB	1:G:4864:GLN:HE21	1.70	1.04
1:C:4861:ALA:CB	1:E:4864:GLN:HE21	1.72	1.03
1:A:4794:TYR:HD2	1:A:4807:CYS:HB2	1.04	1.03
1:A:4823:ARG:CA	1:G:4853:PHE:CZ	2.40	1.03
1:A:4861:ALA:CB	1:C:4864:GLN:HE21	1.72	1.03
1:A:4864:GLN:HE21	1:G:4861:ALA:CB	1.72	1.02
1:A:4791:ARG:C	1:A:4806:LYS:HE2	1.86	1.00
1:E:4849:ILE:CD1	1:G:4819:TYR:HA	1.91	1.00
1:A:4849:ILE:CD1	1:C:4819:TYR:HA	1.92	1.00
1:A:4819:TYR:HA	1:G:4849:ILE:CD1	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4853:PHE:HZ	1:C:4823:ARG:CA	1.75	0.99
1:C:4849:ILE:CD1	1:E:4819:TYR:HA	1.92	0.98
1:A:4823:ARG:CA	1:G:4853:PHE:HZ	1.75	0.97
1:E:4853:PHE:HZ	1:G:4823:ARG:CA	1.74	0.97
1:C:4853:PHE:HZ	1:E:4823:ARG:CA	1.74	0.97
1:C:4811:LEU:CD1	1:E:4520:PHE:CE1	2.49	0.96
1:A:4823:ARG:HA	1:G:4853:PHE:HZ	0.94	0.96
1:A:4520:PHE:CE1	1:G:4811:LEU:CD1	2.49	0.94
1:E:4811:LEU:CD1	1:G:4520:PHE:CE1	2.50	0.93
1:A:4811:LEU:CD1	1:C:4520:PHE:CE1	2.52	0.93
1:E:4853:PHE:HE2	1:G:4823:ARG:CB	1.82	0.93
1:E:4853:PHE:CE2	1:G:4823:ARG:CB	2.52	0.92
1:A:4853:PHE:CE2	1:C:4823:ARG:CB	2.53	0.92
1:C:4853:PHE:CE2	1:E:4823:ARG:CB	2.53	0.92
1:A:4520:PHE:HE1	1:G:4811:LEU:CD1	1.82	0.92
1:A:4823:ARG:CB	1:G:4853:PHE:HE2	1.84	0.91
1:C:4853:PHE:HE2	1:E:4823:ARG:CB	1.84	0.91
1:A:4823:ARG:CB	1:G:4853:PHE:CE2	2.53	0.90
1:A:4853:PHE:HE2	1:C:4823:ARG:CB	1.84	0.90
1:C:4811:LEU:CD1	1:E:4520:PHE:HE1	1.83	0.89
1:E:4861:ALA:HB2	1:G:4864:GLN:HE21	1.37	0.88
1:E:4811:LEU:CD1	1:G:4520:PHE:HE1	1.84	0.88
1:C:4861:ALA:HB2	1:E:4864:GLN:HE21	1.38	0.88
1:A:4861:ALA:HB2	1:C:4864:GLN:HE21	1.38	0.87
1:A:4767:GLN:HE22	1:C:4871:PHE:HE1	1.24	0.85
1:A:4794:TYR:HD2	1:A:4807:CYS:HB3	1.39	0.85
1:A:4864:GLN:HE21	1:G:4861:ALA:HB2	1.38	0.85
1:A:207:PHE:CZ	1:C:2326:ILE:CG2	2.60	0.84
1:A:4787:PHE:HE1	1:A:4808:ASP:O	1.60	0.84
1:E:207:PHE:CZ	1:G:2326:ILE:CG2	2.60	0.84
1:E:207:PHE:CZ	1:G:2326:ILE:HG23	2.13	0.84
1:A:2326:ILE:HG23	1:G:207:PHE:CZ	2.13	0.83
1:A:4871:PHE:HE1	1:G:4767:GLN:HE22	1.25	0.83
1:A:4811:LEU:HD12	1:C:4519:LEU:HD12	1.60	0.83
1:C:4849:ILE:HD11	1:E:4819:TYR:CA	2.08	0.83
1:A:207:PHE:CZ	1:C:2326:ILE:HG23	2.12	0.83
1:E:4849:ILE:HD11	1:G:4819:TYR:CA	2.07	0.83
1:C:207:PHE:CZ	1:E:2326:ILE:HG23	2.13	0.83
1:A:2326:ILE:CG2	1:G:207:PHE:CZ	2.61	0.83
1:A:4811:LEU:CD1	1:C:4520:PHE:CD1	2.61	0.82
1:C:207:PHE:CZ	1:E:2326:ILE:CG2	2.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4861:ALA:HB1	1:G:4864:GLN:HE21	1.42	0.82
1:G:4787:PHE:HE1	1:G:4808:ASP:O	1.62	0.82
1:C:4787:PHE:HE1	1:C:4808:ASP:O	1.62	0.81
1:E:4787:PHE:HE1	1:E:4808:ASP:O	1.62	0.81
1:A:4861:ALA:HB1	1:C:4864:GLN:HE21	1.43	0.81
1:C:4767:GLN:HE22	1:E:4871:PHE:HE1	1.24	0.81
1:C:4861:ALA:HB1	1:E:4864:GLN:HE21	1.43	0.81
1:G:2344:LEU:O	1:G:2348:MET:HB2	1.80	0.81
1:A:2344:LEU:O	1:A:2348:MET:HB2	1.80	0.81
1:C:4853:PHE:HZ	1:E:4823:ARG:HA	0.93	0.81
1:E:4861:ALA:HB2	1:G:4864:GLN:NE2	1.96	0.81
1:A:4849:ILE:HD11	1:C:4819:TYR:CA	2.08	0.80
1:A:4864:GLN:HE21	1:G:4861:ALA:HB1	1.44	0.80
1:C:187:SER:O	1:E:2419:ARG:CD	2.29	0.80
1:C:2344:LEU:O	1:C:2348:MET:HB2	1.80	0.80
1:E:2344:LEU:O	1:E:2348:MET:HB2	1.80	0.80
1:A:2419:ARG:CD	1:G:187:SER:O	2.29	0.80
1:A:187:SER:O	1:C:2419:ARG:CD	2.29	0.80
1:E:187:SER:O	1:G:2419:ARG:CD	2.28	0.80
1:G:1425:THR:N	1:G:1509:CYS:HG	1.80	0.80
1:C:4861:ALA:HB2	1:E:4864:GLN:NE2	1.97	0.80
1:E:4767:GLN:HE22	1:G:4871:PHE:HE1	1.25	0.80
1:A:4861:ALA:HB2	1:C:4864:GLN:NE2	1.97	0.79
1:A:4819:TYR:CA	1:G:4849:ILE:HD11	2.08	0.79
1:E:4853:PHE:HZ	1:G:4823:ARG:HA	0.92	0.79
1:C:1425:THR:N	1:C:1509:CYS:HG	1.81	0.79
1:E:1425:THR:N	1:E:1509:CYS:HG	1.81	0.78
1:A:4853:PHE:HZ	1:C:4823:ARG:HA	0.93	0.78
1:E:123:HIS:HD2	1:E:126:SER:H	1.32	0.78
1:C:4811:LEU:HD12	1:E:4519:LEU:HD12	1.66	0.78
1:A:4519:LEU:CD1	1:G:4811:LEU:HD12	2.14	0.78
1:C:123:HIS:HD2	1:C:126:SER:H	1.32	0.78
1:A:4864:GLN:NE2	1:G:4861:ALA:HB2	1.98	0.77
1:A:1425:THR:N	1:A:1509:CYS:HG	1.82	0.77
1:A:4892:CYS:SG	1:A:4909:HIS:HE1	1.96	0.77
1:C:4811:LEU:HD12	1:E:4519:LEU:CD1	2.14	0.76
1:G:123:HIS:HD2	1:G:126:SER:H	1.32	0.76
1:A:4519:LEU:HD12	1:G:4811:LEU:HD12	1.67	0.76
1:A:4519:LEU:O	1:G:4810:MET:CB	2.34	0.76
1:A:123:HIS:HD2	1:A:126:SER:H	1.32	0.76
1:E:4811:LEU:HD12	1:G:4519:LEU:CD1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4811:LEU:HD12	1:G:4519:LEU:HD12	1.68	0.76
1:A:2326:ILE:CG2	1:G:207:PHE:CE2	2.70	0.75
1:C:4767:GLN:OE1	1:E:4875:ARG:NH2	2.21	0.74
1:C:4892:CYS:SG	1:C:4909:HIS:HE1	1.96	0.74
1:G:1218:GLY:HA3	1:G:1240:ALA:H	1.52	0.74
1:C:1218:GLY:HA3	1:C:1240:ALA:H	1.52	0.74
1:A:4787:PHE:CE1	1:A:4808:ASP:O	2.40	0.74
1:C:4810:MET:CB	1:E:4519:LEU:O	2.35	0.74
1:A:4520:PHE:CD1	1:G:4811:LEU:CD1	2.71	0.74
1:E:4862:ILE:HG22	1:G:4868:ILE:HG12	1.70	0.74
1:E:4767:GLN:OE1	1:G:4875:ARG:NH2	2.21	0.73
1:A:4811:LEU:HD12	1:C:4519:LEU:CD1	2.17	0.73
1:A:4767:GLN:OE1	1:C:4875:ARG:NH2	2.20	0.73
1:A:4875:ARG:NH2	1:G:4767:GLN:OE1	2.21	0.73
1:E:1218:GLY:HA3	1:E:1240:ALA:H	1.52	0.73
1:C:207:PHE:CE2	1:E:2326:ILE:CG2	2.71	0.73
1:C:4811:LEU:CD1	1:E:4520:PHE:CD1	2.71	0.73
1:A:1218:GLY:HA3	1:A:1240:ALA:H	1.52	0.73
1:G:4892:CYS:SG	1:G:4909:HIS:HE1	1.96	0.73
1:E:4810:MET:CB	1:G:4519:LEU:O	2.37	0.72
1:A:4108:GLU:HB3	1:A:4148:ARG:HH12	1.54	0.72
1:E:207:PHE:CE2	1:G:2326:ILE:CG2	2.69	0.72
1:E:4108:GLU:HB3	1:E:4148:ARG:HH12	1.54	0.72
1:A:4862:ILE:HG22	1:C:4868:ILE:HG12	1.71	0.72
1:C:4108:GLU:HB3	1:C:4148:ARG:HH12	1.54	0.72
1:E:4811:LEU:CD1	1:G:4520:PHE:CD1	2.73	0.72
1:A:4868:ILE:HG12	1:G:4862:ILE:HG22	1.72	0.72
1:E:4787:PHE:CE1	1:E:4808:ASP:O	2.43	0.71
1:G:4108:GLU:HB3	1:G:4148:ARG:HH12	1.54	0.71
1:C:4862:ILE:HG22	1:E:4868:ILE:HG12	1.71	0.71
1:A:207:PHE:CE2	1:C:2326:ILE:CG2	2.70	0.71
1:E:4892:CYS:SG	1:E:4909:HIS:HE1	1.96	0.70
1:E:1114:ARG:HB2	1:E:1206:SER:HB3	1.74	0.69
1:C:4787:PHE:CE1	1:C:4808:ASP:O	2.43	0.69
1:G:4787:PHE:CE1	1:G:4808:ASP:O	2.43	0.69
1:A:4767:GLN:NE2	1:C:4871:PHE:CE1	2.53	0.69
1:C:1114:ARG:HB2	1:C:1206:SER:HB3	1.74	0.69
1:G:1114:ARG:HB2	1:G:1206:SER:HB3	1.74	0.69
1:C:4767:GLN:NE2	1:E:4871:PHE:CE1	2.53	0.68
1:A:1114:ARG:HB2	1:A:1206:SER:HB3	1.74	0.68
1:C:590:LYS:H	1:C:593:HIS:HD2	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4792:LYS:N	1:A:4806:LYS:HE2	2.09	0.67
1:A:590:LYS:H	1:A:593:HIS:HD2	1.42	0.67
1:G:590:LYS:H	1:G:593:HIS:HD2	1.42	0.67
1:E:590:LYS:H	1:E:593:HIS:HD2	1.42	0.67
1:E:4861:ALA:CB	1:G:4864:GLN:NE2	2.51	0.66
1:G:748:LEU:HB2	1:G:750:ARG:HG3	1.77	0.66
1:A:748:LEU:HB2	1:A:750:ARG:HG3	1.77	0.66
1:A:3845:GLN:HB2	1:A:3920:THR:HG22	1.78	0.66
1:A:716:ASN:HA	1:A:722:LEU:HD13	1.79	0.66
1:A:1425:THR:N	1:A:1510:VAL:O	2.29	0.66
1:E:1425:THR:N	1:E:1510:VAL:O	2.29	0.66
1:E:4853:PHE:CE2	1:G:4823:ARG:CA	2.79	0.66
1:E:4767:GLN:NE2	1:G:4871:PHE:CE1	2.53	0.65
1:G:1239:PHE:O	1:G:1807:ARG:NH1	2.30	0.65
1:C:748:LEU:HB2	1:C:750:ARG:HG3	1.77	0.65
1:E:4949:CYS:SG	1:E:4950:TRP:N	2.70	0.65
1:G:1425:THR:N	1:G:1510:VAL:O	2.29	0.65
1:G:716:ASN:HA	1:G:722:LEU:HD13	1.79	0.65
1:C:716:ASN:HA	1:C:722:LEU:HD13	1.79	0.65
1:A:1239:PHE:O	1:A:1807:ARG:NH1	2.30	0.65
1:C:4949:CYS:SG	1:C:4950:TRP:N	2.70	0.65
1:C:3845:GLN:HB2	1:C:3920:THR:HG22	1.78	0.65
1:E:3845:GLN:HB2	1:E:3920:THR:HG22	1.78	0.65
1:E:4843:TYR:O	1:E:4847:PHE:HB2	1.97	0.65
1:G:3845:GLN:HB2	1:G:3920:THR:HG22	1.78	0.65
1:G:4949:CYS:SG	1:G:4950:TRP:N	2.70	0.65
1:C:1239:PHE:O	1:C:1807:ARG:NH1	2.30	0.65
1:C:1425:THR:N	1:C:1510:VAL:O	2.29	0.65
1:E:748:LEU:HB2	1:E:750:ARG:HG3	1.77	0.65
1:A:4871:PHE:CE1	1:G:4767:GLN:NE2	2.54	0.64
1:A:4949:CYS:SG	1:A:4950:TRP:N	2.70	0.64
1:C:4843:TYR:O	1:C:4847:PHE:HB2	1.97	0.64
1:G:150:GLN:NE2	1:G:158:CYS:SG	2.70	0.64
1:A:4823:ARG:CA	1:G:4853:PHE:CE2	2.81	0.64
1:E:1239:PHE:O	1:E:1807:ARG:NH1	2.30	0.64
1:E:716:ASN:HA	1:E:722:LEU:HD13	1.79	0.64
1:A:1425:THR:N	1:A:1509:CYS:SG	2.71	0.64
1:A:4811:LEU:HD11	1:C:4520:PHE:CD1	2.25	0.64
2:B:7:ILE:H	2:B:72:ALA:HA	1.63	0.64
1:C:1425:THR:N	1:C:1509:CYS:SG	2.71	0.63
2:H:7:ILE:H	2:H:72:ALA:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4843:TYR:O	1:G:4847:PHE:HB2	1.97	0.63
1:A:4853:PHE:CZ	1:C:4823:ARG:CB	2.80	0.63
1:A:4864:GLN:NE2	1:G:4861:ALA:CB	2.53	0.63
1:A:1431:ARG:HE	1:A:1505:LEU:HD21	1.64	0.63
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.81	0.63
1:A:4794:TYR:CG	1:A:4807:CYS:HB2	2.31	0.63
2:F:7:ILE:H	2:F:72:ALA:HA	1.62	0.63
1:G:1469:LEU:HG	1:G:1480:ILE:HD11	1.81	0.63
1:A:4843:TYR:O	1:A:4847:PHE:HB2	1.97	0.63
1:C:1431:ARG:HE	1:C:1505:LEU:HD21	1.64	0.63
1:E:1431:ARG:HE	1:E:1505:LEU:HD21	1.64	0.63
1:E:4623:SER:O	1:E:4630:GLN:NE2	2.32	0.63
1:G:1431:ARG:HE	1:G:1505:LEU:HD21	1.64	0.63
2:D:7:ILE:H	2:D:72:ALA:HA	1.62	0.63
1:G:1425:THR:N	1:G:1509:CYS:SG	2.71	0.63
1:C:4623:SER:O	1:C:4630:GLN:NE2	2.32	0.62
1:C:4853:PHE:CE2	1:E:4823:ARG:CA	2.81	0.62
1:A:1671:ARG:HH22	2:B:88:PRO:HB2	1.64	0.62
1:C:618:CYS:SG	1:C:629:GLN:NE2	2.73	0.62
1:C:3955:MET:HE3	1:C:3959:LEU:HD11	1.80	0.62
1:G:4623:SER:O	1:G:4630:GLN:NE2	2.32	0.62
1:G:2722:ILE:HG12	1:G:2780:LEU:HD13	1.82	0.62
1:E:1671:ARG:HH22	2:F:88:PRO:HB2	1.64	0.62
1:E:3955:MET:HE3	1:E:3959:LEU:HD11	1.80	0.62
1:A:618:CYS:SG	1:A:629:GLN:NE2	2.73	0.62
1:A:4811:LEU:CD1	1:C:4520:PHE:HD1	2.12	0.62
1:A:4888:LYS:HG2	1:A:4895:GLY:HA3	1.82	0.62
1:C:2722:ILE:HG12	1:C:2780:LEU:HD13	1.82	0.62
1:E:150:GLN:NE2	1:E:158:CYS:SG	2.70	0.62
1:E:1092:LYS:H	1:E:1250:TRP:HZ3	1.48	0.62
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.48	0.62
1:A:4623:SER:O	1:A:4630:GLN:NE2	2.32	0.62
1:A:4823:ARG:CB	1:G:4853:PHE:CZ	2.80	0.62
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.70	0.62
1:C:4005:VAL:HG11	1:C:4115:ARG:HE	1.65	0.62
1:G:1092:LYS:H	1:G:1250:TRP:HZ3	1.48	0.62
1:A:4853:PHE:CE2	1:C:4823:ARG:CA	2.81	0.62
1:C:1092:LYS:H	1:C:1250:TRP:HZ3	1.48	0.62
1:C:4853:PHE:CZ	1:E:4823:ARG:CB	2.80	0.62
1:G:1671:ARG:HH22	2:H:88:PRO:HB2	1.64	0.62
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1425:THR:N	1:E:1509:CYS:SG	2.71	0.62
1:E:1469:LEU:HG	1:E:1480:ILE:HD11	1.81	0.62
1:G:3955:MET:HE3	1:G:3959:LEU:HD11	1.80	0.62
1:A:3955:MET:HE3	1:A:3959:LEU:HD11	1.80	0.61
1:C:2013:ASP:O	1:C:2027:ARG:NH1	2.33	0.61
1:E:618:CYS:SG	1:E:629:GLN:NE2	2.73	0.61
1:A:2013:ASP:O	1:A:2027:ARG:NH1	2.33	0.61
1:E:2013:ASP:O	1:E:2027:ARG:NH1	2.33	0.61
1:E:4005:VAL:HG11	1:E:4115:ARG:HE	1.65	0.61
1:E:4185:GLU:O	1:E:4186:LYS:C	2.44	0.61
1:G:4888:LYS:HG2	1:G:4895:GLY:HA3	1.82	0.61
1:A:4005:VAL:HG11	1:A:4115:ARG:HE	1.65	0.61
1:C:1671:ARG:HH22	2:D:88:PRO:HB2	1.64	0.61
1:C:4185:GLU:O	1:C:4186:LYS:C	2.43	0.61
1:E:4888:LYS:HG2	1:E:4895:GLY:HA3	1.82	0.61
1:E:2722:ILE:HG12	1:E:2780:LEU:HD13	1.82	0.61
1:G:4005:VAL:HG11	1:G:4115:ARG:HE	1.65	0.61
1:G:618:CYS:SG	1:G:629:GLN:NE2	2.73	0.61
1:A:102:MET:O	1:A:106:GLN:HB2	2.01	0.61
1:C:102:MET:O	1:C:106:GLN:HB2	2.01	0.61
1:C:4888:LYS:HG2	1:C:4895:GLY:HA3	1.82	0.61
1:G:102:MET:O	1:G:106:GLN:HB2	2.01	0.61
1:G:2013:ASP:O	1:G:2027:ARG:NH1	2.33	0.61
1:A:2715:PRO:HD2	1:A:2718:LEU:HD12	1.83	0.61
1:A:4185:GLU:O	1:A:4186:LYS:C	2.43	0.61
1:C:1610:ARG:NH1	1:C:1612:SER:OG	2.34	0.61
1:E:2715:PRO:HD2	1:E:2718:LEU:HD12	1.83	0.61
1:A:1610:ARG:NH1	1:A:1612:SER:OG	2.34	0.61
1:E:1610:ARG:NH1	1:E:1612:SER:OG	2.34	0.61
1:G:1610:ARG:NH1	1:G:1612:SER:OG	2.34	0.61
1:C:1099:GLY:H	1:C:1169:THR:HG23	1.66	0.60
1:G:764:PRO:HG2	1:G:781:ASN:HA	1.84	0.60
1:A:2722:ILE:HG12	1:A:2780:LEU:HD13	1.82	0.60
1:A:4794:TYR:CB	1:A:4807:CYS:HB2	2.31	0.60
1:G:2715:PRO:HD2	1:G:2718:LEU:HD12	1.83	0.60
1:G:4807:CYS:O	1:G:4813:CYS:SG	2.60	0.60
1:C:4811:LEU:HD13	1:E:4520:PHE:CD1	2.36	0.60
1:E:4807:CYS:O	1:E:4813:CYS:SG	2.59	0.60
1:G:3841:PHE:HB3	1:G:3920:THR:HG21	1.84	0.60
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.67	0.60
1:E:1099:GLY:H	1:E:1169:THR:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1445:TRP:H	1:E:1487:MET:HB2	1.67	0.60
1:E:1844:GLN:HA	1:E:1847:GLU:HB2	1.84	0.60
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.83	0.60
1:C:2715:PRO:HD2	1:C:2718:LEU:HD12	1.83	0.60
1:A:1844:GLN:HA	1:A:1847:GLU:HB2	1.84	0.60
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	1.84	0.60
1:E:764:PRO:HG2	1:E:781:ASN:HA	1.84	0.60
1:G:1258:PHE:HA	1:G:1595:LEU:HA	1.84	0.60
1:G:4185:GLU:O	1:G:4186:LYS:C	2.43	0.60
1:A:1308:ILE:HD12	1:A:1539:LEU:HB2	1.84	0.59
1:C:764:PRO:HG2	1:C:781:ASN:HA	1.84	0.59
1:E:102:MET:O	1:E:106:GLN:HB2	2.01	0.59
1:E:1258:PHE:HA	1:E:1595:LEU:HA	1.84	0.59
1:E:1308:ILE:HD12	1:E:1539:LEU:HB2	1.84	0.59
1:G:679:VAL:HA	1:G:800:VAL:HG12	1.83	0.59
1:G:1445:TRP:H	1:G:1487:MET:HB2	1.67	0.59
1:G:1844:GLN:HA	1:G:1847:GLU:HB2	1.84	0.59
1:C:1844:GLN:HA	1:C:1847:GLU:HB2	1.84	0.59
1:C:3743:GLN:NE2	1:C:3781:TYR:OH	2.34	0.59
1:C:4767:GLN:NE2	1:E:4871:PHE:HE1	1.97	0.59
1:E:186:VAL:O	1:G:2419:ARG:NH1	2.35	0.59
1:G:1246:ASP:OD2	1:G:1605:LYS:NZ	2.36	0.59
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.67	0.59
1:C:4807:CYS:O	1:C:4813:CYS:SG	2.60	0.59
1:C:2421:ARG:HH21	1:C:2425:ARG:HH21	1.50	0.59
1:E:679:VAL:HA	1:E:800:VAL:HG12	1.82	0.59
1:A:1099:GLY:H	1:A:1169:THR:HG23	1.66	0.59
1:A:1246:ASP:OD2	1:A:1605:LYS:NZ	2.36	0.59
1:A:2419:ARG:NH1	1:G:186:VAL:O	2.36	0.59
1:C:1246:ASP:OD2	1:C:1605:LYS:NZ	2.36	0.59
1:E:1246:ASP:OD2	1:E:1605:LYS:NZ	2.36	0.59
1:G:1308:ILE:HD12	1:G:1539:LEU:HB2	1.84	0.59
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.83	0.59
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	1.84	0.59
1:A:4871:PHE:HE1	1:G:4767:GLN:NE2	1.99	0.59
1:E:3841:PHE:HB3	1:E:3920:THR:HG21	1.84	0.59
1:A:4520:PHE:CD1	1:G:4811:LEU:HD13	2.36	0.59
1:G:1589:GLN:NE2	1:G:1634:GLU:OE1	2.36	0.59
1:A:186:VAL:O	1:C:2419:ARG:NH1	2.35	0.59
1:A:4738:PHE:CB	1:G:4788:ASN:OD1	2.51	0.59
1:A:4788:ASN:OD1	1:C:4738:PHE:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:O	1:E:2419:ARG:NH1	2.36	0.59
1:G:1620:GLN:HE21	1:G:1622:LEU:HD21	1.68	0.59
1:C:1589:GLN:NE2	1:C:1634:GLU:OE1	2.36	0.59
1:C:1258:PHE:HA	1:C:1595:LEU:HA	1.84	0.58
1:C:274:LEU:O	1:C:299:HIS:ND1	2.36	0.58
1:C:1443:VAL:HG22	1:C:1543:VAL:HG22	1.85	0.58
1:C:4788:ASN:OD1	1:E:4738:PHE:CB	2.51	0.58
1:E:1620:GLN:HE21	1:E:1622:LEU:HD21	1.68	0.58
1:E:4853:PHE:CZ	1:G:4823:ARG:CB	2.79	0.58
1:A:673:TRP:HA	1:A:820:ALA:HB3	1.86	0.58
1:A:3973:MET:HG3	1:A:4095:ILE:HD11	1.85	0.58
1:E:2421:ARG:HH21	1:E:2425:ARG:HH21	1.50	0.58
1:G:1099:GLY:H	1:G:1169:THR:HG23	1.66	0.58
1:A:1258:PHE:HA	1:A:1595:LEU:HA	1.84	0.58
1:A:1589:GLN:NE2	1:A:1634:GLU:OE1	2.36	0.58
1:C:673:TRP:HA	1:C:820:ALA:HB3	1.86	0.58
1:E:274:LEU:O	1:E:299:HIS:ND1	2.36	0.58
1:E:1443:VAL:HG22	1:E:1543:VAL:HG22	1.85	0.58
1:G:1905:LEU:HB2	1:G:2081:LEU:HD12	1.85	0.58
1:A:764:PRO:HG2	1:A:781:ASN:HA	1.84	0.58
1:A:1443:VAL:HG22	1:A:1543:VAL:HG22	1.85	0.58
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.70	0.58
1:A:1905:LEU:HB2	1:A:2081:LEU:HD12	1.85	0.58
1:C:930:ASN:HA	1:C:933:LEU:HB2	1.86	0.58
1:C:1308:ILE:HD12	1:C:1539:LEU:HB2	1.84	0.58
1:G:3973:MET:HG3	1:G:4095:ILE:HD11	1.85	0.58
1:A:2421:ARG:HH21	1:A:2425:ARG:HH21	1.50	0.58
1:E:3904:GLN:NE2	1:E:3965:GLN:OE1	2.37	0.58
1:A:76:ARG:HG3	1:C:3891:TRP:CD2	2.39	0.58
1:A:1620:GLN:HE21	1:A:1622:LEU:HD21	1.68	0.58
1:A:4767:GLN:NE2	1:C:4871:PHE:HE1	1.97	0.58
1:G:930:ASN:HA	1:G:933:LEU:HB2	1.86	0.58
1:A:903:GLN:HB3	1:A:914:GLN:HG2	1.86	0.57
1:E:930:ASN:HA	1:E:933:LEU:HB2	1.86	0.57
1:A:3904:GLN:NE2	1:A:3965:GLN:OE1	2.37	0.57
1:C:2421:ARG:NH2	1:C:2476:VAL:O	2.38	0.57
1:E:673:TRP:HA	1:E:820:ALA:HB3	1.86	0.57
1:E:1589:GLN:NE2	1:E:1634:GLU:OE1	2.36	0.57
1:E:2093:TYR:HD2	1:E:3641:LEU:HD12	1.70	0.57
1:E:4767:GLN:NE2	1:G:4871:PHE:HE1	1.98	0.57
1:G:1443:VAL:HG22	1:G:1543:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:TRP:CD2	1:G:76:ARG:HG3	2.40	0.57
1:A:4835:PRO:HB2	1:A:4841:GLU:HG3	1.86	0.57
1:C:1620:GLN:HE21	1:C:1622:LEU:HD21	1.68	0.57
1:E:76:ARG:HG3	1:G:3891:TRP:CD2	2.39	0.57
1:E:4811:LEU:HD13	1:G:4520:PHE:CD1	2.38	0.57
1:C:2093:TYR:HD2	1:C:3641:LEU:HD12	1.70	0.57
1:G:673:TRP:HA	1:G:820:ALA:HB3	1.86	0.57
1:G:903:GLN:HB3	1:G:914:GLN:HG2	1.86	0.57
1:C:682:THR:HA	1:C:798:ILE:HG12	1.87	0.57
1:C:903:GLN:HB3	1:C:914:GLN:HG2	1.86	0.57
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.36	0.57
1:C:3973:MET:HG3	1:C:4095:ILE:HD11	1.85	0.57
1:G:165:ALA:HB2	1:G:182:ILE:HG12	1.87	0.57
1:G:2421:ARG:HH21	1:G:2425:ARG:HH21	1.51	0.57
1:G:3743:GLN:NE2	1:G:3781:TYR:OH	2.34	0.57
1:A:930:ASN:HA	1:A:933:LEU:HB2	1.86	0.57
1:E:3973:MET:HG3	1:E:4095:ILE:HD11	1.85	0.57
1:G:3904:GLN:NE2	1:G:3965:GLN:OE1	2.37	0.57
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.36	0.57
1:E:2421:ARG:NH2	1:E:2476:VAL:O	2.38	0.57
1:E:4788:ASN:OD1	1:G:4738:PHE:CB	2.53	0.57
1:G:682:THR:HA	1:G:798:ILE:HG12	1.87	0.57
1:A:682:THR:HA	1:A:798:ILE:HG12	1.87	0.57
1:C:4113:ASP:HB2	1:C:4117:GLN:HE21	1.70	0.57
1:E:682:THR:HA	1:E:798:ILE:HG12	1.87	0.57
1:G:2421:ARG:NH2	1:G:2476:VAL:O	2.37	0.57
1:G:4113:ASP:HB2	1:G:4117:GLN:HE21	1.70	0.57
1:A:2421:ARG:NH2	1:A:2476:VAL:O	2.37	0.56
1:A:4113:ASP:HB2	1:A:4117:GLN:HE21	1.70	0.56
1:C:1905:LEU:HB2	1:C:2081:LEU:HD12	1.86	0.56
1:C:3880:LEU:HD23	1:C:3944:ALA:HB2	1.87	0.56
1:G:4835:PRO:HB2	1:G:4841:GLU:HG3	1.86	0.56
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.87	0.56
1:C:1110:ALA:O	1:C:1211:GLN:NE2	2.38	0.56
1:E:1905:LEU:HB2	1:E:2081:LEU:HD12	1.85	0.56
1:A:2093:TYR:HD2	1:A:3641:LEU:HD12	1.70	0.56
1:A:3880:LEU:HD23	1:A:3944:ALA:HB2	1.87	0.56
1:C:76:ARG:HG3	1:E:3891:TRP:CD2	2.40	0.56
1:C:238:HIS:HA	1:C:403:LEU:HD22	1.87	0.56
1:G:2011:GLU:O	1:G:2027:ARG:NH2	2.39	0.56
1:C:3904:GLN:NE2	1:C:3965:GLN:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:HIS:HA	1:E:403:LEU:HD22	1.87	0.56
1:G:2093:TYR:HD2	1:G:3641:LEU:HD12	1.70	0.56
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.39	0.56
1:C:374:TYR:HA	1:C:391:ALA:HA	1.87	0.56
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.39	0.56
1:C:4835:PRO:HB2	1:C:4841:GLU:HG3	1.86	0.56
1:E:165:ALA:HB2	1:E:182:ILE:HG12	1.87	0.56
1:E:3729:GLN:O	1:E:3733:HIS:ND1	2.36	0.56
1:E:4113:ASP:HB2	1:E:4117:GLN:HE21	1.70	0.56
1:A:165:ALA:HB2	1:A:182:ILE:HG12	1.87	0.56
1:A:274:LEU:O	1:A:299:HIS:ND1	2.37	0.56
1:C:279:THR:HG1	1:C:285:SER:HG	1.54	0.56
1:A:2011:GLU:O	1:A:2027:ARG:NH2	2.39	0.56
1:C:4889:CYS:HB2	4:C:5101:ATP:HN61	1.71	0.56
1:E:355:LYS:O	1:E:359:SER:OG	2.24	0.56
1:E:374:TYR:HA	1:E:391:ALA:HA	1.87	0.56
1:G:3729:GLN:O	1:G:3733:HIS:ND1	2.36	0.56
1:A:3680:LYS:NZ	1:A:3684:GLU:OE2	2.39	0.56
1:E:903:GLN:HB3	1:E:914:GLN:HG2	1.86	0.56
1:G:355:LYS:O	1:G:359:SER:OG	2.24	0.56
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.88	0.56
1:A:3918:PHE:O	1:A:3922:THR:OG1	2.22	0.56
1:E:4835:PRO:HB2	1:E:4841:GLU:HG3	1.86	0.56
1:A:374:TYR:HA	1:A:391:ALA:HA	1.87	0.56
1:A:4889:CYS:HB2	4:A:5101:ATP:HN61	1.71	0.56
1:E:1209:VAL:N	1:E:1211:GLN:OE1	2.39	0.56
1:E:1601:ASN:ND2	1:E:1643:GLU:OE2	2.39	0.56
1:E:2011:GLU:O	1:E:2027:ARG:NH2	2.39	0.56
1:G:843:GLU:HA	1:G:848:ARG:HG2	1.87	0.56
1:G:1601:ASN:ND2	1:G:1643:GLU:OE2	2.39	0.56
1:G:3680:LYS:NZ	1:G:3684:GLU:OE2	2.39	0.56
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.39	0.55
1:C:165:ALA:HB2	1:C:182:ILE:HG12	1.87	0.55
1:C:2011:GLU:O	1:C:2027:ARG:NH2	2.39	0.55
1:C:3680:LYS:NZ	1:C:3684:GLU:OE2	2.39	0.55
1:E:243:GLU:HA	1:E:264:GLY:HA2	1.87	0.55
1:E:694:ARG:HG2	1:E:716:ASN:HB3	1.89	0.55
1:E:3680:LYS:NZ	1:E:3684:GLU:OE2	2.39	0.55
1:G:374:TYR:HA	1:G:391:ALA:HA	1.87	0.55
1:A:238:HIS:HA	1:A:403:LEU:HD22	1.87	0.55
1:A:4811:LEU:HD13	1:C:4520:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:GLU:HA	1:G:264:GLY:HA2	1.87	0.55
1:A:196:TYR:HA	1:A:201:LEU:HD23	1.89	0.55
1:A:3743:GLN:NE2	1:A:3781:TYR:OH	2.34	0.55
1:C:196:TYR:HA	1:C:201:LEU:HD23	1.89	0.55
1:C:355:LYS:O	1:C:359:SER:OG	2.24	0.55
1:C:694:ARG:HG2	1:C:716:ASN:HB3	1.88	0.55
1:G:694:ARG:HG2	1:G:716:ASN:HB3	1.89	0.55
1:G:1119:ARG:NH2	1:G:1196:ASP:O	2.39	0.55
1:A:3803:VAL:O	1:A:3832:GLN:NE2	2.40	0.55
1:E:4889:CYS:HB2	4:E:5101:ATP:HN61	1.71	0.55
1:G:238:HIS:HA	1:G:403:LEU:HD22	1.87	0.55
1:A:694:ARG:HG2	1:A:716:ASN:HB3	1.89	0.55
1:E:3880:LEU:HD23	1:E:3944:ALA:HB2	1.87	0.55
1:G:196:TYR:HA	1:G:201:LEU:HD23	1.89	0.55
1:G:3880:LEU:HD23	1:G:3944:ALA:HB2	1.87	0.55
1:A:3993:ASN:HD22	1:A:4110:MET:HA	1.72	0.55
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.89	0.55
1:E:2832:VAL:O	1:E:2895:LYS:NZ	2.34	0.55
1:G:274:LEU:O	1:G:299:HIS:ND1	2.36	0.55
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.89	0.55
1:A:355:LYS:O	1:A:359:SER:OG	2.24	0.55
1:C:3993:ASN:HD22	1:C:4110:MET:HA	1.72	0.55
1:G:299:HIS:NE2	1:G:301:THR:OG1	2.37	0.55
1:C:646:THR:OG1	1:C:1684:GLN:NE2	2.40	0.55
1:E:150:GLN:HE21	1:E:158:CYS:HG	1.55	0.55
1:E:218:SER:HB3	1:E:286:GLY:HA3	1.89	0.55
1:E:843:GLU:HA	1:E:848:ARG:HG2	1.87	0.55
1:G:218:SER:HB3	1:G:286:GLY:HA3	1.89	0.55
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.87	0.54
1:A:4810:MET:CB	1:C:4519:LEU:O	2.55	0.54
1:C:1718:ARG:NH1	1:C:1830:ILE:O	2.41	0.54
1:E:646:THR:OG1	1:E:1684:GLN:NE2	2.40	0.54
1:G:2007:HIS:O	1:G:2011:GLU:CB	2.55	0.54
1:C:801:ARG:NH2	1:C:810:GLU:OE1	2.41	0.54
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.88	0.54
1:E:196:TYR:HA	1:E:201:LEU:HD23	1.88	0.54
1:E:2007:HIS:O	1:E:2011:GLU:CB	2.55	0.54
1:G:281:ARG:NH2	1:G:284:TRP:O	2.40	0.54
1:G:3803:VAL:O	1:G:3832:GLN:NE2	2.40	0.54
1:G:4889:CYS:HB2	4:G:5101:ATP:HN61	1.71	0.54
1:A:801:ARG:NH2	1:A:810:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4811:LEU:CD1	1:C:4520:PHE:HE1	1.93	0.54
1:C:3803:VAL:O	1:C:3832:GLN:NE2	2.40	0.54
1:G:646:THR:OG1	1:G:1684:GLN:NE2	2.40	0.54
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.39	0.54
1:G:1718:ARG:NH1	1:G:1830:ILE:O	2.41	0.54
1:A:279:THR:HG1	1:A:285:SER:HG	1.55	0.54
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.39	0.54
1:E:1119:ARG:NH2	1:E:1196:ASP:O	2.39	0.54
1:A:1306:MET:SD	1:A:1575:HIS:NE2	2.81	0.54
1:A:2007:HIS:O	1:A:2011:GLU:CB	2.55	0.54
1:C:244:CYS:SG	1:C:245:LEU:N	2.81	0.54
1:A:244:CYS:SG	1:A:245:LEU:N	2.81	0.54
1:C:2007:HIS:O	1:C:2011:GLU:CB	2.55	0.54
1:C:4811:LEU:HD13	1:E:4520:PHE:CE1	2.41	0.54
1:E:244:CYS:SG	1:E:245:LEU:N	2.81	0.54
1:E:1143:GLN:HA	1:E:1151:HIS:HA	1.90	0.54
1:G:1846:ILE:HG23	1:G:1894:LEU:HB3	1.89	0.54
1:A:281:ARG:NH2	1:A:284:TRP:O	2.40	0.54
1:C:1209:VAL:N	1:C:1211:GLN:OE1	2.39	0.54
1:G:244:CYS:SG	1:G:245:LEU:N	2.81	0.54
1:G:1306:MET:SD	1:G:1575:HIS:NE2	2.81	0.54
1:G:3663:ASP:OD2	1:G:3735:ARG:NH2	2.41	0.54
1:A:646:THR:OG1	1:A:1684:GLN:NE2	2.40	0.54
1:A:3886:ILE:HD11	1:A:3910:ALA:HB1	1.89	0.54
1:C:281:ARG:NH2	1:C:284:TRP:O	2.40	0.54
1:E:506:HIS:NE2	1:E:534:TYR:OH	2.37	0.54
1:E:3803:VAL:O	1:E:3832:GLN:NE2	2.40	0.54
1:E:3993:ASN:HD22	1:E:4110:MET:HA	1.72	0.54
1:C:777:GLY:O	1:C:1468:THR:OG1	2.26	0.54
1:C:2192:LYS:O	1:C:2196:ASN:ND2	2.41	0.54
1:C:3886:ILE:HD11	1:C:3910:ALA:HB1	1.89	0.54
1:E:281:ARG:NH2	1:E:284:TRP:O	2.40	0.54
1:E:3663:ASP:OD2	1:E:3735:ARG:NH2	2.41	0.54
1:A:1846:ILE:HG23	1:A:1894:LEU:HB3	1.89	0.53
1:C:1143:GLN:HA	1:C:1151:HIS:HA	1.90	0.53
1:E:801:ARG:NH2	1:E:810:GLU:OE1	2.41	0.53
1:E:1718:ARG:NH1	1:E:1830:ILE:O	2.41	0.53
1:E:235:ARG:NH2	1:E:268:SER:O	2.41	0.53
1:G:801:ARG:NH2	1:G:810:GLU:OE1	2.41	0.53
1:A:2856:LYS:O	1:A:2860:GLU:HB2	2.09	0.53
1:E:1846:ILE:HG23	1:E:1894:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2192:LYS:O	1:G:2196:ASN:ND2	2.41	0.53
1:G:3993:ASN:HD22	1:G:4110:MET:HA	1.72	0.53
1:A:673:TRP:HB2	1:A:759:LEU:HB3	1.91	0.53
1:A:1110:ALA:O	1:A:1211:GLN:NE2	2.38	0.53
1:A:2192:LYS:O	1:A:2196:ASN:ND2	2.41	0.53
1:E:188:SER:HB2	1:E:190:ARG:HH21	1.74	0.53
1:E:3743:GLN:NE2	1:E:3781:TYR:OH	2.34	0.53
1:G:188:SER:HB2	1:G:190:ARG:HH21	1.74	0.53
1:G:1184:ASP:OD2	1:G:1188:SER:OG	2.26	0.53
1:A:1718:ARG:NH1	1:A:1830:ILE:O	2.41	0.53
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.74	0.53
1:C:673:TRP:HB2	1:C:759:LEU:HB3	1.91	0.53
1:C:728:ASP:HB2	1:C:748:LEU:HA	1.91	0.53
1:C:1306:MET:SD	1:C:1575:HIS:NE2	2.81	0.53
1:C:1846:ILE:HG23	1:C:1894:LEU:HB3	1.89	0.53
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.41	0.53
1:E:2856:LYS:O	1:E:2860:GLU:HB2	2.09	0.53
1:A:299:HIS:NE2	1:A:301:THR:OG1	2.37	0.53
1:A:4811:LEU:CD1	1:C:4519:LEU:HD12	2.37	0.53
1:C:235:ARG:NH2	1:C:268:SER:O	2.41	0.53
1:E:2192:LYS:O	1:E:2196:ASN:ND2	2.41	0.53
1:G:1252:SER:HB2	1:G:1598:ARG:HD3	1.90	0.53
1:A:322:ALA:HB1	1:A:327:THR:HG21	1.91	0.53
1:G:2856:LYS:O	1:G:2860:GLU:HB2	2.09	0.53
1:A:777:GLY:O	1:A:1468:THR:OG1	2.26	0.53
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.26	0.53
1:A:1252:SER:HB2	1:A:1598:ARG:HD3	1.91	0.53
1:C:780:GLU:O	1:C:1466:THR:OG1	2.27	0.53
1:C:3761:LYS:NZ	1:C:3835:GLU:OE2	2.37	0.53
1:E:1306:MET:SD	1:E:1575:HIS:NE2	2.81	0.53
1:G:235:ARG:NH2	1:G:268:SER:O	2.41	0.53
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.41	0.53
1:C:322:ALA:HB1	1:C:327:THR:HG21	1.91	0.53
1:E:122:ARG:HE	1:E:127:GLY:HA2	1.74	0.53
1:E:3886:ILE:HD11	1:E:3910:ALA:HB1	1.89	0.53
1:G:777:GLY:O	1:G:1468:THR:OG1	2.26	0.53
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.74	0.53
1:A:1143:GLN:HA	1:A:1151:HIS:HA	1.90	0.53
1:C:1630:LEU:HD22	1:C:1641:ILE:HD13	1.91	0.53
1:E:4175:PHE:O	1:E:4179:ASN:HB2	2.09	0.53
1:G:1143:GLN:HA	1:G:1151:HIS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.39	0.52
1:A:4175:PHE:O	1:A:4179:ASN:HB2	2.09	0.52
1:A:4811:LEU:CD1	1:C:4519:LEU:CD1	2.87	0.52
1:C:2231:ALA:HA	1:C:2236:ARG:H	1.75	0.52
1:G:1630:LEU:HD22	1:G:1641:ILE:HD13	1.91	0.52
1:A:680:ASP:HB2	1:A:799:LYS:HG3	1.92	0.52
1:A:4042:GLY:HA3	1:A:4080:ASP:HA	1.92	0.52
1:C:122:ARG:HE	1:C:127:GLY:HA2	1.74	0.52
1:A:3748:SER:O	1:A:3793:SER:OG	2.28	0.52
1:C:3918:PHE:O	1:C:3922:THR:OG1	2.22	0.52
1:C:4042:GLY:HA3	1:C:4080:ASP:HA	1.92	0.52
1:E:322:ALA:HB1	1:E:327:THR:HG21	1.91	0.52
1:E:1110:ALA:O	1:E:1211:GLN:NE2	2.38	0.52
1:E:3918:PHE:O	1:E:3922:THR:OG1	2.22	0.52
1:G:2231:ALA:HA	1:G:2236:ARG:H	1.75	0.52
1:G:3886:ILE:HD11	1:G:3910:ALA:HB1	1.89	0.52
1:G:4175:PHE:O	1:G:4179:ASN:HB2	2.09	0.52
1:A:728:ASP:HB2	1:A:748:LEU:HA	1.91	0.52
1:C:680:ASP:HB2	1:C:799:LYS:HG3	1.92	0.52
1:E:680:ASP:HB2	1:E:799:LYS:HG3	1.92	0.52
1:G:4794:TYR:HB2	1:G:4806:LYS:HD2	1.91	0.52
1:A:1471:ASP:H	1:A:1474:GLY:H	1.57	0.52
1:C:1471:ASP:H	1:C:1474:GLY:H	1.57	0.52
1:E:335:LYS:NZ	1:E:396:GLU:O	2.34	0.52
1:E:673:TRP:HB2	1:E:759:LEU:HB3	1.91	0.52
1:G:562:LEU:HD21	1:G:600:LEU:HD22	1.91	0.52
1:G:673:TRP:HB2	1:G:759:LEU:HB3	1.91	0.52
1:A:4791:ARG:O	1:A:4806:LYS:HE2	2.08	0.52
1:C:4594:LEU:O	1:C:4596:VAL:N	2.43	0.52
1:E:777:GLY:O	1:E:1468:THR:OG1	2.27	0.52
1:E:1630:LEU:HD22	1:E:1641:ILE:HD13	1.91	0.52
1:G:680:ASP:HB2	1:G:799:LYS:HG3	1.92	0.52
1:G:1471:ASP:H	1:G:1474:GLY:H	1.57	0.52
1:A:1630:LEU:HD22	1:A:1641:ILE:HD13	1.91	0.52
1:E:1184:ASP:OD2	1:E:1188:SER:OG	2.26	0.52
1:G:122:ARG:HE	1:G:127:GLY:HA2	1.75	0.52
1:G:322:ALA:HB1	1:G:327:THR:HG21	1.91	0.52
1:A:122:ARG:HE	1:A:127:GLY:HA2	1.74	0.52
1:E:728:ASP:HB2	1:E:748:LEU:HA	1.91	0.52
1:E:1153:GLY:HA3	1:E:1182:LEU:HD13	1.92	0.52
1:E:4794:TYR:HB2	1:E:4806:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2231:ALA:HA	1:A:2236:ARG:H	1.75	0.52
1:C:2832:VAL:O	1:C:2895:LYS:NZ	2.34	0.52
1:E:562:LEU:HD21	1:E:600:LEU:HD22	1.91	0.52
1:C:2856:LYS:O	1:C:2860:GLU:HB2	2.09	0.52
1:C:4794:TYR:HB2	1:C:4806:LYS:HD2	1.91	0.52
1:G:780:GLU:O	1:G:1466:THR:OG1	2.27	0.52
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.34	0.51
1:C:1257:GLN:OE1	1:C:1637:ARG:NH2	2.44	0.51
1:E:281:ARG:NH1	1:E:346:VAL:O	2.42	0.51
1:E:652:VAL:HA	1:E:795:SER:HB2	1.92	0.51
1:E:4594:LEU:O	1:E:4596:VAL:N	2.43	0.51
1:G:2308:PHE:HA	1:G:2313:SER:HA	1.92	0.51
1:E:1471:ASP:H	1:E:1474:GLY:H	1.57	0.51
1:E:2231:ALA:HA	1:E:2236:ARG:H	1.75	0.51
1:E:2308:PHE:HA	1:E:2313:SER:HA	1.92	0.51
1:G:1110:ALA:O	1:G:1211:GLN:NE2	2.38	0.51
1:G:2832:VAL:O	1:G:2895:LYS:NZ	2.34	0.51
2:H:6:THR:OG1	2:H:70:GLN:NE2	2.43	0.51
1:A:602:ASP:O	1:A:1576:LYS:NZ	2.43	0.51
1:C:1252:SER:HB2	1:C:1598:ARG:HD3	1.91	0.51
1:E:2127:ILE:HD11	1:E:2143:MET:HG3	1.91	0.51
1:A:750:ARG:N	1:A:753:ASP:OD2	2.44	0.51
1:A:4594:LEU:O	1:A:4596:VAL:N	2.43	0.51
1:C:652:VAL:HA	1:C:795:SER:HB2	1.92	0.51
1:E:2345:LEU:HD21	1:E:2435:GLY:HA3	1.93	0.51
1:G:279:THR:HG1	1:G:285:SER:HG	1.56	0.51
1:G:602:ASP:O	1:G:1576:LYS:NZ	2.43	0.51
1:A:1153:GLY:HA3	1:A:1182:LEU:HD13	1.91	0.51
1:A:2345:LEU:HD21	1:A:2435:GLY:HA3	1.93	0.51
1:A:4138:GLU:HG2	1:A:4148:ARG:HG2	1.92	0.51
1:C:2127:ILE:HD11	1:C:2143:MET:HG3	1.91	0.51
1:C:2345:LEU:HD21	1:C:2435:GLY:HA3	1.93	0.51
1:C:4175:PHE:O	1:C:4179:ASN:HB2	2.09	0.51
1:G:750:ARG:N	1:G:753:ASP:OD2	2.44	0.51
1:A:562:LEU:HD21	1:A:600:LEU:HD22	1.91	0.51
2:B:6:THR:OG1	2:B:70:GLN:NE2	2.43	0.51
1:C:602:ASP:O	1:C:1576:LYS:NZ	2.43	0.51
1:E:1252:SER:HB2	1:E:1598:ARG:HD3	1.91	0.51
1:E:1690:GLU:OE2	1:E:1790:LYS:NZ	2.35	0.51
2:F:6:THR:OG1	2:F:70:GLN:NE2	2.43	0.51
1:G:2345:LEU:HD21	1:G:2435:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4594:LEU:O	1:G:4596:VAL:N	2.43	0.51
1:A:780:GLU:O	1:A:1466:THR:OG1	2.27	0.51
1:C:1153:GLY:HA3	1:C:1182:LEU:HD13	1.91	0.51
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.26	0.51
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.44	0.51
1:E:1257:GLN:OE1	1:E:1637:ARG:NH2	2.44	0.51
1:G:652:VAL:HA	1:G:795:SER:HB2	1.92	0.51
1:G:4042:GLY:HA3	1:G:4080:ASP:HA	1.92	0.51
1:A:2161:ASN:OD1	1:A:2164:ARG:NH2	2.44	0.51
2:D:6:THR:OG1	2:D:70:GLN:NE2	2.43	0.51
1:E:602:ASP:O	1:E:1576:LYS:NZ	2.43	0.51
1:G:281:ARG:NH1	1:G:346:VAL:O	2.42	0.51
1:G:728:ASP:HB2	1:G:748:LEU:HA	1.91	0.51
1:G:2127:ILE:HD11	1:G:2143:MET:HG3	1.91	0.51
1:G:2161:ASN:OD1	1:G:2164:ARG:NH2	2.44	0.51
1:A:4559:HIS:CE1	1:G:4791:ARG:NH2	2.79	0.51
1:C:562:LEU:HD21	1:C:600:LEU:HD22	1.91	0.51
1:E:299:HIS:NE2	1:E:301:THR:OG1	2.37	0.51
1:E:750:ARG:N	1:E:753:ASP:OD2	2.44	0.51
1:E:4042:GLY:HA3	1:E:4080:ASP:HA	1.92	0.51
1:E:4138:GLU:HG2	1:E:4148:ARG:HG2	1.92	0.51
1:G:1257:GLN:OE1	1:G:1637:ARG:NH2	2.44	0.51
1:G:4138:GLU:HG2	1:G:4148:ARG:HG2	1.92	0.51
1:A:235:ARG:NH2	1:A:268:SER:O	2.41	0.51
1:A:281:ARG:NH1	1:A:346:VAL:O	2.42	0.51
1:E:1272:ARG:NH2	1:E:1590:PHE:O	2.44	0.51
1:G:1153:GLY:HA3	1:G:1182:LEU:HD13	1.91	0.51
1:A:2127:ILE:HD11	1:A:2143:MET:HG3	1.91	0.50
1:A:2308:PHE:HA	1:A:2313:SER:HA	1.92	0.50
1:C:750:ARG:N	1:C:753:ASP:OD2	2.44	0.50
1:E:1250:TRP:HB3	1:E:1600:PRO:HB2	1.93	0.50
1:E:1942:ARG:HH22	1:E:3612:LEU:HD23	1.76	0.50
1:G:1272:ARG:NH2	1:G:1590:PHE:O	2.44	0.50
1:C:1942:ARG:HH22	1:C:3612:LEU:HD23	1.76	0.50
1:C:4005:VAL:HG21	1:C:4115:ARG:HG3	1.94	0.50
1:E:4811:LEU:HD13	1:G:4520:PHE:CE1	2.42	0.50
1:G:898:ILE:HG21	1:G:973:THR:HA	1.94	0.50
1:G:1509:CYS:N	1:G:1519:THR:OG1	2.45	0.50
1:A:1509:CYS:N	1:A:1519:THR:OG1	2.44	0.50
1:C:1605:LYS:HD3	1:C:1606:VAL:HG23	1.94	0.50
1:C:2161:ASN:OD1	1:C:2164:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:747:HIS:CE1	1:E:750:ARG:HD2	2.46	0.50
1:E:1084:ARG:N	1:E:1127:GLU:OE2	2.44	0.50
1:E:1487:MET:HE1	1:E:1531:TYR:HB2	1.94	0.50
1:G:1084:ARG:N	1:G:1127:GLU:OE2	2.44	0.50
1:G:1773:ASN:HD21	1:G:1776:TYR:HB3	1.77	0.50
1:A:652:VAL:HA	1:A:795:SER:HB2	1.92	0.50
1:A:1942:ARG:HH22	1:A:3612:LEU:HD23	1.76	0.50
1:A:4520:PHE:CE1	1:G:4811:LEU:HD13	2.41	0.50
1:C:747:HIS:CE1	1:C:750:ARG:HD2	2.46	0.50
1:C:1084:ARG:N	1:C:1127:GLU:OE2	2.44	0.50
1:C:1487:MET:HE1	1:C:1531:TYR:HB2	1.94	0.50
1:A:1922:ARG:HH22	1:A:2039:TYR:HE1	1.60	0.50
1:C:294:PRO:HB3	1:C:330:THR:HG22	1.93	0.50
1:E:898:ILE:HG21	1:E:973:THR:HA	1.94	0.50
1:E:4005:VAL:HG21	1:E:4115:ARG:HG3	1.94	0.50
1:A:747:HIS:CE1	1:A:750:ARG:HD2	2.46	0.50
1:C:898:ILE:HG21	1:C:973:THR:HA	1.94	0.50
1:C:4138:GLU:HG2	1:C:4148:ARG:HG2	1.92	0.50
1:E:1773:ASN:HD21	1:E:1776:TYR:HB3	1.77	0.50
1:G:1922:ARG:HH22	1:G:2039:TYR:HE1	1.60	0.50
1:G:2743:ILE:N	1:G:2753:LYS:O	2.43	0.50
1:A:1257:GLN:OE1	1:A:1637:ARG:NH2	2.44	0.50
1:E:1605:LYS:HD3	1:E:1606:VAL:HG23	1.94	0.50
1:E:2161:ASN:OD1	1:E:2164:ARG:NH2	2.44	0.50
1:G:875:PRO:HB2	1:G:878:LEU:HB2	1.93	0.50
1:G:1605:LYS:HD3	1:G:1606:VAL:HG23	1.94	0.50
1:G:3918:PHE:O	1:G:3922:THR:OG1	2.22	0.50
1:A:294:PRO:HB3	1:A:330:THR:HG22	1.93	0.50
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.35	0.50
1:C:2308:PHE:HA	1:C:2313:SER:HA	1.92	0.50
1:E:279:THR:HG1	1:E:285:SER:HG	1.53	0.50
1:E:1703:TYR:HD2	1:E:1820:PRO:HB2	1.77	0.50
1:G:1703:TYR:HD2	1:G:1820:PRO:HB2	1.77	0.50
1:G:1942:ARG:HH22	1:G:3612:LEU:HD23	1.76	0.50
1:A:1487:MET:HE1	1:A:1531:TYR:HB2	1.94	0.50
1:A:1773:ASN:HD21	1:A:1776:TYR:HB3	1.77	0.50
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.94	0.50
1:C:3748:SER:O	1:C:3793:SER:OG	2.28	0.50
1:E:780:GLU:O	1:E:1466:THR:OG1	2.27	0.50
1:E:1922:ARG:HH22	1:E:2039:TYR:HE1	1.60	0.50
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4753:THR:O	1:A:4756:THR:OG1	2.29	0.49
1:G:294:PRO:HB3	1:G:330:THR:HG22	1.93	0.49
1:G:2764:LEU:HB2	1:G:2769:LYS:HE3	1.94	0.49
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.44	0.49
1:A:1605:LYS:HD3	1:A:1606:VAL:HG23	1.94	0.49
1:A:1751:ILE:HB	1:A:1753:LEU:HD22	1.95	0.49
1:A:2764:LEU:HB2	1:A:2769:LYS:HE3	1.94	0.49
1:C:299:HIS:NE2	1:C:301:THR:OG1	2.37	0.49
1:A:875:PRO:HB2	1:A:878:LEU:HB2	1.93	0.49
1:A:4794:TYR:CD2	1:A:4807:CYS:HB3	2.26	0.49
1:C:1509:CYS:N	1:C:1519:THR:OG1	2.45	0.49
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.77	0.49
1:C:1751:ILE:HB	1:C:1753:LEU:HD22	1.95	0.49
1:C:1922:ARG:HH22	1:C:2039:TYR:HE1	1.60	0.49
1:E:1509:CYS:N	1:E:1519:THR:OG1	2.45	0.49
1:G:4005:VAL:HG21	1:G:4115:ARG:HG3	1.94	0.49
1:A:898:ILE:HG21	1:A:973:THR:HA	1.94	0.49
1:A:4005:VAL:HG21	1:A:4115:ARG:HG3	1.94	0.49
1:C:3803:VAL:HG21	1:C:3881:ARG:HD2	1.95	0.49
1:C:4849:ILE:HG12	1:E:4819:TYR:HD1	1.78	0.49
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.94	0.49
1:A:1250:TRP:HB3	1:A:1600:PRO:HB2	1.93	0.49
1:A:2419:ARG:O	1:A:2422:SER:OG	2.30	0.49
1:A:3872:ILE:HA	1:A:3875:THR:HG22	1.95	0.49
1:A:4791:ARG:NH2	1:C:4559:HIS:CE1	2.81	0.49
1:C:238:HIS:N	1:C:243:GLU:O	2.44	0.49
1:C:1250:TRP:HB3	1:C:1600:PRO:HB2	1.93	0.49
1:C:1690:GLU:OE2	1:C:1790:LYS:NZ	2.35	0.49
1:C:2764:LEU:HB2	1:C:2769:LYS:HE3	1.94	0.49
1:E:3803:VAL:HG21	1:E:3881:ARG:HD2	1.95	0.49
1:E:4722:TYR:HD2	1:E:4723:LEU:HD12	1.78	0.49
1:G:1487:MET:HE1	1:G:1531:TYR:HB2	1.94	0.49
1:A:187:SER:O	1:C:2419:ARG:CG	2.61	0.49
1:A:4794:TYR:O	1:A:4806:LYS:HA	2.12	0.49
1:C:2737:LYS:O	1:C:2741:GLY:N	2.46	0.49
1:C:4722:TYR:HD2	1:C:4723:LEU:HD12	1.78	0.49
1:E:35:LEU:HD13	1:E:49:LEU:HD22	1.94	0.49
1:E:294:PRO:HB3	1:E:330:THR:HG22	1.93	0.49
1:E:903:GLN:H	1:E:914:GLN:HA	1.78	0.49
1:E:1267:HIS:NE2	1:E:1293:GLN:OE1	2.45	0.49
1:G:1090:ALA:HA	1:G:1249:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4011:VAL:HG12	1:G:4015:LEU:HD23	1.94	0.49
1:A:190:ARG:HG2	1:A:207:PHE:HE1	1.78	0.49
1:A:1084:ARG:N	1:A:1127:GLU:OE2	2.44	0.49
1:A:2743:ILE:N	1:A:2753:LYS:O	2.43	0.49
1:A:4559:HIS:NE2	1:G:4791:ARG:NH2	2.61	0.49
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.94	0.49
1:C:1773:ASN:HD21	1:C:1776:TYR:HB3	1.77	0.49
1:E:1751:ILE:HB	1:E:1753:LEU:HD22	1.95	0.49
1:E:4011:VAL:HG12	1:E:4015:LEU:HD23	1.94	0.49
1:G:747:HIS:CE1	1:G:750:ARG:HD2	2.46	0.49
1:A:238:HIS:N	1:A:243:GLU:O	2.44	0.49
1:G:1261:VAL:HG22	1:G:1594:VAL:HG23	1.94	0.49
1:C:1090:ALA:HA	1:C:1249:MET:HG2	1.94	0.49
1:C:2743:ILE:N	1:C:2753:LYS:O	2.43	0.49
1:E:875:PRO:HB2	1:E:878:LEU:HB2	1.93	0.49
1:G:1250:TRP:HB3	1:G:1600:PRO:HB2	1.93	0.49
1:G:1751:ILE:HB	1:G:1753:LEU:HD22	1.95	0.49
1:A:4849:ILE:HG12	1:C:4819:TYR:HD1	1.78	0.49
1:E:2404:ALA:HB2	1:E:2475:ARG:HH21	1.78	0.49
1:E:2764:LEU:HB2	1:E:2769:LYS:HE3	1.94	0.49
1:G:443:SER:HA	1:G:444:THR:HA	1.56	0.49
1:G:903:GLN:H	1:G:914:GLN:HA	1.77	0.49
1:G:1125:ASP:OD1	1:G:1597:SER:OG	2.31	0.49
1:A:1090:ALA:HA	1:A:1249:MET:HG2	1.94	0.48
1:A:3803:VAL:HG21	1:A:3881:ARG:HD2	1.95	0.48
1:C:875:PRO:HB2	1:C:878:LEU:HB2	1.93	0.48
1:E:119:ILE:HD13	1:E:162:ILE:HD11	1.95	0.48
1:E:3748:SER:O	1:E:3793:SER:OG	2.28	0.48
1:E:4849:ILE:HG12	1:G:4819:TYR:HD1	1.76	0.48
1:A:4722:TYR:HD2	1:A:4723:LEU:HD12	1.78	0.48
1:C:187:SER:O	1:E:2419:ARG:CG	2.62	0.48
1:E:1090:ALA:HA	1:E:1249:MET:HG2	1.94	0.48
1:G:3871:ILE:O	1:G:3874:SER:OG	2.26	0.48
1:C:2404:ALA:HB2	1:C:2475:ARG:HH21	1.78	0.48
1:C:4791:ARG:NH2	1:E:4559:HIS:NE2	2.61	0.48
1:E:1261:VAL:HG22	1:E:1594:VAL:HG23	1.94	0.48
1:E:3761:LYS:NZ	1:E:3835:GLU:OE2	2.37	0.48
1:E:4791:ARG:NH2	1:G:4559:HIS:CE1	2.81	0.48
1:G:3872:ILE:HA	1:G:3875:THR:HG22	1.94	0.48
1:G:4722:TYR:HD2	1:G:4723:LEU:HD12	1.78	0.48
1:A:1297:THR:HB	1:A:1547:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2737:LYS:O	1:A:2741:GLY:N	2.46	0.48
1:A:4011:VAL:HG12	1:A:4015:LEU:HD23	1.94	0.48
1:C:119:ILE:HD13	1:C:162:ILE:HD11	1.95	0.48
1:C:4791:ARG:NH2	1:E:4559:HIS:CE1	2.81	0.48
1:E:3872:ILE:HA	1:E:3875:THR:HG22	1.95	0.48
1:E:4568:TYR:O	1:E:4572:THR:OG1	2.30	0.48
1:G:1297:THR:HB	1:G:1547:ALA:HB3	1.96	0.48
1:G:2737:LYS:O	1:G:2741:GLY:N	2.46	0.48
1:A:176:ARG:N	1:A:179:ASP:OD2	2.46	0.48
1:A:4792:LYS:CA	1:A:4806:LYS:HE2	2.42	0.48
1:C:903:GLN:H	1:C:914:GLN:HA	1.77	0.48
1:C:4753:THR:O	1:C:4756:THR:OG1	2.29	0.48
1:E:190:ARG:HG2	1:E:207:PHE:HE1	1.78	0.48
1:E:238:HIS:N	1:E:243:GLU:O	2.44	0.48
1:E:601:LEU:HD11	1:E:642:LEU:HB3	1.96	0.48
1:G:3803:VAL:HG21	1:G:3881:ARG:HD2	1.95	0.48
1:C:281:ARG:NH1	1:C:346:VAL:O	2.42	0.48
1:C:3872:ILE:HA	1:C:3875:THR:HG22	1.95	0.48
1:C:4861:ALA:CB	1:E:4864:GLN:NE2	2.53	0.48
1:E:1125:ASP:OD1	1:E:1597:SER:OG	2.31	0.48
1:E:1509:CYS:SG	1:E:1510:VAL:N	2.87	0.48
1:E:2737:LYS:O	1:E:2741:GLY:N	2.46	0.48
1:G:20:VAL:HG12	1:G:216:PRO:HA	1.94	0.48
1:G:190:ARG:HG2	1:G:207:PHE:HE1	1.78	0.48
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.94	0.48
1:C:1261:VAL:HG22	1:C:1594:VAL:HG23	1.94	0.48
1:C:4011:VAL:HG12	1:C:4015:LEU:HD23	1.94	0.48
1:E:1929:PHE:HZ	1:E:2030:LEU:HB3	1.79	0.48
1:G:590:LYS:H	1:G:593:HIS:CD2	2.29	0.48
1:G:2404:ALA:HB2	1:G:2475:ARG:HH21	1.78	0.48
1:G:4647:ASP:OD1	1:G:4648:LYS:N	2.47	0.48
1:G:4753:THR:O	1:G:4756:THR:OG1	2.29	0.48
1:A:119:ILE:HD13	1:A:162:ILE:HD11	1.95	0.48
1:A:1509:CYS:SG	1:A:1510:VAL:N	2.87	0.48
1:A:4037:ASP:OD1	1:A:4037:ASP:N	2.47	0.48
1:C:190:ARG:HG2	1:C:207:PHE:HE1	1.78	0.48
1:C:601:LEU:HD11	1:C:642:LEU:HB3	1.96	0.48
1:C:4037:ASP:OD1	1:C:4037:ASP:N	2.47	0.48
1:E:20:VAL:HG12	1:E:216:PRO:HA	1.94	0.48
1:E:544:ASN:HD22	1:E:547:ASN:HD21	1.62	0.48
1:G:119:ILE:HD13	1:G:162:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1929:PHE:HZ	1:G:2030:LEU:HB3	1.79	0.48
1:A:903:GLN:H	1:A:914:GLN:HA	1.77	0.48
1:A:4148:ARG:NH2	1:A:4150:TYR:OH	2.47	0.48
1:E:187:SER:O	1:G:2419:ARG:CG	2.61	0.48
1:A:1261:VAL:HG22	1:A:1594:VAL:HG23	1.94	0.48
1:A:1267:HIS:NE2	1:A:1293:GLN:OE1	2.45	0.48
1:A:1511:VAL:HG13	1:A:1516:GLY:HA2	1.96	0.48
1:A:2404:ALA:HB2	1:A:2475:ARG:HH21	1.78	0.48
1:C:1509:CYS:SG	1:C:1510:VAL:N	2.87	0.48
1:C:2829:MET:HE1	1:C:2896:PHE:HB2	1.96	0.48
1:C:4148:ARG:NH2	1:C:4150:TYR:OH	2.47	0.48
1:E:1682:GLU:HA	1:E:1685:LEU:HD13	1.96	0.48
1:E:4647:ASP:OD1	1:E:4648:LYS:N	2.47	0.48
1:G:1267:HIS:NE2	1:G:1293:GLN:OE1	2.45	0.48
1:G:2419:ARG:O	1:G:2422:SER:OG	2.30	0.48
1:A:877:HIS:HB3	1:A:952:ILE:HG13	1.95	0.47
1:A:1176:THR:HG22	1:A:1181:ILE:HG12	1.96	0.47
1:A:3761:LYS:NZ	1:A:3835:GLU:OE2	2.37	0.47
1:A:4791:ARG:NH2	1:C:4559:HIS:NE2	2.62	0.47
1:C:1267:HIS:NE2	1:C:1293:GLN:OE1	2.45	0.47
1:C:1297:THR:HB	1:C:1547:ALA:HB3	1.96	0.47
1:C:1511:VAL:HG13	1:C:1516:GLY:HA2	1.96	0.47
1:E:2419:ARG:O	1:E:2422:SER:OG	2.30	0.47
1:G:1176:THR:HG22	1:G:1181:ILE:HG12	1.96	0.47
1:A:2419:ARG:CG	1:G:187:SER:O	2.61	0.47
1:C:892:LEU:HD11	1:C:983:LEU:HD22	1.96	0.47
1:C:1176:THR:HG22	1:C:1181:ILE:HG12	1.96	0.47
1:E:280:LEU:HD11	1:E:294:PRO:HG2	1.96	0.47
1:E:4148:ARG:NH2	1:E:4150:TYR:OH	2.47	0.47
1:A:892:LEU:HD11	1:A:983:LEU:HD22	1.96	0.47
1:A:1929:PHE:HZ	1:A:2030:LEU:HB3	1.79	0.47
1:C:1682:GLU:HA	1:C:1685:LEU:HD13	1.96	0.47
1:C:4161:TRP:HD1	1:C:4201:MET:HE1	1.79	0.47
1:E:1176:THR:HG22	1:E:1181:ILE:HG12	1.96	0.47
1:G:280:LEU:HD11	1:G:294:PRO:HG2	1.96	0.47
1:G:4148:ARG:NH2	1:G:4150:TYR:OH	2.47	0.47
1:A:568:SER:O	1:A:572:LEU:HB2	2.15	0.47
1:A:601:LEU:HD11	1:A:642:LEU:HB3	1.96	0.47
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.97	0.47
1:A:4647:ASP:OD1	1:A:4648:LYS:N	2.47	0.47
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:877:HIS:HB3	1:E:952:ILE:HG13	1.95	0.47
1:E:1297:THR:HB	1:E:1547:ALA:HB3	1.96	0.47
1:G:176:ARG:N	1:G:179:ASP:OD2	2.46	0.47
1:G:892:LEU:HD11	1:G:983:LEU:HD22	1.96	0.47
1:A:4819:TYR:HD1	1:G:4849:ILE:HG12	1.78	0.47
1:C:568:SER:O	1:C:572:LEU:HB2	2.15	0.47
1:C:2832:VAL:H	1:C:2895:LYS:HD3	1.80	0.47
1:E:2829:MET:HE1	1:E:2896:PHE:HB2	1.96	0.47
1:E:4161:TRP:HD1	1:E:4201:MET:HE1	1.79	0.47
1:G:2177:VAL:HG22	1:G:2221:TYR:HE2	1.80	0.47
1:A:1256:PRO:HD2	1:A:1451:HIS:HB3	1.96	0.47
1:C:661:LEU:O	1:C:788:PHE:N	2.39	0.47
1:C:1929:PHE:HZ	1:C:2030:LEU:HB3	1.79	0.47
1:C:2860:GLU:O	1:C:2864:LYS:NZ	2.42	0.47
1:E:568:SER:O	1:E:572:LEU:HB2	2.15	0.47
1:E:892:LEU:HD11	1:E:983:LEU:HD22	1.96	0.47
1:E:2707:VAL:HG21	1:E:2786:TRP:HE1	1.80	0.47
1:G:35:LEU:HD13	1:G:49:LEU:HD22	1.95	0.47
1:G:544:ASN:HD22	1:G:547:ASN:HD21	1.62	0.47
1:G:1511:VAL:HG13	1:G:1516:GLY:HA2	1.96	0.47
1:A:277:LEU:HD23	1:A:297:LEU:HD21	1.97	0.47
1:A:695:VAL:HA	1:A:792:VAL:HG22	1.97	0.47
1:A:2623:CYS:O	1:A:2627:GLY:N	2.47	0.47
1:A:2832:VAL:H	1:A:2895:LYS:HD3	1.80	0.47
1:A:3862:GLN:NE2	1:A:3869:VAL:O	2.48	0.47
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.97	0.47
1:C:288:HIS:HD2	1:C:352:SER:HB3	1.80	0.47
1:E:288:HIS:HD2	1:E:352:SER:HB3	1.80	0.47
1:E:1256:PRO:HD2	1:E:1451:HIS:HB3	1.96	0.47
1:E:1511:VAL:HG13	1:E:1516:GLY:HA2	1.96	0.47
1:E:2876:ASP:OD1	1:E:2876:ASP:N	2.48	0.47
1:E:3862:GLN:NE2	1:E:3869:VAL:O	2.48	0.47
1:G:277:LEU:HD23	1:G:297:LEU:HD21	1.97	0.47
1:G:568:SER:O	1:G:572:LEU:HB2	2.15	0.47
1:G:1256:PRO:HD2	1:G:1451:HIS:HB3	1.96	0.47
1:G:3862:GLN:NE2	1:G:3869:VAL:O	2.48	0.47
1:A:733:TRP:CD1	1:A:738:ALA:HB2	2.50	0.47
1:C:695:VAL:HA	1:C:792:VAL:HG22	1.97	0.47
1:C:877:HIS:HB3	1:C:952:ILE:HG13	1.95	0.47
1:C:4647:ASP:OD1	1:C:4648:LYS:N	2.47	0.47
1:G:601:LEU:HD11	1:G:642:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1689:ILE:HG12	1:C:1703:TYR:HE1	1.80	0.47
1:G:1703:TYR:CD2	1:G:1820:PRO:HB2	2.50	0.47
1:G:2829:MET:HE1	1:G:2896:PHE:HB2	1.96	0.47
1:A:1125:ASP:OD1	1:A:1597:SER:OG	2.31	0.47
1:A:4161:TRP:HD1	1:A:4201:MET:HE1	1.79	0.47
1:C:733:TRP:CD1	1:C:738:ALA:HB2	2.50	0.47
1:C:2707:VAL:HG21	1:C:2786:TRP:HE1	1.80	0.47
1:E:2743:ILE:N	1:E:2753:LYS:O	2.43	0.47
1:G:733:TRP:CD1	1:G:738:ALA:HB2	2.50	0.47
1:G:2707:VAL:HG21	1:G:2786:TRP:HE1	1.80	0.47
1:G:3748:SER:O	1:G:3793:SER:OG	2.28	0.47
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.97	0.46
1:A:1682:GLU:HA	1:A:1685:LEU:HD13	1.96	0.46
1:C:590:LYS:H	1:C:593:HIS:CD2	2.29	0.46
1:C:1256:PRO:HD2	1:C:1451:HIS:HB3	1.96	0.46
1:C:1703:TYR:CD2	1:C:1820:PRO:HB2	2.50	0.46
1:C:3862:GLN:NE2	1:C:3869:VAL:O	2.48	0.46
1:C:3871:ILE:O	1:C:3874:SER:OG	2.26	0.46
1:E:277:LEU:HD23	1:E:297:LEU:HD21	1.97	0.46
1:E:695:VAL:HA	1:E:792:VAL:HG22	1.97	0.46
1:E:733:TRP:CD1	1:E:738:ALA:HB2	2.50	0.46
1:E:756:SER:HB3	1:E:769:ARG:HB2	1.97	0.46
1:E:1703:TYR:CD2	1:E:1820:PRO:HB2	2.50	0.46
1:E:2832:VAL:H	1:E:2895:LYS:HD3	1.80	0.46
1:G:695:VAL:HA	1:G:792:VAL:HG22	1.97	0.46
1:G:4037:ASP:OD1	1:G:4037:ASP:N	2.47	0.46
1:A:411:GLU:HA	1:A:414:ARG:HB2	1.97	0.46
1:A:1484:ASN:H	1:A:1486:TYR:HA	1.81	0.46
1:C:544:ASN:HD22	1:C:547:ASN:HD21	1.62	0.46
1:E:1689:ILE:HG12	1:E:1703:TYR:HE1	1.80	0.46
1:G:756:SER:HB3	1:G:769:ARG:HB2	1.97	0.46
1:A:280:LEU:HD11	1:A:294:PRO:HG2	1.96	0.46
1:A:544:ASN:HD22	1:A:547:ASN:HD21	1.62	0.46
1:A:1703:TYR:CD2	1:A:1820:PRO:HB2	2.50	0.46
1:A:2829:MET:HE1	1:A:2896:PHE:HB2	1.96	0.46
1:A:4861:ALA:CB	1:C:4864:GLN:NE2	2.53	0.46
1:C:280:LEU:HD11	1:C:294:PRO:HG2	1.96	0.46
1:C:416:ALA:HA	1:C:419:ILE:HD12	1.98	0.46
1:E:1640:ASP:OD1	1:E:1640:ASP:N	2.47	0.46
1:A:288:HIS:CD2	1:A:352:SER:HB3	2.51	0.46
1:C:411:GLU:HA	1:C:414:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4791:ARG:NH2	1:G:4559:HIS:NE2	2.63	0.46
1:G:416:ALA:HA	1:G:419:ILE:HD12	1.98	0.46
1:G:877:HIS:HB3	1:G:952:ILE:HG13	1.95	0.46
1:G:1682:GLU:HA	1:G:1685:LEU:HD13	1.95	0.46
1:G:2832:VAL:H	1:G:2895:LYS:HD3	1.80	0.46
1:G:2857:LYS:HG2	1:G:2869:HIS:HB2	1.98	0.46
1:A:2857:LYS:HG2	1:A:2869:HIS:HB2	1.98	0.46
1:G:180:ASP:HB3	1:G:211:LEU:HD22	1.97	0.46
1:G:1484:ASN:H	1:G:1486:TYR:HA	1.80	0.46
1:G:2860:GLU:O	1:G:2864:LYS:NZ	2.42	0.46
1:A:180:ASP:HB3	1:A:211:LEU:HD22	1.97	0.46
1:A:288:HIS:HD2	1:A:352:SER:HB3	1.80	0.46
1:A:2177:VAL:HG22	1:A:2221:TYR:HE2	1.80	0.46
1:C:277:LEU:HD23	1:C:297:LEU:HD21	1.97	0.46
1:E:2177:VAL:HG22	1:E:2221:TYR:HE2	1.80	0.46
1:A:416:ALA:HA	1:A:419:ILE:HD12	1.98	0.46
1:A:1272:ARG:HH12	1:A:1588:VAL:HA	1.80	0.46
1:A:1640:ASP:N	1:A:1640:ASP:OD1	2.47	0.46
1:A:2860:GLU:O	1:A:2864:LYS:NZ	2.42	0.46
1:C:1272:ARG:HH12	1:C:1588:VAL:HA	1.80	0.46
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.97	0.46
1:G:1689:ILE:HG12	1:G:1703:TYR:HE1	1.80	0.46
1:C:2857:LYS:HG2	1:C:2869:HIS:HB2	1.98	0.46
1:C:4105:ASN:OD1	1:C:4109:HIS:ND1	2.49	0.46
1:E:416:ALA:HA	1:E:419:ILE:HD12	1.98	0.46
1:G:288:HIS:HD2	1:G:352:SER:HB3	1.80	0.46
1:G:4161:TRP:HD1	1:G:4201:MET:HE1	1.79	0.46
1:C:4918:ASN:O	1:C:4922:PHE:HB2	2.16	0.46
1:E:1090:ALA:HB3	1:E:1203:PRO:HD2	1.98	0.46
1:A:2707:VAL:HG21	1:A:2786:TRP:HE1	1.80	0.46
1:C:1114:ARG:HB3	1:C:1128:LEU:HD22	1.97	0.46
1:C:2177:VAL:HG22	1:C:2221:TYR:HE2	1.80	0.46
1:A:108:GLY:HA3	1:A:109:GLY:HA3	1.67	0.45
1:A:1035:TYR:HA	1:A:1038:LEU:HG	1.98	0.45
1:A:1090:ALA:HB3	1:A:1203:PRO:HD2	1.97	0.45
1:C:1125:ASP:OD1	1:C:1597:SER:OG	2.31	0.45
1:C:1738:LEU:HD22	1:C:1739:PHE:H	1.81	0.45
1:E:411:GLU:HA	1:E:414:ARG:HB2	1.98	0.45
1:E:443:SER:HA	1:E:444:THR:HA	1.56	0.45
1:E:2349:GLU:OE2	1:E:2438:SER:OG	2.34	0.45
1:E:4105:ASN:OD1	1:E:4109:HIS:ND1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2072:GLN:NE2	1:A:3647:LYS:O	2.50	0.45
1:C:288:HIS:CD2	1:C:352:SER:HB3	2.51	0.45
1:G:1035:TYR:HA	1:G:1038:LEU:HG	1.98	0.45
1:A:661:LEU:O	1:A:788:PHE:N	2.39	0.45
1:A:1043:LYS:HB2	1:A:1047:LYS:HE3	1.99	0.45
1:A:3956:GLN:HE21	1:A:3976:GLN:HE22	1.64	0.45
1:E:1738:LEU:HD22	1:E:1739:PHE:H	1.81	0.45
1:E:4037:ASP:OD1	1:E:4037:ASP:N	2.47	0.45
1:G:288:HIS:CD2	1:G:352:SER:HB3	2.51	0.45
1:A:1689:ILE:HG12	1:A:1703:TYR:HE1	1.80	0.45
1:A:1738:LEU:HD22	1:A:1739:PHE:H	1.81	0.45
1:A:2349:GLU:OE2	1:A:2438:SER:OG	2.34	0.45
1:C:1304:LEU:HD23	1:C:1305:SER:H	1.81	0.45
1:C:2623:CYS:O	1:C:2627:GLY:N	2.47	0.45
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.52	0.45
1:E:176:ARG:N	1:E:179:ASP:OD2	2.46	0.45
1:E:2857:LYS:HG2	1:E:2869:HIS:HB2	1.98	0.45
1:G:1043:LYS:HB2	1:G:1047:LYS:HE3	1.99	0.45
1:G:1509:CYS:SG	1:G:1510:VAL:N	2.87	0.45
1:G:1629:SER:HA	1:G:1640:ASP:HA	1.97	0.45
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.98	0.45
1:C:170:SER:OG	1:C:171:GLU:N	2.50	0.45
1:C:1640:ASP:N	1:C:1640:ASP:OD1	2.47	0.45
1:C:2349:GLU:OE2	1:C:2438:SER:OG	2.34	0.45
1:C:2419:ARG:O	1:C:2422:SER:OG	2.30	0.45
1:E:246:THR:OG1	1:E:272:ARG:NH1	2.50	0.45
1:A:1114:ARG:HB3	1:A:1128:LEU:HD22	1.97	0.45
1:A:1116:GLY:HA3	1:A:1136:ALA:HA	1.99	0.45
1:A:1304:LEU:HD23	1:A:1305:SER:H	1.81	0.45
1:A:4105:ASN:OD1	1:A:4109:HIS:ND1	2.49	0.45
2:D:49:ARG:HB3	2:D:52:LYS:HE2	1.99	0.45
1:E:180:ASP:HB3	1:E:211:LEU:HD22	1.97	0.45
1:E:4918:ASN:O	1:E:4922:PHE:HB2	2.16	0.45
1:G:411:GLU:HA	1:G:414:ARG:HB2	1.97	0.45
1:G:748:LEU:HD13	1:G:750:ARG:HE	1.82	0.45
1:G:1090:ALA:HB3	1:G:1203:PRO:HD2	1.98	0.45
1:G:2072:GLN:NE2	1:G:3647:LYS:O	2.50	0.45
1:G:2349:GLU:OE2	1:G:2438:SER:OG	2.34	0.45
1:A:1013:ARG:O	1:A:1027:ARG:N	2.50	0.45
1:C:2315:GLU:OE2	1:C:3814:LYS:NZ	2.44	0.45
1:C:3800:SER:OG	1:C:3801:CYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:748:LEU:HD13	1:E:750:ARG:HE	1.82	0.45
1:E:1272:ARG:HH12	1:E:1588:VAL:HA	1.81	0.45
1:E:3730:ALA:HA	1:E:3733:HIS:CE1	2.52	0.45
1:G:1304:LEU:HD23	1:G:1305:SER:H	1.81	0.45
1:A:2466:LYS:NZ	1:A:2492:GLY:O	2.50	0.45
1:C:748:LEU:HD13	1:C:750:ARG:HE	1.82	0.45
1:C:2072:GLN:NE2	1:C:3647:LYS:O	2.50	0.45
1:C:2710:SER:HB3	1:C:2781:LYS:HD3	1.99	0.45
1:E:288:HIS:CD2	1:E:352:SER:HB3	2.51	0.45
1:E:1629:SER:HA	1:E:1640:ASP:HA	1.97	0.45
1:G:1013:ARG:O	1:G:1027:ARG:N	2.50	0.45
1:G:1272:ARG:HH12	1:G:1588:VAL:HA	1.80	0.45
1:C:41:GLY:H	1:C:44:ASN:HB3	1.82	0.45
1:C:1085:PHE:N	1:C:1127:GLU:OE2	2.47	0.45
1:E:1114:ARG:HB3	1:E:1128:LEU:HD22	1.97	0.45
1:E:1756:SER:OG	1:E:1920:ARG:NH2	2.50	0.45
1:G:238:HIS:N	1:G:243:GLU:O	2.44	0.45
1:G:394:HIS:HD2	1:G:397:GLY:H	1.65	0.45
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.98	0.45
1:G:1114:ARG:HB3	1:G:1128:LEU:HD22	1.98	0.45
1:G:1116:GLY:HA3	1:G:1136:ALA:HA	1.99	0.45
1:A:246:THR:OG1	1:A:272:ARG:NH1	2.50	0.45
1:A:2710:SER:HB3	1:A:2781:LYS:HD3	1.99	0.45
1:C:246:THR:OG1	1:C:272:ARG:NH1	2.50	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.98	0.45
1:C:1035:TYR:HA	1:C:1038:LEU:HG	1.98	0.45
1:E:1304:LEU:HD23	1:E:1305:SER:H	1.81	0.45
1:G:1738:LEU:HD22	1:G:1739:PHE:H	1.81	0.45
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.52	0.44
1:A:3845:GLN:HE21	1:A:3923:GLU:HG3	1.82	0.44
1:C:1043:LYS:HB2	1:C:1047:LYS:HE3	1.99	0.44
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	1.98	0.44
1:C:1243:THR:HG23	1:C:1807:ARG:HD2	2.00	0.44
1:C:1484:ASN:H	1:C:1486:TYR:HA	1.81	0.44
1:E:766:ILE:HB	1:E:779:PHE:HB2	1.98	0.44
1:E:1013:ARG:O	1:E:1027:ARG:N	2.50	0.44
1:E:1114:ARG:HD3	1:E:1128:LEU:HB3	1.99	0.44
1:G:1118:SER:HB2	1:G:1122:CYS:SG	2.58	0.44
1:G:1640:ASP:OD1	1:G:1640:ASP:N	2.47	0.44
1:G:4105:ASN:OD1	1:G:4109:HIS:ND1	2.49	0.44
1:A:2876:ASP:OD1	1:A:2876:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4809:ASP:HB3	1:A:4812:THR:HG23	2.00	0.44
1:A:4918:ASN:O	1:A:4922:PHE:HB2	2.16	0.44
1:C:618:CYS:O	1:C:629:GLN:NE2	2.51	0.44
1:C:1116:GLY:HA3	1:C:1136:ALA:HA	1.99	0.44
1:E:1245:ARG:HH21	1:E:1810:VAL:HG22	1.82	0.44
1:E:2072:GLN:NE2	1:E:3647:LYS:O	2.50	0.44
1:E:2226:SER:HB2	1:E:2241:LEU:HB2	1.99	0.44
1:E:3956:GLN:HE21	1:E:3976:GLN:HE22	1.64	0.44
1:G:41:GLY:H	1:G:44:ASN:HB3	1.82	0.44
1:G:3730:ALA:HA	1:G:3733:HIS:CE1	2.52	0.44
2:H:67:SER:N	2:H:70:GLN:OE1	2.51	0.44
1:A:41:GLY:H	1:A:44:ASN:HB3	1.82	0.44
1:A:1118:SER:HB2	1:A:1122:CYS:SG	2.58	0.44
1:C:915:HIS:CE1	1:C:917:CYS:HB2	2.53	0.44
1:E:1243:THR:HG23	1:E:1807:ARG:HD2	1.99	0.44
1:G:1245:ARG:HH21	1:G:1810:VAL:HG22	1.82	0.44
1:G:3845:GLN:HE21	1:G:3923:GLU:HG3	1.82	0.44
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.51	0.44
1:A:3871:ILE:O	1:A:3874:SER:OG	2.26	0.44
1:A:4886:GLU:OE1	4:A:5101:ATP:O2'	2.32	0.44
1:C:1013:ARG:O	1:C:1027:ARG:N	2.50	0.44
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.51	0.44
1:C:3845:GLN:HE21	1:C:3923:GLU:HG3	1.82	0.44
1:C:3956:GLN:HE21	1:C:3976:GLN:HE22	1.64	0.44
1:E:19:GLU:OE1	1:E:218:SER:OG	2.36	0.44
1:E:661:LEU:O	1:E:788:PHE:N	2.39	0.44
1:E:694:ARG:HB3	1:E:716:ASN:HD22	1.83	0.44
1:E:924:LEU:HB2	1:E:929:ARG:HB2	2.00	0.44
1:G:246:THR:OG1	1:G:272:ARG:NH1	2.50	0.44
1:G:364:GLN:HE21	1:G:369:GLY:HA2	1.83	0.44
1:G:694:ARG:HB3	1:G:716:ASN:HD22	1.83	0.44
1:G:1085:PHE:N	1:G:1127:GLU:OE2	2.47	0.44
1:G:3956:GLN:HE21	1:G:3976:GLN:HE22	1.64	0.44
1:A:19:GLU:OE1	1:A:218:SER:OG	2.36	0.44
1:A:1176:THR:HA	1:A:1181:ILE:HA	2.00	0.44
1:A:1226:TYR:HA	1:A:1229:ILE:HD12	1.99	0.44
1:E:328:ALA:HB3	1:E:366:ILE:HD11	2.00	0.44
1:E:915:HIS:CE1	1:E:917:CYS:HB2	2.53	0.44
1:E:1043:LYS:HB2	1:E:1047:LYS:HE3	1.99	0.44
1:E:3845:GLN:HE21	1:E:3923:GLU:HG3	1.82	0.44
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:924:LEU:HB2	1:G:929:ARG:HB2	2.00	0.44
1:G:1114:ARG:HD3	1:G:1128:LEU:HB3	1.99	0.44
1:G:1117:TRP:HE1	1:G:1164:CYS:HB3	1.83	0.44
1:G:1243:THR:HG23	1:G:1807:ARG:HD2	1.99	0.44
1:G:4918:ASN:O	1:G:4922:PHE:HB2	2.16	0.44
2:H:26:TYR:HB2	2:H:101:VAL:HG22	2.00	0.44
1:A:328:ALA:HB3	1:A:366:ILE:HD11	2.00	0.44
1:A:394:HIS:HD2	1:A:397:GLY:H	1.65	0.44
1:A:748:LEU:HD13	1:A:750:ARG:HE	1.82	0.44
2:B:26:TYR:HB2	2:B:101:VAL:HG22	2.00	0.44
2:B:49:ARG:HB3	2:B:52:LYS:HE2	1.99	0.44
2:B:67:SER:N	2:B:70:GLN:OE1	2.51	0.44
1:C:298:ARG:HE	1:C:303:GLY:HA2	1.83	0.44
1:C:694:ARG:HB3	1:C:716:ASN:HD22	1.83	0.44
1:C:1166:VAL:HA	1:C:1173:MET:HG3	2.00	0.44
1:E:41:GLY:H	1:E:44:ASN:HB3	1.82	0.44
1:E:1118:SER:HB2	1:E:1122:CYS:SG	2.57	0.44
1:E:4201:MET:HE2	1:E:4201:MET:HB2	1.92	0.44
2:F:26:TYR:HB2	2:F:101:VAL:HG22	2.00	0.44
2:F:67:SER:N	2:F:70:GLN:OE1	2.51	0.44
1:G:19:GLU:OE1	1:G:218:SER:OG	2.36	0.44
1:G:328:ALA:HB3	1:G:366:ILE:HD11	2.00	0.44
1:G:1176:THR:HA	1:G:1181:ILE:HA	2.00	0.44
1:G:2226:SER:HB2	1:G:2241:LEU:HB2	1.99	0.44
1:G:2710:SER:HB3	1:G:2781:LYS:HD3	1.99	0.44
1:G:4186:LYS:HE2	1:G:4186:LYS:HB3	1.84	0.44
1:A:1243:THR:HG23	1:A:1807:ARG:HD2	2.00	0.44
1:A:2226:SER:HB2	1:A:2241:LEU:HB2	1.99	0.44
1:A:4642:PRO:HG2	1:A:4648:LYS:HA	2.00	0.44
1:A:4794:TYR:HB2	1:A:4807:CYS:H	1.82	0.44
1:C:1114:ARG:HD3	1:C:1128:LEU:HB3	1.99	0.44
1:E:170:SER:OG	1:E:171:GLU:N	2.50	0.44
1:E:1035:TYR:HA	1:E:1038:LEU:HG	1.98	0.44
1:E:1484:ASN:H	1:E:1486:TYR:HA	1.80	0.44
1:E:2301:ASP:OD1	1:E:2304:ARG:NH2	2.51	0.44
1:E:2710:SER:HB3	1:E:2781:LYS:HD3	1.99	0.44
1:E:4191:VAL:HG21	1:E:4950:TRP:CZ3	2.53	0.44
1:G:1690:GLU:OE2	1:G:1790:LYS:NZ	2.34	0.44
1:G:1938:GLN:HE22	1:G:3611:ASN:HB2	1.83	0.44
2:H:49:ARG:HB3	2:H:52:LYS:HE2	1.99	0.44
1:A:618:CYS:O	1:A:629:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.53	0.44
1:A:1117:TRP:HH2	1:A:1239:PHE:HZ	1.66	0.44
1:A:1166:VAL:HA	1:A:1173:MET:HG3	2.00	0.44
1:C:1176:THR:HA	1:C:1181:ILE:HA	2.00	0.44
1:C:1518:LEU:HD23	1:C:1518:LEU:HA	1.87	0.44
1:C:2226:SER:HB2	1:C:2241:LEU:HB2	1.99	0.44
1:C:3687:PHE:HA	1:C:3690:MET:HB2	2.00	0.44
1:C:4191:VAL:HG21	1:C:4950:TRP:CZ3	2.53	0.44
2:D:67:SER:N	2:D:70:GLN:OE1	2.51	0.44
1:E:76:ARG:HG3	1:G:3891:TRP:CE3	2.53	0.44
1:E:394:HIS:HD2	1:E:397:GLY:H	1.65	0.44
1:E:1116:GLY:HA3	1:E:1136:ALA:HA	1.99	0.44
1:E:1938:GLN:HE22	1:E:3611:ASN:HB2	1.83	0.44
1:G:618:CYS:O	1:G:629:GLN:NE2	2.51	0.44
1:G:4899:PHE:CE2	1:G:4909:HIS:HB2	2.53	0.44
1:A:694:ARG:HB3	1:A:716:ASN:HD22	1.83	0.44
1:A:718:VAL:HA	1:A:736:CYS:N	2.33	0.44
1:A:1114:ARG:HD3	1:A:1128:LEU:HB3	1.99	0.44
1:A:2461:PHE:O	1:A:2465:HIS:NE2	2.51	0.44
1:C:924:LEU:HB2	1:C:929:ARG:HB2	2.00	0.44
1:C:4186:LYS:HE2	1:C:4186:LYS:HB3	1.84	0.44
1:C:4811:LEU:CD1	1:E:4520:PHE:HD1	2.29	0.44
1:E:108:GLY:HA3	1:E:109:GLY:HA3	1.67	0.44
1:E:364:GLN:HE21	1:E:369:GLY:HA2	1.83	0.44
1:E:657:PRO:HA	1:E:834:VAL:HA	1.99	0.44
1:E:4611:LEU:HD21	1:E:4617:TYR:HD2	1.83	0.44
1:G:1117:TRP:HH2	1:G:1239:PHE:HZ	1.66	0.44
1:G:3687:PHE:HA	1:G:3690:MET:HB2	2.00	0.44
1:A:1117:TRP:HE1	1:A:1164:CYS:HB3	1.83	0.43
1:A:4191:VAL:HG21	1:A:4950:TRP:CZ3	2.53	0.43
1:A:4792:LYS:HA	1:A:4806:LYS:HE2	1.99	0.43
1:C:3742:LEU:HD12	1:C:3742:LEU:HA	1.86	0.43
1:C:4201:MET:HE2	1:C:4201:MET:HB2	1.92	0.43
1:E:2623:CYS:O	1:E:2627:GLY:N	2.47	0.43
1:E:3687:PHE:HA	1:E:3690:MET:HB2	2.00	0.43
2:F:49:ARG:HB3	2:F:52:LYS:HE2	1.99	0.43
1:G:73:LEU:HB3	1:G:77:ALA:HB3	2.00	0.43
1:G:1166:VAL:HA	1:G:1173:MET:HG3	2.00	0.43
1:G:4611:LEU:HD21	1:G:4617:TYR:HD2	1.83	0.43
1:G:4642:PRO:HG2	1:G:4648:LYS:HA	2.00	0.43
1:G:4737:ASN:OD1	1:G:4737:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3760:LEU:HD23	1:A:3760:LEU:HA	1.82	0.43
1:A:4899:PHE:CE2	1:A:4909:HIS:HB2	2.53	0.43
1:C:4899:PHE:CE2	1:C:4909:HIS:HB2	2.53	0.43
2:D:26:TYR:HB2	2:D:101:VAL:HG22	2.00	0.43
1:E:1678:SER:OG	2:F:36:PHE:O	2.31	0.43
1:E:2466:LYS:NZ	1:E:2492:GLY:O	2.50	0.43
2:F:23:VAL:HG12	2:F:104:LEU:HD12	2.00	0.43
1:G:298:ARG:HE	1:G:303:GLY:HA2	1.83	0.43
1:G:1226:TYR:HA	1:G:1229:ILE:HD12	1.99	0.43
1:G:2217:ASP:N	1:G:2217:ASP:OD1	2.50	0.43
1:G:2461:PHE:O	1:G:2465:HIS:NE2	2.51	0.43
1:G:4191:VAL:HG21	1:G:4950:TRP:CZ3	2.53	0.43
1:A:76:ARG:HG3	1:C:3891:TRP:CE3	2.54	0.43
1:C:4611:LEU:HD21	1:C:4617:TYR:HD2	1.83	0.43
1:E:73:LEU:HB3	1:E:77:ALA:HB3	2.00	0.43
1:E:1176:THR:HA	1:E:1181:ILE:HA	2.00	0.43
1:G:115:TYR:CG	1:G:164:PRO:HG3	2.53	0.43
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.83	0.43
1:A:924:LEU:HB2	1:A:929:ARG:HB2	2.00	0.43
1:A:3877:ASP:HA	1:A:3880:LEU:HD12	2.01	0.43
1:A:4611:LEU:HD21	1:A:4617:TYR:HD2	1.83	0.43
1:C:1117:TRP:HE1	1:C:1164:CYS:HB3	1.83	0.43
1:C:1118:SER:HB2	1:C:1122:CYS:SG	2.58	0.43
1:E:1166:VAL:HA	1:E:1173:MET:HG3	2.00	0.43
1:E:2124:LEU:HA	1:E:2127:ILE:HG22	2.01	0.43
1:E:4753:THR:O	1:E:4756:THR:OG1	2.29	0.43
2:H:15:PHE:HA	2:H:16:PRO:HD3	1.85	0.43
1:A:303:GLY:N	1:A:420:ARG:HH22	2.17	0.43
1:C:115:TYR:CG	1:C:164:PRO:HG3	2.53	0.43
1:C:394:HIS:HD2	1:C:397:GLY:H	1.65	0.43
1:C:1226:TYR:HA	1:C:1229:ILE:HD12	1.99	0.43
1:C:2124:LEU:HA	1:C:2127:ILE:HG22	2.01	0.43
2:D:23:VAL:HG12	2:D:104:LEU:HD12	2.00	0.43
1:E:896:ASN:ND2	1:E:1052:GLU:OE2	2.44	0.43
1:E:1785:ASP:HA	1:E:1788:LYS:HG2	2.00	0.43
1:E:4737:ASN:OD1	1:E:4737:ASN:N	2.50	0.43
1:E:4899:PHE:CE2	1:E:4909:HIS:HB2	2.53	0.43
1:G:50:GLU:OE2	1:G:61:ASP:N	2.50	0.43
1:G:551:PHE:HD1	1:G:551:PHE:HA	1.67	0.43
1:G:2301:ASP:OD1	1:G:2304:ARG:NH2	2.51	0.43
1:C:19:GLU:OE1	1:C:218:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:GLY:N	1:C:420:ARG:HH22	2.17	0.43
1:C:657:PRO:HA	1:C:834:VAL:HA	1.99	0.43
1:C:1245:ARG:HH21	1:C:1810:VAL:HG22	1.82	0.43
1:C:3761:LYS:NZ	1:C:3839:ASP:OD2	2.47	0.43
1:C:3877:ASP:HA	1:C:3880:LEU:HD12	2.01	0.43
2:D:15:PHE:HA	2:D:16:PRO:HD3	1.85	0.43
1:E:3877:ASP:HA	1:E:3880:LEU:HD12	2.01	0.43
2:F:19:GLY:H	2:F:49:ARG:HD2	1.84	0.43
2:H:23:VAL:HG12	2:H:104:LEU:HD12	2.00	0.43
1:A:115:TYR:CG	1:A:164:PRO:HG3	2.53	0.43
1:A:1785:ASP:HA	1:A:1788:LYS:HG2	2.00	0.43
1:A:3777:LYS:HE3	1:A:3777:LYS:HB2	1.84	0.43
1:C:328:ALA:HB3	1:C:366:ILE:HD11	2.00	0.43
1:E:298:ARG:HE	1:E:303:GLY:HA2	1.83	0.43
1:E:2143:MET:HE1	1:E:2193:MET:HG3	2.01	0.43
1:E:3983:LEU:HD23	1:E:4102:LEU:HD11	2.00	0.43
1:G:34:LYS:H	1:G:53:SER:HG	1.62	0.43
1:A:657:PRO:HA	1:A:834:VAL:HA	1.99	0.43
1:A:1938:GLN:HE22	1:A:3611:ASN:HB2	1.83	0.43
1:C:76:ARG:HG3	1:E:3891:TRP:CE3	2.54	0.43
1:C:718:VAL:HA	1:C:736:CYS:N	2.33	0.43
1:C:864:PRO:HB3	1:C:1034:PRO:HB3	2.01	0.43
1:C:1117:TRP:HH2	1:C:1239:PHE:HZ	1.66	0.43
1:C:1678:SER:HB2	1:C:1768:PHE:CZ	2.54	0.43
1:C:1758:ARG:HD3	1:C:1920:ARG:HH22	1.84	0.43
1:C:4642:PRO:HG2	1:C:4648:LYS:HA	2.00	0.43
1:E:303:GLY:N	1:E:420:ARG:HH22	2.17	0.43
1:E:1117:TRP:HE1	1:E:1164:CYS:HB3	1.83	0.43
1:E:1226:TYR:HA	1:E:1229:ILE:HD12	1.99	0.43
1:E:1433:PHE:HD2	1:E:1551:ASN:HB3	1.83	0.43
1:E:1609:SER:N	1:E:1623:GLU:OE2	2.52	0.43
1:E:1758:ARG:HD3	1:E:1920:ARG:HH22	1.84	0.43
1:G:303:GLY:N	1:G:420:ARG:HH22	2.17	0.43
1:G:657:PRO:HA	1:G:834:VAL:HA	1.99	0.43
1:G:3970:LYS:HA	1:G:3973:MET:HE2	2.01	0.43
1:A:896:ASN:ND2	1:A:1052:GLU:OE2	2.44	0.43
1:A:1245:ARG:HH21	1:A:1810:VAL:HG22	1.82	0.43
1:A:3687:PHE:HA	1:A:3690:MET:HB2	2.00	0.43
1:C:1785:ASP:HA	1:C:1788:LYS:HG2	2.00	0.43
1:E:618:CYS:O	1:E:629:GLN:NE2	2.51	0.43
1:E:864:PRO:HB3	1:E:1034:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1117:TRP:HH2	1:E:1239:PHE:HZ	1.66	0.43
1:G:1576:LYS:HE3	1:G:1587:HIS:CD2	2.54	0.43
1:G:1609:SER:N	1:G:1623:GLU:OE2	2.52	0.43
1:G:2466:LYS:NZ	1:G:2492:GLY:O	2.50	0.43
1:G:4597:PRO:HA	1:G:4600:ILE:HG22	2.01	0.43
1:A:3891:TRP:CE3	1:G:76:ARG:HG3	2.53	0.43
1:A:3983:LEU:HD23	1:A:4102:LEU:HD11	2.00	0.43
1:A:4093:LYS:HE2	1:A:4093:LYS:HB3	1.87	0.43
1:A:4597:PRO:HA	1:A:4600:ILE:HG22	2.01	0.43
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.83	0.43
1:C:650:ASN:HA	1:C:1626:GLN:HA	2.01	0.43
1:C:4696:SER:OG	1:C:4697:ALA:N	2.52	0.43
1:G:2315:GLU:OE2	1:G:3814:LYS:NZ	2.44	0.43
1:G:2623:CYS:O	1:G:2627:GLY:N	2.47	0.43
1:G:3877:ASP:HA	1:G:3880:LEU:HD12	2.01	0.43
1:G:4923:LEU:HD12	1:G:4923:LEU:HA	1.92	0.43
2:H:19:GLY:H	2:H:49:ARG:HD2	1.84	0.43
1:A:2083:ARG:HD3	1:A:3688:LEU:HD22	2.01	0.42
1:A:4024:LEU:HA	1:A:4027:LEU:HD12	2.00	0.42
1:A:4929:LYS:NZ	1:A:4938:GLU:OE2	2.47	0.42
1:C:73:LEU:HB3	1:C:77:ALA:HB3	2.00	0.42
1:C:267:VAL:O	1:C:273:SER:OG	2.35	0.42
1:C:2461:PHE:O	1:C:2465:HIS:NE2	2.51	0.42
1:E:2725:TYR:O	1:E:2729:SER:OG	2.37	0.42
1:G:1785:ASP:HA	1:G:1788:LYS:HG2	2.00	0.42
2:H:74:LEU:HB2	2:H:99:PHE:HB2	2.01	0.42
1:A:1644:LEU:HD21	1:A:1651:LEU:HA	2.01	0.42
1:A:2124:LEU:HA	1:A:2127:ILE:HG22	2.01	0.42
1:C:2083:ARG:HD3	1:C:3688:LEU:HD22	2.01	0.42
1:C:4597:PRO:HA	1:C:4600:ILE:HG22	2.01	0.42
1:E:650:ASN:HA	1:E:1626:GLN:HA	2.01	0.42
1:E:1644:LEU:HD21	1:E:1651:LEU:HA	2.01	0.42
1:E:1678:SER:HB2	1:E:1768:PHE:CZ	2.54	0.42
1:E:2217:ASP:N	1:E:2217:ASP:OD1	2.50	0.42
1:E:2461:PHE:O	1:E:2465:HIS:NE2	2.51	0.42
1:G:896:ASN:ND2	1:G:1052:GLU:OE2	2.44	0.42
1:G:2116:ASP:OD2	1:G:2154:LYS:N	2.52	0.42
1:G:4022:LEU:HD13	1:G:4025:LYS:HE3	2.01	0.42
1:G:4024:LEU:HD11	1:G:4084:PHE:HE2	1.84	0.42
1:C:176:ARG:N	1:C:179:ASP:OD2	2.46	0.42
1:C:1108:VAL:HG12	1:C:1109:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1644:LEU:HD21	1:C:1651:LEU:HA	2.01	0.42
1:C:2143:MET:HE1	1:C:2193:MET:HG3	2.01	0.42
1:C:2466:LYS:NZ	1:C:2492:GLY:O	2.50	0.42
1:C:2761:TYR:OH	1:C:2773:ARG:NH2	2.44	0.42
2:D:19:GLY:H	2:D:49:ARG:HD2	1.84	0.42
1:E:115:TYR:CG	1:E:164:PRO:HG3	2.53	0.42
1:E:3970:LYS:HA	1:E:3973:MET:HE2	2.01	0.42
1:G:2124:LEU:HA	1:G:2127:ILE:HG22	2.01	0.42
1:A:1678:SER:HB2	1:A:1768:PHE:CZ	2.54	0.42
1:A:3970:LYS:HA	1:A:3973:MET:HE2	2.01	0.42
1:C:1267:HIS:HB3	1:C:1294:ASN:HD21	1.85	0.42
1:C:1576:LYS:HE3	1:C:1587:HIS:CD2	2.54	0.42
1:C:1609:SER:N	1:C:1623:GLU:OE2	2.52	0.42
1:E:2116:ASP:OD2	1:E:2154:LYS:N	2.52	0.42
1:E:4597:PRO:HA	1:E:4600:ILE:HG22	2.01	0.42
2:F:74:LEU:HB2	2:F:99:PHE:HB2	2.01	0.42
1:G:718:VAL:HA	1:G:736:CYS:N	2.33	0.42
1:G:1433:PHE:HD2	1:G:1551:ASN:HB3	1.83	0.42
1:G:1644:LEU:HD21	1:G:1651:LEU:HA	2.01	0.42
1:A:318:ASP:HB3	1:A:319:LYS:H	1.68	0.42
1:A:650:ASN:HA	1:A:1626:GLN:HA	2.01	0.42
1:A:1108:VAL:HG12	1:A:1109:THR:HG23	2.02	0.42
1:A:1433:PHE:HD2	1:A:1551:ASN:HB3	1.83	0.42
1:A:1756:SER:OG	1:A:1920:ARG:NH2	2.50	0.42
1:A:1758:ARG:HD3	1:A:1920:ARG:HH22	1.84	0.42
1:A:2127:ILE:HD12	1:A:2127:ILE:HA	1.92	0.42
1:A:4126:VAL:O	1:A:4130:PHE:N	2.53	0.42
2:B:15:PHE:HA	2:B:16:PRO:HD3	1.85	0.42
1:C:1433:PHE:HD2	1:C:1551:ASN:HB3	1.83	0.42
1:E:718:VAL:HA	1:E:736:CYS:N	2.33	0.42
1:E:4024:LEU:HD11	1:E:4084:PHE:HE2	1.84	0.42
1:G:1678:SER:HB2	1:G:1768:PHE:CZ	2.54	0.42
1:G:2143:MET:HE1	1:G:2193:MET:HG3	2.01	0.42
1:G:2725:TYR:O	1:G:2729:SER:OG	2.37	0.42
1:G:4605:LYS:HG3	1:G:4645:TYR:HE1	1.84	0.42
1:A:590:LYS:H	1:A:593:HIS:CD2	2.29	0.42
1:A:1678:SER:OG	2:B:36:PHE:O	2.31	0.42
1:A:4767:GLN:NE2	1:C:4871:PHE:CZ	2.82	0.42
2:B:74:LEU:HB2	2:B:99:PHE:HB2	2.01	0.42
1:C:50:GLU:OE2	1:C:61:ASP:N	2.50	0.42
1:C:1938:GLN:HE22	1:C:3611:ASN:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2790:ILE:HG12	1:C:2904:VAL:HG22	2.02	0.42
1:E:228:LEU:HD12	1:E:354:ILE:HB	2.02	0.42
1:E:235:ARG:HE	1:E:274:LEU:HD23	1.84	0.42
1:E:4642:PRO:HG2	1:E:4648:LYS:HA	2.00	0.42
2:F:26:TYR:O	2:F:39:SER:OG	2.35	0.42
1:G:228:LEU:HD12	1:G:354:ILE:HB	2.02	0.42
1:A:73:LEU:HB3	1:A:77:ALA:HB3	2.00	0.42
1:A:79:GLN:HA	1:A:82:LEU:HB2	2.02	0.42
1:A:415:THR:HG21	1:A:485:ARG:HG2	2.02	0.42
1:A:1609:SER:N	1:A:1623:GLU:OE2	2.52	0.42
1:A:3990:ASN:HD22	1:A:3994:GLY:HA3	1.85	0.42
1:A:4022:LEU:HD13	1:A:4025:LYS:HE3	2.01	0.42
1:C:235:ARG:HE	1:C:274:LEU:HD23	1.84	0.42
1:C:2217:ASP:OD1	1:C:2217:ASP:N	2.50	0.42
1:C:2717:LYS:H	1:C:2717:LYS:HG2	1.50	0.42
1:C:3777:LYS:HE3	1:C:3777:LYS:HB2	1.84	0.42
1:C:3990:ASN:HD22	1:C:3994:GLY:HA3	1.85	0.42
1:C:4568:TYR:O	1:C:4572:THR:OG1	2.30	0.42
1:E:394:HIS:CD2	1:E:396:GLU:H	2.37	0.42
1:E:415:THR:HG21	1:E:485:ARG:HG2	2.02	0.42
1:E:1576:LYS:HE3	1:E:1587:HIS:CD2	2.54	0.42
1:E:3977:LYS:HE2	1:E:3977:LYS:HB3	1.90	0.42
1:G:394:HIS:CD2	1:G:396:GLU:H	2.37	0.42
1:G:1243:THR:HG21	1:G:1808:ASP:HB3	2.02	0.42
1:G:1256:PRO:O	1:G:1451:HIS:ND1	2.39	0.42
1:G:1758:ARG:HD3	1:G:1920:ARG:HH22	1.84	0.42
1:G:4085:VAL:O	1:G:4089:HIS:CB	2.68	0.42
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.83	0.42
1:A:394:HIS:CD2	1:A:396:GLU:H	2.37	0.42
1:A:4871:PHE:CZ	1:G:4767:GLN:NE2	2.83	0.42
2:B:19:GLY:H	2:B:49:ARG:HD2	1.84	0.42
1:C:4024:LEU:HA	1:C:4027:LEU:HD12	2.00	0.42
1:E:79:GLN:HA	1:E:82:LEU:HB2	2.02	0.42
1:E:801:ARG:HH21	1:E:1616:GLY:HA2	1.85	0.42
1:E:2083:ARG:HD3	1:E:3688:LEU:HD22	2.01	0.42
1:E:3990:ASN:HD22	1:E:3994:GLY:HA3	1.85	0.42
1:G:864:PRO:HB3	1:G:1034:PRO:HB3	2.01	0.42
1:G:4024:LEU:HA	1:G:4027:LEU:HD12	2.00	0.42
1:A:2293:PRO:HB2	1:A:2294:VAL:H	1.60	0.42
1:A:4085:VAL:O	1:A:4089:HIS:CB	2.68	0.42
2:B:23:VAL:HG12	2:B:104:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:HIS:CD2	1:C:396:GLU:H	2.37	0.42
1:C:2876:ASP:OD1	1:C:2876:ASP:N	2.48	0.42
1:C:4085:VAL:O	1:C:4089:HIS:CB	2.68	0.42
1:C:4737:ASN:OD1	1:C:4737:ASN:N	2.50	0.42
2:D:74:LEU:HB2	2:D:99:PHE:HB2	2.01	0.42
1:E:1108:VAL:HG12	1:E:1109:THR:HG23	2.02	0.42
1:E:4024:LEU:HA	1:E:4027:LEU:HD12	2.00	0.42
1:G:235:ARG:HE	1:G:274:LEU:HD23	1.84	0.42
1:G:650:ASN:H	1:G:689:GLU:CD	2.28	0.42
1:G:650:ASN:HA	1:G:1626:GLN:HA	2.02	0.42
1:G:4126:VAL:O	1:G:4130:PHE:N	2.53	0.42
1:A:551:PHE:HD1	1:A:551:PHE:HA	1.67	0.42
1:A:1576:LYS:HE3	1:A:1587:HIS:CD2	2.54	0.42
1:C:4095:ILE:HD13	1:C:4095:ILE:HG21	1.81	0.42
1:C:4605:LYS:HG3	1:C:4645:TYR:HE1	1.84	0.42
1:E:50:GLU:OE2	1:E:61:ASP:N	2.50	0.42
1:E:318:ASP:HB3	1:E:319:LYS:H	1.68	0.42
1:E:4022:LEU:HD13	1:E:4025:LYS:HE3	2.01	0.42
1:A:228:LEU:HD12	1:A:354:ILE:HB	2.02	0.41
1:A:235:ARG:HE	1:A:274:LEU:HD23	1.84	0.41
1:A:864:PRO:HB3	1:A:1034:PRO:HB3	2.01	0.41
1:C:1165:MET:HB3	1:C:1236:TYR:CZ	2.55	0.41
1:C:3729:GLN:HE22	1:C:3769:GLY:H	1.68	0.41
1:C:4655:MET:HB2	1:C:4670:LEU:HD13	2.02	0.41
1:E:614:LEU:HD12	1:E:614:LEU:HA	1.92	0.41
1:E:1165:MET:HB3	1:E:1236:TYR:CZ	2.55	0.41
1:E:4126:VAL:O	1:E:4130:PHE:N	2.53	0.41
1:G:682:THR:HG21	1:G:750:ARG:HA	2.02	0.41
1:G:3916:GLN:O	1:G:3920:THR:HG23	2.20	0.41
1:A:2143:MET:HE1	1:A:2193:MET:HG3	2.01	0.41
1:C:79:GLN:HA	1:C:82:LEU:HB2	2.02	0.41
1:C:4126:VAL:O	1:C:4130:PHE:N	2.53	0.41
1:C:4499:ASN:HD21	1:C:4502:ASN:HD22	1.69	0.41
1:E:2315:GLU:OE2	1:E:3814:LYS:NZ	2.44	0.41
1:E:2860:GLU:O	1:E:2864:LYS:NZ	2.42	0.41
1:E:4655:MET:HB2	1:E:4670:LEU:HD13	2.02	0.41
1:G:661:LEU:O	1:G:788:PHE:N	2.39	0.41
1:A:50:GLU:OE2	1:A:61:ASP:N	2.50	0.41
1:A:544:ASN:HD22	1:A:547:ASN:ND2	2.18	0.41
1:A:650:ASN:H	1:A:689:GLU:CD	2.28	0.41
1:A:682:THR:HG21	1:A:750:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:HIS:HB3	1:A:1294:ASN:HD21	1.85	0.41
1:A:2790:ILE:HG12	1:A:2904:VAL:HG22	2.02	0.41
1:A:3729:GLN:HE22	1:A:3769:GLY:H	1.68	0.41
1:A:4186:LYS:HE2	1:A:4186:LYS:HB3	1.84	0.41
1:A:4189:LEU:HA	1:A:4192:ASN:HD22	1.86	0.41
1:C:801:ARG:HH21	1:C:1616:GLY:HA2	1.85	0.41
1:E:590:LYS:H	1:E:593:HIS:CD2	2.29	0.41
1:E:1267:HIS:HB3	1:E:1294:ASN:HD21	1.85	0.41
1:G:79:GLN:HA	1:G:82:LEU:HB2	2.02	0.41
1:G:2083:ARG:HD3	1:G:3688:LEU:HD22	2.01	0.41
1:G:3800:SER:OG	1:G:3801:CYS:N	2.48	0.41
1:G:3983:LEU:HD23	1:G:4102:LEU:HD11	2.00	0.41
1:G:4929:LYS:NZ	1:G:4938:GLU:OE2	2.47	0.41
1:A:2725:TYR:O	1:A:2729:SER:OG	2.37	0.41
1:A:4655:MET:HB2	1:A:4670:LEU:HD13	2.02	0.41
1:A:4791:ARG:HD3	1:C:4559:HIS:HE1	1.86	0.41
1:C:228:LEU:HD12	1:C:354:ILE:HB	2.02	0.41
1:C:2116:ASP:OD2	1:C:2154:LYS:N	2.52	0.41
1:C:3970:LYS:HA	1:C:3973:MET:HE2	2.01	0.41
1:C:3983:LEU:HD23	1:C:4102:LEU:HD11	2.00	0.41
1:E:544:ASN:HD22	1:E:547:ASN:ND2	2.18	0.41
1:E:650:ASN:H	1:E:689:GLU:CD	2.28	0.41
1:E:4085:VAL:O	1:E:4089:HIS:CB	2.68	0.41
1:G:415:THR:HG21	1:G:485:ARG:HG2	2.02	0.41
1:A:889:ILE:HA	1:A:1056:THR:HG21	2.03	0.41
1:A:4024:LEU:HD11	1:A:4084:PHE:HE2	1.84	0.41
1:A:4170:LYS:HE2	1:A:4170:LYS:HB3	1.93	0.41
1:A:4605:LYS:HG3	1:A:4645:TYR:HE1	1.84	0.41
1:A:4793:PHE:HD1	1:A:4833:GLU:HB3	1.86	0.41
1:C:4024:LEU:HD11	1:C:4084:PHE:HE2	1.84	0.41
1:E:228:LEU:HD21	1:E:405:LEU:HD13	2.03	0.41
1:E:2790:ILE:HG12	1:E:2904:VAL:HG22	2.02	0.41
1:E:3916:GLN:O	1:E:3920:THR:HG23	2.20	0.41
1:E:4605:LYS:HG3	1:E:4645:TYR:HE1	1.84	0.41
1:E:4665:ASP:OD1	1:E:4665:ASP:N	2.52	0.41
1:G:2717:LYS:H	1:G:2717:LYS:HG2	1.50	0.41
1:G:3777:LYS:HB2	1:G:3777:LYS:HE3	1.84	0.41
1:G:4189:LEU:HA	1:G:4192:ASN:HD22	1.86	0.41
1:G:4499:ASN:HD21	1:G:4502:ASN:HD22	1.68	0.41
1:G:4655:MET:HB2	1:G:4670:LEU:HD13	2.02	0.41
1:A:1243:THR:HG21	1:A:1808:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2217:ASP:OD1	1:A:2217:ASP:N	2.50	0.41
1:C:4189:LEU:HA	1:C:4192:ASN:HD22	1.86	0.41
1:E:2201:LEU:HD23	1:E:2201:LEU:HA	1.91	0.41
1:E:3831:LEU:HA	1:E:3832:GLN:HA	1.85	0.41
1:E:3926:GLN:HE21	1:E:4935:THR:HA	1.85	0.41
1:E:4080:ASP:HB2	1:E:4083:GLU:HB2	2.03	0.41
1:E:4499:ASN:HD21	1:E:4502:ASN:HD22	1.69	0.41
1:G:889:ILE:HA	1:G:1056:THR:HG21	2.03	0.41
1:G:2790:ILE:HG12	1:G:2904:VAL:HG22	2.02	0.41
1:A:1165:MET:HB3	1:A:1236:TYR:CZ	2.55	0.41
1:A:4559:HIS:HE1	1:G:4791:ARG:HD3	1.86	0.41
1:C:318:ASP:HB3	1:C:319:LYS:H	1.68	0.41
1:C:415:THR:HG21	1:C:485:ARG:HG2	2.02	0.41
1:C:4022:LEU:HD13	1:C:4025:LYS:HE3	2.01	0.41
1:E:1705:LEU:HA	1:E:1705:LEU:HD23	1.89	0.41
1:E:2761:TYR:OH	1:E:2773:ARG:NH2	2.44	0.41
1:G:544:ASN:HD22	1:G:547:ASN:ND2	2.18	0.41
1:G:1106:GLU:HB3	1:G:1214:ARG:HD2	2.03	0.41
1:G:4080:ASP:HB2	1:G:4083:GLU:HB2	2.03	0.41
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	2.03	0.41
1:A:4499:ASN:HD21	1:A:4502:ASN:HD22	1.69	0.41
1:A:4794:TYR:HB2	1:A:4807:CYS:HB2	2.03	0.41
1:C:1106:GLU:HB3	1:C:1214:ARG:HD2	2.03	0.41
1:C:3916:GLN:O	1:C:3920:THR:HG23	2.20	0.41
1:E:1243:THR:HG21	1:E:1808:ASP:HB3	2.02	0.41
1:E:4189:LEU:HA	1:E:4192:ASN:HD22	1.86	0.41
1:E:4637:ASN:ND2	1:E:4669:GLU:OE1	2.50	0.41
1:G:801:ARG:HH21	1:G:1616:GLY:HA2	1.85	0.41
1:G:1165:MET:HB3	1:G:1236:TYR:CZ	2.55	0.41
1:A:443:SER:HA	1:A:444:THR:HA	1.56	0.41
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.93	0.41
1:A:1106:GLU:HB3	1:A:1214:ARG:HD2	2.03	0.41
1:A:3916:GLN:O	1:A:3920:THR:HG23	2.21	0.41
1:C:544:ASN:HD22	1:C:547:ASN:ND2	2.18	0.41
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	2.03	0.41
1:C:3926:GLN:HE21	1:C:4935:THR:HA	1.86	0.41
1:E:1106:GLU:HB3	1:E:1214:ARG:HD2	2.03	0.41
1:E:4929:LYS:NZ	1:E:4938:GLU:OE2	2.47	0.41
1:G:1470:GLY:HA2	1:G:1474:GLY:HA2	2.03	0.41
1:A:801:ARG:HH21	1:A:1616:GLY:HA2	1.85	0.41
1:A:4637:ASN:ND2	1:A:4669:GLU:OE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4737:ASN:OD1	1:A:4737:ASN:N	2.50	0.41
1:C:731:HIS:CE1	1:C:738:ALA:HB1	2.56	0.41
1:E:2464:ASP:OD1	1:E:2464:ASP:N	2.51	0.41
1:E:3732:LEU:HD23	1:E:3732:LEU:HA	1.85	0.41
1:G:375:GLN:HE21	1:G:392:ILE:HD13	1.86	0.41
1:G:731:HIS:CE1	1:G:738:ALA:HB1	2.56	0.41
1:G:929:ARG:O	1:G:933:LEU:N	2.44	0.41
1:G:1108:VAL:HG12	1:G:1109:THR:HG23	2.02	0.41
1:G:1267:HIS:HB3	1:G:1294:ASN:HD21	1.85	0.41
1:G:4136:ARG:HH11	1:G:4136:ARG:HD3	1.76	0.41
1:A:228:LEU:HD21	1:A:405:LEU:HD13	2.03	0.40
1:A:375:GLN:HE21	1:A:392:ILE:HD13	1.86	0.40
1:A:731:HIS:CE1	1:A:738:ALA:HB1	2.56	0.40
1:A:2315:GLU:OE2	1:A:3814:LYS:NZ	2.44	0.40
2:B:25:HIS:HB3	2:B:40:ARG:NE	2.36	0.40
1:C:108:GLY:HA3	1:C:109:GLY:HA3	1.67	0.40
1:C:4637:ASN:ND2	1:C:4669:GLU:OE1	2.50	0.40
1:C:4791:ARG:HD3	1:E:4559:HIS:HE1	1.86	0.40
1:E:1831:MET:HE2	1:E:1831:MET:HB3	1.98	0.40
1:E:4000:MET:HE3	1:E:4000:MET:HB2	1.89	0.40
1:A:371:TRP:N	1:A:394:HIS:O	2.53	0.40
1:C:682:THR:HG21	1:C:750:ARG:HA	2.02	0.40
1:C:2463:PRO:HB2	1:C:2519:ARG:HD2	2.03	0.40
1:C:4665:ASP:OD1	1:C:4665:ASP:N	2.52	0.40
1:G:3729:GLN:HE22	1:G:3769:GLY:H	1.68	0.40
1:G:3761:LYS:NZ	1:G:3835:GLU:OE2	2.37	0.40
1:G:3970:LYS:HB2	1:G:3970:LYS:HE2	1.90	0.40
1:A:1611:ILE:O	1:A:1620:GLN:N	2.55	0.40
1:A:1937:LEU:HD13	1:A:1937:LEU:HA	1.96	0.40
1:C:1678:SER:OG	2:D:36:PHE:O	2.31	0.40
1:C:4793:PHE:HD1	1:C:4833:GLU:HB3	1.86	0.40
1:C:4923:LEU:HD12	1:C:4923:LEU:HA	1.92	0.40
1:E:2463:PRO:HB2	1:E:2519:ARG:HD2	2.03	0.40
1:E:3729:GLN:HE22	1:E:3769:GLY:H	1.68	0.40
1:E:4071:ALA:HB1	1:E:4079:LEU:HD22	2.03	0.40
1:E:4093:LYS:HE2	1:E:4093:LYS:HB3	1.87	0.40
1:A:4000:MET:HE3	1:A:4000:MET:HB2	1.89	0.40
1:C:375:GLN:HE21	1:C:392:ILE:HD13	1.86	0.40
1:C:1243:THR:HG21	1:C:1808:ASP:HB3	2.02	0.40
1:E:681:HIS:HD2	1:E:799:LYS:HD3	1.87	0.40
1:E:2127:ILE:HD12	1:E:2127:ILE:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:99:PHE:HB3	2:F:101:VAL:HG23	2.04	0.40
1:G:228:LEU:HD21	1:G:405:LEU:HD13	2.03	0.40
1:G:3903:GLY:O	1:G:3907:PHE:HB2	2.21	0.40
1:G:3990:ASN:HD22	1:G:3994:GLY:HA3	1.85	0.40
1:G:4793:PHE:HD1	1:G:4833:GLU:HB3	1.86	0.40
1:A:565:LEU:HA	1:A:604:HIS:CE1	2.57	0.40
1:A:1518:LEU:HD23	1:A:1518:LEU:HA	1.87	0.40
1:C:3983:LEU:HD12	1:C:3983:LEU:HA	1.95	0.40
1:C:4080:ASP:HB2	1:C:4083:GLU:HB2	2.03	0.40
1:E:1470:GLY:HA2	1:E:1474:GLY:HA2	2.03	0.40
1:G:170:SER:OG	1:G:171:GLU:N	2.50	0.40
1:G:1104:GLU:OE2	1:G:1216:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	36	71
1	C	3356/4968 (68%)	2915 (87%)	432 (13%)	9 (0%)	36	71
1	E	3356/4968 (68%)	2910 (87%)	437 (13%)	9 (0%)	36	71
1	G	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	36	71
2	B	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13844/20304 (68%)	12025 (87%)	1783 (13%)	36 (0%)	37	71

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4595	LYS
1	A	4645	TYR
1	C	4595	LYS
1	C	4645	TYR
1	E	4595	LYS
1	E	4645	TYR
1	G	4595	LYS
1	G	4645	TYR
1	A	102	MET
1	A	143	LEU
1	A	2233	PRO
1	C	102	MET
1	C	143	LEU
1	C	2233	PRO
1	E	102	MET
1	E	143	LEU
1	E	2233	PRO
1	G	102	MET
1	G	143	LEU
1	G	2233	PRO
1	A	730	LEU
1	A	853	PRO
1	C	730	LEU
1	C	853	PRO
1	E	730	LEU
1	E	853	PRO
1	G	730	LEU
1	G	853	PRO
1	A	1848	PRO
1	A	3803	VAL
1	C	1848	PRO
1	C	3803	VAL
1	E	1848	PRO
1	E	3803	VAL
1	G	1848	PRO
1	G	3803	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	2681/4355 (62%)	2654 (99%)	27 (1%)	68	75
1	C	2680/4355 (62%)	2656 (99%)	24 (1%)	70	75
1	E	2682/4355 (62%)	2656 (99%)	26 (1%)	68	75
1	G	2681/4355 (62%)	2655 (99%)	26 (1%)	68	75
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	11076/17776 (62%)	10973 (99%)	103 (1%)	68	75

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	VAL
1	A	541	ILE
1	A	551	PHE
1	A	625	VAL
1	A	791	VAL
1	A	854	THR
1	A	907	VAL
1	A	925	PRO
1	A	950	VAL
1	A	989	THR
1	A	990	PRO
1	A	1042	THR
1	A	1304	LEU
1	A	1619	VAL
1	A	1632	ILE
1	A	1738	LEU
1	A	1771	ILE
1	A	2118	ILE
1	A	2324	LEU
1	A	3726	LEU
1	A	3847	LEU
1	A	3893	TYR
1	A	4185	GLU
1	A	4521	TYR
1	A	4807	CYS

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Mol	Chain	Res	Type
1	A	4811	LEU
1	A	4813	CYS
1	C	445	VAL
1	C	541	ILE
1	C	551	PHE
1	C	625	VAL
1	C	791	VAL
1	C	854	THR
1	C	925	PRO
1	C	989	THR
1	C	990	PRO
1	C	1042	THR
1	C	1304	LEU
1	C	1619	VAL
1	C	1632	ILE
1	C	1738	LEU
1	C	1771	ILE
1	C	2118	ILE
1	C	2324	LEU
1	C	3726	LEU
1	C	3847	LEU
1	C	3893	TYR
1	C	4185	GLU
1	C	4521	TYR
1	C	4807	CYS
1	C	4811	LEU
1	E	445	VAL
1	E	541	ILE
1	E	551	PHE
1	E	625	VAL
1	E	791	VAL
1	E	854	THR
1	E	907	VAL
1	E	925	PRO
1	E	950	VAL
1	E	989	THR
1	E	990	PRO
1	E	1042	THR
1	E	1304	LEU
1	E	1619	VAL
1	E	1632	ILE
1	E	1738	LEU

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Mol	Chain	Res	Type
1	E	1771	ILE
1	E	2118	ILE
1	E	2324	LEU
1	E	3726	LEU
1	E	3847	LEU
1	E	3893	TYR
1	E	4185	GLU
1	E	4521	TYR
1	E	4807	CYS
1	E	4811	LEU
1	G	445	VAL
1	G	541	ILE
1	G	551	PHE
1	G	625	VAL
1	G	791	VAL
1	G	854	THR
1	G	907	VAL
1	G	925	PRO
1	G	950	VAL
1	G	989	THR
1	G	990	PRO
1	G	1042	THR
1	G	1304	LEU
1	G	1619	VAL
1	G	1632	ILE
1	G	1738	LEU
1	G	1771	ILE
1	G	2118	ILE
1	G	2324	LEU
1	G	3726	LEU
1	G	3847	LEU
1	G	3893	TYR
1	G	4185	GLU
1	G	4521	TYR
1	G	4807	CYS
1	G	4811	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (251) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	84	ASN
1	A	123	HIS
1	A	252	HIS
1	A	261	HIS
1	A	293	GLN
1	A	375	GLN
1	A	394	HIS
1	A	477	ASN
1	A	487	ASN
1	A	547	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	629	GLN
1	A	658	ASN
1	A	681	HIS
1	A	746	GLN
1	A	747	HIS
1	A	888	ASN
1	A	915	HIS
1	A	1233	GLN
1	A	1242	ASN
1	A	1554	GLN
1	A	1587	HIS
1	A	1620	GLN
1	A	1656	HIS
1	A	1669	ASN
1	A	1670	HIS
1	A	1684	GLN
1	A	1722	ASN
1	A	1844	GLN
1	A	1918	GLN
1	A	1921	HIS
1	A	1938	GLN
1	A	1940	ASN
1	A	2119	ASN
1	A	2317	ASN
1	A	2755	GLN
1	A	2839	HIS
1	A	3611	ASN
1	A	3666	HIS

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Mol	Chain	Res	Type
1	A	3813	ASN
1	A	3851	HIS
1	A	3870	ASN
1	A	3906	ASN
1	A	3916	GLN
1	A	3956	GLN
1	A	3961	GLN
1	A	3990	ASN
1	A	3993	ASN
1	A	4058	HIS
1	A	4117	GLN
1	A	4131	GLN
1	A	4499	ASN
1	A	4559	HIS
1	A	4639	GLN
1	A	4764	ASN
1	A	4864	GLN
1	A	4914	HIS
1	A	4962	GLN
2	B	25	HIS
2	B	31	GLN
1	C	12	GLN
1	C	84	ASN
1	C	123	HIS
1	C	252	HIS
1	C	261	HIS
1	C	375	GLN
1	C	394	HIS
1	C	477	ASN
1	C	547	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	629	GLN
1	C	658	ASN
1	C	681	HIS
1	C	746	GLN
1	C	747	HIS
1	C	888	ASN
1	C	915	HIS
1	C	1242	ASN
1	C	1554	GLN

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Mol	Chain	Res	Type
1	C	1587	HIS
1	C	1620	GLN
1	C	1656	HIS
1	C	1669	ASN
1	C	1670	HIS
1	C	1684	GLN
1	C	1722	ASN
1	C	1844	GLN
1	C	1918	GLN
1	C	1921	HIS
1	C	1938	GLN
1	C	1940	ASN
1	C	2317	ASN
1	C	2755	GLN
1	C	2839	HIS
1	C	3611	ASN
1	C	3666	HIS
1	C	3813	ASN
1	C	3851	HIS
1	C	3870	ASN
1	C	3906	ASN
1	C	3916	GLN
1	C	3956	GLN
1	C	3961	GLN
1	C	3990	ASN
1	C	3993	ASN
1	C	4058	HIS
1	C	4117	GLN
1	C	4131	GLN
1	C	4499	ASN
1	C	4559	HIS
1	C	4639	GLN
1	C	4764	ASN
1	C	4864	GLN
1	C	4914	HIS
1	C	4962	GLN
2	D	25	HIS
1	E	12	GLN
1	E	44	ASN
1	E	71	GLN
1	E	84	ASN
1	E	150	GLN

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Mol	Chain	Res	Type
1	E	252	HIS
1	E	261	HIS
1	E	293	GLN
1	E	364	GLN
1	E	375	GLN
1	E	394	HIS
1	E	477	ASN
1	E	547	ASN
1	E	593	HIS
1	E	604	HIS
1	E	628	ASN
1	E	629	GLN
1	E	658	ASN
1	E	681	HIS
1	E	746	GLN
1	E	747	HIS
1	E	888	ASN
1	E	915	HIS
1	E	1242	ASN
1	E	1554	GLN
1	E	1587	HIS
1	E	1620	GLN
1	E	1656	HIS
1	E	1669	ASN
1	E	1670	HIS
1	E	1684	GLN
1	E	1722	ASN
1	E	1844	GLN
1	E	1918	GLN
1	E	1921	HIS
1	E	1938	GLN
1	E	1940	ASN
1	E	2211	ASN
1	E	2317	ASN
1	E	2755	GLN
1	E	2839	HIS
1	E	3611	ASN
1	E	3666	HIS
1	E	3813	ASN
1	E	3851	HIS
1	E	3870	ASN
1	E	3906	ASN

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Mol	Chain	Res	Type
1	E	3916	GLN
1	E	3956	GLN
1	E	3961	GLN
1	E	3990	ASN
1	E	3993	ASN
1	E	4058	HIS
1	E	4117	GLN
1	E	4131	GLN
1	E	4499	ASN
1	E	4559	HIS
1	E	4621	GLN
1	E	4639	GLN
1	E	4764	ASN
1	E	4864	GLN
1	E	4914	HIS
1	E	4962	GLN
2	F	25	HIS
2	F	31	GLN
1	G	12	GLN
1	G	71	GLN
1	G	84	ASN
1	G	123	HIS
1	G	252	HIS
1	G	261	HIS
1	G	293	GLN
1	G	364	GLN
1	G	375	GLN
1	G	394	HIS
1	G	477	ASN
1	G	547	ASN
1	G	593	HIS
1	G	604	HIS
1	G	628	ASN
1	G	629	GLN
1	G	658	ASN
1	G	681	HIS
1	G	746	GLN
1	G	747	HIS
1	G	888	ASN
1	G	915	HIS
1	G	1233	GLN
1	G	1242	ASN

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Mol	Chain	Res	Type
1	G	1587	HIS
1	G	1620	GLN
1	G	1656	HIS
1	G	1669	ASN
1	G	1670	HIS
1	G	1684	GLN
1	G	1722	ASN
1	G	1844	GLN
1	G	1918	GLN
1	G	1921	HIS
1	G	1938	GLN
1	G	1940	ASN
1	G	2317	ASN
1	G	2755	GLN
1	G	2839	HIS
1	G	3611	ASN
1	G	3666	HIS
1	G	3813	ASN
1	G	3851	HIS
1	G	3870	ASN
1	G	3906	ASN
1	G	3916	GLN
1	G	3956	GLN
1	G	3961	GLN
1	G	3990	ASN
1	G	3993	ASN
1	G	4058	HIS
1	G	4117	GLN
1	G	4131	GLN
1	G	4499	ASN
1	G	4515	ASN
1	G	4559	HIS
1	G	4639	GLN
1	G	4764	ASN
1	G	4864	GLN
1	G	4914	HIS
1	G	4962	GLN
2	H	25	HIS
2	H	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	CFF	E	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)
6	CFF	A	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)
4	ATP	C	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	A	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	E	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
4	ATP	G	5101	-	32,33,33	1.31	4 (12%)	48,52,52	1.84	8 (16%)
6	CFF	C	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)
6	CFF	G	5103	-	15,15,15	2.01	7 (46%)	23,23,23	2.81	10 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	E	5103	-	-	-	0/2/2/2
6	CFF	A	5103	-	-	-	0/2/2/2
4	ATP	C	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	A	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	E	5101	-	-	6/22/38/38	0/3/3/3
4	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5101	ATP	C5-C4	4.27	1.46	1.39
4	C	5101	ATP	C5-C4	4.27	1.46	1.39
4	E	5101	ATP	C5-C4	4.27	1.46	1.39
4	G	5101	ATP	C5-C4	4.27	1.46	1.39
6	G	5103	CFF	C6-N1	-4.22	1.31	1.40
6	A	5103	CFF	C6-N1	-4.18	1.31	1.40
6	C	5103	CFF	C6-N1	-4.18	1.31	1.40
6	E	5103	CFF	C6-N1	-4.18	1.31	1.40
4	A	5101	ATP	C5-N7	-2.95	1.33	1.39
4	C	5101	ATP	C5-N7	-2.95	1.33	1.39
4	E	5101	ATP	C5-N7	-2.95	1.33	1.39
4	G	5101	ATP	C5-N7	-2.95	1.33	1.39
6	A	5103	CFF	C4-N3	-2.67	1.33	1.38
6	C	5103	CFF	C4-N3	-2.67	1.33	1.38
6	E	5103	CFF	C4-N3	-2.67	1.33	1.38
6	G	5103	CFF	C4-N3	-2.67	1.33	1.38
6	C	5103	CFF	C2-N1	-2.42	1.34	1.39
6	A	5103	CFF	C5-N7	-2.40	1.34	1.38
6	C	5103	CFF	C5-N7	-2.40	1.34	1.38
6	E	5103	CFF	C5-N7	-2.40	1.34	1.38
6	G	5103	CFF	C5-N7	-2.40	1.34	1.38
6	A	5103	CFF	C2-N1	-2.38	1.34	1.39
6	E	5103	CFF	C2-N1	-2.38	1.34	1.39
6	G	5103	CFF	C2-N1	-2.35	1.34	1.39
6	A	5103	CFF	O11-C2	-2.25	1.18	1.22
6	C	5103	CFF	O11-C2	-2.25	1.18	1.22
6	E	5103	CFF	O11-C2	-2.25	1.18	1.22
6	G	5103	CFF	O11-C2	-2.25	1.18	1.22
6	C	5103	CFF	O13-C6	-2.20	1.18	1.23
6	E	5103	CFF	O13-C6	-2.20	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	CFF	C2-N3	-2.18	1.34	1.39
6	E	5103	CFF	C2-N3	-2.18	1.34	1.39
6	G	5103	CFF	C2-N3	-2.18	1.34	1.39
6	A	5103	CFF	O13-C6	-2.17	1.18	1.23
6	G	5103	CFF	O13-C6	-2.17	1.18	1.23
6	C	5103	CFF	C2-N3	-2.15	1.34	1.39
4	A	5101	ATP	C5-C6	2.11	1.46	1.41
4	E	5101	ATP	C5-C6	2.11	1.46	1.41
4	G	5101	ATP	C5-C6	2.11	1.46	1.41
4	C	5101	ATP	C5-C6	2.08	1.46	1.41
4	G	5101	ATP	C8-N9	-2.06	1.34	1.37
4	A	5101	ATP	C8-N9	-2.02	1.34	1.37
4	C	5101	ATP	C8-N9	-2.02	1.34	1.37
4	E	5101	ATP	C8-N9	-2.02	1.34	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	CFF	C14-N7-C8	-7.76	111.77	126.28
6	G	5103	CFF	C14-N7-C8	-7.75	111.77	126.28
6	E	5103	CFF	C14-N7-C8	-7.74	111.80	126.28
6	C	5103	CFF	C14-N7-C8	-7.73	111.82	126.28
4	A	5101	ATP	C5-C4-N3	-6.11	118.31	126.72
4	C	5101	ATP	C5-C4-N3	-6.11	118.31	126.72
4	E	5101	ATP	C5-C4-N3	-6.11	118.31	126.72
4	G	5101	ATP	C5-C4-N3	-6.11	118.31	126.72
4	A	5101	ATP	N3-C4-N9	5.18	135.97	127.17
4	C	5101	ATP	N3-C4-N9	5.18	135.97	127.17
4	E	5101	ATP	N3-C4-N9	5.18	135.97	127.17
4	G	5101	ATP	N3-C4-N9	5.18	135.97	127.17
6	E	5103	CFF	C14-N7-C5	5.03	139.74	127.77
6	A	5103	CFF	C14-N7-C5	5.03	139.73	127.77
6	G	5103	CFF	C14-N7-C5	5.03	139.73	127.77
6	C	5103	CFF	C14-N7-C5	5.02	139.71	127.77
6	G	5103	CFF	C5-C6-N1	4.23	119.81	112.06
6	A	5103	CFF	C5-C6-N1	4.22	119.80	112.06
6	C	5103	CFF	C5-C6-N1	4.22	119.80	112.06
6	E	5103	CFF	C5-C6-N1	4.22	119.80	112.06
4	A	5101	ATP	C2-N3-C4	3.63	120.71	111.83
4	C	5101	ATP	C2-N3-C4	3.63	120.71	111.83
4	E	5101	ATP	C2-N3-C4	3.63	120.71	111.83
4	G	5101	ATP	C2-N3-C4	3.63	120.71	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	CFF	C6-N1-C2	-3.53	119.92	125.66
6	E	5103	CFF	C6-N1-C2	-3.53	119.92	125.66
6	G	5103	CFF	C6-N1-C2	-3.53	119.93	125.66
6	C	5103	CFF	C6-N1-C2	-3.52	119.93	125.66
6	G	5103	CFF	N7-C8-N9	-3.26	107.57	113.48
6	A	5103	CFF	N7-C8-N9	-3.25	107.59	113.48
6	A	5103	CFF	N3-C4-N9	3.25	131.37	126.27
6	C	5103	CFF	N3-C4-N9	3.25	131.37	126.27
6	G	5103	CFF	N3-C4-N9	3.25	131.37	126.27
6	C	5103	CFF	N7-C8-N9	-3.23	107.62	113.48
6	E	5103	CFF	N7-C8-N9	-3.23	107.62	113.48
6	E	5103	CFF	N3-C4-N9	3.23	131.34	126.27
4	A	5101	ATP	N3-C2-N1	-3.08	123.93	128.58
4	C	5101	ATP	N3-C2-N1	-3.07	123.93	128.58
4	E	5101	ATP	N3-C2-N1	-3.07	123.93	128.58
4	G	5101	ATP	N3-C2-N1	-3.07	123.93	128.58
4	A	5101	ATP	O4'-C1'-N9	3.01	113.88	108.09
4	C	5101	ATP	O4'-C1'-N9	3.01	113.88	108.09
4	E	5101	ATP	O4'-C1'-N9	3.01	113.88	108.09
4	G	5101	ATP	O4'-C1'-N9	3.00	113.85	108.09
4	A	5101	ATP	C4-C5-N7	-2.89	107.27	110.58
4	C	5101	ATP	C4-C5-N7	-2.89	107.27	110.58
4	E	5101	ATP	C4-C5-N7	-2.89	107.27	110.58
4	G	5101	ATP	C4-C5-N7	-2.89	107.27	110.58
6	C	5103	CFF	N3-C2-N1	2.81	120.65	117.14
6	A	5103	CFF	N3-C2-N1	2.78	120.61	117.14
6	E	5103	CFF	N3-C2-N1	2.78	120.61	117.14
6	G	5103	CFF	N3-C2-N1	2.76	120.59	117.14
4	G	5101	ATP	C4-N9-C8	2.63	108.50	105.74
6	C	5103	CFF	O13-C6-C5	-2.63	120.99	126.38
6	E	5103	CFF	O13-C6-C5	-2.63	120.99	126.38
6	A	5103	CFF	O13-C6-C5	-2.62	121.01	126.38
6	G	5103	CFF	O13-C6-C5	-2.62	121.01	126.38
4	A	5101	ATP	C4-N9-C8	2.61	108.48	105.74
4	C	5101	ATP	C4-N9-C8	2.61	108.48	105.74
4	E	5101	ATP	C4-N9-C8	2.61	108.48	105.74
6	C	5103	CFF	C6-C5-C4	-2.50	119.76	122.92
6	A	5103	CFF	C6-C5-C4	-2.49	119.78	122.92
6	E	5103	CFF	C6-C5-C4	-2.49	119.78	122.92
6	G	5103	CFF	C6-C5-C4	-2.49	119.78	122.92
4	A	5101	ATP	C5-N7-C8	2.33	107.12	103.45
4	C	5101	ATP	C5-N7-C8	2.33	107.12	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5101	ATP	C5-N7-C8	2.33	107.12	103.45
4	G	5101	ATP	C5-N7-C8	2.32	107.10	103.45
6	G	5103	CFF	C8-N9-C4	2.11	108.05	102.98
6	A	5103	CFF	C8-N9-C4	2.10	108.02	102.98
6	C	5103	CFF	C8-N9-C4	2.10	108.02	102.98
6	E	5103	CFF	C8-N9-C4	2.09	107.98	102.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	O4'-C1'-N9-C8
4	A	5101	ATP	O4'-C1'-N9-C4
4	C	5101	ATP	O4'-C1'-N9-C8
4	C	5101	ATP	O4'-C1'-N9-C4
4	E	5101	ATP	O4'-C1'-N9-C8
4	E	5101	ATP	O4'-C1'-N9-C4
4	G	5101	ATP	O4'-C1'-N9-C8
4	G	5101	ATP	O4'-C1'-N9-C4
4	A	5101	ATP	PB-O3A-PA-O1A
4	A	5101	ATP	PB-O3A-PA-O2A
4	C	5101	ATP	PB-O3A-PA-O1A
4	C	5101	ATP	PB-O3A-PA-O2A
4	E	5101	ATP	PB-O3A-PA-O1A
4	E	5101	ATP	PB-O3A-PA-O2A
4	G	5101	ATP	PB-O3A-PA-O1A
4	G	5101	ATP	PB-O3A-PA-O2A
4	A	5101	ATP	C4'-C5'-O5'-PA
4	E	5101	ATP	C4'-C5'-O5'-PA
4	G	5101	ATP	C4'-C5'-O5'-PA
4	C	5101	ATP	C4'-C5'-O5'-PA
4	A	5101	ATP	O4'-C4'-C5'-O5'
4	C	5101	ATP	O4'-C4'-C5'-O5'
4	E	5101	ATP	O4'-C4'-C5'-O5'
4	G	5101	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

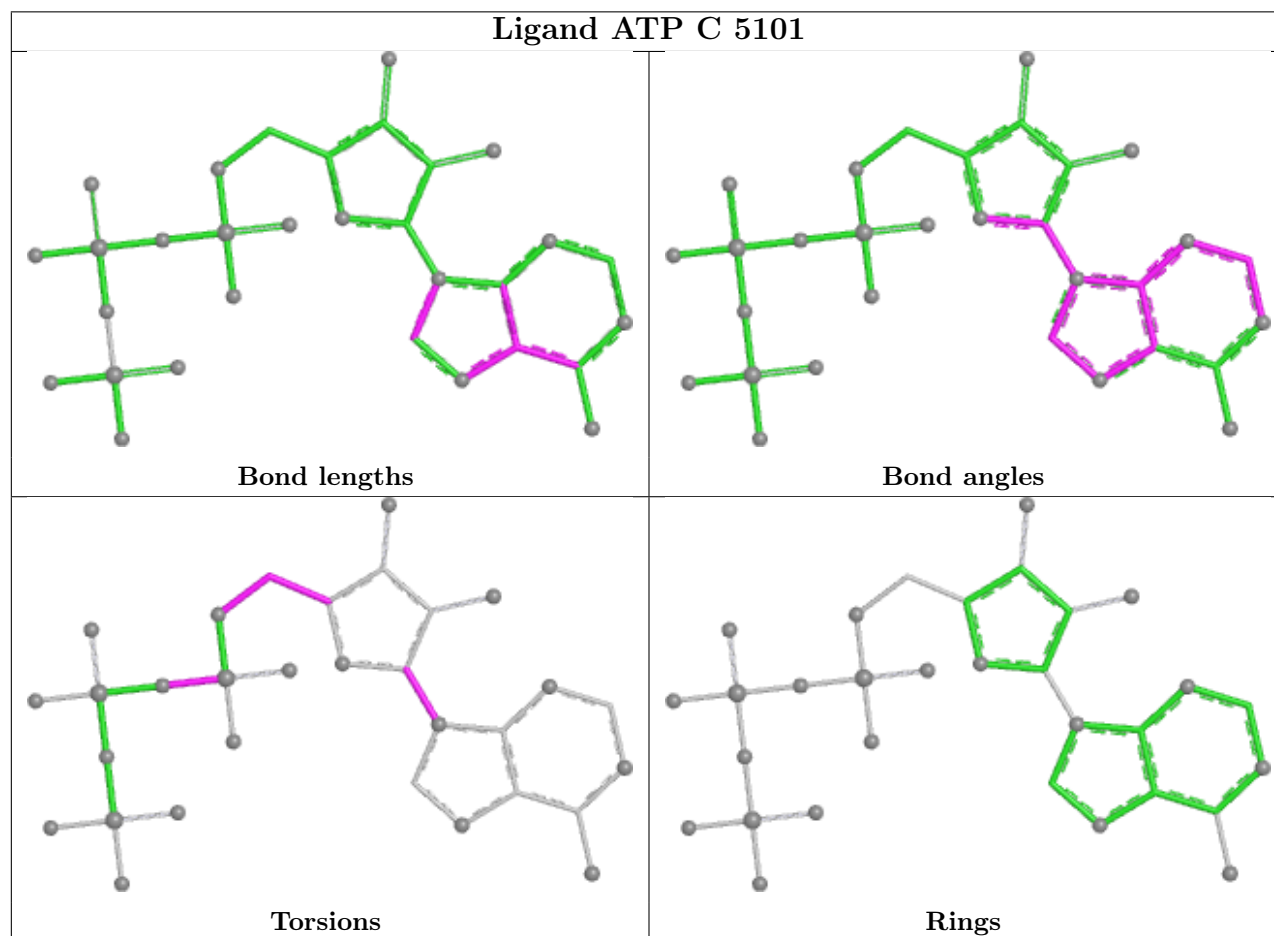
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5101	ATP	1	0

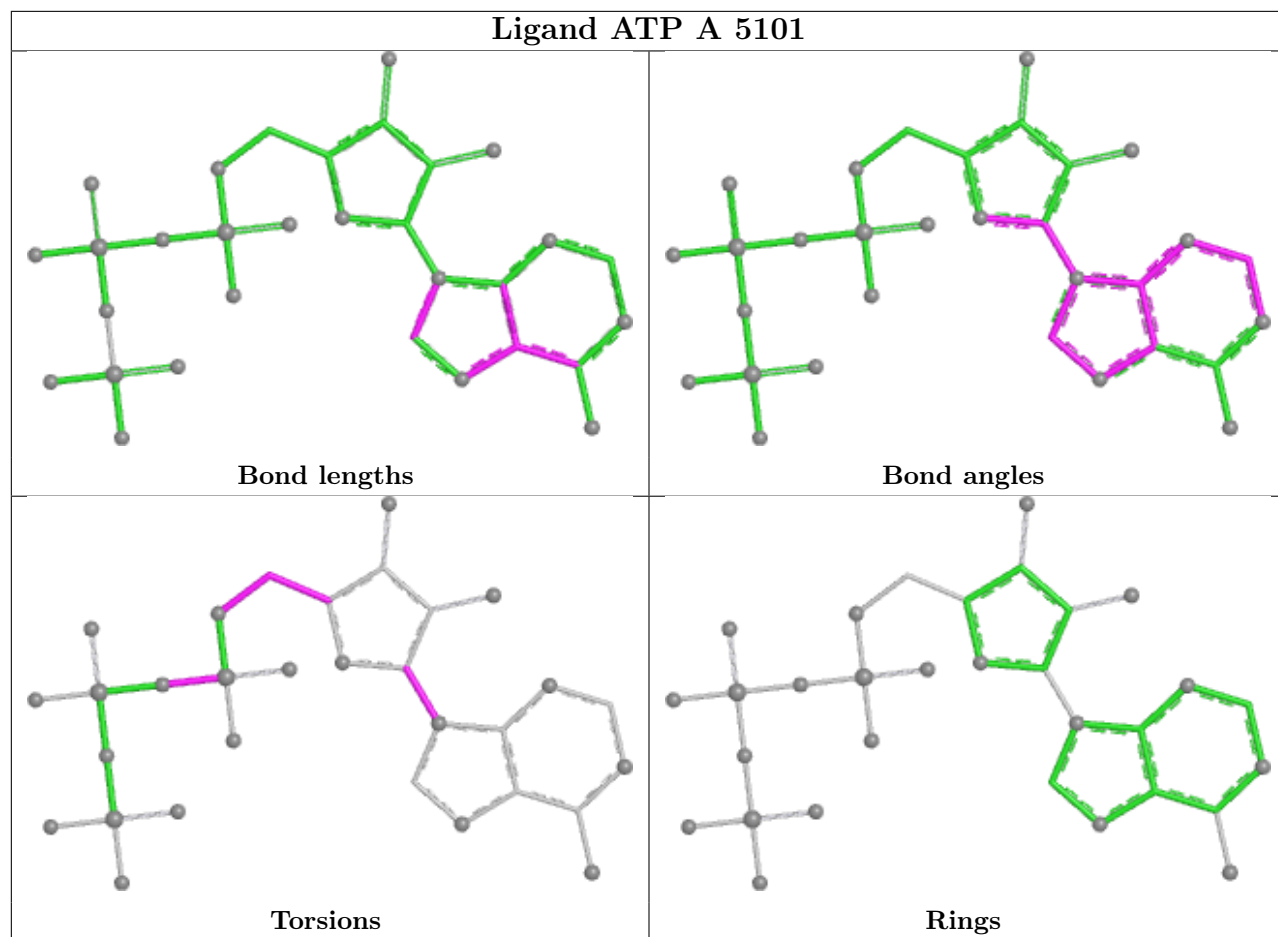
Continued on next page...

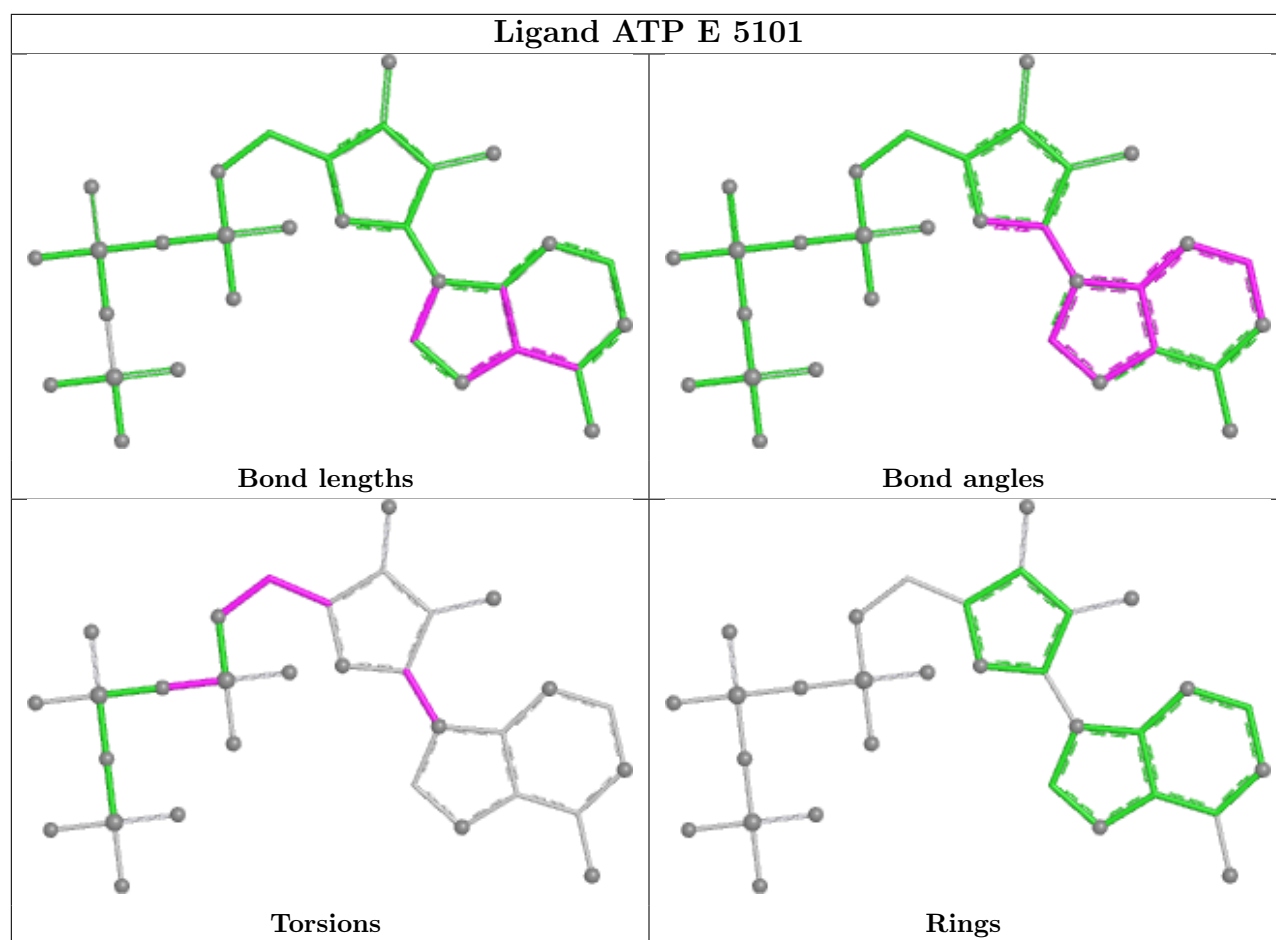
Continued from previous page...

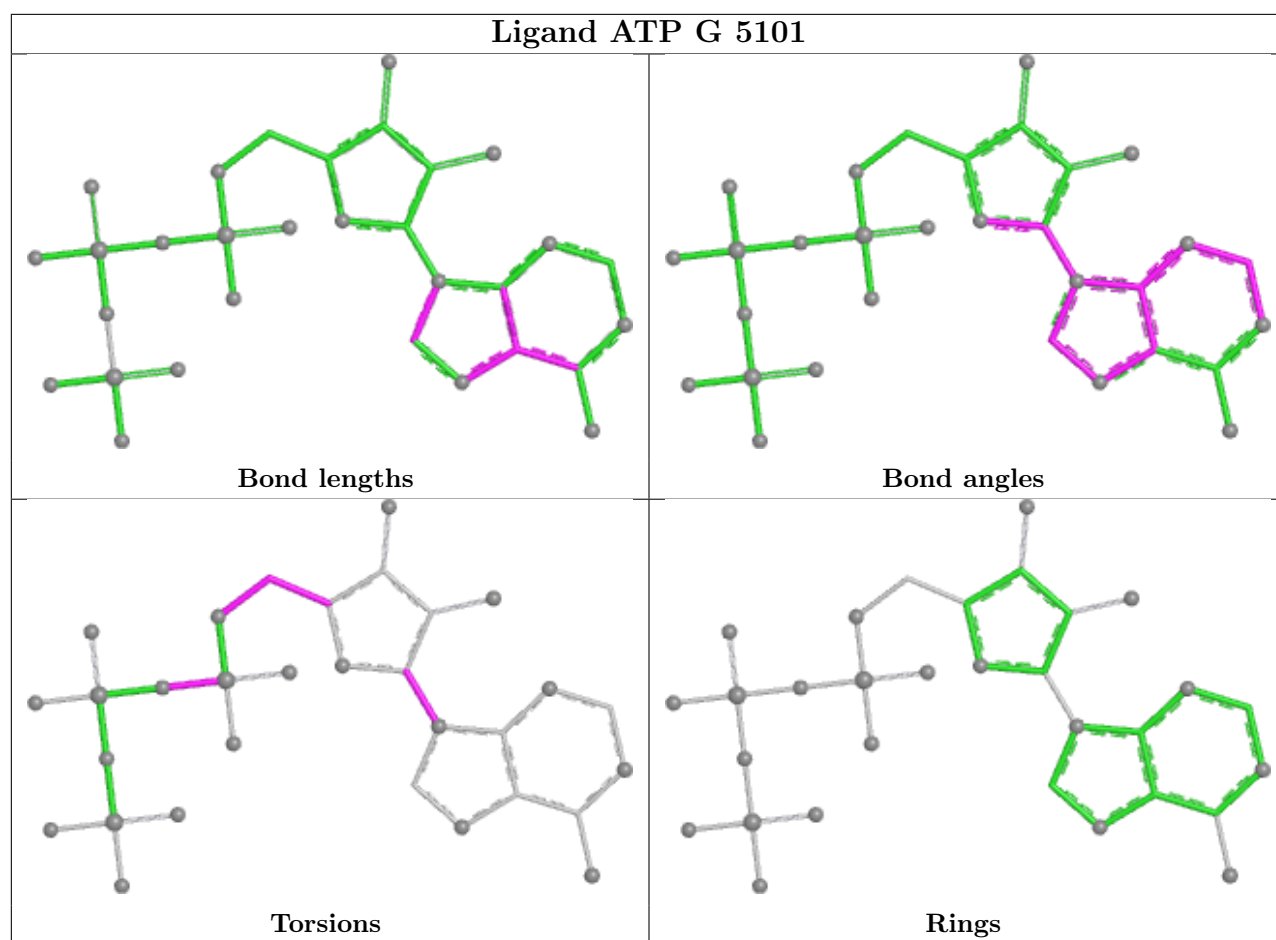
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5101	ATP	2	0
4	E	5101	ATP	1	0
4	G	5101	ATP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

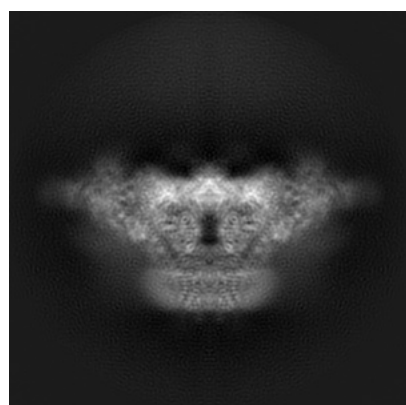
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9831. These allow visual inspection of the internal detail of the map and identification of artifacts.

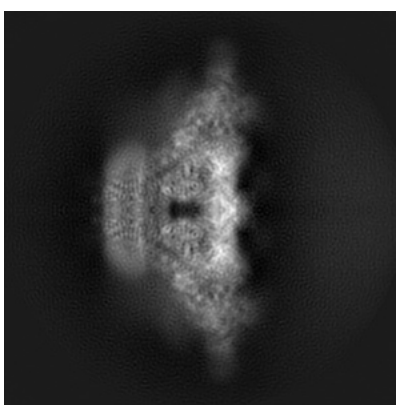
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

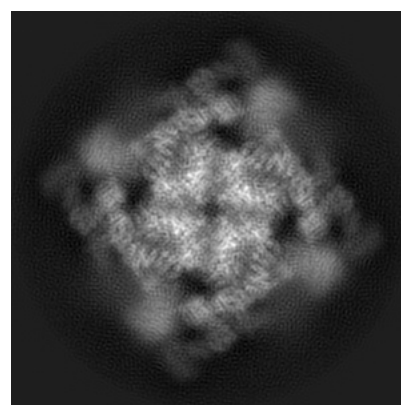
6.1.1 Primary map



X



Y

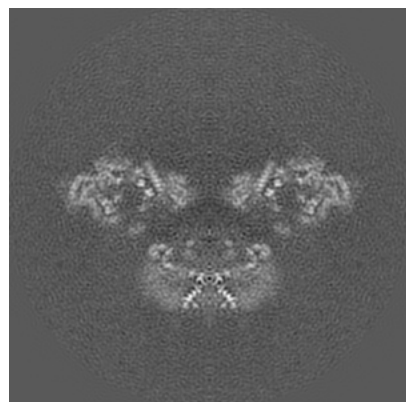


Z

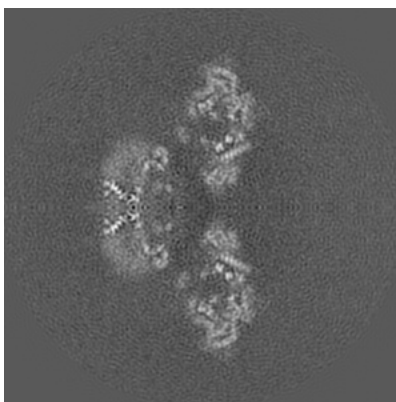
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

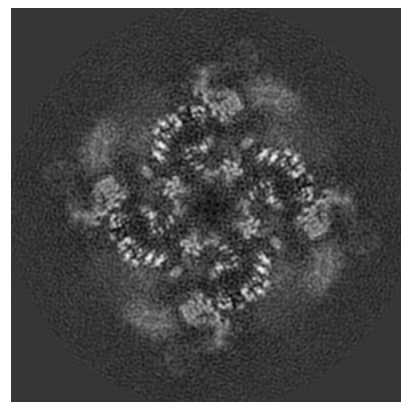
6.2.1 Primary map



X Index: 200



Y Index: 200

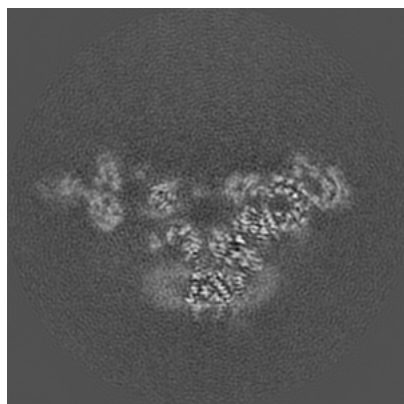


Z Index: 200

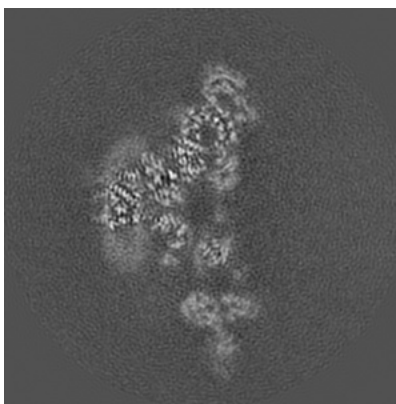
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

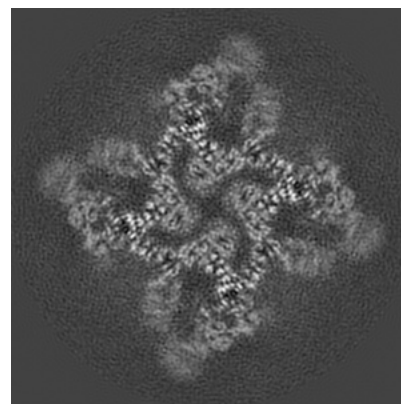
6.3.1 Primary map



X Index: 186



Y Index: 214

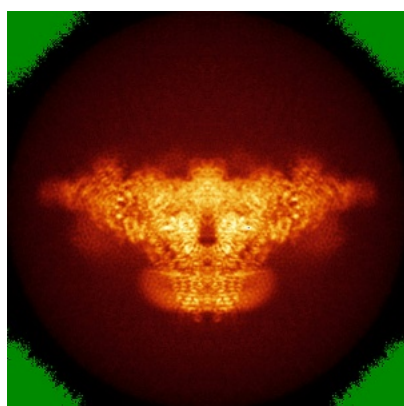


Z Index: 217

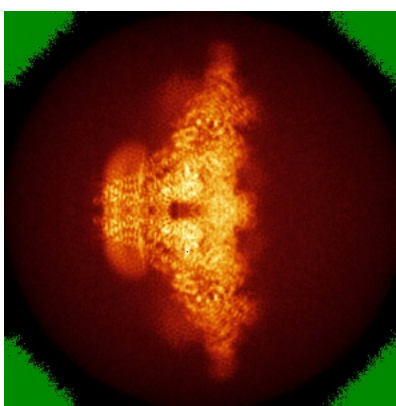
The images above show the largest variance slices of the map in three orthogonal directions.

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

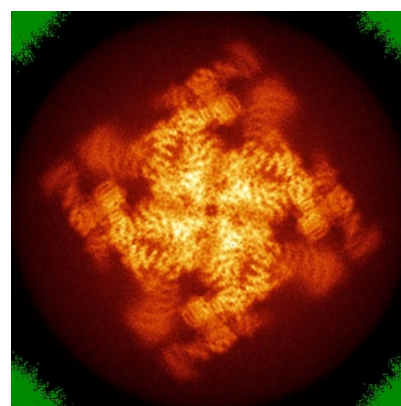
6.4.1 Primary map



X



Y

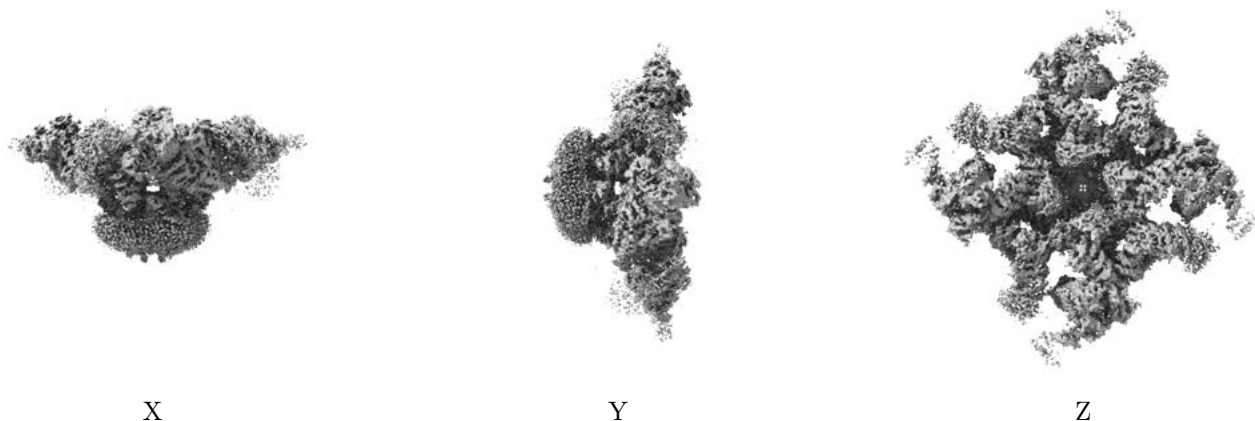


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

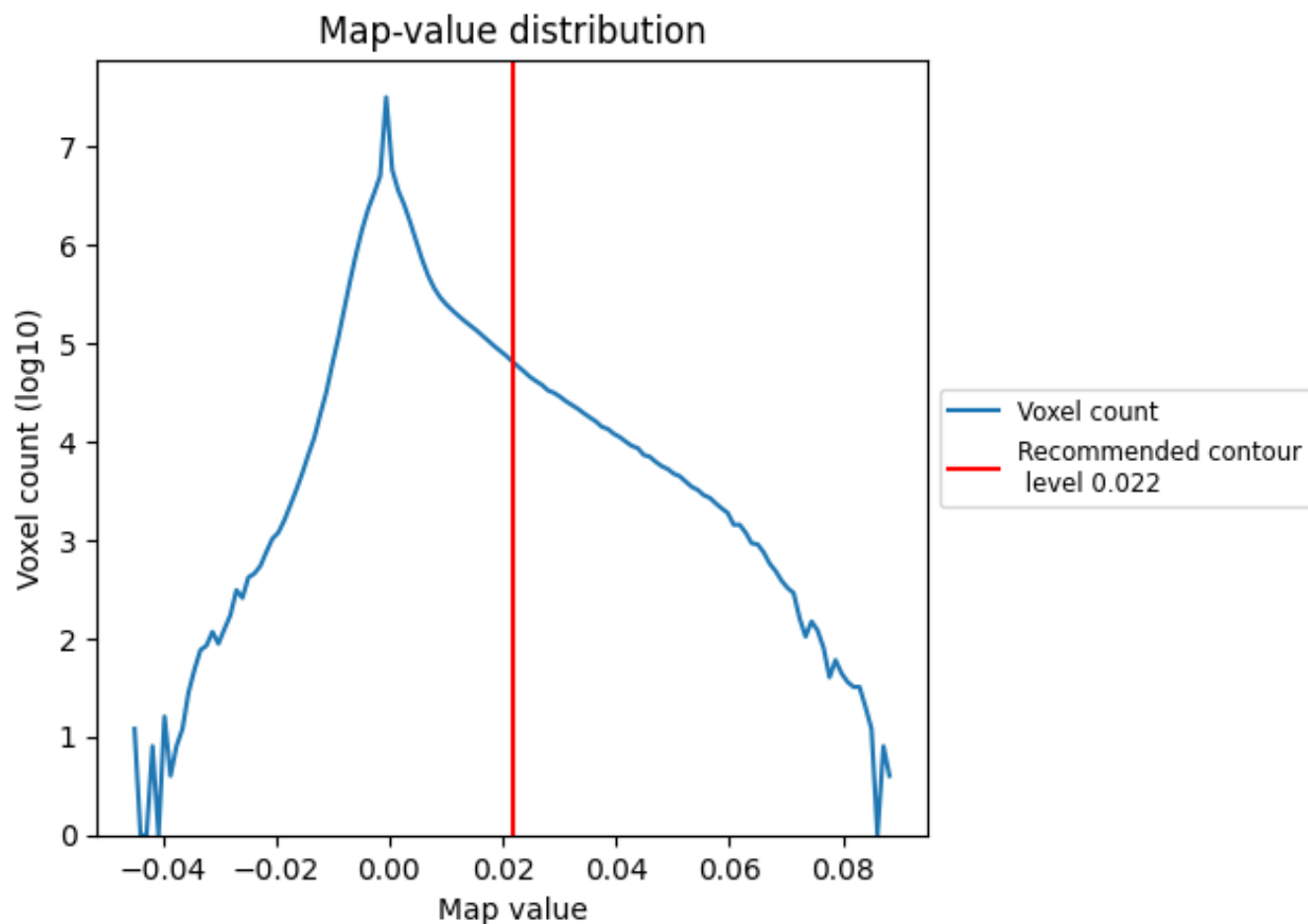
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

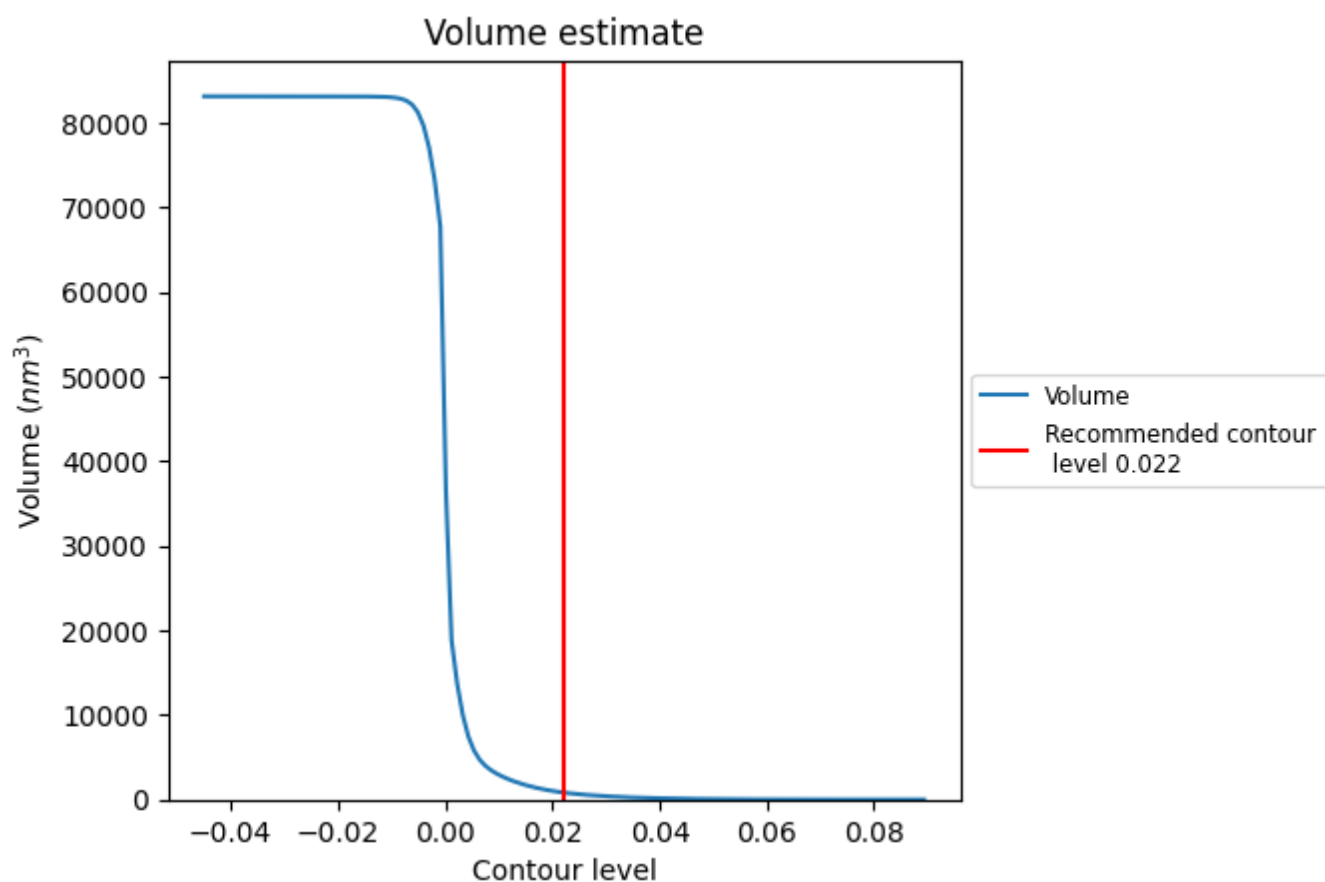
This section contains the results of statistical analysis of the map.

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.

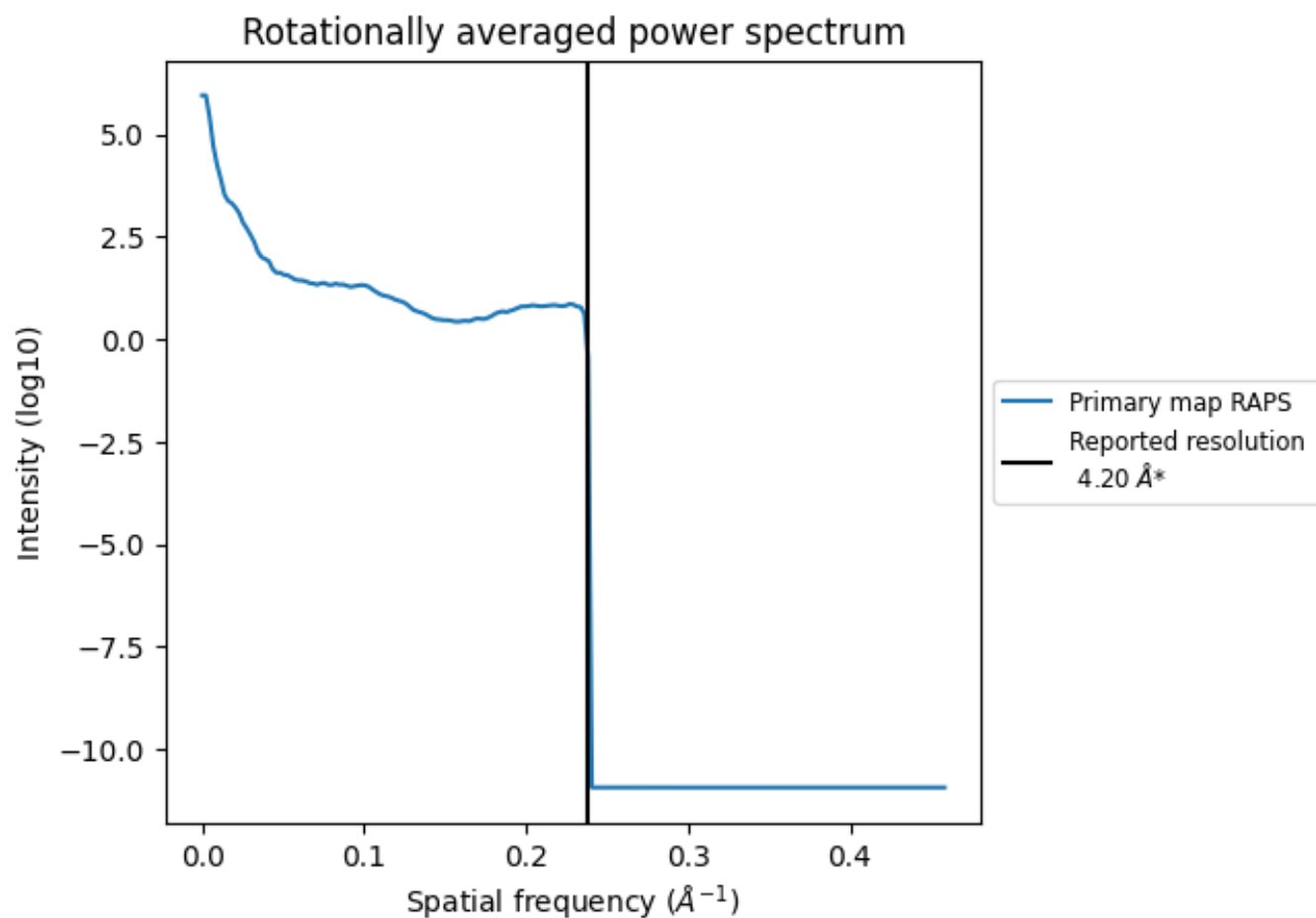
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm³; this corresponds to an approximate mass of 755 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 ⓘ

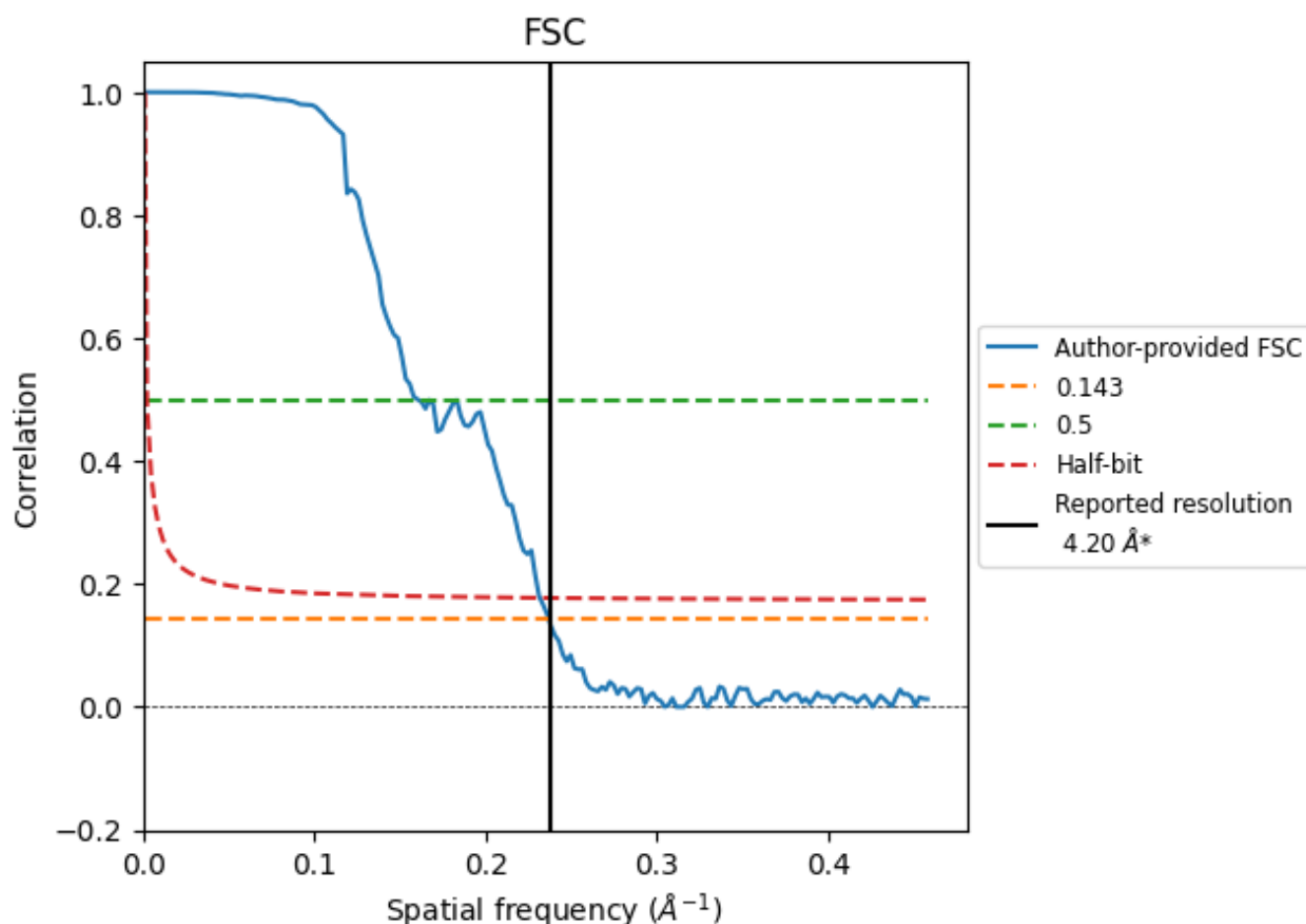


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

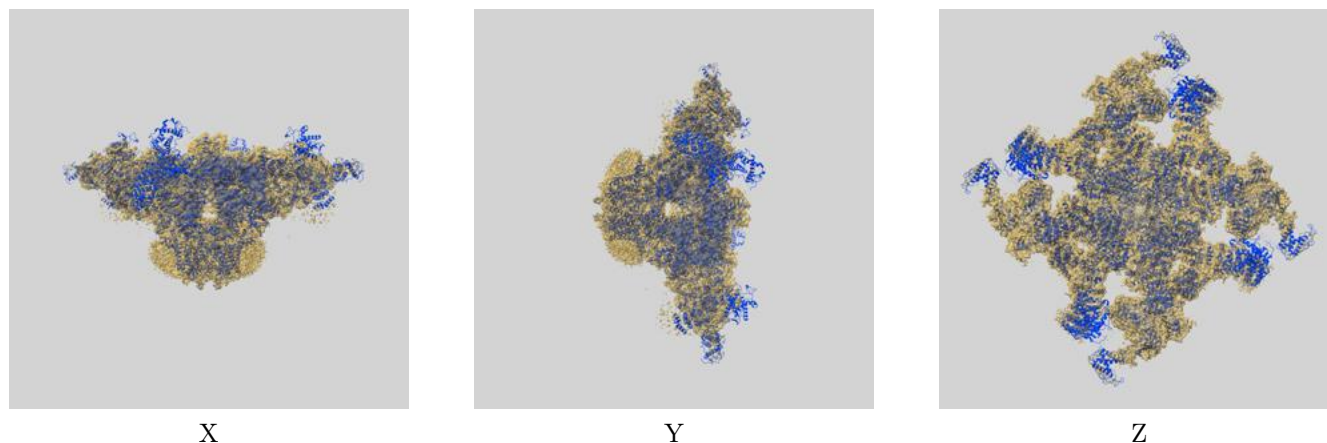
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.23	4.31
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

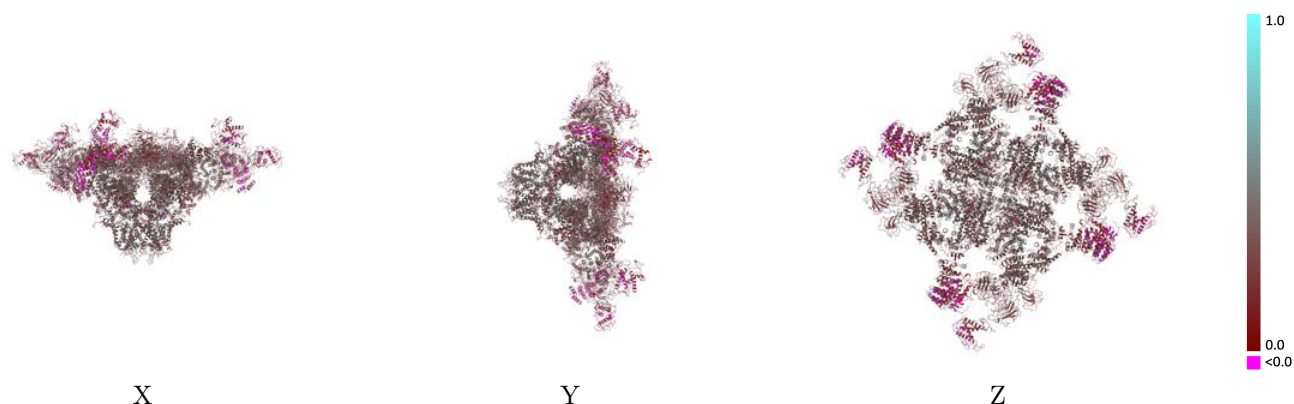
This section contains information regarding the fit between EMDB map EMD-9831 and PDB model 6JI0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



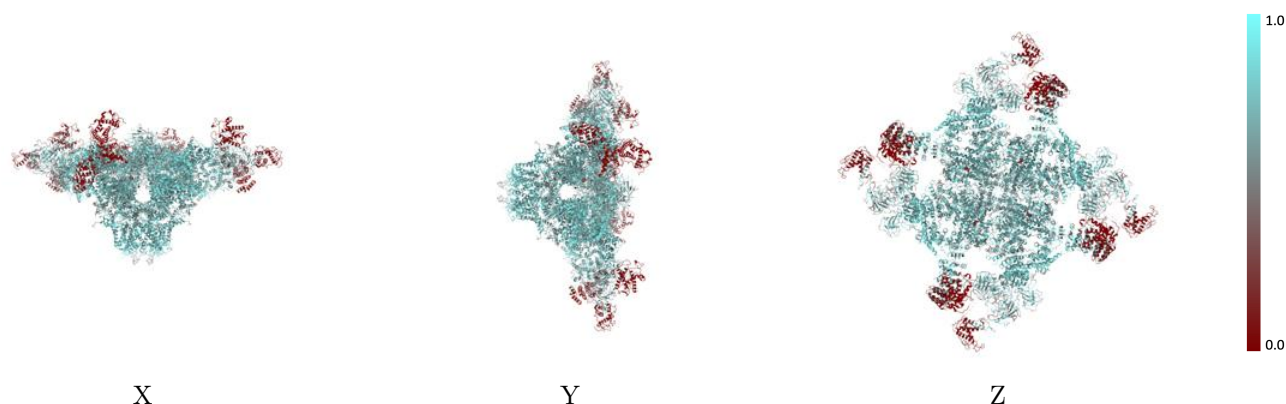
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



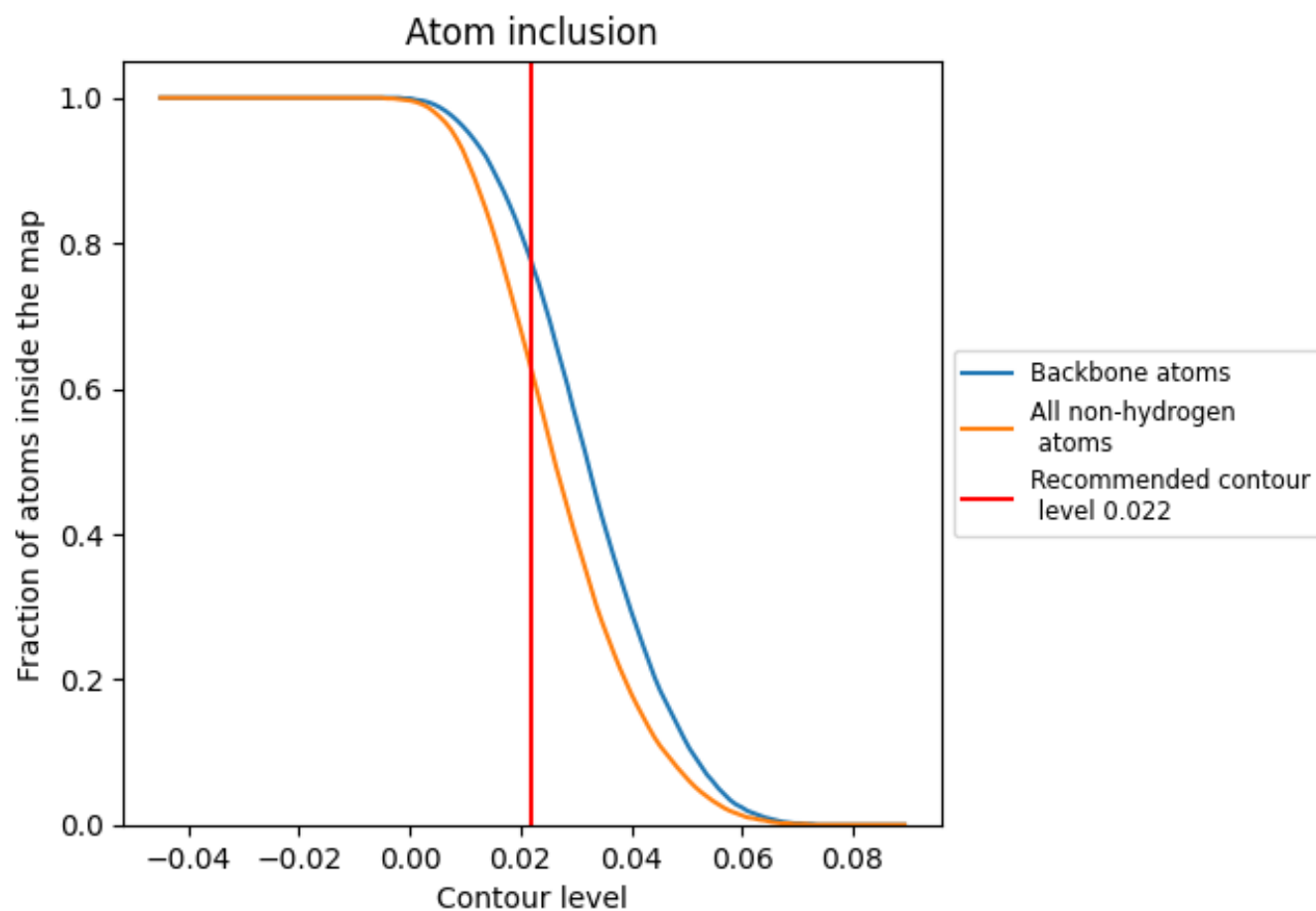
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.3220
A	0.6250	0.3220
B	0.6630	0.3270
C	0.6250	0.3220
D	0.6630	0.3280
E	0.6250	0.3210
F	0.6630	0.3250
G	0.6250	0.3210
H	0.6650	0.3240

