



Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 11:44 PM JST

PDB ID : 6JII
EMDB ID : EMD-9834
Title : Structure of RyR2 (F/A/C/L-Ca²⁺/apo-CaM-M dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-21
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:

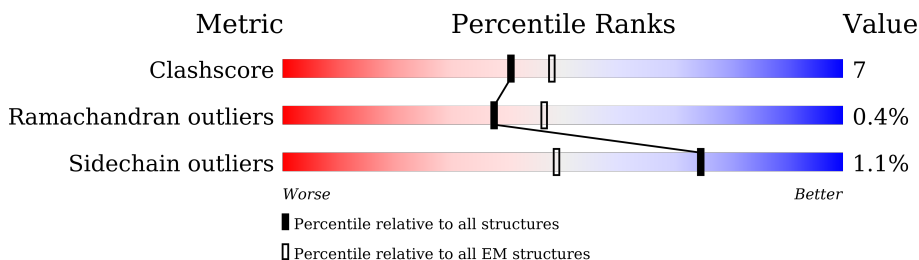
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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.



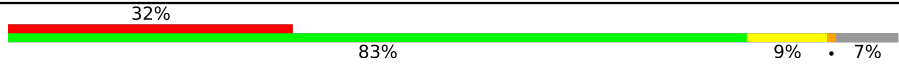

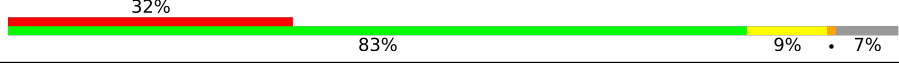
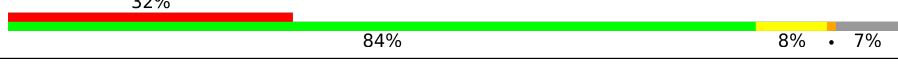
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	108	
1	D	108	
1	G	108	
1	J	108	
2	B	4968	
2	E	4968	
2	H	4968	
2	K	4968	

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Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 115028 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	107	819	516	144	155	4	0	0
1	D	107	819	516	144	155	4	0	0
1	G	107	819	516	144	155	4	0	0
1	J	107	819	516	144	155	4	0	0

- Molecule 2 is a protein called Ryr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	3508	26813	17078	4599	4977	159	0	0
2	E	3508	26813	17078	4599	4977	159	0	0
2	H	3508	26813	17078	4599	4977	159	0	0
2	K	3508	26813	17078	4599	4977	159	0	0

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	138	1078	668	176	225	9	0	0
3	F	138	1078	668	176	225	9	0	0
3	I	138	1078	668	176	225	9	0	0
3	L	138	1078	668	176	225	9	0	0

There are 16 discrepancies between the modelled and reference sequences:

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

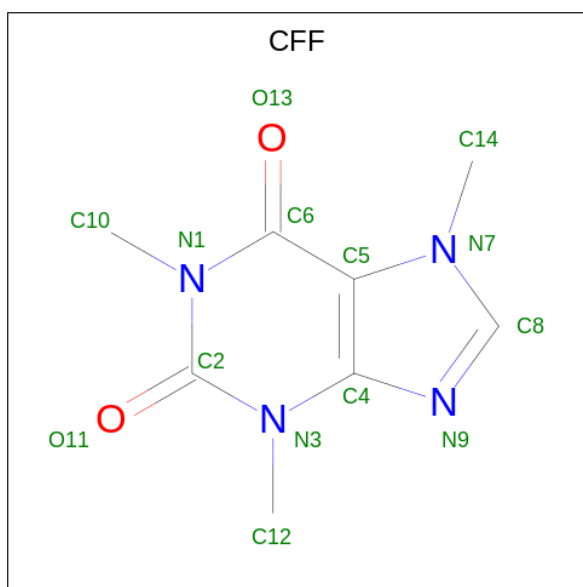
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Zn 1 1	0
4	E	1	Total Zn 1 1	0
4	H	1	Total Zn 1 1	0
4	K	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

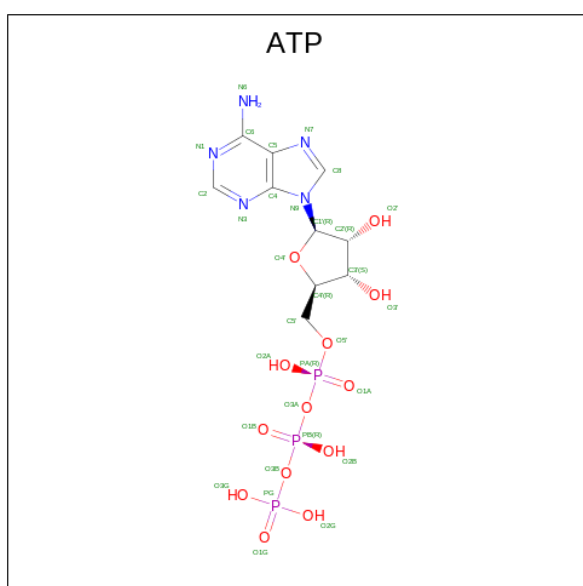
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Ca 1 1	0
5	E	1	Total Ca 1 1	0
5	H	1	Total Ca 1 1	0
5	K	1	Total Ca 1 1	0

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	14	8	4	2	0
6	E	1	14	8	4	2	0
6	H	1	14	8	4	2	0
6	K	1	14	8	4	2	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

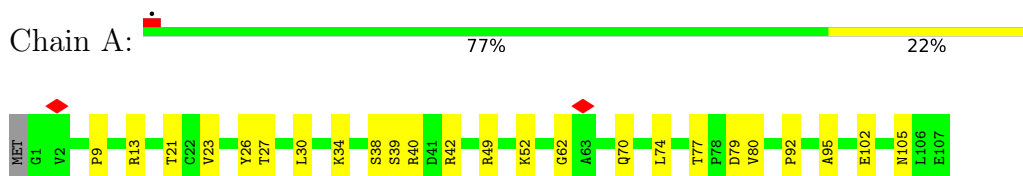


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	31	10	5	13	3	0
7	E	1	31	10	5	13	3	0
7	H	1	31	10	5	13	3	0
7	K	1	31	10	5	13	3	0

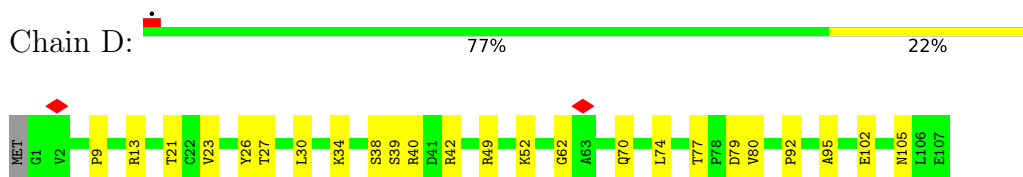
3 Residue-property plots

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.

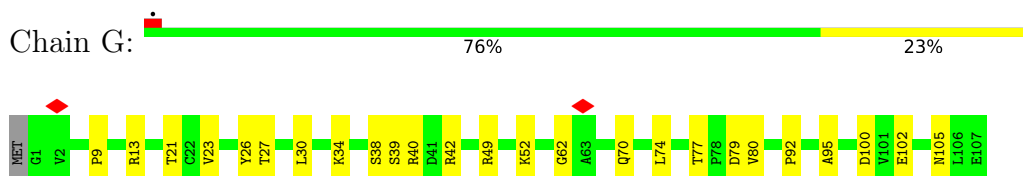
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



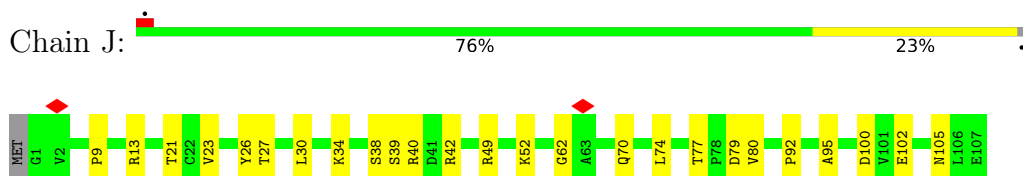
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



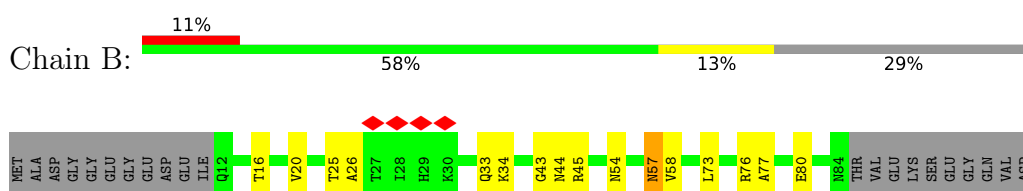
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

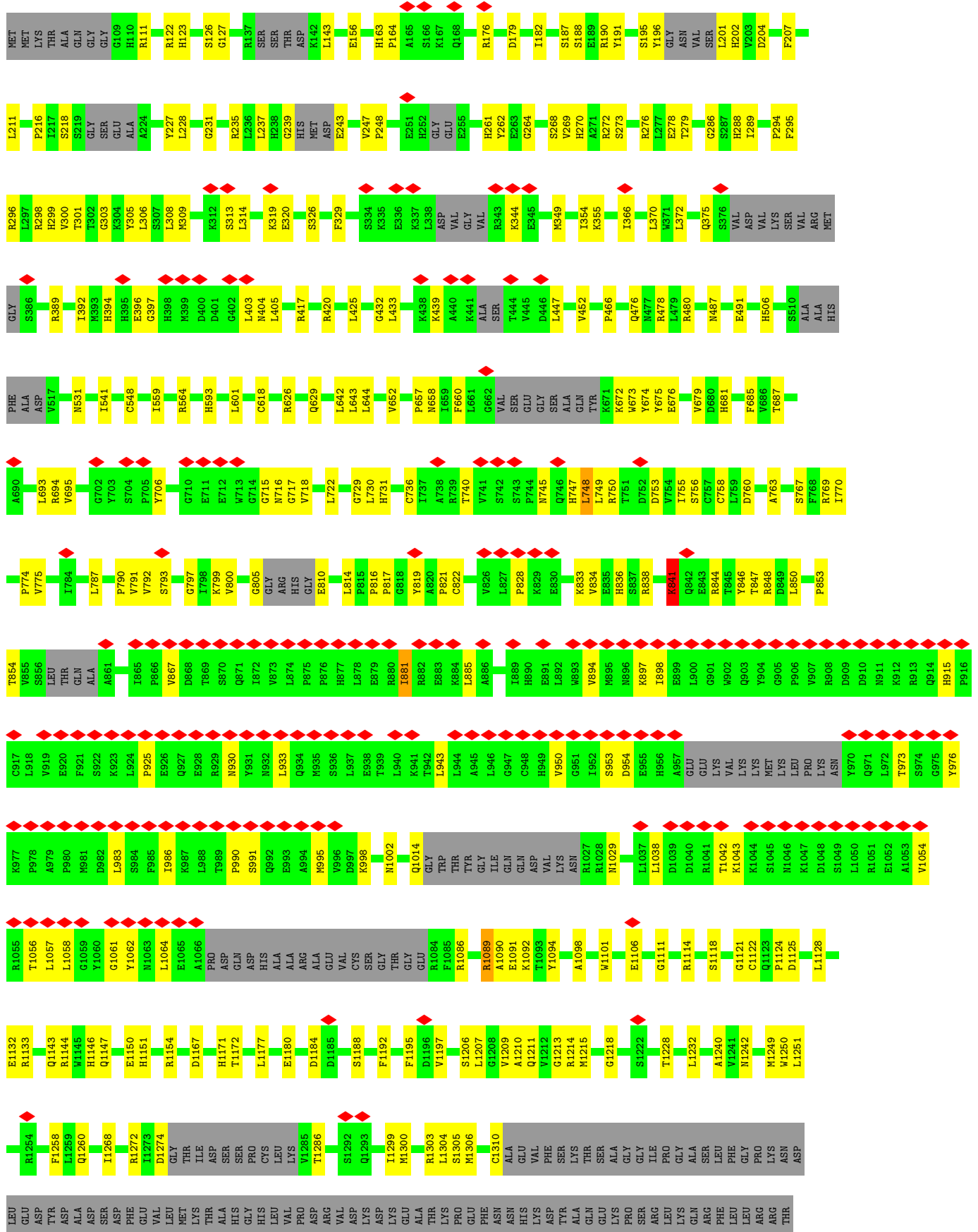


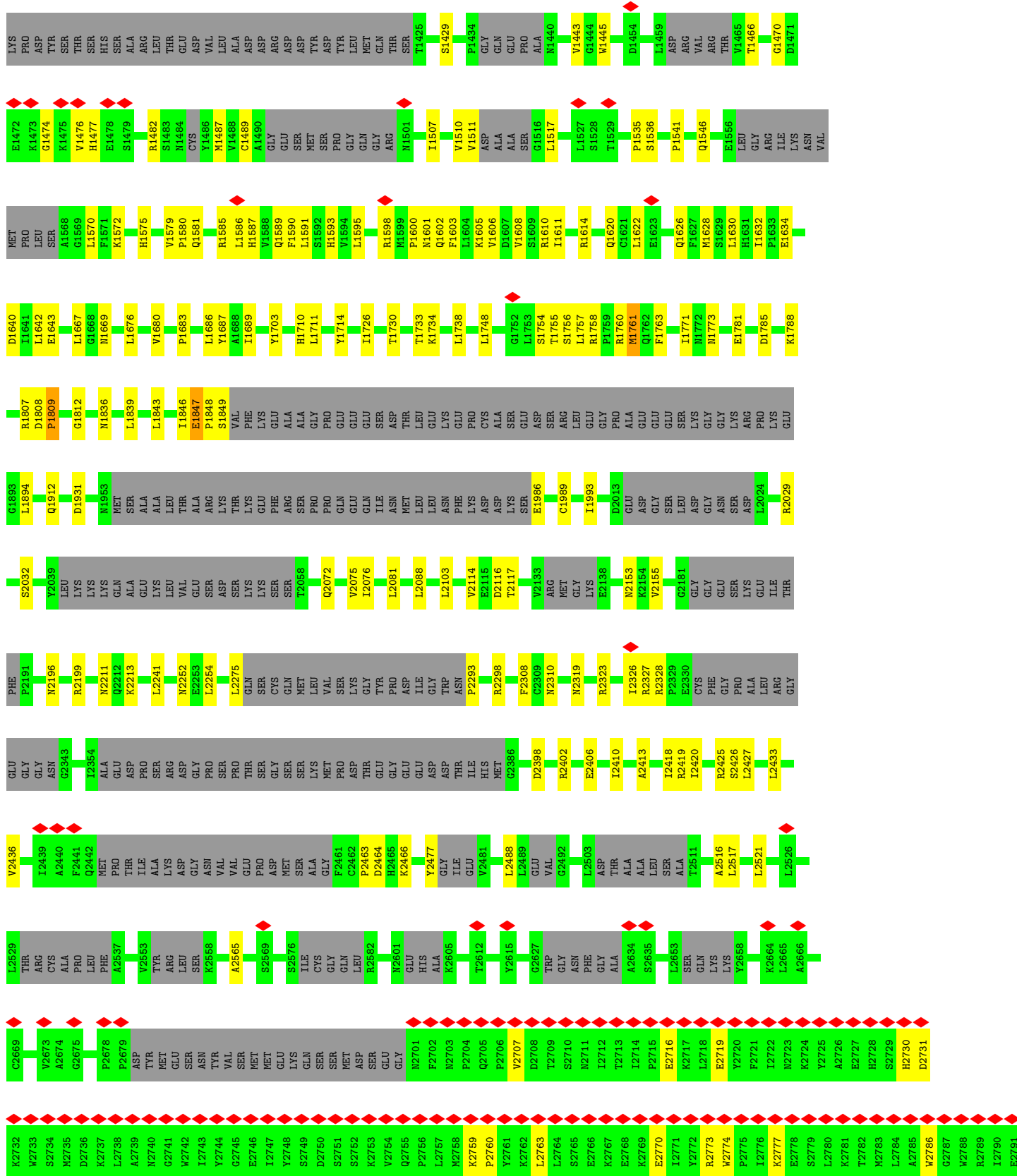
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryr2







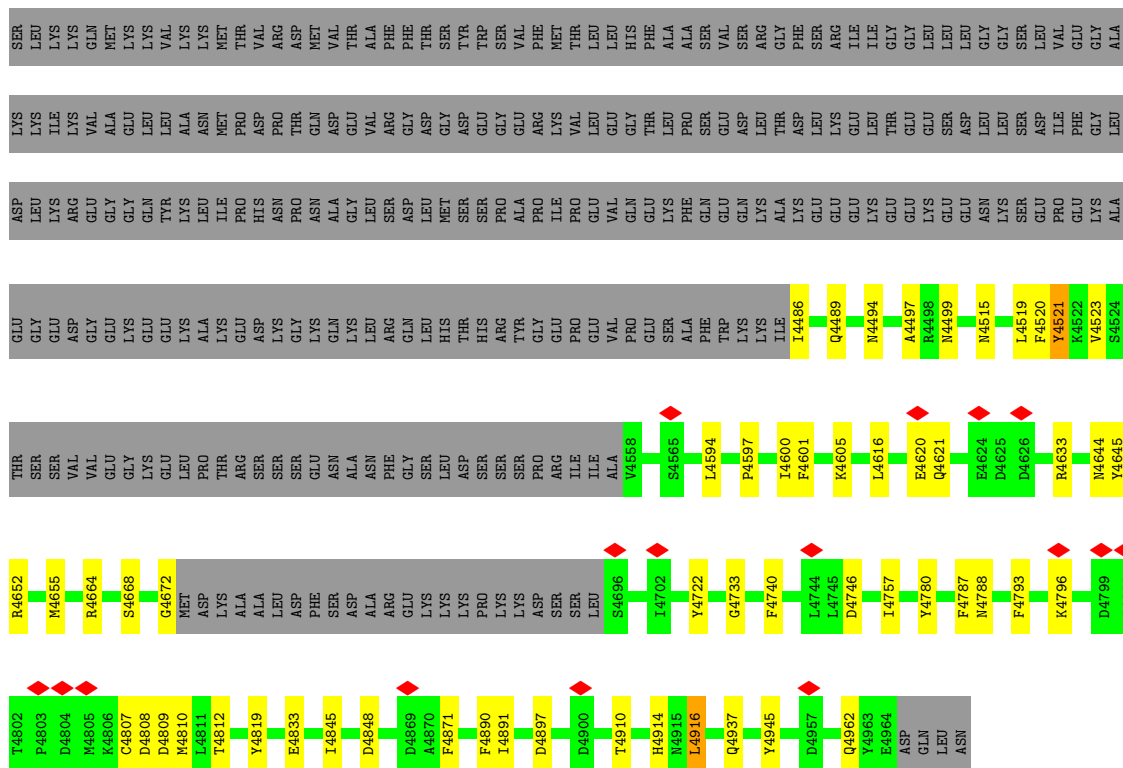
R2792	T2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ARG	ARG	ILE	SER	GLN	GLN	THR	SER	GLN	VAL	VAL	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	L2827	D2828	H2829	S2830	H2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840	H2841	A2842	E2843	H2844	H2845	E2847	H2848	Y2849	H2850	H2851
I2852	W2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	E2862	S2863	K2864	G2865	G2866	G2867	H2868	P2870	L2871	L2872	V2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	I2893	L2894	K2895	F2896	Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU			
GLU	LEU	ASP	THR	PRO	SER	ILE	GLU	PHE	ALA	TYR	SER	GLN	GLN	GLN	VAL	GLU	ALA	HIS	TYR	ILE	LEU	VAL	ASP	GLY	GLU	ALA	HIS	GLN	GLY	PHE	ASP	GLY	ILE	VAL	SER	ARG	CYS	SER	LYS	PHE	PHE	ALA	ALA	LYS	VAL	VAL	LEU	PRO	LEU										
ILE	ASP	TYR	PHE	LYS	ASN	HIS	Y2982	M2999	K3002	E3003	M3004	V3005	THR	SER	SER	LEU	F3009	V3014	R3019	N3025	D3026	A3027	T3028	SER	ILE	VAL	ASN	CYS	L3034	L3037	T3040	A3043	T3049	V3054	K3055	SER	ALA	ALA	ARG	ALA	F3061	L3062	D3063	N3064	A3065	A3066	E3067												
D3068	K3071	T3072	M3073	E3074	N3075	L3076	K3077	Q3080	F3081	T3082	HIS	THR	ARG	ASN	GLN	PRO	LYS	VAL	THR	GLN	ILE	ASN	T3098	T3099	V3100	A3101	L3102	L3103	P3104	M3105	L3106	S3107	S3108	L3109	F3110	E3111	H3112	I3113	G3114	Q3117	F3118	GLY	ASP	LEU	D3124	E3125	D3126	A3065	E3067	L3124	I3125	D3126	W3127	Q3128	V3129	S3130			
C3131	Y3132	R3133	I3134	L3135	T3136	S3137	L3138	Y3139	A3140	L3141	G3142	T3143	S3144	SER	ILE	TYR	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
ARG	GLU	ALA	ARG	LEU	ASN	PRO	THR	ASN	VAL	ASP	VAL	CYS	PRO	ILE	SER	TYR	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
TRP	GLU	HIS	GLY	PRO	GLU	ASN	ASN	ALA	GLU	MET	CYS	THR	ALA	ASN	PRO	LYS	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
VAL	LYS	PRO	GLN	LEU	LEU	LYS	THR	VAL	PRO	MET	GLU	CYS	THR	ALA	ASN	LYS	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
TYR	PRO	LEU	LEU	ILE	ARG	VAL	THR	ASP	TYR	ASN	ASN	GLY	GLU	PRO	ASN	GLY	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
PHE	LEU	ILE	THR	ASP	THR	LYS	SER	LYS	ASP	ALA	VAL	VAL	THR	GLY	ALA	LYS	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
ALA	LEU	ALA	LYS	ASN	ARG	PHE	SER	VAL	LEU	LEU	LYS	THR	THR	GLY	ASP	GLY	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
ARG	VAL	ASP	ILE	ALA	ASN	VAL	VAL	PRO	PHE	GLN	SER	GLY	GLY	GLN	ASP	GLY	V3149	E3150	R3151	R3153	S3154	A3155	G3157	E3158	C3159	L3160	A3161	A3162	F3163	A3164	G3165	A3166	PHE	PRO	VAL	F3171	L3172	E3173	T3174	H3175	L3176	D3177	K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER					
I3642	K3647	P3648	GLY	ALA	ASN	VAL	VAL	PRO	PRO	PHE	GLU	GLY	GLY	GLY	THR	LYS	R3661	V3662	D3663	T3678	E3679	K3680	L3683	E3684	C3700	S3714	L3726	Q3729	A3730	R3731	L3732	H3733	D3734	R3735	A3747	S3748	L3760	K3777	S3593	K3594	Q3595	R3596	K3597	A3602	R3605	K3606	A3607	L3612	A3617	H3635	Y3636								
Q3799	S3800	C3801	S3802	V3803	L3804	D3805	L3806	N3807	A3808	F3809	Q3812	K3820	THR	VAL	GLU	GLY	GLY	GLY	GLY	SER	THR	TYR	TYR	GLY	ASP	L3880	R3881	S3885	I3886	W3891	E3901	Q3902	G3903	Q3904	K3905	N3906	N3919	T3920	L3921	T3922	I3925	L3936	R3940	L3941	A3944	V3951													

VAL	ASP	VAL	LVS	SER	VAL	ARG	MET	GLY	S386	R389	I392	H394	H394	H395	G396	G397	H398	H399	D400	D401	G402	L403	M404	L405	R417	R420	L425	G432	L433	K438	K439	A440	K441	ALA	SER	T444	V445	D446	L447	V452	P466	Q476	H477	R478	L479	R480	M487														
E491	H506	SE510	ALA	ALA	HIS	PHE	ASP	ASP	V517	L530	M531	I541	C548	I559	R564	H593	L601	H608	C618	R626	Q629	L642	L643	L644	V652	P657	M658	I659	F660	G662	VAL	SER	GLU	GLY	GLY	SER	ALA	GLN	TTR	K671	K672	M673	L674																		
Y675	E676	V679	D680	H681	F685	V686	T687	A690	L693	R694	V695	G702	Y703	S704	P705	Y706	G710	E711	E712	M713	G714	G715	N716	G717	V718	L722	G729	L730	H731	C736	I737	A738	R739	T740	V741	S742	S743	P744	N745	Q746	L748	L749	R750	T751	D752	D753	V755	I756	S756												
C757	C758	L759	D760	A763	S767	F768	I770	P774	V775	I784	L787	P790	V791	V792	S793	G797	I798	K799	V800	G805	GLY	ARG	HIS	GLY	E810	L814	P815	P816	P817	G818	Y819	A820	P821	C822	V826	L827	P828	K829	E830	K833	V834	E835	H836	S837	R838	K841															
Q842	E843	R844	T845	Y846	T847	R848	D849	L850	P853	T854	V855	S856	LEU	THR	GLN	ALA	A861	I865	P866	V867	D868	T869	S870	Q871	I872	V873	L874	P875	P876	H877	L878	E879	R880	I881	R882	E883	K884	L885	A886	I889	H890	E891	L892	H893	V894	H895	G896	K897	I898	E899	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	ASP	CS48	H949	V950	G951	N952	S953	D954	E955	H956	A957	GLU	GLU	VAL	VAL	LYS	LYS	MET	LYS	
LEU	PRO	LYS	ASN	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981	D982	L983	F985	I986	K987	L988	T989	P990	Q992	E993	A994	M995	V996	D997	K998	N1002	Q1014	GLY	THR	TRP	LYS	TYR	GLY	ILE	GLN	GLN	ASP	VAL	VAL	ASN	R1027	R1028	M1029	S953	D954	E955	H956	A957	GLU	GLU	VAL	VAL	LYS	LYS	MET	LYS
K1044	S1045	M1046	K1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	R1055	L1056	L1057	L1058	G1059	Y1060	G1061	Y1062	M1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ARG	ALA	GLU	VAL	VAL	CYS	SER	GLY	THR	GLU	R1084	F1085	R1086	R1089	A1090	E1091	K1092	L1093	Y1094	A1098	M1099	H1101	E1106	G1111	R1114							
S1118	G1121	C1122	Q1123	P1124	D1125	L1128	E1132	R1133	Q1143	R1144	W1145	H1146	Q1147	E1150	H1151	R1154	V1162	D1167	H1171	T1172	T1176	L1177	E1180	D1184	D1185	S1188	F1189	L1192	F1195	D1196	V1197	S1206	L1207	G1208	V1209	A1210	Q1211	V1212	G1213	R1214	M1215	G1218																			
S1222	T1228	L1232	A1240	M1242	M1249	W1250	L1251	R1254	F1258	L1259	Q1260	I1268	R1272	D1274	GLY	THR	ILE	ASP	SER	ASP	SER	GLU	HIS	ASP	PRO	CYS	LEU	LEU	LYS	V1285	T1286	S1292	Q1293	L1299	M1300	R1303	L1304	S1305	M1306	C1310	ALA	ASN	ASN	PRO	VAL	PHE	SER	THR	LYS	THR	SER	ALA									
GLY	GLY	ILE	PRO	GLY	ALA	SER	PHE	GLY	PRO	LYS	ASN	ASP	GLU	GLU	TYR	ASP	ALA	ASP	PHE	GLU	VAL	VAL	MET	LYS	THR	ILE	ASP	SER	HIS	ASP	PRO	CYS	LEU	VAL	VAL	PRO	ASP	ASP	VAL	ASP	GLY	GLN	MET	THR	GLU	THR	SER	VAL													
LYS	PRO	ARG	ARG	LYS	GLN	ARG	PHE	LEU	LEU	ARG	ARG	THR	LYS	PRO	TYR	ASP	SER	HIS	ALA	ARG	LEU	ASP	ASP	ASP	ASP	ASP	ASP	THR	ASP	THR	LEU	GLN	PRO	THR	THR	THR	THR	THR	THR	GLY	GLN	GLN	GLY	ASP	ALA	ALA	GLY	PRO	ALA	ALA	VAL	VAL									
D1454	L1459	ASP	VAL	ARG	THR	V1465	T1466	G1470	D1471	E1472	K1473	G1474	K1475	V1476	H1477	E1478	S1479	R1482	S1483	N1484	CYS	Y1486	M1487	V1488	A1490	Q1589	F1590	L1591	S1592	V1594	L1595	R1598	M1599	P1600	N1601	Q1602	F1603	L1604	K1605	D1607	V1606	F1608	S1609	R1610	I1611	R1614	S1528	G1444	T1529	P1535	S1536										
P1541	Q1546	E1556	LEU	GLY	ARG	ILE	LYS	ASN	VAL	MET	PRO	LEU	SER	A1568	G1569	L1570	F1571	K1572	H1575	V1579	P1580	Q1581	R1585	L1586	H1587	V1588	Q1589	F1590	L1591	S1592	V1594	L1595	R1598	M1599	P1600	N1601	Q1602	F1603	L1604	K1605	D1607	V1606	F1608	S1609	R1610	I1611	R1614	Q1620	C1621												

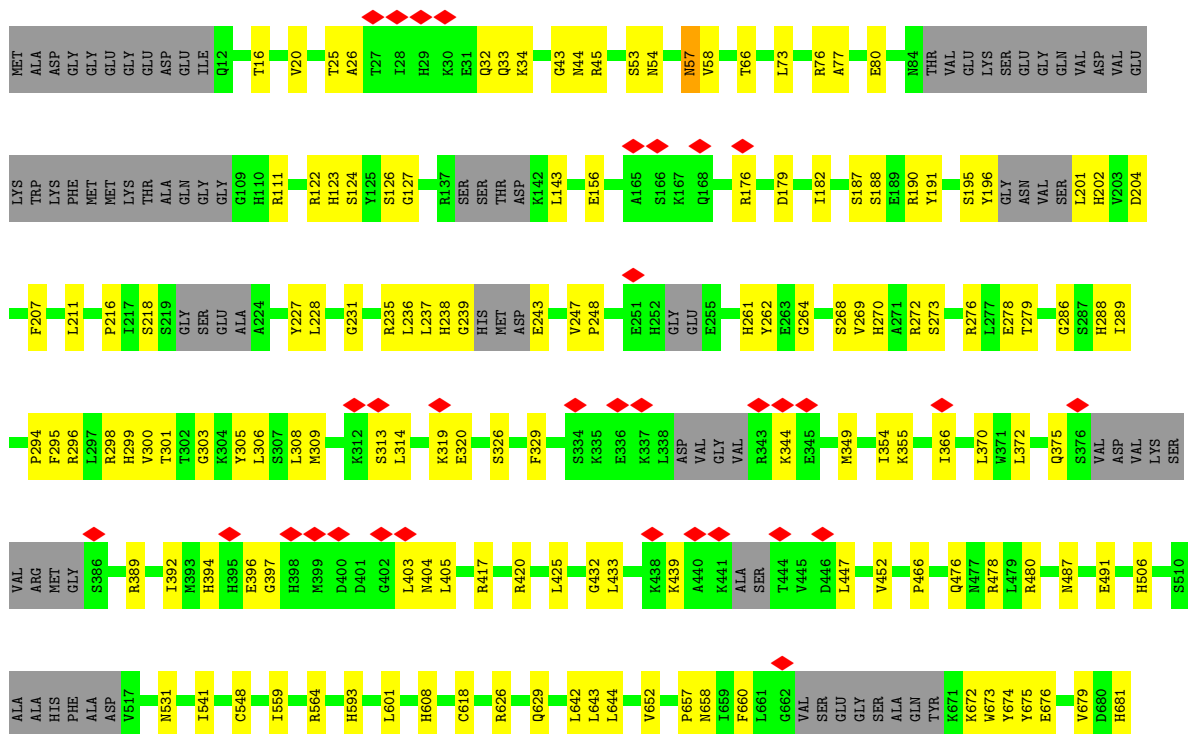
Table listing amino acid residues with their IDs, labels, and validation status. The table is organized into vertical columns, each representing a different residue type or a specific region of the protein. Red diamonds at the top and bottom of certain columns indicate specific validation flags or errors.

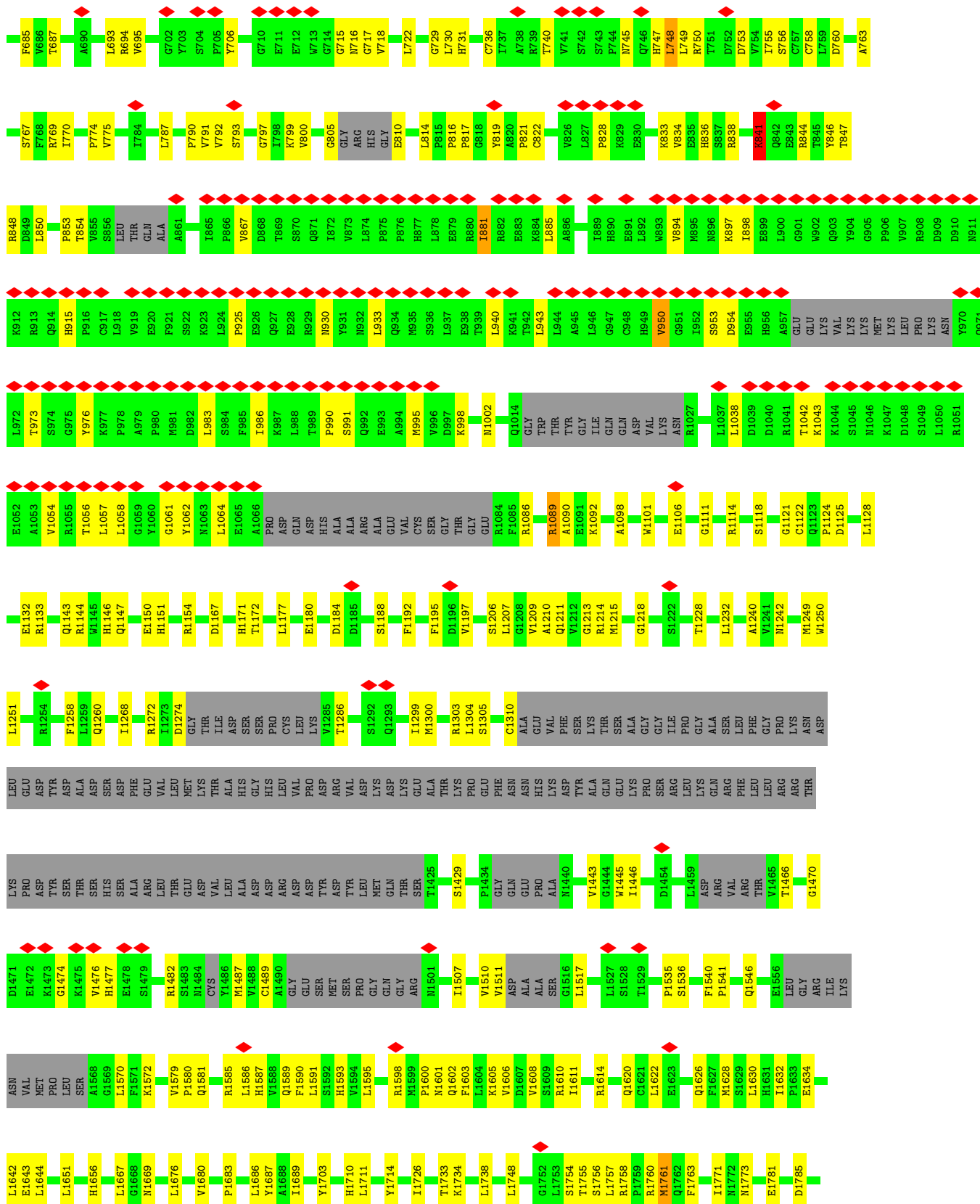
The residues listed include: L1622, E1623, S1754, I1755, I1756, G1757, R1758, P1759, M1628, S1629, M1761, H1630, Q1762, F1763, I1771, M1772, M1773, D1640, I1641, L1642, E1643, L1644, L1651, H1656, L1667, G1668, M1669, L1676, I1846, E1847, P1848, S1849, VAL, P1683, L1686, G1687, H1688, I1689, Y1703, D1704, L1705, H1710, L1711, Y1714, I1726, T1733, K1734, L1738, G1739, P1740, L1748, G1752, L1753.

The table continues with numerous other residues, including: L2410, A2413, I2418, R2419, L2420, R2425, S2426, L2427, L2433, Y2436, I2439, A2440, F2441, G2442, M2601, H2605, K2612, Y2615, G2627, P2700, Q2705, P2706, V2707, D2708, T2709, S2710, M2711, I2712, T2713, I2714, P2715, E2716, K2717.

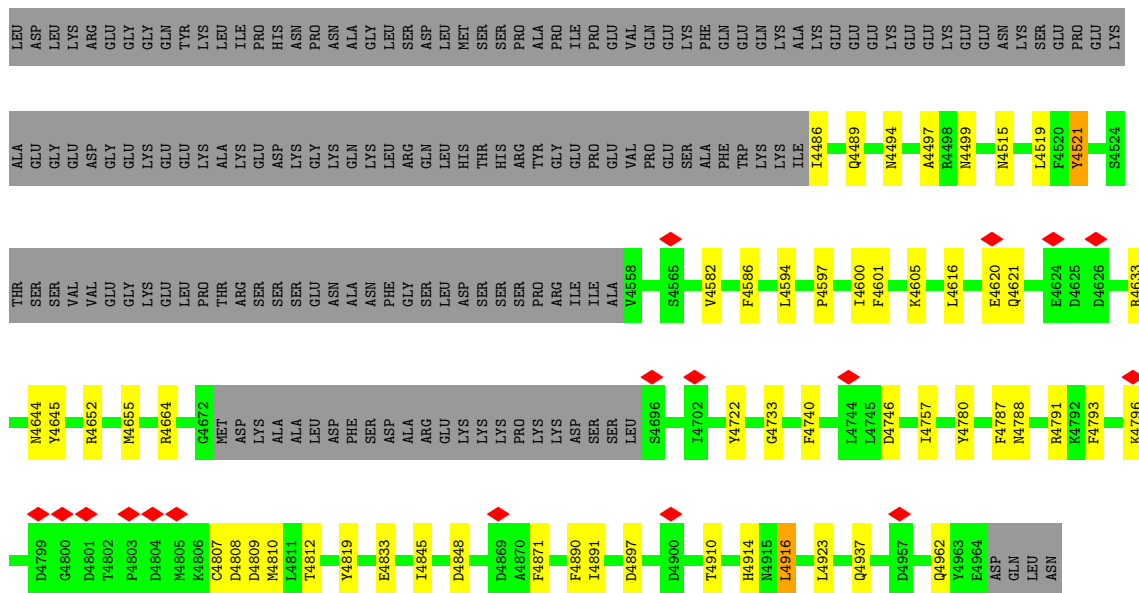


• Molecule 2: Ryr2

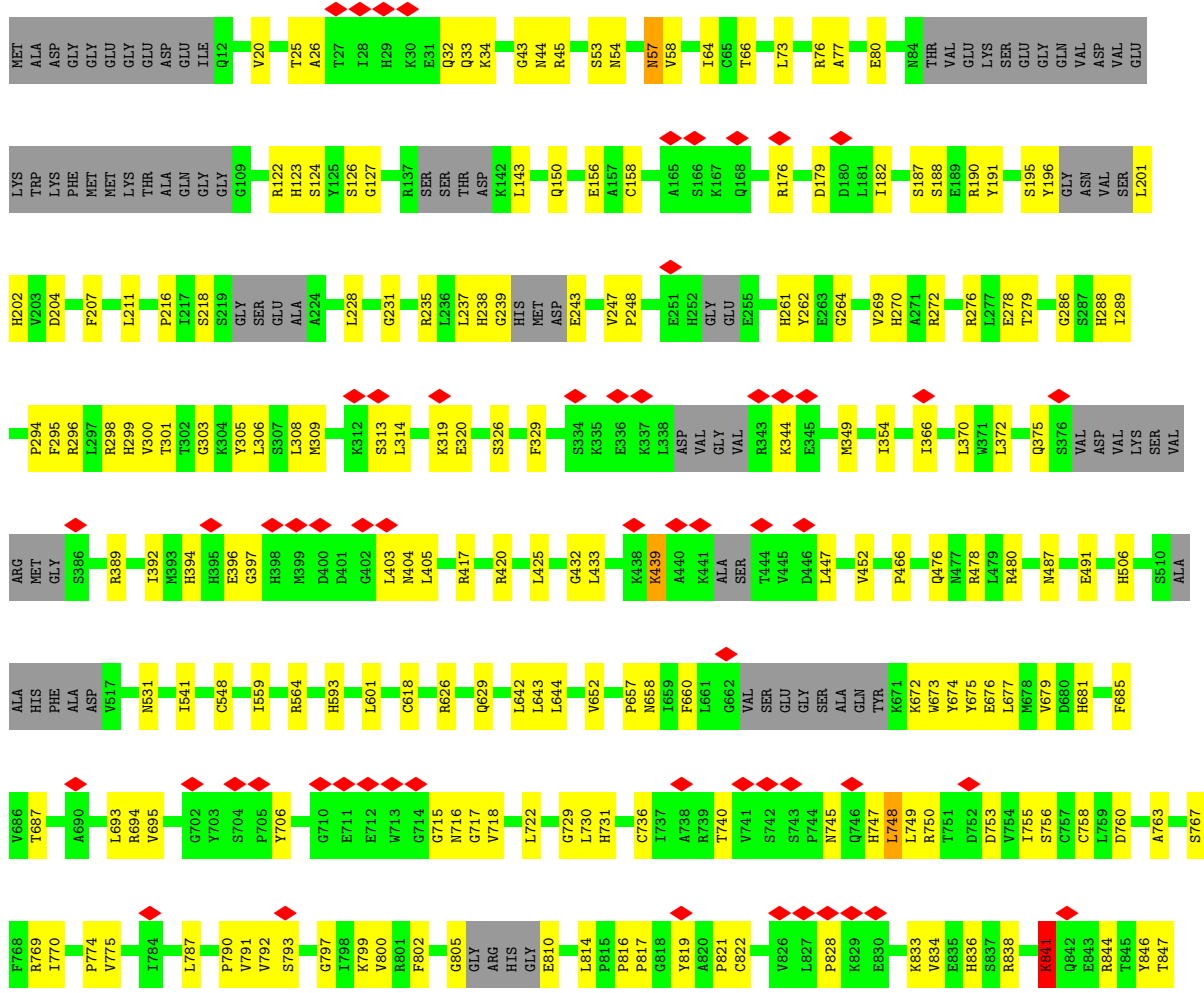


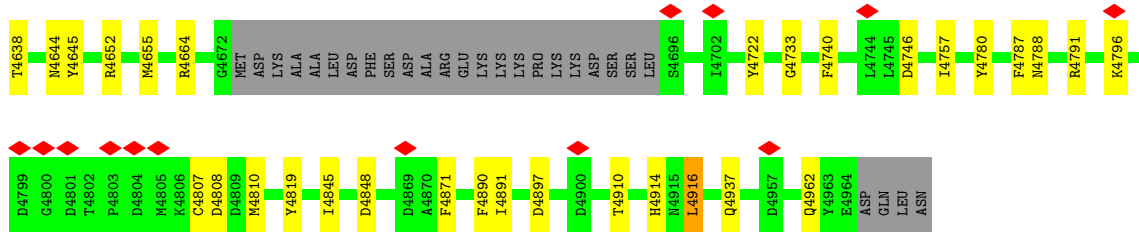


L3062	D3063	H3064	A3065	A3066	E3067	D3068	K3071	T3072	H3073	E3074	H3075	L3076	K3077	A3080	F3081	T3082	HIS	THR	ARG	ASN	ASN	GLN	PRO	LYS	GLY	VAL	THR	ILE	ILE	ASN	TYR	T3098	T3099	V3100	L3102	L3103	F3104	H3105	L3106	S3107	S3108	L3109	F3110	E3111	H3112	I3113	G3114	Q3117	F3118	GLY	GLU	ASP	LEU	ILE	L3124					
E3125	D3126	V3127	Q3128	V3129	S3130	C3131	L3132	R3133	I3134	L3135	S3136	L3138	Y3139	A3140	L3141	G3142	T3143	S3144	LYS	THR	SER	LEU	ILE	TYR	V3149	E3150	R3151	Q3152	L3153	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	LEU	SER	ARG	GLU	ARG	ALA	LEU	ALA	PRO	VAL	GLU	ASP	VAL	PRO	ILE	PRO	LEU	SER	ALA	GLU	LEU	VAL	LEU	GLU	THR	MET	ASP	ALA	LEU	ILE	GLU	TYR	ASN	ARG	LEU	TYR	GLY	VAL	THR	VAL	GLU	VAL	GLU	VAL	PRO	PRO	LEU	LEU	GLN	CYS								
SER	TYR	MET	SER	ASP	TRP	TRP	GLU	HIS	PRO	GLY	ASP	ALA	ASN	PRO	TYR	GLY	GLY	ASN	THR	LEU	GLU	VAL	LEU	ASN	THR	LEU	GLY	GLU	LEU	ILE	ASP	LEU	ILE	GLY	TYR	ASN	ASN	LEU	ASP	GLY	ASP	GLY	TRP	MET	GLU	VAL	ARG	LEU	ALA	VAL	THR	THR	VAL	PHE	SER					
GLN	PRO	ILE	ASN	LYS	VAL	LYS	PRO	GLN	LEU	GLY	ALA	LEU	LYS	THR	HIS	PHE	PRO	ALA	VAL	LEU	LEU	GLU	MET	GLY	GLU	VAL	ALA	GLY	LEU	VAL	SER	ALA	LEU	GLY	GLY	TRP	LEU	ILE	ILE	ASP	GLY	GLN	ASP	VAL	GLY	ASN	PHE	THR	THR	VAL	THR	ALA								
ARG	ASP	LEU	TYR	ALA	PHE	TYR	PRO	LEU	ILE	ASP	ILE	ARG	PHE	VAL	ASP	ASN	THR	LYS	ASN	ARG	ASP	ALA	LYS	TRP	VAL	LEU	GLU	VAL	GLU	VAL	PHE	VAL	ILE	TYR	TRP	GLY	LEU	LEU	ARG	GLU	GLU	GLY	GLN	ASP	VAL	PHE	VAL	VAL	GLN	ASN										
GLU	ILE	ASN	GLU	MET	SER	PHE	LEU	ILE	THR	ASN	ARG	THR	LYS	SER	LEU	MET	LYS	ASN	THR	LYS	ASP	ALA	VAL	VAL	VAL	GLY	LEU	GLY	ARG	VAL	TYR	VAL	GLY	ILE	GLY	TRP	GLY	VAL	LEU	ALA	TYR	LYS	ASN	ALA	ASP	GLY	ASN	ILE	CYS	PRO										
GLY	ASP	GLN	GLU	ILE	LEU	ALA	LEU	LYS	THR	ASN	ARG	THR	LYS	ASP	GLU	GLY	ILE	ILE	ARG	LYS	PRO	GLU	VAL	VAL	VAL	VAL	GLY	GLY	GLU	LEU	GLY	LYS	THR	ILE	LEU	ALA	ALA	TYR	LYS	TYR	ASP	LEU	PRO	ASN	ASN	THR	THR	ASP												
PRO	GLU	THR	VAL	GLU	ARG	VAL	GLY	ALA	VAL	PRO	GLU	ASP	GLY	GLY	THR	LYS	THR	ARG	ARG	ARG	TYR	TYR	TYR	GLU	GLU	GLU	GLU	GLU	ASP	ASP	ASP	GLY	ALA	ALA	VAL	VAL	LYS	LEU	S3593	K3594	Q3595	A3602	R3605	M3606	A3607	L3612														
A3617	H3635	Y3638	I3642	K3647	F3648	ALA	VAL	VAL	PRO	GLU	GLY	GLY	THR	THR	R3661	V3662	D3663	T3678	E3679	K3680	L3683	E3684	C3700	HIS	GLU	GLU	GLU	GLU	ASP	ASP	ASP	ASP	GLY	GLU	GLU	VAL	GLY	GLU	GLU	L3726	Q3729	A3730	R3731	H3733	D3734	R3735	A3747	S3748												
L3760	K3777	Q3799	S3800	C3802	V3803	L3804	L3806	H3807	F3808	F3809	Q3812	K3820	VAL	THR	GLU	GLU	GLY	SER	GLY	GLY	V3829	L3831	Q3832	D3833	L3844	L3871	S3874	L3880	R3881	S3885	I3886	K3891	E3901	Q3902	Q3903	Q3904	R3905	R3906	A3910	L3911	N3919	T3920																		
L3921	I3922	I3925	L3936	R3940	L3941	A3944	V3951	M3955	T4073	D4074	E4075	H4076	E4077	V4085	M3985	L3986	L3987	N3990	N3993	I3996	M4000	M4003	E4006	N4010	V4011	I4014	M4020	F4021	L4022	D4026	L4027	S4030	D4031	K4034	E4035	G4040	K4041	K4046	R4047																					
D4048	F4049	A4052	H4056	E4063	L4067	C4070	A4071	T4073	D4074	E4075	H4076	E4077	V4085	M3985	L3986	L3987	N3990	N3993	I3996	M4000	M4003	E4006	N4010	V4011	I4014	M4020	F4021	L4022	D4026	L4027	S4030	D4031	K4034	E4035	G4040	K4041	K4046	R4047																						
M4192	Q4206	I4207	SER	GLU	ASP	LEU	ASN	GLY	ARG	SER	ALA	ASN	PRO	ASP	THR	GLY	GLU	VAL	THR	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY													
LYS	SER	LEU	LYS	GLN	MET	LYS	VAL	LYS	ASN	ARG	VAL	THR	THR	VAL	ARG	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR									
ALA	LYS	ILE	LYS	VAL	ALA	GLU	LEU	ALA	ASN	MET	PRO	THR	ASP	PRO	GLN	THR	ASP	VAL	THR	GLU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL							

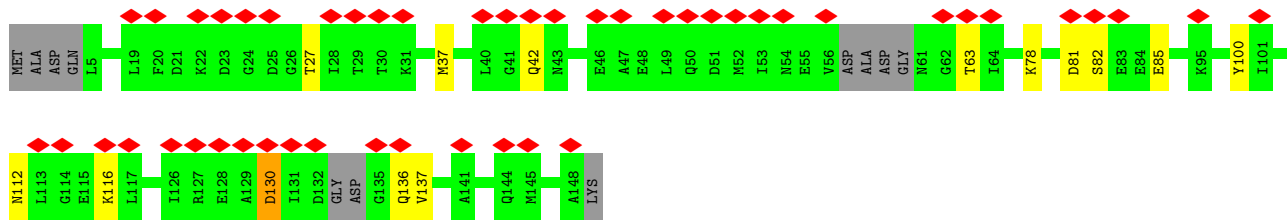
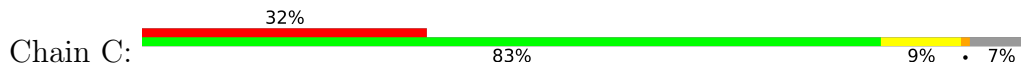


• Molecule 2: Ryr2

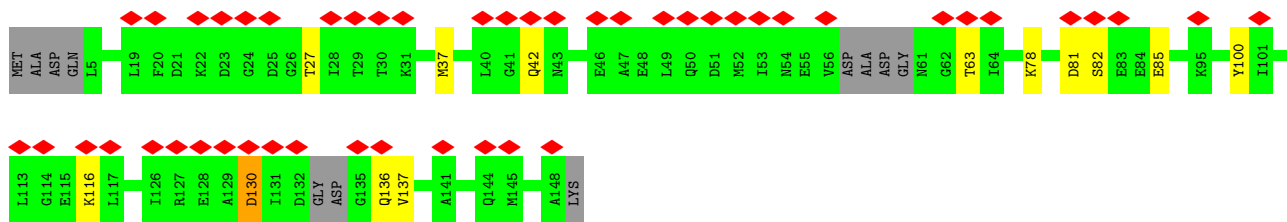
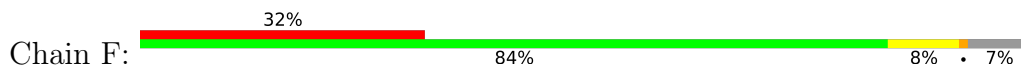




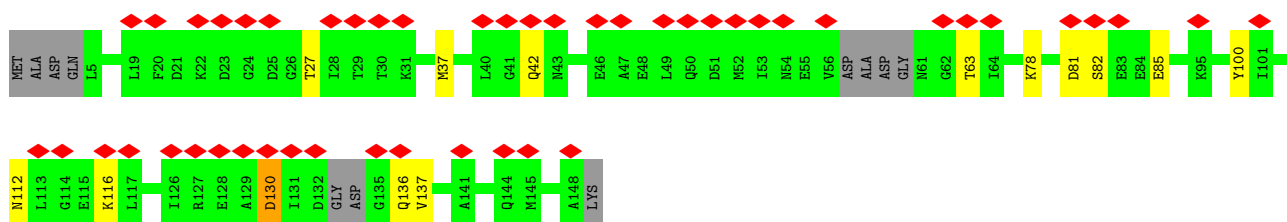
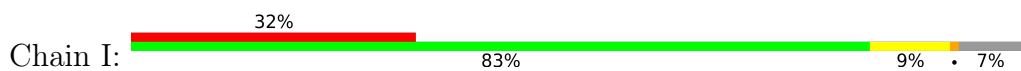
• Molecule 3: Calmodulin-1



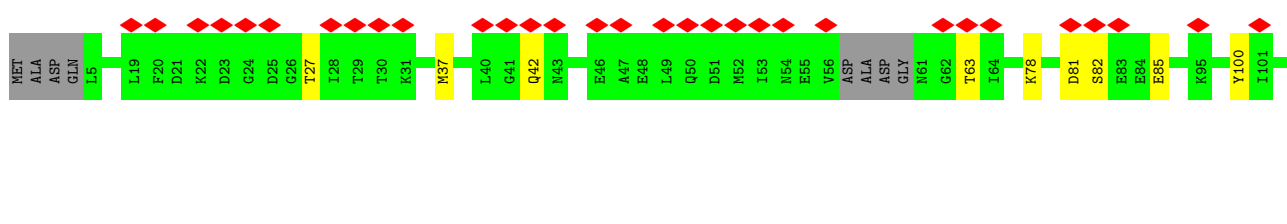
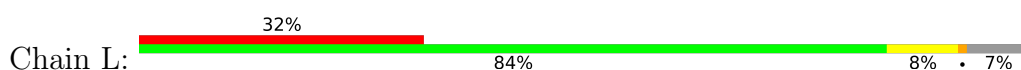
• Molecule 3: Calmodulin-1

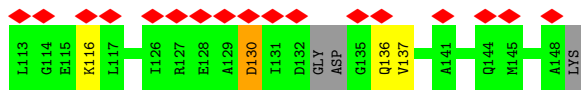


• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69556	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	0.096	Depositor
Minimum map value	-0.036	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: ATP, CFF, ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/835	0.56	0/1123
1	D	0.38	0/835	0.56	0/1123
1	G	0.38	0/835	0.56	0/1123
1	J	0.38	0/835	0.56	0/1123
2	B	0.41	0/27315	0.61	2/36936 (0.0%)
2	E	0.41	0/27315	0.61	2/36936 (0.0%)
2	H	0.41	0/27315	0.61	2/36936 (0.0%)
2	K	0.41	0/27315	0.61	2/36936 (0.0%)
3	C	0.33	0/1088	0.53	0/1459
3	F	0.33	0/1088	0.53	0/1459
3	I	0.33	0/1088	0.53	0/1459
3	L	0.33	0/1088	0.53	0/1459
All	All	0.41	0/116952	0.60	8/158072 (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
2	B	0	24
2	E	0	24
2	H	0	24
2	K	0	24
All	All	0	96

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2517	LEU	CA-CB-CG	6.97	131.33	115.30
2	B	2517	LEU	CA-CB-CG	6.97	131.32	115.30
2	E	2517	LEU	CA-CB-CG	6.95	131.29	115.30
2	K	2517	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	1738	LEU	CA-CB-CG	6.03	129.18	115.30
2	K	1738	LEU	CA-CB-CG	6.02	129.16	115.30
2	H	1738	LEU	CA-CB-CG	6.02	129.14	115.30
2	E	1738	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1476	VAL	Peptide
2	B	1570	LEU	Peptide
2	B	1579	VAL	Peptide
2	B	1748	LEU	Peptide
2	B	1808	ASP	Peptide
2	B	1809	PRO	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	2308	PHE	Peptide
2	B	3612	LEU	Peptide
2	B	3802	SER	Peptide
2	B	3805	ASP	Peptide
2	B	4070	CYS	Peptide
2	B	4163	LYS	Peptide
2	B	685	PHE	Peptide
2	B	729	GLY	Peptide
2	B	748	LEU	Peptide
2	B	791	VAL	Peptide
2	B	816	PRO	Peptide
2	B	817	PRO	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide
2	B	841	LYS	Peptide
2	B	854	THR	Peptide
2	E	1476	VAL	Peptide
2	E	1570	LEU	Peptide
2	E	1579	VAL	Peptide
2	E	1748	LEU	Peptide
2	E	1808	ASP	Peptide
2	E	1809	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	1847	GLU	Peptide
2	E	2075	VAL	Peptide
2	E	2308	PHE	Peptide
2	E	3612	LEU	Peptide
2	E	3802	SER	Peptide
2	E	3805	ASP	Peptide
2	E	4070	CYS	Peptide
2	E	4163	LYS	Peptide
2	E	685	PHE	Peptide
2	E	729	GLY	Peptide
2	E	748	LEU	Peptide
2	E	791	VAL	Peptide
2	E	816	PRO	Peptide
2	E	817	PRO	Peptide
2	E	819	TYR	Peptide
2	E	838	ARG	Peptide
2	E	841	LYS	Peptide
2	E	854	THR	Peptide
2	H	1476	VAL	Peptide
2	H	1570	LEU	Peptide
2	H	1579	VAL	Peptide
2	H	1748	LEU	Peptide
2	H	1808	ASP	Peptide
2	H	1809	PRO	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	2308	PHE	Peptide
2	H	3612	LEU	Peptide
2	H	3802	SER	Peptide
2	H	3805	ASP	Peptide
2	H	4070	CYS	Peptide
2	H	4163	LYS	Peptide
2	H	685	PHE	Peptide
2	H	729	GLY	Peptide
2	H	748	LEU	Peptide
2	H	791	VAL	Peptide
2	H	816	PRO	Peptide
2	H	817	PRO	Peptide
2	H	819	TYR	Peptide
2	H	838	ARG	Peptide
2	H	841	LYS	Peptide
2	H	854	THR	Peptide

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Mol	Chain	Res	Type	Group
2	K	1476	VAL	Peptide
2	K	1570	LEU	Peptide
2	K	1579	VAL	Peptide
2	K	1748	LEU	Peptide
2	K	1808	ASP	Peptide
2	K	1809	PRO	Peptide
2	K	1847	GLU	Peptide
2	K	2075	VAL	Peptide
2	K	2308	PHE	Peptide
2	K	3612	LEU	Peptide
2	K	3802	SER	Peptide
2	K	3805	ASP	Peptide
2	K	4070	CYS	Peptide
2	K	4163	LYS	Peptide
2	K	685	PHE	Peptide
2	K	729	GLY	Peptide
2	K	748	LEU	Peptide
2	K	791	VAL	Peptide
2	K	816	PRO	Peptide
2	K	817	PRO	Peptide
2	K	819	TYR	Peptide
2	K	838	ARG	Peptide
2	K	841	LYS	Peptide
2	K	854	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	819	0	824	13	0
1	D	819	0	824	13	0
1	G	819	0	824	14	0
1	J	819	0	824	14	0
2	B	26813	0	25339	450	0
2	E	26813	0	25339	437	0
2	H	26813	0	25339	441	0
2	K	26813	0	25339	439	0
3	C	1078	0	1032	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1078	0	1032	7	0
3	I	1078	0	1032	8	0
3	L	1078	0	1032	7	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	H	14	0	10	0	0
6	K	14	0	10	0	0
7	B	31	0	12	4	0
7	E	31	0	12	4	0
7	H	31	0	12	5	0
7	K	31	0	12	4	0
All	All	115028	0	108868	1669	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 7.

All (1669) 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)
2:K:1986:GLU:N	2:K:1989:CYS:HG	1.54	1.05
2:B:1986:GLU:N	2:B:1989:CYS:HG	1.54	1.05
2:H:1986:GLU:N	2:H:1989:CYS:HG	1.55	1.03
2:B:4811:LEU:HD13	2:E:4519:LEU:HD21	1.39	1.03
2:E:1986:GLU:N	2:E:1989:CYS:HG	1.56	1.02
2:B:76:ARG:NH2	2:E:3806:LEU:HD11	1.77	1.00
2:E:76:ARG:NH2	2:H:3806:LEU:HD11	1.78	0.98
2:B:3806:LEU:HD11	2:K:76:ARG:NH2	1.77	0.98
2:H:76:ARG:NH2	2:K:3806:LEU:HD11	1.78	0.96
2:E:4848:ASP:CG	2:H:4819:TYR:HE1	1.67	0.96
2:B:207:PHE:CZ	2:E:2326:ILE:HG23	2.00	0.96
2:E:207:PHE:CZ	2:H:2326:ILE:HG23	2.00	0.96
2:B:4819:TYR:HE1	2:K:4848:ASP:CG	1.69	0.95
2:B:4848:ASP:CG	2:E:4819:TYR:HE1	1.68	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2326:ILE:HG23	2:K:207:PHE:CZ	2.01	0.95
2:H:4848:ASP:CG	2:K:4819:TYR:HE1	1.70	0.95
2:H:207:PHE:CZ	2:K:2326:ILE:HG23	2.01	0.93
2:B:1843:LEU:O	2:B:1847:GLU:HB2	1.71	0.91
2:E:76:ARG:HH21	2:H:3806:LEU:HD21	1.36	0.91
2:E:1843:LEU:O	2:E:1847:GLU:HB2	1.71	0.91
2:K:1843:LEU:O	2:K:1847:GLU:HB2	1.71	0.90
2:H:1843:LEU:O	2:H:1847:GLU:HB2	1.71	0.90
2:B:4796:LYS:NZ	2:B:4807:CYS:SG	2.45	0.90
2:H:143:LEU:HD11	2:K:2426:SER:O	1.72	0.90
2:E:143:LEU:HD11	2:H:2426:SER:O	1.72	0.89
2:H:76:ARG:HH21	2:K:3806:LEU:HD21	1.38	0.89
2:B:2426:SER:O	2:K:143:LEU:HD11	1.72	0.88
2:B:3806:LEU:HD21	2:K:76:ARG:HH21	1.38	0.88
2:B:76:ARG:HH21	2:E:3806:LEU:HD21	1.38	0.88
2:B:76:ARG:HH21	2:E:3806:LEU:HD11	1.36	0.87
2:B:143:LEU:HD11	2:E:2426:SER:O	1.73	0.86
2:E:76:ARG:HH21	2:H:3806:LEU:HD11	1.38	0.86
2:E:4848:ASP:CG	2:H:4819:TYR:CE1	2.48	0.86
2:B:4811:LEU:HD13	2:E:4519:LEU:CD2	2.04	0.85
2:B:4848:ASP:CG	2:E:4819:TYR:CE1	2.50	0.85
2:E:76:ARG:NH2	2:H:3806:LEU:HD21	1.91	0.84
2:H:76:ARG:NH2	2:K:3806:LEU:HD21	1.93	0.84
2:B:4819:TYR:CE1	2:K:4848:ASP:CG	2.50	0.84
2:H:4848:ASP:CG	2:K:4819:TYR:CE1	2.51	0.84
2:B:3806:LEU:HD21	2:K:76:ARG:NH2	1.92	0.84
2:B:3806:LEU:HD11	2:K:76:ARG:HH21	1.37	0.83
2:H:76:ARG:HH21	2:K:3806:LEU:HD11	1.37	0.83
2:B:76:ARG:NH2	2:E:3806:LEU:HD21	1.92	0.82
2:H:143:LEU:CD1	2:K:2426:SER:O	2.28	0.81
2:B:2426:SER:O	2:K:143:LEU:CD1	2.28	0.81
2:E:143:LEU:CD1	2:H:2426:SER:O	2.29	0.80
2:B:4848:ASP:OD2	2:E:4819:TYR:CE1	2.35	0.80
2:E:4848:ASP:OD2	2:H:4819:TYR:CE1	2.34	0.80
2:E:143:LEU:HD13	2:H:2426:SER:OG	1.81	0.80
2:B:4819:TYR:CE1	2:K:4848:ASP:OD2	2.35	0.80
2:B:143:LEU:CD1	2:E:2426:SER:O	2.29	0.80
2:H:4848:ASP:OD2	2:K:4819:TYR:CE1	2.36	0.79
2:H:143:LEU:HD13	2:K:2426:SER:OG	1.82	0.78
2:B:143:LEU:HD13	2:E:2426:SER:OG	1.84	0.78
2:B:2426:SER:OG	2:K:143:LEU:HD13	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4787:PHE:HD1	2:B:4808:ASP:O	1.66	0.78
2:K:123:HIS:HD2	2:K:126:SER:H	1.32	0.77
2:H:123:HIS:HD2	2:H:126:SER:H	1.32	0.77
2:B:2419:ARG:HD3	2:K:156:GLU:OE1	1.86	0.76
2:B:156:GLU:OE1	2:E:2419:ARG:HD3	1.85	0.75
2:H:156:GLU:OE1	2:K:2419:ARG:HD3	1.86	0.75
2:B:123:HIS:HD2	2:B:126:SER:H	1.32	0.74
2:B:143:LEU:CD1	2:E:2427:LEU:HD13	2.18	0.74
2:E:123:HIS:HD2	2:E:126:SER:H	1.32	0.74
2:E:156:GLU:OE1	2:H:2419:ARG:HD3	1.88	0.74
2:B:143:LEU:HD11	2:E:2427:LEU:HD13	1.69	0.74
2:B:2427:LEU:HD13	2:K:143:LEU:HD11	1.70	0.73
2:B:2427:LEU:HD13	2:K:143:LEU:CD1	2.19	0.73
2:H:143:LEU:CD1	2:K:2427:LEU:HD13	2.19	0.73
2:E:143:LEU:HD11	2:H:2427:LEU:HD13	1.71	0.72
2:H:143:LEU:HD11	2:K:2427:LEU:HD13	1.71	0.72
2:E:143:LEU:CD1	2:H:2427:LEU:HD13	2.20	0.72
2:B:4519:LEU:O	2:K:4810:MET:CB	2.39	0.71
2:E:207:PHE:CE2	2:H:2326:ILE:HG23	2.26	0.71
2:B:76:ARG:HH21	2:E:3806:LEU:CD1	2.04	0.70
3:F:100:TYR:HB3	3:F:136:GLN:HB3	1.72	0.70
2:H:4810:MET:CB	2:K:4519:LEU:O	2.38	0.70
2:B:207:PHE:CZ	2:E:2326:ILE:CG2	2.74	0.70
3:C:100:TYR:HB3	3:C:136:GLN:HB3	1.72	0.70
2:H:207:PHE:CZ	2:K:2326:ILE:CG2	2.75	0.70
2:E:207:PHE:CZ	2:H:2326:ILE:CG2	2.74	0.70
2:B:299:HIS:HE2	2:B:301:THR:HG1	1.40	0.69
2:H:1605:LYS:HD3	2:H:1606:VAL:HG23	1.74	0.69
3:L:100:TYR:HB3	3:L:136:GLN:HB3	1.72	0.69
2:E:299:HIS:HE2	2:E:301:THR:HG1	1.39	0.69
2:E:4848:ASP:CB	2:H:4819:TYR:HE1	2.04	0.69
3:I:100:TYR:HB3	3:I:136:GLN:HB3	1.72	0.69
2:B:2326:ILE:CG2	2:K:207:PHE:CZ	2.75	0.69
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.57	0.69
2:K:4046:LYS:H	2:K:4077:GLU:HB3	1.57	0.69
2:B:2326:ILE:HG23	2:K:207:PHE:CE2	2.27	0.69
2:B:207:PHE:CE2	2:E:2326:ILE:HG23	2.27	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD1	2.06	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD2	2.06	0.69
2:K:1605:LYS:HD3	2:K:1606:VAL:HG23	1.74	0.69
2:H:207:PHE:CE2	2:K:2326:ILE:HG23	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1089:ARG:HE	2:B:1600:PRO:HB3	1.59	0.68
2:B:3806:LEU:CD1	2:K:76:ARG:HH21	2.05	0.68
2:B:1605:LYS:HD3	2:B:1606:VAL:HG23	1.74	0.68
2:B:2327:ARG:HH21	2:K:191:TYR:HE2	1.42	0.68
2:E:4046:LYS:H	2:E:4077:GLU:HB3	1.57	0.68
2:B:3806:LEU:CD2	2:K:76:ARG:HH21	2.07	0.68
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.57	0.68
2:E:1089:ARG:HE	2:E:1600:PRO:HB3	1.59	0.68
2:E:1605:LYS:HD3	2:E:1606:VAL:HG23	1.74	0.68
2:E:4810:MET:CB	2:H:4519:LEU:O	2.42	0.68
2:H:191:TYR:HE2	2:K:2327:ARG:HH21	1.42	0.68
2:H:4848:ASP:CB	2:K:4819:TYR:HE1	2.06	0.68
2:K:657:PRO:HA	2:K:834:VAL:HA	1.76	0.67
2:B:4848:ASP:CB	2:E:4819:TYR:HE1	2.07	0.67
2:H:1089:ARG:HE	2:H:1600:PRO:HB3	1.59	0.67
2:K:1089:ARG:HE	2:K:1600:PRO:HB3	1.59	0.67
2:B:4819:TYR:HE1	2:K:4848:ASP:CB	2.07	0.67
2:B:850:LEU:HB3	2:B:1207:LEU:HD11	1.77	0.67
2:H:657:PRO:HA	2:H:834:VAL:HA	1.76	0.67
2:K:3951:VAL:O	2:K:3955:MET:HB2	1.95	0.67
2:E:191:TYR:HE2	2:H:2327:ARG:HH21	1.42	0.67
2:B:3951:VAL:O	2:B:3955:MET:HB2	1.95	0.66
2:E:758:CYS:HB3	2:E:767:SER:HB2	1.78	0.66
2:H:758:CYS:HB3	2:H:767:SER:HB2	1.78	0.66
2:E:3951:VAL:O	2:E:3955:MET:HB2	1.95	0.66
2:H:3951:VAL:O	2:H:3955:MET:HB2	1.96	0.66
2:E:657:PRO:HA	2:E:834:VAL:HA	1.76	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD2	2.08	0.66
2:B:191:TYR:HE2	2:E:2327:ARG:HH21	1.42	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD1	2.06	0.66
2:B:207:PHE:CE1	2:E:2326:ILE:CG2	2.79	0.66
2:E:850:LEU:HB3	2:E:1207:LEU:HD11	1.77	0.66
2:B:657:PRO:HA	2:B:834:VAL:HA	1.76	0.65
2:K:758:CYS:HB3	2:K:767:SER:HB2	1.78	0.65
2:B:758:CYS:HB3	2:B:767:SER:HB2	1.78	0.65
2:H:207:PHE:CE1	2:K:2326:ILE:CG2	2.80	0.65
2:K:850:LEU:HB3	2:K:1207:LEU:HD11	1.77	0.65
2:B:2326:ILE:CG2	2:K:207:PHE:CE1	2.79	0.65
2:E:207:PHE:CE1	2:H:2326:ILE:CG2	2.80	0.65
2:K:797:GLY:HA2	2:K:1622:LEU:HA	1.79	0.65
2:B:76:ARG:HH21	2:E:3806:LEU:CD2	2.07	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HB2	2:B:1213:GLY:H	1.62	0.65
2:H:850:LEU:HB3	2:H:1207:LEU:HD11	1.77	0.65
2:H:299:HIS:HE2	2:H:301:THR:HG1	1.39	0.64
2:B:797:GLY:HA2	2:B:1622:LEU:HA	1.79	0.64
2:E:26:ALA:HB3	2:E:33:GLN:HB3	1.80	0.64
2:H:26:ALA:HB3	2:H:33:GLN:HB3	1.80	0.64
2:H:1303:ARG:HH12	2:H:1595:LEU:HB2	1.62	0.64
2:K:1303:ARG:HH12	2:K:1595:LEU:HB2	1.62	0.64
2:E:1303:ARG:HH12	2:E:1595:LEU:HB2	1.62	0.63
2:E:4796:LYS:NZ	2:E:4807:CYS:SG	2.71	0.63
2:K:26:ALA:HB3	2:K:33:GLN:HB3	1.80	0.63
2:E:850:LEU:HB2	2:E:1213:GLY:H	1.62	0.63
2:K:4796:LYS:NZ	2:K:4807:CYS:SG	2.71	0.63
2:B:26:ALA:HB3	2:B:33:GLN:HB3	1.80	0.63
2:H:797:GLY:HA2	2:H:1622:LEU:HA	1.79	0.63
2:H:4146:ILE:HD12	2:H:4962:GLN:HB2	1.81	0.63
2:H:4796:LYS:NZ	2:H:4807:CYS:SG	2.71	0.63
2:H:850:LEU:HB2	2:H:1213:GLY:H	1.62	0.63
2:K:850:LEU:HB2	2:K:1213:GLY:H	1.62	0.63
2:B:1303:ARG:HH12	2:B:1595:LEU:HB2	1.62	0.63
2:E:247:VAL:O	2:E:272:ARG:NH1	2.30	0.63
2:E:797:GLY:HA2	2:E:1622:LEU:HA	1.79	0.63
2:E:4146:ILE:HD12	2:E:4962:GLN:HB2	1.81	0.63
2:H:1299:ILE:HG12	2:H:1546:GLN:HG2	1.81	0.63
2:K:299:HIS:HE2	2:K:301:THR:HG1	1.40	0.63
2:B:1299:ILE:HG12	2:B:1546:GLN:HG2	1.81	0.62
2:K:4146:ILE:HD12	2:K:4962:GLN:HB2	1.81	0.62
2:B:3806:LEU:CD1	2:K:76:ARG:NH2	2.59	0.62
1:G:77:THR:HG22	1:G:79:ASP:H	1.63	0.62
2:K:476:GLN:HE22	2:K:3678:THR:HG22	1.65	0.62
2:B:247:VAL:O	2:B:272:ARG:NH1	2.30	0.62
2:B:80:GLU:HG3	2:E:3891:TRP:HZ3	1.63	0.62
2:B:4811:LEU:HD22	2:E:4520:PHE:CE1	2.35	0.62
1:J:77:THR:HG22	1:J:79:ASP:H	1.63	0.62
2:B:476:GLN:HE22	2:B:3678:THR:HG22	1.65	0.62
1:D:77:THR:HG22	1:D:79:ASP:H	1.63	0.62
2:B:143:LEU:HD12	2:E:2427:LEU:CD1	2.30	0.62
2:B:4146:ILE:HD12	2:B:4962:GLN:HB2	1.81	0.62
2:B:4808:ASP:OD2	2:E:4523:VAL:HG21	1.99	0.62
2:E:80:GLU:HG3	2:H:3891:TRP:HZ3	1.63	0.62
1:A:77:THR:HG22	1:A:79:ASP:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:476:GLN:HE22	2:E:3678:THR:HG22	1.65	0.62
2:H:76:ARG:NH2	2:K:3806:LEU:CD1	2.60	0.61
2:H:476:GLN:HE22	2:H:3678:THR:HG22	1.65	0.61
2:K:4020:MET:CE	2:K:4063:GLU:HB3	2.31	0.61
2:K:4031:ASP:HB3	2:K:4035:GLU:HB2	1.83	0.61
2:B:3891:TRP:HZ3	2:K:80:GLU:HG3	1.64	0.61
2:E:1299:ILE:HG12	2:E:1546:GLN:HG2	1.81	0.61
2:H:4031:ASP:HB3	2:H:4035:GLU:HB2	1.83	0.61
2:K:247:VAL:O	2:K:272:ARG:NH1	2.30	0.61
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.83	0.61
2:B:1114:ARG:HB3	2:B:1128:LEU:HD22	1.83	0.61
2:B:4020:MET:CE	2:B:4063:GLU:HB3	2.30	0.61
2:K:195:SER:HB3	2:K:202:HIS:HB2	1.82	0.61
2:E:694:ARG:HB2	2:E:793:SER:HB2	1.83	0.61
2:E:4020:MET:CE	2:E:4063:GLU:HB3	2.30	0.61
2:K:930:ASN:HA	2:K:933:LEU:HB2	1.83	0.61
2:B:4810:MET:CB	2:E:4519:LEU:O	2.49	0.61
2:E:4022:LEU:HA	2:E:4089:HIS:HE1	1.66	0.61
2:H:195:SER:HB3	2:H:202:HIS:HB2	1.82	0.61
2:H:80:GLU:HG3	2:K:3891:TRP:HZ3	1.65	0.60
2:K:1114:ARG:HB3	2:K:1128:LEU:HD22	1.83	0.60
2:B:4022:LEU:HA	2:B:4089:HIS:HE1	1.66	0.60
2:B:4031:ASP:HB3	2:B:4035:GLU:HB2	1.83	0.60
2:K:1272:ARG:NH1	2:K:1587:HIS:O	2.34	0.60
2:E:4031:ASP:HB3	2:E:4035:GLU:HB2	1.83	0.60
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.83	0.60
2:H:930:ASN:HA	2:H:933:LEU:HB2	1.83	0.60
2:B:195:SER:HB3	2:B:202:HIS:HB2	1.82	0.60
2:E:1114:ARG:HB3	2:E:1128:LEU:HD22	1.83	0.60
2:E:1272:ARG:NH1	2:E:1587:HIS:O	2.34	0.60
2:H:247:VAL:O	2:H:272:ARG:NH1	2.30	0.60
2:H:4020:MET:CE	2:H:4063:GLU:HB3	2.31	0.60
2:K:1299:ILE:HG12	2:K:1546:GLN:HG2	1.81	0.60
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.34	0.60
2:K:1249:MET:H	2:K:1603:PHE:HB2	1.67	0.60
2:B:2427:LEU:CD1	2:K:143:LEU:HD12	2.31	0.60
2:E:195:SER:HB3	2:E:202:HIS:HB2	1.82	0.60
2:E:3663:ASP:OD2	2:E:3735:ARG:NH2	2.35	0.60
2:H:1249:MET:H	2:H:1603:PHE:HB2	1.67	0.60
2:B:3663:ASP:OD2	2:B:3735:ARG:NH2	2.35	0.60
2:E:674:TYR:HB3	2:E:821:PRO:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3663:ASP:OD2	2:K:3735:ARG:NH2	2.35	0.60
2:H:3663:ASP:OD2	2:H:3735:ARG:NH2	2.35	0.60
2:K:4022:LEU:HA	2:K:4089:HIS:HE1	1.66	0.60
2:E:143:LEU:HD12	2:H:2427:LEU:CD1	2.32	0.60
2:H:191:TYR:CE2	2:K:2327:ARG:NH2	2.70	0.60
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.34	0.60
2:K:694:ARG:HB2	2:K:793:SER:HB2	1.83	0.60
2:B:930:ASN:HA	2:B:933:LEU:HB2	1.83	0.59
2:H:674:TYR:HB3	2:H:821:PRO:HA	1.84	0.59
2:E:1249:MET:H	2:E:1603:PHE:HB2	1.67	0.59
2:H:143:LEU:HD12	2:K:2427:LEU:CD1	2.32	0.59
2:H:1114:ARG:HB3	2:H:1128:LEU:HD22	1.83	0.59
2:H:4022:LEU:HA	2:H:4089:HIS:HE1	1.66	0.59
2:B:1171:HIS:ND1	2:B:1195:PHE:O	2.36	0.59
2:B:2327:ARG:NH2	2:K:191:TYR:CE2	2.70	0.59
2:E:191:TYR:CE2	2:H:2327:ARG:NH2	2.71	0.59
2:B:674:TYR:HB3	2:B:821:PRO:HA	1.84	0.59
2:B:1249:MET:H	2:B:1603:PHE:HB2	1.67	0.59
2:K:1090:ALA:HA	2:K:1249:MET:HG2	1.85	0.59
2:B:626:ARG:HD2	2:B:1669:ASN:HD21	1.68	0.59
2:B:1090:ALA:HA	2:B:1249:MET:HG2	1.85	0.59
2:E:930:ASN:HA	2:E:933:LEU:HB2	1.83	0.59
2:K:674:TYR:HB3	2:K:821:PRO:HA	1.84	0.59
2:K:3799:GLN:O	2:K:3881:ARG:NH1	2.35	0.59
2:B:76:ARG:NH2	2:E:3806:LEU:CD1	2.58	0.59
2:B:4791:ARG:HB3	2:B:4808:ASP:HB2	1.83	0.59
2:E:1090:ALA:HA	2:E:1249:MET:HG2	1.85	0.59
2:H:1754:SER:HB2	2:H:1758:ARG:HH12	1.68	0.58
2:B:3799:GLN:O	2:B:3881:ARG:NH1	2.35	0.58
2:E:76:ARG:NH2	2:H:3806:LEU:CD1	2.59	0.58
2:H:1090:ALA:HA	2:H:1249:MET:HG2	1.85	0.58
2:K:25:THR:HG22	2:K:34:LYS:HG2	1.85	0.58
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.85	0.58
2:E:1154:ARG:HH21	2:E:1177:LEU:HD23	1.68	0.58
2:K:1171:HIS:ND1	2:K:1195:PHE:O	2.36	0.58
2:K:1754:SER:HB2	2:K:1758:ARG:HH12	1.69	0.58
2:K:2770:GLU:HA	2:K:2773:ARG:HB2	1.85	0.58
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.69	0.58
2:E:480:ARG:NH2	2:E:3679:GLU:OE2	2.36	0.58
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.85	0.58
2:B:191:TYR:CE2	2:E:2327:ARG:NH2	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:HG1	1:D:49:ARG:HH21	1.48	0.58
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.69	0.58
2:B:1754:SER:HB2	2:B:1758:ARG:HH12	1.69	0.58
2:E:1754:SER:HB2	2:E:1758:ARG:HH12	1.69	0.58
2:E:2770:GLU:HA	2:E:2773:ARG:HB2	1.85	0.58
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.85	0.58
2:K:1154:ARG:HH21	2:K:1177:LEU:HD23	1.68	0.58
2:E:943:LEU:HB3	2:E:950:VAL:HG21	1.86	0.58
2:E:4124:GLU:HG3	2:E:4128:ASN:HD21	1.69	0.58
2:H:1154:ARG:HH21	2:H:1177:LEU:HD23	1.68	0.58
2:H:270:HIS:ND1	2:H:491:GLU:OE1	2.37	0.58
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.36	0.58
2:K:480:ARG:NH2	2:K:3679:GLU:OE2	2.36	0.58
2:K:626:ARG:HD2	2:K:1669:ASN:HD21	1.68	0.58
2:E:626:ARG:HD2	2:E:1669:ASN:HD21	1.68	0.58
2:K:4124:GLU:HG3	2:K:4128:ASN:HD21	1.69	0.58
2:K:706:TYR:OH	2:K:1086:ARG:NH2	2.37	0.58
2:B:270:HIS:ND1	2:B:491:GLU:OE1	2.37	0.57
2:B:943:LEU:HB3	2:B:950:VAL:HG21	1.86	0.57
2:B:2275:LEU:H	2:B:2293:PRO:HD3	1.69	0.57
2:E:3799:GLN:O	2:E:3881:ARG:NH1	2.35	0.57
2:E:3805:ASP:OD2	2:E:3809:PHE:N	2.37	0.57
2:H:943:LEU:HB3	2:H:950:VAL:HG11	1.86	0.57
2:K:248:PRO:HD3	2:K:261:HIS:HD2	1.69	0.57
2:B:1146:HIS:HB2	2:B:1192:PHE:HE1	1.70	0.57
2:E:270:HIS:ND1	2:E:491:GLU:OE1	2.37	0.57
2:E:1171:HIS:ND1	2:E:1195:PHE:O	2.36	0.57
2:H:626:ARG:HD2	2:H:1669:ASN:HD21	1.68	0.57
2:K:300:VAL:O	2:K:420:ARG:NH2	2.37	0.57
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.85	0.57
2:K:375:GLN:HE21	2:K:392:ILE:HD13	1.69	0.57
2:E:706:TYR:OH	2:E:1086:ARG:NH2	2.37	0.57
2:H:2436:VAL:O	2:H:2466:LYS:NZ	2.38	0.57
2:E:1628:MET:HB2	2:E:1687:TYR:HE2	1.70	0.57
2:H:300:VAL:O	2:H:420:ARG:NH2	2.37	0.57
2:B:300:VAL:O	2:B:420:ARG:NH2	2.37	0.57
2:B:375:GLN:HE21	2:B:392:ILE:HD13	1.69	0.57
2:E:248:PRO:HD3	2:E:261:HIS:HD2	1.69	0.57
2:E:375:GLN:HE21	2:E:392:ILE:HD13	1.69	0.57
2:E:2436:VAL:O	2:E:2466:LYS:NZ	2.38	0.57
2:B:2436:VAL:O	2:B:2466:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:867:VAL:O	2:E:1002:ASN:ND2	2.38	0.57
2:H:1171:HIS:ND1	2:H:1195:PHE:O	2.36	0.57
2:H:1628:MET:HB2	2:H:1687:TYR:HE2	1.70	0.57
2:H:3799:GLN:O	2:H:3881:ARG:NH1	2.35	0.57
2:K:1146:HIS:HB2	2:K:1192:PHE:HE1	1.70	0.57
2:B:248:PRO:HD3	2:B:261:HIS:HD2	1.69	0.57
2:E:25:THR:HG22	2:E:34:LYS:HG2	1.85	0.57
2:E:2275:LEU:H	2:E:2293:PRO:HD3	1.69	0.57
2:K:270:HIS:ND1	2:K:491:GLU:OE1	2.37	0.57
2:K:3805:ASP:OD2	2:K:3809:PHE:N	2.37	0.57
2:E:300:VAL:O	2:E:420:ARG:NH2	2.37	0.57
2:E:954:ASP:HB2	2:E:1061:GLY:HA3	1.87	0.57
2:H:706:TYR:OH	2:H:1086:ARG:NH2	2.37	0.57
2:K:4192:ASN:OD1	2:K:4605:LYS:NZ	2.29	0.57
2:K:4890:PHE:H	7:K:6003:ATP:HN61	1.53	0.57
2:B:278:GLU:HB2	2:B:296:ARG:HB2	1.87	0.56
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.36	0.56
2:B:1154:ARG:HH21	2:B:1177:LEU:HD23	1.68	0.56
2:H:375:GLN:HE21	2:H:392:ILE:HD13	1.69	0.56
1:J:23:VAL:HB	1:J:105:ASN:H	1.70	0.56
2:B:867:VAL:O	2:B:1002:ASN:ND2	2.38	0.56
2:B:3901:GLU:OE1	2:B:3902:GLN:NE2	2.39	0.56
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.23	0.56
2:H:3805:ASP:OD2	2:H:3809:PHE:N	2.37	0.56
2:K:1628:MET:HB2	2:K:1687:TYR:HE2	1.70	0.56
2:K:2275:LEU:H	2:K:2293:PRO:HD3	1.69	0.56
2:B:954:ASP:HB2	2:B:1061:GLY:HA3	1.87	0.56
2:B:3805:ASP:OD2	2:B:3809:PHE:N	2.37	0.56
2:E:1146:HIS:HB2	2:E:1192:PHE:HE1	1.70	0.56
2:E:2834:LEU:HD11	2:E:2894:LEU:HB3	1.88	0.56
2:E:4159:THR:O	2:E:4163:LYS:NZ	2.37	0.56
1:G:23:VAL:HB	1:G:105:ASN:H	1.70	0.56
2:H:248:PRO:HD3	2:H:261:HIS:HD2	1.69	0.56
2:H:867:VAL:O	2:H:1002:ASN:ND2	2.38	0.56
2:H:4890:PHE:H	7:H:6003:ATP:HN61	1.53	0.56
2:K:867:VAL:O	2:K:1002:ASN:ND2	2.38	0.56
2:K:3901:GLU:OE1	2:K:3902:GLN:NE2	2.39	0.56
2:B:2464:ASP:OD1	2:B:2464:ASP:N	2.36	0.56
2:E:2521:LEU:HD22	2:E:2565:ALA:HB2	1.88	0.56
2:E:2707:VAL:HG21	2:E:2786:TRP:HE1	1.71	0.56
2:H:954:ASP:HB2	2:H:1061:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3901:GLU:OE1	2:H:3902:GLN:NE2	2.39	0.56
2:H:4159:THR:O	2:H:4163:LYS:NZ	2.37	0.56
2:K:943:LEU:HB3	2:K:950:VAL:HG11	1.86	0.56
2:B:4791:ARG:CB	2:B:4808:ASP:CB	2.84	0.56
2:B:4890:PHE:H	7:B:6003:ATP:HN61	1.53	0.56
2:E:3901:GLU:OE1	2:E:3902:GLN:NE2	2.39	0.56
2:H:2275:LEU:H	2:H:2293:PRO:HD3	1.69	0.56
2:H:2707:VAL:HG21	2:H:2786:TRP:HE1	1.71	0.56
2:K:954:ASP:HB2	2:K:1061:GLY:HA3	1.87	0.56
1:D:23:VAL:HB	1:D:105:ASN:H	1.70	0.56
2:E:1144:ARG:NH2	2:E:1150:GLU:OE1	2.39	0.56
2:K:2436:VAL:O	2:K:2466:LYS:NZ	2.38	0.56
2:B:4168:GLU:HB2	2:B:4171:ARG:NH1	2.20	0.56
2:E:278:GLU:HB2	2:E:296:ARG:HB2	1.87	0.56
2:H:2521:LEU:HD22	2:H:2565:ALA:HB2	1.87	0.56
2:K:1144:ARG:NH2	2:K:1150:GLU:OE1	2.39	0.56
1:A:23:VAL:HB	1:A:105:ASN:H	1.70	0.56
2:B:1628:MET:HB2	2:B:1687:TYR:HE2	1.70	0.56
2:B:2834:LEU:HD11	2:B:2894:LEU:HB3	1.88	0.56
2:H:1303:ARG:HH22	2:H:1595:LEU:HD13	1.71	0.56
2:K:833:LYS:HA	2:K:1614:ARG:HH12	1.71	0.56
2:H:1144:ARG:NH2	2:H:1150:GLU:OE1	2.39	0.56
2:B:706:TYR:OH	2:B:1086:ARG:NH2	2.37	0.56
2:B:1303:ARG:HH22	2:B:1595:LEU:HD13	1.71	0.56
2:H:278:GLU:HB2	2:H:296:ARG:HB2	1.87	0.56
2:H:1146:HIS:HB2	2:H:1192:PHE:HE1	1.70	0.56
2:B:2426:SER:HG	2:K:143:LEU:HD13	1.70	0.55
2:K:278:GLU:HB2	2:K:296:ARG:HB2	1.87	0.55
2:K:4085:VAL:O	2:K:4089:HIS:N	2.40	0.55
2:B:1144:ARG:NH2	2:B:1150:GLU:OE1	2.39	0.55
2:B:2521:LEU:HD22	2:B:2565:ALA:HB2	1.87	0.55
2:E:4890:PHE:H	7:E:6003:ATP:HN61	1.54	0.55
2:K:417:ARG:HH11	2:K:420:ARG:HH11	1.55	0.55
2:B:289:ILE:HG22	2:B:354:ILE:HD12	1.88	0.55
2:B:417:ARG:HH11	2:B:420:ARG:HH11	1.54	0.55
2:H:2834:LEU:HD11	2:H:2894:LEU:HB3	1.88	0.55
2:H:289:ILE:HG22	2:H:354:ILE:HD12	1.88	0.55
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.72	0.55
2:K:1303:ARG:HH22	2:K:1595:LEU:HD13	1.71	0.55
2:E:833:LYS:HA	2:E:1614:ARG:HH12	1.71	0.55
2:H:231:GLY:O	2:H:276:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:289:ILE:HG22	2:K:354:ILE:HD12	1.88	0.55
2:K:2521:LEU:HD22	2:K:2565:ALA:HB2	1.87	0.55
2:B:833:LYS:HA	2:B:1614:ARG:HH12	1.71	0.55
2:E:1303:ARG:HH22	2:E:1595:LEU:HD13	1.71	0.55
2:E:3919:ASN:O	2:E:3922:THR:OG1	2.23	0.55
2:B:2707:VAL:HG21	2:B:2786:TRP:HE1	1.71	0.54
2:E:289:ILE:HG22	2:E:354:ILE:HD12	1.88	0.54
2:H:833:LYS:HA	2:H:1614:ARG:HH12	1.71	0.54
2:K:231:GLY:O	2:K:276:ARG:NH1	2.40	0.54
2:K:298:ARG:HE	2:K:303:GLY:HA2	1.72	0.54
2:K:2834:LEU:HD11	2:K:2894:LEU:HB3	1.88	0.54
2:B:841:LYS:HB2	2:B:848:ARG:HD3	1.90	0.54
2:E:1572:LYS:HE2	2:E:1585:ARG:HB3	1.90	0.54
2:K:288:HIS:ND1	2:K:349:MET:O	2.40	0.54
2:K:841:LYS:HB2	2:K:848:ARG:HD3	1.90	0.54
2:B:1572:LYS:HE2	2:B:1585:ARG:HB3	1.90	0.54
2:H:1242:ASN:HB2	2:H:1807:ARG:HG2	1.90	0.54
2:K:2707:VAL:HG21	2:K:2786:TRP:HE1	1.71	0.54
2:H:1303:ARG:HB2	2:H:1593:HIS:HB2	1.90	0.54
2:B:288:HIS:ND1	2:B:349:MET:O	2.40	0.54
2:B:3800:SER:OG	2:B:3801:CYS:N	2.41	0.54
2:B:4791:ARG:HB2	2:B:4808:ASP:CB	2.38	0.54
2:E:231:GLY:O	2:E:276:ARG:NH1	2.40	0.54
2:B:626:ARG:NH2	2:B:1667:LEU:O	2.41	0.54
2:H:143:LEU:CD1	2:K:2427:LEU:CD1	2.86	0.54
2:H:841:LYS:HB2	2:H:848:ARG:HD3	1.90	0.54
2:K:626:ARG:NH2	2:K:1667:LEU:O	2.41	0.54
2:K:1242:ASN:HB2	2:K:1807:ARG:HG2	1.90	0.54
2:E:674:TYR:OH	2:E:676:GLU:OE2	2.21	0.54
2:H:288:HIS:ND1	2:H:349:MET:O	2.40	0.54
2:B:231:GLY:O	2:B:276:ARG:NH1	2.40	0.54
2:H:417:ARG:HH11	2:H:420:ARG:HH11	1.55	0.54
2:H:1272:ARG:HG3	2:H:1586:LEU:HD13	1.90	0.54
2:B:756:SER:HB3	2:B:769:ARG:H	1.73	0.54
2:B:2413:ALA:HB1	2:B:2418:ILE:HD11	1.90	0.54
2:E:841:LYS:HB2	2:E:848:ARG:HD3	1.90	0.54
2:E:4497:ALA:HB1	2:E:4594:LEU:HD13	1.90	0.54
2:H:626:ARG:NH2	2:H:1667:LEU:O	2.41	0.54
2:H:681:HIS:HB2	2:H:799:LYS:HG2	1.90	0.54
2:B:4085:VAL:O	2:B:4089:HIS:N	2.40	0.53
2:B:156:GLU:OE1	2:E:2419:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4159:THR:O	2:B:4163:LYS:NZ	2.37	0.53
2:E:417:ARG:HH11	2:E:420:ARG:HH11	1.55	0.53
2:E:844:ARG:HG2	2:E:846:TYR:H	1.74	0.53
2:H:207:PHE:CE1	2:K:2326:ILE:HG23	2.43	0.53
2:K:1572:LYS:HE2	2:K:1585:ARG:HB3	1.90	0.53
2:K:2464:ASP:OD1	2:K:2464:ASP:N	2.36	0.53
2:B:1429:SER:HA	2:B:1507:ILE:HG12	1.90	0.53
2:E:288:HIS:ND1	2:E:349:MET:O	2.40	0.53
2:K:309:MET:O	2:K:313:SER:N	2.42	0.53
2:E:298:ARG:HE	2:E:303:GLY:HA2	1.72	0.53
2:E:626:ARG:NH2	2:E:1667:LEU:O	2.41	0.53
2:E:2413:ALA:HB1	2:E:2418:ILE:HD11	1.91	0.53
2:E:1242:ASN:HB2	2:E:1807:ARG:HG2	1.90	0.53
2:E:1303:ARG:HB2	2:E:1593:HIS:HB2	1.90	0.53
2:H:1572:LYS:HE2	2:H:1585:ARG:HB3	1.90	0.53
2:K:1429:SER:HA	2:K:1507:ILE:HG12	1.91	0.53
2:B:681:HIS:HB2	2:B:799:LYS:HG2	1.90	0.53
2:E:1272:ARG:HG3	2:E:1586:LEU:HD13	1.90	0.53
2:K:1272:ARG:NH2	2:K:1590:PHE:O	2.42	0.53
2:B:1242:ASN:HB2	2:B:1807:ARG:HG2	1.90	0.53
2:B:4020:MET:CE	2:B:4067:LEU:HD13	2.39	0.53
2:B:4497:ALA:HB1	2:B:4594:LEU:HD13	1.90	0.53
2:E:66:THR:HG1	2:E:124:SER:HG	1.53	0.53
2:E:143:LEU:CD1	2:H:2427:LEU:CD1	2.86	0.53
2:H:309:MET:O	2:H:313:SER:N	2.42	0.53
2:H:756:SER:HB3	2:H:769:ARG:H	1.73	0.53
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.42	0.53
2:K:681:HIS:HB2	2:K:799:LYS:HG2	1.90	0.53
2:K:844:ARG:HG2	2:K:846:TYR:H	1.74	0.53
2:B:844:ARG:HG2	2:B:846:TYR:H	1.74	0.53
2:K:1272:ARG:HG3	2:K:1586:LEU:HD13	1.90	0.53
2:K:2413:ALA:HB1	2:K:2418:ILE:HD11	1.90	0.53
2:K:4020:MET:CE	2:K:4067:LEU:HD13	2.39	0.53
2:B:4787:PHE:CD1	2:B:4808:ASP:O	2.56	0.53
2:E:156:GLU:OE1	2:H:2419:ARG:NH1	2.42	0.53
2:E:681:HIS:HB2	2:E:799:LYS:HG2	1.90	0.53
2:K:674:TYR:OH	2:K:676:GLU:OE2	2.21	0.53
2:B:309:MET:O	2:B:313:SER:N	2.42	0.53
2:B:1303:ARG:HB2	2:B:1593:HIS:HB2	1.90	0.53
2:E:1429:SER:HA	2:E:1507:ILE:HG12	1.91	0.53
2:H:2413:ALA:HB1	2:H:2418:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:466:PRO:HB3	2:K:478:ARG:HD2	1.91	0.53
2:K:2406:GLU:O	2:K:2410:ILE:N	2.42	0.53
2:E:309:MET:O	2:E:313:SER:N	2.42	0.52
2:E:716:ASN:HA	2:E:722:LEU:HD13	1.91	0.52
2:E:4020:MET:CE	2:E:4067:LEU:HD13	2.39	0.52
2:E:4085:VAL:O	2:E:4089:HIS:N	2.40	0.52
2:E:4605:LYS:HG3	2:E:4645:TYR:HE1	1.73	0.52
2:H:466:PRO:HB3	2:H:478:ARG:HD2	1.91	0.52
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	1.91	0.52
2:H:4020:MET:CE	2:H:4067:LEU:HD13	2.39	0.52
2:K:2116:ASP:OD1	2:K:2153:ASN:ND2	2.43	0.52
2:K:4159:THR:O	2:K:4163:LYS:NZ	2.37	0.52
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.72	0.52
2:B:1272:ARG:HG3	2:B:1586:LEU:HD13	1.90	0.52
2:B:4605:LYS:HG3	2:B:4645:TYR:HE1	1.73	0.52
2:E:756:SER:HB3	2:E:769:ARG:H	1.74	0.52
2:K:1250:TRP:HB3	2:K:1600:PRO:HB2	1.91	0.52
2:E:308:LEU:HD21	2:E:370:LEU:HD12	1.91	0.52
2:K:66:THR:OG1	2:K:124:SER:OG	2.25	0.52
2:K:756:SER:HB3	2:K:769:ARG:H	1.74	0.52
2:K:3800:SER:OG	2:K:3801:CYS:N	2.41	0.52
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.42	0.52
2:H:308:LEU:HD21	2:H:370:LEU:HD12	1.91	0.52
2:H:844:ARG:HG2	2:H:846:TYR:H	1.74	0.52
2:H:1114:ARG:NH1	2:H:1128:LEU:O	2.43	0.52
2:H:4085:VAL:O	2:H:4089:HIS:N	2.40	0.52
2:K:4605:LYS:HG3	2:K:4645:TYR:HE1	1.73	0.52
2:B:716:ASN:HA	2:B:722:LEU:HD13	1.91	0.52
2:B:2419:ARG:NH1	2:K:156:GLU:OE1	2.42	0.52
2:E:1250:TRP:HB3	2:E:1600:PRO:HB2	1.91	0.52
2:H:1429:SER:HA	2:H:1507:ILE:HG12	1.91	0.52
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.23	0.52
2:K:3729:GLN:O	2:K:3733:HIS:ND1	2.43	0.52
2:H:716:ASN:HA	2:H:722:LEU:HD13	1.91	0.52
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.43	0.52
2:K:1114:ARG:NH1	2:K:1128:LEU:O	2.43	0.52
1:G:21:THR:HG1	1:G:49:ARG:HH21	1.54	0.52
2:H:4605:LYS:HG3	2:H:4645:TYR:HE1	1.73	0.52
2:K:644:LEU:HD22	2:K:1632:ILE:HG22	1.92	0.52
2:K:4497:ALA:HB1	2:K:4594:LEU:HD13	1.90	0.52
2:B:4192:ASN:OD1	2:B:4605:LYS:NZ	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3800:SER:OG	2:E:3801:CYS:N	2.41	0.52
2:H:687:THR:HG23	2:H:1626:GLN:HE21	1.75	0.52
2:K:1303:ARG:HB2	2:K:1593:HIS:HB2	1.90	0.52
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.43	0.51
2:B:2406:GLU:O	2:B:2410:ILE:N	2.42	0.51
2:E:466:PRO:HB3	2:E:478:ARG:HD2	1.91	0.51
2:E:1114:ARG:NH1	2:E:1128:LEU:O	2.43	0.51
2:E:2116:ASP:OD1	2:E:2153:ASN:ND2	2.43	0.51
2:E:2730:HIS:NE2	2:E:2759:LYS:O	2.43	0.51
2:K:1260:GLN:HG2	2:K:1591:LEU:HD13	1.92	0.51
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	1.92	0.51
2:B:2427:LEU:CD1	2:K:143:LEU:CD1	2.86	0.51
2:E:279:THR:O	2:E:296:ARG:NH2	2.43	0.51
2:E:805:GLY:HA2	2:E:810:GLU:HB2	1.92	0.51
2:E:1272:ARG:NH2	2:E:1590:PHE:O	2.42	0.51
2:E:2406:GLU:O	2:E:2410:ILE:N	2.42	0.51
2:H:4497:ALA:HB1	2:H:4594:LEU:HD13	1.90	0.51
2:B:279:THR:O	2:B:296:ARG:NH2	2.43	0.51
2:K:559:ILE:HD13	2:K:593:HIS:HB3	1.93	0.51
2:B:176:ARG:N	2:B:179:ASP:OD2	2.44	0.51
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.93	0.51
2:B:2730:HIS:NE2	2:B:2759:LYS:O	2.43	0.51
2:E:559:ILE:HD13	2:E:593:HIS:HB3	1.93	0.51
2:K:1209:VAL:N	2:K:1211:GLN:OE1	2.44	0.51
2:B:687:THR:HG23	2:B:1626:GLN:HE21	1.75	0.51
2:B:1209:VAL:N	2:B:1211:GLN:OE1	2.44	0.51
2:K:1111:GLY:HA3	2:K:1211:GLN:HE21	1.76	0.51
2:B:466:PRO:HB3	2:B:478:ARG:HD2	1.91	0.51
2:E:20:VAL:HG12	2:E:216:PRO:HA	1.93	0.51
2:E:644:LEU:HD22	2:E:1632:ILE:HG22	1.92	0.51
2:H:20:VAL:HG12	2:H:216:PRO:HA	1.93	0.51
2:H:182:ILE:HD11	2:H:211:LEU:HD23	1.92	0.51
2:H:279:THR:O	2:H:296:ARG:NH2	2.43	0.51
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.93	0.51
2:K:308:LEU:HD21	2:K:370:LEU:HD12	1.91	0.51
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.92	0.51
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.43	0.51
1:D:27:THR:HA	1:D:38:SER:HA	1.93	0.51
2:K:176:ARG:N	2:K:179:ASP:OD2	2.44	0.51
2:B:308:LEU:HD21	2:B:370:LEU:HD12	1.91	0.51
2:B:760:ASP:HB2	2:B:763:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:TYR:HA	2:E:201:LEU:HD23	1.92	0.51
2:E:4192:ASN:OD1	2:E:4605:LYS:NZ	2.29	0.51
2:H:176:ARG:N	2:H:179:ASP:OD2	2.44	0.51
2:H:196:TYR:HA	2:H:201:LEU:HD23	1.92	0.51
1:J:9:PRO:HA	1:J:70:GLN:HG3	1.92	0.51
2:K:805:GLY:HA2	2:K:810:GLU:HB2	1.92	0.51
1:D:9:PRO:HA	1:D:70:GLN:HG3	1.92	0.51
2:E:1209:VAL:N	2:E:1211:GLN:OE1	2.44	0.51
2:H:1209:VAL:N	2:H:1211:GLN:OE1	2.44	0.51
2:K:687:THR:HG23	2:K:1626:GLN:HE21	1.75	0.51
2:K:2730:HIS:NE2	2:K:2759:LYS:O	2.43	0.51
2:B:3729:GLN:O	2:B:3733:HIS:ND1	2.43	0.51
2:E:182:ILE:HD11	2:E:211:LEU:HD23	1.92	0.51
2:E:672:LYS:HA	2:E:760:ASP:HA	1.93	0.51
2:E:760:ASP:HB2	2:E:763:ALA:HB3	1.93	0.51
2:E:4020:MET:HE2	2:E:4063:GLU:HB3	1.93	0.51
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.38	0.51
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.92	0.51
2:K:196:TYR:HA	2:K:201:LEU:HD23	1.92	0.51
2:K:672:LYS:HA	2:K:760:ASP:HA	1.93	0.51
2:K:716:ASN:HA	2:K:722:LEU:HD13	1.91	0.51
1:A:9:PRO:HA	1:A:70:GLN:HG3	1.92	0.50
2:B:143:LEU:CD1	2:E:2427:LEU:CD1	2.85	0.50
2:B:672:LYS:HA	2:B:760:ASP:HA	1.93	0.50
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.92	0.50
3:C:27:THR:HA	3:C:63:THR:HB	1.94	0.50
2:E:1847:GLU:OE1	2:E:1849:SER:OG	2.25	0.50
2:E:4486:ILE:HG22	2:E:4489:GLN:H	1.77	0.50
2:H:156:GLU:OE1	2:K:2419:ARG:NH1	2.43	0.50
2:K:644:LEU:HB3	2:K:1630:LEU:HD12	1.94	0.50
2:K:1114:ARG:HB2	2:K:1206:SER:HB3	1.92	0.50
2:K:3919:ASN:O	2:K:3922:THR:OG1	2.23	0.50
2:B:196:TYR:HA	2:B:201:LEU:HD23	1.92	0.50
2:B:1038:LEU:HD12	2:B:1043:LYS:HE3	1.94	0.50
2:E:43:GLY:H	2:E:45:ARG:HH12	1.59	0.50
2:E:1038:LEU:HD12	2:E:1043:LYS:HE3	1.94	0.50
2:H:2114:VAL:O	2:H:2117:THR:OG1	2.28	0.50
2:K:4616:LEU:HA	2:K:4620:GLU:HB2	1.93	0.50
3:L:27:THR:HA	3:L:63:THR:HB	1.94	0.50
2:B:1303:ARG:O	2:B:1593:HIS:N	2.45	0.50
2:E:687:THR:HG23	2:E:1626:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1771:ILE:HG22	2:E:1773:ASN:H	1.76	0.50
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.76	0.50
1:J:27:THR:HA	1:J:38:SER:HA	1.93	0.50
2:B:43:GLY:H	2:B:45:ARG:HH12	1.59	0.50
2:E:644:LEU:HB3	2:E:1630:LEU:HD12	1.94	0.50
2:E:1114:ARG:HB2	2:E:1206:SER:HB3	1.92	0.50
2:H:43:GLY:H	2:H:45:ARG:HH12	1.59	0.50
2:H:805:GLY:HA2	2:H:810:GLU:HB2	1.92	0.50
2:K:279:THR:O	2:K:296:ARG:NH2	2.43	0.50
2:B:295:PHE:N	2:B:329:PHE:O	2.44	0.50
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.76	0.50
2:E:1260:GLN:HG2	2:E:1591:LEU:HD13	1.92	0.50
2:E:4167:LYS:NZ	7:E:6003:ATP:O2B	2.44	0.50
1:G:27:THR:HA	1:G:38:SER:HA	1.93	0.50
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.92	0.50
2:H:672:LYS:HA	2:H:760:ASP:HA	1.92	0.50
2:H:1303:ARG:O	2:H:1593:HIS:N	2.45	0.50
2:H:4486:ILE:HG22	2:H:4489:GLN:H	1.77	0.50
2:K:182:ILE:HD11	2:K:211:LEU:HD23	1.92	0.50
2:K:295:PHE:N	2:K:329:PHE:O	2.44	0.50
2:K:760:ASP:HB2	2:K:763:ALA:HB3	1.93	0.50
2:K:1303:ARG:O	2:K:1593:HIS:N	2.45	0.50
2:B:805:GLY:HA2	2:B:810:GLU:HB2	1.92	0.50
2:E:176:ARG:N	2:E:179:ASP:OD2	2.44	0.50
3:F:27:THR:HA	3:F:63:THR:HB	1.94	0.50
1:G:9:PRO:HA	1:G:70:GLN:HG3	1.92	0.50
2:H:1038:LEU:HD12	2:H:1043:LYS:HE3	1.94	0.50
2:H:4616:LEU:HA	2:H:4620:GLU:HB2	1.93	0.50
2:K:20:VAL:HG12	2:K:216:PRO:HA	1.93	0.50
2:H:1171:HIS:HE1	2:H:1197:VAL:H	1.60	0.50
2:B:20:VAL:HG12	2:B:216:PRO:HA	1.93	0.50
2:B:182:ILE:HD11	2:B:211:LEU:HD23	1.92	0.50
2:B:1260:GLN:HG2	2:B:1591:LEU:HD13	1.92	0.50
2:B:2832:VAL:O	2:B:2895:LYS:NZ	2.38	0.50
2:B:3803:VAL:HG22	2:B:3881:ARG:HH21	1.77	0.50
2:E:1611:ILE:HB	2:E:1620:GLN:HB3	1.94	0.50
2:E:4616:LEU:HA	2:E:4620:GLU:HB2	1.93	0.50
2:H:1304:LEU:HB3	2:H:1541:PRO:HG2	1.94	0.50
2:H:2730:HIS:NE2	2:H:2759:LYS:O	2.43	0.50
2:K:1171:HIS:HE1	2:K:1197:VAL:H	1.60	0.50
2:B:693:LEU:HD13	2:B:749:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1304:LEU:HB3	2:B:1541:PRO:HG2	1.94	0.50
2:E:1111:GLY:HA3	2:E:1211:GLN:HE21	1.76	0.50
2:H:1847:GLU:OE1	2:H:1849:SER:OG	2.25	0.50
3:I:27:THR:HA	3:I:63:THR:HB	1.94	0.50
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.30	0.49
2:B:1611:ILE:HB	2:B:1620:GLN:HB3	1.94	0.49
2:B:1771:ILE:HG22	2:B:1773:ASN:H	1.76	0.49
2:B:4486:ILE:HG22	2:B:4489:GLN:H	1.77	0.49
2:B:4521:TYR:HB3	2:K:4787:PHE:CZ	2.47	0.49
2:H:1771:ILE:HG22	2:H:1773:ASN:H	1.76	0.49
2:K:3803:VAL:HG22	2:K:3881:ARG:HH21	1.77	0.49
2:H:693:LEU:HD13	2:H:749:LEU:HD22	1.94	0.49
2:H:4787:PHE:CZ	2:K:4521:TYR:HB3	2.46	0.49
2:K:4486:ILE:HG22	2:K:4489:GLN:H	1.77	0.49
2:B:1154:ARG:NH2	2:B:1180:GLU:OE1	2.46	0.49
2:B:4616:LEU:HA	2:B:4620:GLU:HB2	1.93	0.49
2:H:295:PHE:N	2:H:329:PHE:O	2.44	0.49
2:H:1443:VAL:HB	2:H:1489:CYS:HB2	1.94	0.49
2:K:693:LEU:HD13	2:K:749:LEU:HD22	1.94	0.49
2:K:748:LEU:HD22	2:K:750:ARG:HE	1.78	0.49
2:K:1038:LEU:HD12	2:K:1043:LYS:HE3	1.94	0.49
2:K:1304:LEU:HB3	2:K:1541:PRO:HG2	1.94	0.49
2:B:644:LEU:HB3	2:B:1630:LEU:HD12	1.94	0.49
2:B:4168:GLU:CB	2:B:4171:ARG:NH1	2.75	0.49
2:B:4722:TYR:OH	2:B:4746:ASP:OD1	2.23	0.49
2:H:760:ASP:HB2	2:H:763:ALA:HB3	1.93	0.49
2:K:2114:VAL:O	2:K:2117:THR:OG1	2.28	0.49
2:B:4167:LYS:NZ	7:B:6003:ATP:O2B	2.44	0.49
2:H:991:SER:OG	2:H:1064:LEU:O	2.30	0.49
2:H:1260:GLN:HG2	2:H:1591:LEU:HD13	1.92	0.49
2:H:1611:ILE:HB	2:H:1620:GLN:HB3	1.94	0.49
2:K:1443:VAL:HB	2:K:1489:CYS:HB2	1.94	0.49
2:K:1611:ILE:HB	2:K:1620:GLN:HB3	1.94	0.49
2:K:1771:ILE:HG22	2:K:1773:ASN:H	1.76	0.49
2:B:748:LEU:HD22	2:B:750:ARG:HE	1.78	0.49
2:B:1171:HIS:HE1	2:B:1197:VAL:H	1.60	0.49
2:E:1304:LEU:HB3	2:E:1541:PRO:HG2	1.94	0.49
2:H:1154:ARG:NH2	2:H:1180:GLU:OE1	2.46	0.49
2:B:991:SER:OG	2:B:1064:LEU:O	2.30	0.49
2:B:1242:ASN:HD22	2:B:1807:ARG:HD2	1.78	0.49
2:B:4787:PHE:CZ	2:E:4521:TYR:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1184:ASP:N	2:E:1188:SER:O	2.45	0.49
2:H:3803:VAL:HG22	2:H:3881:ARG:HH21	1.77	0.49
2:K:1242:ASN:HD22	2:K:1807:ARG:HD2	1.78	0.49
2:K:1847:GLU:OE1	2:K:1849:SER:OG	2.25	0.49
1:A:27:THR:HA	1:A:38:SER:HA	1.93	0.49
2:E:3803:VAL:HG22	2:E:3881:ARG:HH21	1.77	0.49
2:E:4164:PRO:HB2	2:E:4165:GLN:HG3	1.95	0.49
2:E:4207:ILE:HD12	2:E:4494:ASN:HD22	1.78	0.49
2:E:295:PHE:N	2:E:329:PHE:O	2.44	0.49
2:E:991:SER:OG	2:E:1064:LEU:O	2.30	0.49
2:H:748:LEU:HD22	2:H:750:ARG:HE	1.77	0.49
2:H:2832:VAL:O	2:H:2895:LYS:NZ	2.38	0.49
2:H:4164:PRO:HB2	2:H:4165:GLN:HG3	1.95	0.49
2:B:76:ARG:NH2	2:E:3806:LEU:CD2	2.71	0.49
2:B:4207:ILE:HD12	2:B:4494:ASN:HD22	1.78	0.49
2:B:4910:THR:HG21	7:B:6003:ATP:C5	2.48	0.49
2:E:1154:ARG:NH2	2:E:1180:GLU:OE1	2.46	0.49
2:H:1589:GLN:NE2	2:H:1634:GLU:OE1	2.46	0.49
2:H:3977:LYS:HB2	2:H:4095:ILE:HG13	1.95	0.49
2:K:991:SER:OG	2:K:1064:LEU:O	2.30	0.49
2:B:1125:ASP:HA	2:B:1598:ARG:HH11	1.78	0.48
2:B:4791:ARG:HB2	2:B:4808:ASP:HB3	1.96	0.48
2:E:693:LEU:HD13	2:E:749:LEU:HD22	1.94	0.48
2:E:1171:HIS:HE1	2:E:1197:VAL:H	1.60	0.48
2:E:3729:GLN:O	2:E:3733:HIS:ND1	2.43	0.48
1:G:49:ARG:HB3	1:G:52:LYS:HE2	1.95	0.48
2:H:644:LEU:HB3	2:H:1630:LEU:HD12	1.94	0.48
2:H:1125:ASP:HA	2:H:1598:ARG:HH11	1.78	0.48
2:H:4207:ILE:HD12	2:H:4494:ASN:HD22	1.78	0.48
2:H:4655:MET:O	2:H:4664:ARG:NH1	2.46	0.48
2:K:43:GLY:H	2:K:45:ARG:HH12	1.59	0.48
2:K:2832:VAL:O	2:K:2895:LYS:NZ	2.38	0.48
1:A:49:ARG:HB3	1:A:52:LYS:HE2	1.95	0.48
2:B:674:TYR:OH	2:B:676:GLU:OE2	2.21	0.48
1:D:49:ARG:HB3	1:D:52:LYS:HE2	1.95	0.48
2:E:953:SER:OG	2:E:1061:GLY:O	2.32	0.48
2:E:1303:ARG:O	2:E:1593:HIS:N	2.45	0.48
2:E:3977:LYS:HB2	2:E:4095:ILE:HG13	1.95	0.48
2:H:4910:THR:HG21	7:H:6003:ATP:C5	2.48	0.48
1:J:49:ARG:HB3	1:J:52:LYS:HE2	1.95	0.48
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:GLY:O	2:B:243:GLU:N	2.46	0.48
2:B:1589:GLN:NE2	2:B:1634:GLU:OE1	2.46	0.48
2:B:4164:PRO:HB2	2:B:4165:GLN:HG3	1.95	0.48
2:E:1251:LEU:O	2:E:1601:ASN:N	2.47	0.48
2:H:1242:ASN:HD22	2:H:1807:ARG:HD2	1.78	0.48
2:K:218:SER:HB3	2:K:286:GLY:HA3	1.96	0.48
2:K:1733:THR:HG22	2:K:1755:THR:HB	1.96	0.48
2:K:3593:SER:O	2:K:3597:LYS:NZ	2.42	0.48
2:K:4207:ILE:HD12	2:K:4494:ASN:HD22	1.78	0.48
2:E:1443:VAL:HB	2:E:1489:CYS:HB2	1.94	0.48
2:E:4910:THR:HG21	7:E:6003:ATP:C5	2.48	0.48
2:H:58:VAL:HG22	2:H:320:GLU:HA	1.96	0.48
2:H:673:TRP:HE3	2:H:822:CYS:HA	1.78	0.48
3:I:37:MET:HB3	3:I:42:GLN:HB2	1.96	0.48
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.96	0.48
2:K:1154:ARG:NH2	2:K:1180:GLU:OE1	2.46	0.48
2:B:718:VAL:HA	2:B:736:CYS:N	2.29	0.48
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.95	0.48
2:H:799:LYS:HB3	2:H:1620:GLN:HG3	1.95	0.48
2:K:673:TRP:HE3	2:K:822:CYS:HA	1.78	0.48
2:K:4891:ILE:HD13	2:K:4914:HIS:HB3	1.95	0.48
2:K:4910:THR:HG21	7:K:6003:ATP:C5	2.48	0.48
2:B:1733:THR:HG22	2:B:1755:THR:HB	1.96	0.48
2:E:673:TRP:HE3	2:E:822:CYS:HA	1.78	0.48
2:E:748:LEU:HD22	2:E:750:ARG:HE	1.78	0.48
2:H:674:TYR:OH	2:H:676:GLU:OE2	2.21	0.48
2:H:1733:THR:HG22	2:H:1755:THR:HB	1.96	0.48
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.96	0.48
2:K:239:GLY:O	2:K:243:GLU:N	2.47	0.48
2:E:1242:ASN:HD22	2:E:1807:ARG:HD2	1.78	0.48
2:E:1733:THR:HG22	2:E:1755:THR:HB	1.96	0.48
2:E:4022:LEU:HD12	2:E:4089:HIS:CE1	2.49	0.48
2:H:239:GLY:O	2:H:243:GLU:N	2.46	0.48
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.95	0.48
2:K:718:VAL:HA	2:K:736:CYS:N	2.29	0.48
2:K:1589:GLN:NE2	2:K:1634:GLU:OE1	2.46	0.48
2:K:4164:PRO:HB2	2:K:4165:GLN:HG3	1.95	0.48
2:B:58:VAL:HG22	2:B:320:GLU:HA	1.96	0.48
2:B:1443:VAL:HB	2:B:1489:CYS:HB2	1.94	0.48
2:E:218:SER:HB3	2:E:286:GLY:HA3	1.96	0.48
2:E:1589:GLN:NE2	2:E:1634:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:GLY:HA3	1:G:74:LEU:HD21	1.96	0.48
2:K:847:THR:OG1	2:K:1215:MET:O	2.32	0.48
2:K:3977:LYS:HB2	2:K:4095:ILE:HG13	1.95	0.48
2:B:1106:GLU:O	2:B:1214:ARG:N	2.47	0.48
2:B:4655:MET:O	2:B:4664:ARG:NH1	2.46	0.48
2:E:239:GLY:O	2:E:243:GLU:N	2.46	0.48
2:E:4722:TYR:OH	2:E:4746:ASP:OD1	2.23	0.48
2:K:799:LYS:HB3	2:K:1620:GLN:HG3	1.95	0.48
2:K:1445:TRP:H	2:K:1487:MET:HB2	1.79	0.48
2:K:4655:MET:O	2:K:4664:ARG:NH1	2.46	0.48
3:L:37:MET:HB3	3:L:42:GLN:HB2	1.96	0.48
2:B:799:LYS:HB3	2:B:1620:GLN:HG3	1.95	0.47
2:B:3977:LYS:HB2	2:B:4095:ILE:HG13	1.95	0.47
2:E:541:ILE:HG23	2:E:548:CYS:HB3	1.96	0.47
2:E:1106:GLU:O	2:E:1214:ARG:N	2.47	0.47
2:E:2114:VAL:O	2:E:2117:THR:OG1	2.28	0.47
3:F:37:MET:HB3	3:F:42:GLN:HB2	1.96	0.47
2:H:1251:LEU:O	2:H:1601:ASN:N	2.47	0.47
2:H:2464:ASP:OD1	2:H:2464:ASP:N	2.36	0.47
2:K:1106:GLU:O	2:K:1214:ARG:N	2.47	0.47
2:K:1143:GLN:HA	2:K:1151:HIS:HA	1.96	0.47
2:K:4167:LYS:NZ	7:K:6003:ATP:O2B	2.44	0.47
2:B:4791:ARG:HB3	2:B:4808:ASP:CB	2.43	0.47
1:D:62:GLY:HA3	1:D:74:LEU:HD21	1.96	0.47
2:E:4848:ASP:CB	2:H:4819:TYR:CE1	2.93	0.47
2:H:143:LEU:HD12	2:K:2427:LEU:HD13	1.93	0.47
2:H:1106:GLU:O	2:H:1214:ARG:N	2.47	0.47
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.96	0.47
2:H:1184:ASP:N	2:H:1188:SER:O	2.45	0.47
2:B:235:ARG:NH2	2:B:269:VAL:O	2.39	0.47
2:E:433:LEU:HD12	2:E:447:LEU:HD11	1.97	0.47
2:H:847:THR:OG1	2:H:1215:MET:O	2.32	0.47
2:H:2072:GLN:NE2	2:H:3647:LYS:O	2.47	0.47
2:H:4621:GLN:HE22	2:H:4633:ARG:HH12	1.62	0.47
2:K:58:VAL:HG22	2:K:320:GLU:HA	1.96	0.47
2:K:953:SER:OG	2:K:1061:GLY:O	2.32	0.47
2:K:3936:LEU:HD21	2:K:3941:LEU:HD22	1.96	0.47
2:K:4621:GLN:HE22	2:K:4633:ARG:HH12	1.62	0.47
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.96	0.47
2:B:953:SER:OG	2:B:1061:GLY:O	2.32	0.47
2:B:1445:TRP:H	2:B:1487:MET:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4655:MET:O	2:E:4664:ARG:NH1	2.46	0.47
2:E:4845:ILE:HG23	2:H:4819:TYR:HB2	1.97	0.47
2:H:2029:ARG:O	2:H:2032:SER:OG	2.28	0.47
2:K:1125:ASP:HA	2:K:1598:ARG:HH11	1.78	0.47
2:K:3904:GLN:NE2	2:K:3965:GLN:OE1	2.48	0.47
2:B:731:HIS:CG	2:B:740:THR:HA	2.50	0.47
2:B:1218:GLY:HA3	2:B:1240:ALA:H	1.79	0.47
2:E:1218:GLY:HA3	2:E:1240:ALA:H	1.78	0.47
2:E:2832:VAL:O	2:E:2895:LYS:NZ	2.38	0.47
2:E:4891:ILE:HD13	2:E:4914:HIS:HB3	1.95	0.47
2:H:143:LEU:HD13	2:K:2426:SER:O	2.13	0.47
2:H:1218:GLY:HA3	2:H:1240:ALA:H	1.78	0.47
2:H:1445:TRP:H	2:H:1487:MET:HB2	1.79	0.47
2:H:4020:MET:HE2	2:H:4063:GLU:HB3	1.96	0.47
2:H:4022:LEU:HD12	2:H:4089:HIS:CE1	2.49	0.47
2:B:433:LEU:HD12	2:B:447:LEU:HD11	1.97	0.47
2:B:673:TRP:HE3	2:B:822:CYS:HA	1.78	0.47
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.96	0.47
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.48	0.47
2:B:4621:GLN:HE22	2:B:4633:ARG:HH12	1.62	0.47
3:C:78:LYS:HA	3:C:81:ASP:HB2	1.97	0.47
2:E:188:SER:HB2	2:E:190:ARG:HH21	1.80	0.47
2:E:1125:ASP:HA	2:E:1598:ARG:HH11	1.78	0.47
2:E:1445:TRP:H	2:E:1487:MET:HB2	1.79	0.47
2:H:3729:GLN:O	2:H:3733:HIS:ND1	2.43	0.47
2:K:4010:ASN:OD1	2:K:4010:ASN:N	2.48	0.47
2:B:1184:ASP:N	2:B:1188:SER:O	2.45	0.47
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.80	0.47
2:B:2072:GLN:NE2	2:B:3647:LYS:O	2.47	0.47
2:B:4022:LEU:HD12	2:B:4089:HIS:CE1	2.49	0.47
3:C:37:MET:HB3	3:C:42:GLN:HB2	1.96	0.47
1:D:26:TYR:N	1:D:39:SER:OG	2.47	0.47
2:E:731:HIS:CG	2:E:740:THR:HA	2.50	0.47
2:E:1602:GLN:HE22	2:E:1642:LEU:HB3	1.80	0.47
2:E:4193:PHE:O	2:E:4197:THR:OG1	2.25	0.47
2:E:4787:PHE:CZ	2:H:4521:TYR:HB3	2.49	0.47
1:G:26:TYR:N	1:G:39:SER:OG	2.47	0.47
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.80	0.47
2:K:731:HIS:CG	2:K:740:THR:HA	2.50	0.47
2:K:2029:ARG:O	2:K:2032:SER:OG	2.28	0.47
2:K:2072:GLN:NE2	2:K:3647:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:GLU:HB2	2:B:187:SER:HB3	1.97	0.47
2:B:1847:GLU:OE1	2:B:1849:SER:OG	2.25	0.47
2:E:306:LEU:HD11	2:E:314:LEU:HG	1.97	0.47
2:E:3904:GLN:NE2	2:E:3965:GLN:OE1	2.48	0.47
2:H:953:SER:OG	2:H:1061:GLY:O	2.32	0.47
2:H:995:MET:HG2	2:H:998:LYS:HD2	1.97	0.47
2:K:541:ILE:HG23	2:K:548:CYS:HB3	1.96	0.47
2:K:995:MET:HG2	2:K:998:LYS:HD2	1.97	0.47
2:K:1167:ASP:OD2	2:K:1172:THR:OG1	2.32	0.47
2:B:2029:ARG:O	2:B:2032:SER:OG	2.27	0.47
2:B:3936:LEU:HD21	2:B:3941:LEU:HD22	1.96	0.47
2:E:4621:GLN:HE22	2:E:4633:ARG:HH12	1.62	0.47
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.96	0.47
2:H:433:LEU:HD12	2:H:447:LEU:HD11	1.97	0.47
2:H:541:ILE:HG23	2:H:548:CYS:HB3	1.96	0.47
2:K:4022:LEU:HD12	2:K:4089:HIS:CE1	2.49	0.47
2:B:4010:ASN:OD1	2:B:4010:ASN:N	2.48	0.47
1:G:40:ARG:NH2	1:G:102:GLU:OE1	2.48	0.47
2:H:306:LEU:HD11	2:H:314:LEU:HG	1.97	0.47
2:H:4010:ASN:OD1	2:H:4010:ASN:N	2.48	0.47
2:E:799:LYS:HB3	2:E:1620:GLN:HG3	1.95	0.46
2:E:2072:GLN:NE2	2:E:3647:LYS:O	2.47	0.46
2:H:731:HIS:CG	2:H:740:THR:HA	2.50	0.46
2:H:2406:GLU:O	2:H:2410:ILE:N	2.42	0.46
2:K:1218:GLY:HA3	2:K:1240:ALA:H	1.79	0.46
2:B:204:ASP:N	2:B:204:ASP:OD1	2.48	0.46
2:B:268:SER:O	2:B:273:SER:OG	2.31	0.46
2:B:541:ILE:HG23	2:B:548:CYS:HB3	1.96	0.46
2:B:995:MET:HG2	2:B:998:LYS:HD2	1.97	0.46
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.80	0.46
2:E:262:TYR:HB2	2:E:389:ARG:HB3	1.96	0.46
2:E:718:VAL:HA	2:E:736:CYS:N	2.29	0.46
2:E:836:HIS:CE1	2:E:1610:ARG:HD2	2.51	0.46
2:E:1608:VAL:HG12	2:E:1610:ARG:HB2	1.97	0.46
2:H:718:VAL:HA	2:H:736:CYS:N	2.29	0.46
2:K:188:SER:HB2	2:K:190:ARG:HH21	1.80	0.46
2:K:1602:GLN:HE22	2:K:1642:LEU:HB3	1.80	0.46
1:A:40:ARG:NH2	1:A:102:GLU:OE1	2.48	0.46
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.80	0.46
2:E:204:ASP:OD1	2:E:204:ASP:N	2.48	0.46
2:E:1132:GLU:HB3	2:E:1147:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:78:LYS:HA	3:F:81:ASP:HB2	1.97	0.46
2:H:836:HIS:CE1	2:H:1610:ARG:HD2	2.51	0.46
1:A:26:TYR:N	1:A:39:SER:OG	2.47	0.46
2:B:1676:LEU:O	2:B:1680:VAL:N	2.47	0.46
2:E:58:VAL:HG22	2:E:320:GLU:HA	1.96	0.46
2:E:156:GLU:HB2	2:E:187:SER:HB3	1.97	0.46
1:G:92:PRO:HG2	1:G:95:ALA:HB2	1.98	0.46
2:H:679:VAL:HA	2:H:800:VAL:HG12	1.97	0.46
2:H:1676:LEU:O	2:H:1680:VAL:N	2.47	0.46
2:H:1912:GLN:HB2	2:H:2088:LEU:HD11	1.98	0.46
2:H:3680:LYS:NZ	2:H:3684:GLU:OE2	2.47	0.46
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.48	0.46
2:K:433:LEU:HD12	2:K:447:LEU:HD11	1.97	0.46
1:A:21:THR:HG1	1:A:49:ARG:HH21	1.59	0.46
1:D:92:PRO:HG2	1:D:95:ALA:HB2	1.98	0.46
2:E:1143:GLN:HA	2:E:1151:HIS:HA	1.96	0.46
2:E:2319:ASN:OD1	2:E:2323:ARG:NH2	2.49	0.46
2:E:3936:LEU:HD21	2:E:3941:LEU:HD22	1.96	0.46
2:H:1608:VAL:HG12	2:H:1610:ARG:HB2	1.97	0.46
2:H:3683:LEU:HD12	2:H:3748:SER:HB3	1.98	0.46
2:K:1184:ASP:OD2	2:K:1188:SER:OG	2.30	0.46
2:K:4000:MET:HA	2:K:4003:MET:HG2	1.98	0.46
2:K:4808:ASP:OD1	2:K:4808:ASP:N	2.47	0.46
3:L:78:LYS:HA	3:L:81:ASP:HB2	1.97	0.46
2:B:1608:VAL:HG12	2:B:1610:ARG:HB2	1.96	0.46
2:B:2114:VAL:O	2:B:2117:THR:OG1	2.28	0.46
2:B:3607:ALA:HB3	3:C:85:GLU:HG2	1.98	0.46
2:B:3808:ALA:O	2:B:3812:GLN:HB2	2.16	0.46
2:E:995:MET:HG2	2:E:998:LYS:HD2	1.97	0.46
2:E:3683:LEU:HD12	2:E:3748:SER:HB3	1.98	0.46
2:H:122:ARG:HH21	2:H:127:GLY:HA2	1.81	0.46
2:H:288:HIS:N	2:H:349:MET:O	2.47	0.46
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.30	0.46
2:H:4167:LYS:NZ	7:H:6003:ATP:O2B	2.44	0.46
1:J:92:PRO:HG2	1:J:95:ALA:HB2	1.98	0.46
2:K:306:LEU:HD11	2:K:314:LEU:HG	1.97	0.46
2:E:4757:ILE:HG23	2:E:4871:PHE:HZ	1.81	0.46
2:H:1470:GLY:HA2	2:H:1474:GLY:HA2	1.98	0.46
2:H:4000:MET:HA	2:H:4003:MET:HG2	1.98	0.46
2:H:4192:ASN:OD1	2:H:4605:LYS:NZ	2.29	0.46
2:K:3680:LYS:NZ	2:K:3684:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1912:GLN:HB2	2:B:2088:LEU:HD11	1.97	0.46
2:B:2319:ASN:OD1	2:B:2323:ARG:NH2	2.49	0.46
2:E:394:HIS:HD2	2:E:397:GLY:H	1.63	0.46
2:E:1098:ALA:O	2:E:1101:TRP:NE1	2.38	0.46
2:E:1756:SER:OG	2:E:1757:LEU:N	2.49	0.46
2:E:1912:GLN:HB2	2:E:2088:LEU:HD11	1.98	0.46
2:E:3607:ALA:HB3	3:F:85:GLU:HG2	1.98	0.46
2:H:156:GLU:HB2	2:H:187:SER:HB3	1.97	0.46
2:H:204:ASP:OD1	2:H:204:ASP:N	2.48	0.46
2:H:2117:THR:HG22	2:H:2155:VAL:HG11	1.98	0.46
2:H:3607:ALA:HB3	3:I:85:GLU:HG2	1.98	0.46
2:K:288:HIS:N	2:K:349:MET:O	2.47	0.46
2:K:836:HIS:CE1	2:K:1610:ARG:HD2	2.51	0.46
2:K:1132:GLU:HB3	2:K:1147:GLN:HE21	1.80	0.46
2:K:3683:LEU:HD12	2:K:3748:SER:HB3	1.98	0.46
1:A:92:PRO:HG2	1:A:95:ALA:HB2	1.98	0.46
2:B:122:ARG:HH21	2:B:127:GLY:HA2	1.81	0.46
2:B:836:HIS:CE1	2:B:1610:ARG:HD2	2.51	0.46
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.80	0.46
2:H:2252:ASN:HD22	2:H:3595:GLN:HG3	1.81	0.46
2:H:3936:LEU:HD21	2:H:3941:LEU:HD22	1.96	0.46
2:K:262:TYR:HB2	2:K:389:ARG:HB3	1.96	0.46
2:K:1098:ALA:O	2:K:1101:TRP:NE1	2.38	0.46
2:K:2252:ASN:HD22	2:K:3595:GLN:HG3	1.81	0.46
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.96	0.46
2:B:306:LEU:HD11	2:B:314:LEU:HG	1.97	0.46
2:K:235:ARG:NH2	2:K:269:VAL:O	2.39	0.46
2:K:894:VAL:HG11	2:K:976:TYR:HD2	1.81	0.46
2:K:897:LYS:HE2	2:K:915:HIS:CG	2.51	0.46
2:K:1608:VAL:HG12	2:K:1610:ARG:HB2	1.96	0.46
2:K:1912:GLN:HB2	2:K:2088:LEU:HD11	1.98	0.46
2:K:3607:ALA:HB3	3:L:85:GLU:HG2	1.98	0.46
2:B:986:ILE:HB	2:B:1058:LEU:HB3	1.98	0.45
2:B:3806:LEU:CD2	2:K:76:ARG:NH2	2.72	0.45
2:E:2252:ASN:HD22	2:E:3595:GLN:HG3	1.81	0.45
2:E:2425:ARG:HH12	2:E:2477:TYR:HA	1.81	0.45
2:E:3993:ASN:HD22	2:E:4110:MET:HG3	1.81	0.45
2:H:894:VAL:HG11	2:H:976:TYR:HD2	1.81	0.45
2:H:1132:GLU:HB3	2:H:1147:GLN:HE21	1.80	0.45
1:J:26:TYR:N	1:J:39:SER:OG	2.47	0.45
2:K:3993:ASN:HD22	2:K:4110:MET:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4147:GLU:OE1	2:K:4937:GLN:NE2	2.49	0.45
2:B:894:VAL:HG11	2:B:976:TYR:HD2	1.81	0.45
2:B:2252:ASN:HD22	2:B:3595:GLN:HG3	1.81	0.45
2:E:288:HIS:N	2:E:349:MET:O	2.47	0.45
2:E:986:ILE:HB	2:E:1058:LEU:HB3	1.98	0.45
2:E:1511:VAL:HA	2:E:1517:LEU:H	1.81	0.45
2:E:2464:ASP:OD1	2:E:2464:ASP:N	2.36	0.45
2:H:1763:PHE:HB3	2:H:1781:GLU:HB3	1.98	0.45
3:I:78:LYS:HA	3:I:81:ASP:HB2	1.97	0.45
2:K:679:VAL:HA	2:K:800:VAL:HG12	1.97	0.45
2:K:769:ARG:HA	2:K:775:VAL:HG23	1.99	0.45
2:K:1251:LEU:O	2:K:1601:ASN:N	2.47	0.45
2:K:1763:PHE:HB3	2:K:1781:GLU:HB3	1.98	0.45
2:K:4757:ILE:HG23	2:K:4871:PHE:HZ	1.81	0.45
2:B:80:GLU:HG3	2:E:3891:TRP:CZ3	2.49	0.45
2:B:769:ARG:HA	2:B:775:VAL:HG23	1.99	0.45
2:B:4147:GLU:OE1	2:B:4937:GLN:NE2	2.49	0.45
2:E:76:ARG:HH21	2:H:3806:LEU:CG	2.29	0.45
2:E:897:LYS:HE2	2:E:915:HIS:CG	2.52	0.45
2:E:2117:THR:HG22	2:E:2155:VAL:HG11	1.98	0.45
2:E:3808:ALA:O	2:E:3812:GLN:HB2	2.16	0.45
2:H:66:THR:OG1	2:H:124:SER:OG	2.25	0.45
2:H:4722:TYR:OH	2:H:4746:ASP:OD1	2.23	0.45
2:H:4845:ILE:HG23	2:K:4819:TYR:HB2	1.99	0.45
2:K:156:GLU:HB2	2:K:187:SER:HB3	1.97	0.45
2:K:4722:TYR:OH	2:K:4746:ASP:OD1	2.23	0.45
2:K:4733:GLY:HA3	2:K:4740:PHE:HD1	1.82	0.45
2:B:394:HIS:HD2	2:B:397:GLY:H	1.63	0.45
2:B:4020:MET:HE2	2:B:4063:GLU:HB3	1.98	0.45
2:E:76:ARG:HH22	2:H:3806:LEU:HD11	1.75	0.45
2:E:268:SER:O	2:E:273:SER:OG	2.31	0.45
2:E:1763:PHE:HB3	2:E:1781:GLU:HB3	1.98	0.45
2:H:394:HIS:HD2	2:H:397:GLY:H	1.63	0.45
2:H:3984:LEU:HB2	2:H:4102:LEU:HD12	1.99	0.45
2:H:4147:GLU:OE1	2:H:4937:GLN:NE2	2.49	0.45
2:K:1710:HIS:HB2	2:K:1711:LEU:HD12	1.99	0.45
2:B:847:THR:OG1	2:B:1215:MET:O	2.32	0.45
2:B:1251:LEU:O	2:B:1601:ASN:N	2.47	0.45
2:B:1470:GLY:HA2	2:B:1474:GLY:HA2	1.98	0.45
2:B:1511:VAL:HA	2:B:1517:LEU:H	1.81	0.45
2:B:1726:ILE:HG13	2:B:1757:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1763:PHE:HB3	2:B:1781:GLU:HB3	1.98	0.45
2:B:2425:ARG:HH12	2:B:2477:TYR:HA	1.81	0.45
2:B:3993:ASN:HD22	2:B:4110:MET:HG3	1.81	0.45
2:E:770:ILE:HG12	2:E:775:VAL:HG21	1.99	0.45
2:E:847:THR:OG1	2:E:1215:MET:O	2.32	0.45
2:E:1710:HIS:HB2	2:E:1711:LEU:HD12	1.99	0.45
2:H:643:LEU:H	2:H:643:LEU:HG	1.60	0.45
2:K:3808:ALA:O	2:K:3812:GLN:HB2	2.16	0.45
2:B:897:LYS:HE2	2:B:915:HIS:CG	2.51	0.45
2:B:1710:HIS:HB2	2:B:1711:LEU:HD12	1.99	0.45
2:B:2117:THR:HG22	2:B:2155:VAL:HG11	1.98	0.45
2:B:2426:SER:O	2:K:143:LEU:HD13	2.13	0.45
2:B:3683:LEU:HD12	2:B:3748:SER:HB3	1.98	0.45
2:B:4819:TYR:CE1	2:K:4848:ASP:CB	2.95	0.45
2:E:1986:GLU:N	2:E:1989:CYS:SG	2.73	0.45
2:H:76:ARG:HH22	2:K:3806:LEU:HD11	1.76	0.45
2:H:1726:ILE:HG13	2:H:1757:LEU:HD23	1.98	0.45
2:H:3993:ASN:HD22	2:H:4110:MET:HG3	1.81	0.45
2:K:305:TYR:HE2	2:K:319:LYS:HG2	1.81	0.45
2:K:394:HIS:HD2	2:K:397:GLY:H	1.63	0.45
2:K:1470:GLY:HA2	2:K:1474:GLY:HA2	1.98	0.45
2:K:1756:SER:OG	2:K:1757:LEU:N	2.49	0.45
2:B:1756:SER:OG	2:B:1757:LEU:N	2.49	0.45
2:B:4897:ASP:N	2:B:4897:ASP:OD1	2.50	0.45
2:E:122:ARG:HH21	2:E:127:GLY:HA2	1.81	0.45
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.79	0.45
2:H:1511:VAL:HA	2:H:1517:LEU:H	1.81	0.45
2:H:2425:ARG:HH12	2:H:2477:TYR:HA	1.81	0.45
2:H:4733:GLY:HA3	2:H:4740:PHE:HD1	1.82	0.45
2:K:308:LEU:N	2:K:326:SER:O	2.49	0.45
2:K:1184:ASP:N	2:K:1188:SER:O	2.45	0.45
2:K:1640:ASP:OD1	2:K:1640:ASP:N	2.44	0.45
2:K:4897:ASP:OD1	2:K:4897:ASP:N	2.50	0.45
2:B:16:THR:OG1	2:B:111:ARG:O	2.29	0.45
2:B:4000:MET:HA	2:B:4003:MET:HG2	1.98	0.45
2:B:4168:GLU:HA	2:B:4171:ARG:CZ	2.46	0.45
2:E:679:VAL:HA	2:E:800:VAL:HG12	1.97	0.45
2:E:769:ARG:HA	2:E:775:VAL:HG23	1.99	0.45
2:E:3984:LEU:HB2	2:E:4102:LEU:HD12	1.99	0.45
2:H:235:ARG:NH2	2:H:269:VAL:O	2.39	0.45
2:H:769:ARG:HA	2:H:775:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1756:SER:OG	2:H:1757:LEU:N	2.49	0.45
2:H:3808:ALA:O	2:H:3812:GLN:HB2	2.16	0.45
2:H:3921:LEU:HD23	2:H:3921:LEU:HA	1.73	0.45
2:K:204:ASP:OD1	2:K:204:ASP:N	2.48	0.45
2:K:986:ILE:HB	2:K:1058:LEU:HB3	1.98	0.45
2:K:2319:ASN:OD1	2:K:2323:ARG:NH2	2.49	0.45
2:B:76:ARG:HH21	2:E:3806:LEU:CG	2.30	0.45
2:B:770:ILE:HG12	2:B:775:VAL:HG21	1.99	0.45
2:B:3680:LYS:NZ	2:B:3684:GLU:OE2	2.47	0.45
2:B:4733:GLY:HA3	2:B:4740:PHE:HD1	1.82	0.45
2:B:4757:ILE:HG23	2:B:4871:PHE:HZ	1.81	0.45
2:E:1184:ASP:OD2	2:E:1188:SER:OG	2.30	0.45
2:E:4897:ASP:N	2:E:4897:ASP:OD1	2.50	0.45
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.81	0.45
2:H:4022:LEU:HA	2:H:4089:HIS:CE1	2.50	0.45
2:K:122:ARG:HH21	2:K:127:GLY:HA2	1.81	0.45
2:K:4022:LEU:HA	2:K:4089:HIS:CE1	2.50	0.45
2:B:660:PHE:HB3	2:B:787:LEU:HD22	1.99	0.45
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.97	0.45
2:B:695:VAL:HA	2:B:792:VAL:HG22	1.99	0.45
2:E:80:GLU:HG3	2:H:3891:TRP:CZ3	2.49	0.45
2:E:3970:LYS:HB3	2:E:3970:LYS:HE2	1.82	0.45
2:E:4733:GLY:HA3	2:E:4740:PHE:HD1	1.82	0.45
2:K:54:ASN:HB3	2:K:57:ASN:HB3	1.99	0.45
2:K:394:HIS:CD2	2:K:396:GLU:H	2.35	0.45
3:L:130:ASP:O	3:L:137:VAL:HG22	2.17	0.45
2:B:1167:ASP:OD2	2:B:1172:THR:OG1	2.32	0.44
2:E:1470:GLY:HA2	2:E:1474:GLY:HA2	1.98	0.44
2:E:4000:MET:HA	2:E:4003:MET:HG2	1.98	0.44
2:E:4022:LEU:HA	2:E:4089:HIS:CE1	2.50	0.44
2:E:4147:GLU:OE1	2:E:4937:GLN:NE2	2.49	0.44
2:E:4808:ASP:OD1	2:E:4808:ASP:N	2.47	0.44
2:H:986:ILE:HB	2:H:1058:LEU:HB3	1.98	0.44
2:H:1710:HIS:HB2	2:H:1711:LEU:HD12	1.98	0.44
2:H:4897:ASP:OD1	2:H:4897:ASP:N	2.50	0.44
2:K:1726:ILE:HG13	2:K:1757:LEU:HD23	1.98	0.44
2:K:2117:THR:HG22	2:K:2155:VAL:HG11	1.98	0.44
2:B:54:ASN:HB3	2:B:57:ASN:HB3	1.99	0.44
2:B:143:LEU:HD12	2:E:2427:LEU:HD11	2.00	0.44
2:B:288:HIS:N	2:B:349:MET:O	2.47	0.44
2:B:643:LEU:H	2:B:643:LEU:HG	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:ALA:N	2:B:1211:GLN:OE1	2.50	0.44
2:B:4022:LEU:HA	2:B:4089:HIS:CE1	2.50	0.44
3:C:130:ASP:O	3:C:137:VAL:HG22	2.17	0.44
2:E:305:TYR:HE2	2:E:319:LYS:HG2	1.81	0.44
2:E:660:PHE:HB3	2:E:787:LEU:HD22	2.00	0.44
2:E:894:VAL:HG11	2:E:976:TYR:HD2	1.81	0.44
2:E:1726:ILE:HG13	2:E:1757:LEU:HD23	1.98	0.44
2:E:2891:GLN:HG2	2:E:2894:LEU:HD12	1.99	0.44
2:H:695:VAL:HA	2:H:792:VAL:HG22	1.99	0.44
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.99	0.44
2:H:2319:ASN:OD1	2:H:2323:ARG:NH2	2.48	0.44
2:K:1258:PHE:HB3	2:K:1303:ARG:NH1	2.33	0.44
2:K:3642:ILE:HG22	2:K:3731:ARG:HD3	1.99	0.44
2:K:3844:LEU:HD23	2:K:3844:LEU:HA	1.79	0.44
2:B:76:ARG:HH22	2:E:3806:LEU:HD11	1.74	0.44
2:B:394:HIS:CD2	2:B:396:GLU:H	2.35	0.44
2:B:2760:PRO:HD2	2:B:2763:LEU:HD12	1.99	0.44
2:E:750:ARG:N	2:E:753:ASP:OD2	2.46	0.44
2:E:4010:ASN:OD1	2:E:4010:ASN:N	2.48	0.44
3:F:130:ASP:O	3:F:137:VAL:HG22	2.17	0.44
2:H:191:TYR:OH	2:K:2327:ARG:CZ	2.66	0.44
2:H:2891:GLN:HG2	2:H:2894:LEU:HD12	1.99	0.44
3:I:130:ASP:O	3:I:137:VAL:HG22	2.17	0.44
2:K:1162:VAL:O	2:K:1176:THR:OG1	2.33	0.44
2:K:1511:VAL:HA	2:K:1517:LEU:H	1.81	0.44
2:K:2425:ARG:HH12	2:K:2477:TYR:HA	1.81	0.44
2:K:2760:PRO:HD2	2:K:2763:LEU:HD12	1.99	0.44
2:B:1640:ASP:OD1	2:B:1640:ASP:N	2.44	0.44
2:B:2891:GLN:HG2	2:B:2894:LEU:HD12	1.99	0.44
2:B:3806:LEU:HD11	2:K:76:ARG:HH22	1.75	0.44
2:B:4175:PHE:O	2:B:4179:ASN:ND2	2.51	0.44
2:E:294:PRO:HB3	2:E:366:ILE:HD11	1.99	0.44
2:E:3642:ILE:HG22	2:E:3731:ARG:HD3	1.99	0.44
2:H:308:LEU:N	2:H:326:SER:O	2.49	0.44
2:H:1601:ASN:ND2	2:H:1643:GLU:OE2	2.36	0.44
2:H:3760:LEU:HD23	2:H:3760:LEU:HA	1.81	0.44
2:H:4757:ILE:HG23	2:H:4871:PHE:HZ	1.81	0.44
2:K:3984:LEU:HB2	2:K:4102:LEU:HD12	1.99	0.44
2:B:674:TYR:HE2	2:B:814:LEU:HB2	1.83	0.44
2:B:2880:ALA:O	2:B:2884:ALA:N	2.49	0.44
2:E:394:HIS:CD2	2:E:396:GLU:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2398:ASP:OD1	2:E:2402:ARG:NH2	2.50	0.44
2:H:394:HIS:CD2	2:H:396:GLU:H	2.35	0.44
2:H:660:PHE:HB3	2:H:787:LEU:HD22	1.99	0.44
2:H:3844:LEU:HD23	2:H:3844:LEU:HA	1.79	0.44
2:H:4175:PHE:O	2:H:4179:ASN:ND2	2.51	0.44
1:J:40:ARG:NH2	1:J:102:GLU:OE1	2.48	0.44
2:K:1121:GLY:O	2:K:1133:ARG:NH1	2.51	0.44
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.82	0.44
2:B:1258:PHE:HB3	2:B:1303:ARG:NH1	2.33	0.44
2:B:2327:ARG:CZ	2:K:191:TYR:OH	2.66	0.44
2:E:238:HIS:N	2:E:243:GLU:O	2.43	0.44
2:E:674:TYR:HE2	2:E:814:LEU:HB2	1.83	0.44
2:E:4136:ARG:HH21	2:E:4148:ARG:CZ	2.31	0.44
2:H:2770:GLU:O	2:H:2774:TRP:HB2	2.18	0.44
2:H:4136:ARG:HH21	2:H:4148:ARG:CZ	2.31	0.44
2:K:4601:PHE:HD1	2:K:4644:ASN:HB3	1.83	0.44
2:B:506:HIS:NE2	2:B:564:ARG:HG2	2.33	0.44
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.51	0.44
2:E:76:ARG:NH2	2:H:3806:LEU:CD2	2.70	0.44
2:E:1121:GLY:O	2:E:1133:ARG:NH1	2.51	0.44
2:E:1167:ASP:OD2	2:E:1172:THR:OG1	2.32	0.44
2:E:1258:PHE:HB3	2:E:1303:ARG:NH1	2.33	0.44
2:E:2880:ALA:O	2:E:2884:ALA:N	2.49	0.44
2:H:76:ARG:HH21	2:K:3806:LEU:CG	2.31	0.44
2:H:1305:SER:HB2	2:H:1591:LEU:HB2	2.00	0.44
2:K:32:GLN:O	2:K:53:SER:OG	2.28	0.44
2:K:4136:ARG:HH21	2:K:4148:ARG:CZ	2.31	0.44
2:K:4175:PHE:O	2:K:4179:ASN:ND2	2.51	0.44
2:B:308:LEU:N	2:B:326:SER:O	2.49	0.44
2:B:3806:LEU:CG	2:K:76:ARG:HH21	2.30	0.44
2:B:3984:LEU:HB2	2:B:4102:LEU:HD12	1.99	0.44
2:B:4791:ARG:CB	2:B:4808:ASP:HB3	2.47	0.44
1:D:30:LEU:HD12	1:D:34:LYS:HB2	2.00	0.44
1:D:40:ARG:NH2	1:D:102:GLU:OE1	2.48	0.44
2:H:294:PRO:HB3	2:H:366:ILE:HD11	2.00	0.44
2:H:770:ILE:HG12	2:H:775:VAL:HG21	1.99	0.44
2:H:897:LYS:HE2	2:H:915:HIS:CG	2.52	0.44
2:K:660:PHE:HB3	2:K:787:LEU:HD22	1.99	0.44
2:K:770:ILE:HG12	2:K:775:VAL:HG21	1.99	0.44
2:K:3921:LEU:HD23	2:K:3921:LEU:HA	1.73	0.44
2:K:4020:MET:HE2	2:K:4063:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:TYR:OH	2:E:2327:ARG:CZ	2.65	0.44
2:B:1274:ASP:HB2	2:B:1286:THR:HA	2.00	0.44
2:E:54:ASN:HB3	2:E:57:ASN:HB3	1.99	0.44
2:E:695:VAL:HA	2:E:792:VAL:HG22	1.99	0.44
2:E:3680:LYS:NZ	2:E:3684:GLU:OE2	2.47	0.44
2:H:3642:ILE:HG22	2:H:3731:ARG:HD3	1.99	0.44
2:H:4601:PHE:HD1	2:H:4644:ASN:HB3	1.83	0.44
2:K:748:LEU:HB2	2:K:750:ARG:HG3	1.99	0.44
2:K:2891:GLN:HG2	2:K:2894:LEU:HD12	1.99	0.44
2:E:228:LEU:HD11	2:E:405:LEU:HD13	2.00	0.43
2:E:769:ARG:HG2	2:E:774:PRO:HA	2.00	0.43
2:E:2856:LYS:O	2:E:2860:GLU:HB2	2.18	0.43
2:H:694:ARG:HG2	2:H:716:ASN:HB3	2.00	0.43
2:H:750:ARG:N	2:H:753:ASP:OD2	2.46	0.43
2:H:769:ARG:HG2	2:H:774:PRO:HA	2.00	0.43
2:K:1305:SER:HB2	2:K:1591:LEU:HB2	2.00	0.43
2:K:2770:GLU:O	2:K:2774:TRP:HB2	2.18	0.43
2:K:3880:LEU:HD23	2:K:3944:ALA:HB2	2.00	0.43
2:B:694:ARG:HG2	2:B:716:ASN:HB3	2.00	0.43
2:B:3593:SER:O	2:B:3597:LYS:NZ	2.42	0.43
2:B:4020:MET:HE1	2:B:4063:GLU:HB3	2.00	0.43
2:B:4819:TYR:HB2	2:K:4845:ILE:HG23	2.00	0.43
2:E:506:HIS:NE2	2:E:564:ARG:HG2	2.33	0.43
2:E:748:LEU:HB2	2:E:750:ARG:HG3	1.99	0.43
1:J:30:LEU:HD12	1:J:34:LYS:HB2	2.00	0.43
2:K:1757:LEU:HD13	2:K:1757:LEU:HA	1.88	0.43
2:B:2241:LEU:HD12	2:B:2298:ARG:HG3	2.01	0.43
2:B:4845:ILE:HG23	2:E:4819:TYR:HB2	2.00	0.43
2:E:143:LEU:HD13	2:H:2426:SER:O	2.14	0.43
2:E:898:ILE:HD13	2:E:973:THR:HG22	2.00	0.43
2:H:2241:LEU:HD12	2:H:2298:ARG:HG3	2.00	0.43
2:H:2856:LYS:O	2:H:2860:GLU:HB2	2.18	0.43
2:K:694:ARG:HG2	2:K:716:ASN:HB3	2.00	0.43
2:K:2856:LYS:O	2:K:2860:GLU:HB2	2.18	0.43
2:B:769:ARG:HG2	2:B:774:PRO:HA	2.00	0.43
2:B:4601:PHE:HD1	2:B:4644:ASN:HB3	1.83	0.43
2:E:2241:LEU:HD12	2:E:2298:ARG:HG3	2.01	0.43
2:H:54:ASN:HB3	2:H:57:ASN:HB3	1.99	0.43
2:H:718:VAL:HA	2:H:736:CYS:H	1.83	0.43
2:H:1057:LEU:O	2:H:1062:TYR:N	2.51	0.43
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1258:PHE:HB3	2:H:1303:ARG:NH1	2.33	0.43
2:K:674:TYR:HE2	2:K:814:LEU:HB2	1.83	0.43
2:K:695:VAL:HA	2:K:792:VAL:HG22	1.99	0.43
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.38	0.43
2:E:4011:VAL:HA	2:E:4014:ILE:HG12	2.00	0.43
2:H:674:TYR:HE2	2:H:814:LEU:HB2	1.83	0.43
2:H:1734:LYS:HE2	2:H:1931:ASP:HB3	2.00	0.43
2:H:2397:ILE:HD12	2:H:2397:ILE:HA	1.94	0.43
2:H:2760:PRO:HD2	2:H:2763:LEU:HD12	1.99	0.43
2:H:2880:ALA:O	2:H:2884:ALA:N	2.49	0.43
2:H:3800:SER:OG	2:H:3801:CYS:N	2.41	0.43
2:H:4848:ASP:CB	2:K:4819:TYR:CE1	2.95	0.43
2:K:718:VAL:HA	2:K:736:CYS:H	1.83	0.43
2:K:2241:LEU:HD12	2:K:2298:ARG:HG3	2.00	0.43
2:K:2463:PRO:HB3	2:K:2516:ALA:HB2	2.01	0.43
2:B:4523:VAL:HG21	2:K:4791:ARG:HD2	2.00	0.43
2:B:4780:TYR:OH	2:E:4515:ASN:HB3	2.19	0.43
2:E:2760:PRO:HD2	2:E:2763:LEU:HD12	1.99	0.43
2:E:4175:PHE:O	2:E:4179:ASN:ND2	2.51	0.43
2:E:4601:PHE:HD1	2:E:4644:ASN:HB3	1.83	0.43
1:G:30:LEU:HD12	1:G:34:LYS:HB2	2.00	0.43
2:H:1274:ASP:HB2	2:H:1286:THR:HA	2.00	0.43
2:H:2252:ASN:HB2	2:H:2310:ASN:HD21	1.84	0.43
2:K:769:ARG:HG2	2:K:774:PRO:HA	2.00	0.43
2:K:1305:SER:HA	2:K:1593:HIS:HD2	1.84	0.43
2:K:2398:ASP:OD1	2:K:2402:ARG:NH2	2.50	0.43
2:K:2731:ASP:HB3	2:K:2826:ALA:HB2	2.01	0.43
2:K:4020:MET:HE1	2:K:4063:GLU:HB3	2.01	0.43
2:B:294:PRO:HB3	2:B:366:ILE:HD11	1.99	0.43
2:B:601:LEU:HG	2:B:642:LEU:HD23	2.01	0.43
2:B:1734:LYS:HE2	2:B:1931:ASP:HB3	2.00	0.43
2:B:3921:LEU:HD23	2:B:3921:LEU:HA	1.73	0.43
2:E:601:LEU:HG	2:E:642:LEU:HD23	2.01	0.43
2:E:1057:LEU:O	2:E:1062:TYR:N	2.51	0.43
2:E:1305:SER:HA	2:E:1593:HIS:HD2	1.84	0.43
2:E:2252:ASN:HB2	2:E:2310:ASN:HD21	1.84	0.43
2:H:425:LEU:HD21	2:H:452:VAL:HG13	2.01	0.43
2:H:1228:THR:HA	2:H:1232:LEU:HD12	2.01	0.43
2:H:1785:ASP:OD1	2:H:1788:LYS:NZ	2.51	0.43
2:H:1986:GLU:N	2:H:1989:CYS:SG	2.73	0.43
2:K:652:VAL:HG11	2:K:715:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1310:CYS:HB2	2:K:1536:SER:HA	2.01	0.43
2:K:1785:ASP:OD1	2:K:1788:LYS:NZ	2.50	0.43
2:B:228:LEU:HD11	2:B:405:LEU:HD13	2.00	0.43
2:B:1714:TYR:CD1	2:B:1761:MET:HB3	2.54	0.43
2:B:2463:PRO:HB3	2:B:2516:ALA:HB2	2.01	0.43
2:B:3642:ILE:HG22	2:B:3731:ARG:HD3	1.99	0.43
2:B:4136:ARG:HH21	2:B:4148:ARG:CZ	2.31	0.43
2:E:308:LEU:N	2:E:326:SER:O	2.49	0.43
2:E:1601:ASN:ND2	2:E:1643:GLU:OE2	2.36	0.43
2:H:2759:LYS:HA	2:H:2760:PRO:HD3	1.92	0.43
2:H:3986:MET:HG2	2:H:3996:ILE:HD11	2.01	0.43
2:K:898:ILE:HD13	2:K:973:THR:HG22	2.00	0.43
2:K:1676:LEU:O	2:K:1680:VAL:N	2.47	0.43
2:K:4787:PHE:HD1	2:K:4808:ASP:O	2.02	0.43
2:B:898:ILE:HD13	2:B:973:THR:HG22	2.00	0.43
2:B:2770:GLU:O	2:B:2774:TRP:HB2	2.18	0.43
2:B:3891:TRP:CZ3	2:K:80:GLU:HG3	2.50	0.43
2:E:3612:LEU:HD23	2:E:3617:ALA:HB2	2.01	0.43
2:H:228:LEU:HD11	2:H:405:LEU:HD13	2.00	0.43
2:H:506:HIS:NE2	2:H:564:ARG:HG2	2.33	0.43
2:H:898:ILE:HD13	2:H:973:THR:HG22	2.00	0.43
2:K:506:HIS:NE2	2:K:564:ARG:HG2	2.33	0.43
2:K:1274:ASP:HB2	2:K:1286:THR:HA	2.00	0.43
2:K:3612:LEU:HD23	2:K:3617:ALA:HB2	2.01	0.43
2:B:718:VAL:HA	2:B:736:CYS:H	1.83	0.43
2:B:1305:SER:HB2	2:B:1591:LEU:HB2	2.00	0.43
2:B:2252:ASN:HB2	2:B:2310:ASN:HD21	1.84	0.43
2:B:2427:LEU:HD11	2:K:143:LEU:HD12	2.01	0.43
2:B:3760:LEU:HD23	2:B:3760:LEU:HA	1.81	0.43
2:E:425:LEU:HD21	2:E:452:VAL:HG13	2.01	0.43
2:E:940:LEU:HD23	2:E:940:LEU:HA	1.89	0.43
2:E:1274:ASP:HB2	2:E:1286:THR:HA	2.00	0.43
2:E:2770:GLU:O	2:E:2774:TRP:HB2	2.18	0.43
2:H:601:LEU:HG	2:H:642:LEU:HD23	2.01	0.43
2:H:1305:SER:HA	2:H:1593:HIS:HD2	1.84	0.43
2:H:1310:CYS:HB2	2:H:1536:SER:HA	2.01	0.43
2:H:1836:ASN:HA	2:H:1839:LEU:HB2	2.01	0.43
2:H:2076:ILE:HG21	2:H:2081:LEU:HD22	2.00	0.43
2:H:2731:ASP:HB3	2:H:2826:ALA:HB2	2.01	0.43
2:K:601:LEU:HG	2:K:642:LEU:HD23	2.01	0.43
2:K:1601:ASN:ND2	2:K:1643:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD12	1:A:34:LYS:HB2	2.00	0.42
2:B:243:GLU:HA	2:B:264:GLY:HA2	2.01	0.42
2:B:4011:VAL:HA	2:B:4014:ILE:HG12	2.00	0.42
2:B:4515:ASN:HB3	2:K:4780:TYR:OH	2.19	0.42
1:D:9:PRO:HD2	2:E:748:LEU:HD11	2.01	0.42
2:E:64:ILE:H	2:E:64:ILE:HG13	1.74	0.42
2:E:191:TYR:OH	2:H:2327:ARG:CZ	2.67	0.42
2:E:235:ARG:NH2	2:E:269:VAL:O	2.39	0.42
2:E:243:GLU:HA	2:E:264:GLY:HA2	2.00	0.42
2:E:1228:THR:HA	2:E:1232:LEU:HD12	2.01	0.42
2:E:1310:CYS:HB2	2:E:1536:SER:HA	2.01	0.42
2:E:1714:TYR:CD1	2:E:1761:MET:HB3	2.54	0.42
2:E:2076:ILE:HG21	2:E:2081:LEU:HD22	2.01	0.42
2:E:2716:GLU:HA	2:E:2719:GLU:HB2	2.01	0.42
2:E:2731:ASP:HB3	2:E:2826:ALA:HB2	2.01	0.42
2:E:3880:LEU:HD23	2:E:3944:ALA:HB2	2.00	0.42
2:E:4787:PHE:HD1	2:E:4808:ASP:O	2.02	0.42
2:H:1466:THR:HG22	2:H:1482:ARG:HG2	2.01	0.42
2:H:3777:LYS:HE3	2:H:3777:LYS:HB2	1.87	0.42
2:H:3871:ILE:O	2:H:3874:SER:OG	2.26	0.42
2:K:238:HIS:N	2:K:243:GLU:O	2.43	0.42
2:K:1210:ALA:N	2:K:1211:GLN:OE1	2.50	0.42
2:K:1836:ASN:HA	2:K:1839:LEU:HB2	2.01	0.42
2:K:4635:VAL:O	2:K:4638:THR:OG1	2.33	0.42
2:B:1057:LEU:O	2:B:1062:TYR:N	2.51	0.42
2:B:1305:SER:HA	2:B:1593:HIS:HD2	1.84	0.42
2:B:1310:CYS:HB2	2:B:1536:SER:HA	2.01	0.42
2:B:2759:LYS:HA	2:B:2760:PRO:HD3	1.92	0.42
2:B:4168:GLU:HB2	2:B:4171:ARG:HH12	1.84	0.42
2:B:4193:PHE:O	2:B:4197:THR:OG1	2.25	0.42
1:D:77:THR:HB	1:D:80:VAL:HG23	2.01	0.42
2:E:694:ARG:HG2	2:E:716:ASN:HB3	2.00	0.42
2:E:2834:LEU:HD13	2:E:2838:LEU:HB3	2.01	0.42
2:H:243:GLU:HA	2:H:264:GLY:HA2	2.01	0.42
2:H:3605:ARG:HH12	3:I:82:SER:HB3	1.85	0.42
2:H:3612:LEU:HD23	2:H:3617:ALA:HB2	2.01	0.42
2:H:4787:PHE:HD1	2:H:4808:ASP:O	2.02	0.42
2:H:4890:PHE:H	7:H:6003:ATP:N6	2.17	0.42
2:K:243:GLU:HA	2:K:264:GLY:HA2	2.01	0.42
2:K:425:LEU:HD21	2:K:452:VAL:HG13	2.01	0.42
2:K:1714:TYR:CD1	2:K:1761:MET:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2252:ASN:HB2	2:K:2310:ASN:HD21	1.84	0.42
2:K:2834:LEU:HD13	2:K:2838:LEU:HB3	2.01	0.42
2:K:4011:VAL:HA	2:K:4014:ILE:HG12	2.00	0.42
2:B:143:LEU:HD13	2:E:2426:SER:O	2.13	0.42
2:B:237:LEU:HB2	2:B:404:ASN:HB3	2.02	0.42
2:B:675:TYR:CE1	2:B:790:PRO:HB3	2.54	0.42
2:B:676:GLU:HG3	2:B:814:LEU:HB3	2.01	0.42
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.99	0.42
2:B:2731:ASP:HB3	2:B:2826:ALA:HB2	2.01	0.42
2:B:2856:LYS:O	2:B:2860:GLU:HB2	2.18	0.42
2:B:3612:LEU:HD23	2:B:3617:ALA:HB2	2.01	0.42
2:E:2433:LEU:HD22	2:E:2488:LEU:HD22	2.01	0.42
2:E:4597:PRO:HA	2:E:4600:ILE:HG22	2.01	0.42
1:G:77:THR:HB	1:G:80:VAL:HG23	2.01	0.42
2:H:652:VAL:HG11	2:H:715:GLY:HA2	2.01	0.42
2:H:1092:LYS:H	2:H:1250:TRP:HZ3	1.67	0.42
2:H:2463:PRO:HB3	2:H:2516:ALA:HB2	2.00	0.42
1:J:21:THR:HG1	1:J:49:ARG:HH21	1.59	0.42
2:K:1730:THR:O	2:K:1733:THR:OG1	2.28	0.42
2:K:1734:LYS:HE2	2:K:1931:ASP:HB3	2.00	0.42
2:K:3986:MET:HG2	2:K:3996:ILE:HD11	2.01	0.42
2:B:294:PRO:HD3	2:B:344:LYS:HE3	2.02	0.42
2:B:1228:THR:HA	2:B:1232:LEU:HD12	2.01	0.42
2:B:3605:ARG:HH12	3:C:82:SER:HB3	1.85	0.42
2:E:143:LEU:HD12	2:H:2427:LEU:HD11	2.01	0.42
2:E:294:PRO:HD3	2:E:344:LYS:HE3	2.02	0.42
2:E:652:VAL:HG11	2:E:715:GLY:HA2	2.01	0.42
2:E:1734:LYS:HE2	2:E:1931:ASP:HB3	2.00	0.42
2:E:3987:LEU:HG	2:E:3990:ASN:HD21	1.85	0.42
2:H:1167:ASP:OD2	2:H:1172:THR:OG1	2.32	0.42
2:K:294:PRO:HB3	2:K:366:ILE:HD11	1.99	0.42
2:K:675:TYR:CE1	2:K:790:PRO:HB3	2.54	0.42
2:K:4020:MET:HE2	2:K:4067:LEU:HD13	2.01	0.42
2:B:394:HIS:CD2	2:B:397:GLY:H	2.38	0.42
2:B:745:ASN:HB3	2:B:747:HIS:HB2	2.02	0.42
2:B:2076:ILE:HG21	2:B:2081:LEU:HD22	2.00	0.42
2:B:2433:LEU:HD22	2:B:2488:LEU:HD22	2.01	0.42
2:B:2716:GLU:HA	2:B:2719:GLU:HB2	2.01	0.42
2:B:3986:MET:HG2	2:B:3996:ILE:HD11	2.01	0.42
2:E:439:LYS:HE3	2:E:439:LYS:HB3	1.91	0.42
2:E:618:CYS:SG	2:E:629:GLN:NE2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:718:VAL:HA	2:E:736:CYS:H	1.83	0.42
2:E:745:ASN:HB3	2:E:747:HIS:HB2	2.02	0.42
2:E:755:ILE:HA	2:E:770:ILE:HD13	2.02	0.42
2:E:1305:SER:HB2	2:E:1591:LEU:HB2	2.00	0.42
2:H:3880:LEU:HD23	2:H:3944:ALA:HB2	2.00	0.42
2:H:4791:ARG:HD2	2:K:4523:VAL:HG21	2.00	0.42
2:K:618:CYS:SG	2:K:629:GLN:NE2	2.93	0.42
2:K:1092:LYS:H	2:K:1250:TRP:HZ3	1.67	0.42
2:K:3605:ARG:HH12	3:L:82:SER:HB3	1.85	0.42
2:B:1836:ASN:HA	2:B:1839:LEU:HB2	2.01	0.42
2:B:1986:GLU:N	2:B:1989:CYS:SG	2.73	0.42
2:B:3880:LEU:HD23	2:B:3944:ALA:HB2	2.00	0.42
2:B:4635:VAL:O	2:B:4638:THR:OG1	2.33	0.42
2:E:3921:LEU:HD23	2:E:3921:LEU:HA	1.73	0.42
2:H:32:GLN:O	2:H:53:SER:OG	2.28	0.42
2:H:268:SER:O	2:H:273:SER:OG	2.31	0.42
2:H:676:GLU:HG3	2:H:814:LEU:HB3	2.01	0.42
2:H:1124:PRO:HG2	2:H:1598:ARG:HG3	2.01	0.42
2:H:2433:LEU:HD22	2:H:2488:LEU:HD22	2.01	0.42
2:H:3987:LEU:HG	2:H:3990:ASN:HD21	1.85	0.42
2:K:228:LEU:HD11	2:K:405:LEU:HD13	2.00	0.42
2:K:1466:THR:HG22	2:K:1482:ARG:HG2	2.01	0.42
2:K:1732:GLU:O	2:K:1735:SER:OG	2.32	0.42
2:B:73:LEU:HB3	2:B:77:ALA:HB3	2.02	0.42
2:B:675:TYR:CZ	2:B:790:PRO:HB3	2.55	0.42
2:B:983:LEU:HD23	2:B:1056:THR:HA	2.02	0.42
2:B:1124:PRO:HG2	2:B:1598:ARG:HG3	2.01	0.42
2:B:2834:LEU:HD13	2:B:2838:LEU:HB3	2.01	0.42
2:B:4020:MET:HE2	2:B:4067:LEU:HD13	2.01	0.42
2:E:16:THR:OG1	2:E:111:ARG:O	2.29	0.42
2:E:675:TYR:CE1	2:E:790:PRO:HB3	2.54	0.42
2:E:1676:LEU:O	2:E:1680:VAL:N	2.47	0.42
2:E:2463:PRO:HB3	2:E:2516:ALA:HB2	2.01	0.42
2:H:618:CYS:SG	2:H:629:GLN:NE2	2.93	0.42
2:H:675:TYR:CE1	2:H:790:PRO:HB3	2.54	0.42
2:H:1210:ALA:N	2:H:1211:GLN:OE1	2.51	0.42
2:H:1676:LEU:HD23	2:H:1676:LEU:HA	1.89	0.42
2:K:237:LEU:HB2	2:K:404:ASN:HB3	2.02	0.42
2:K:294:PRO:HD3	2:K:344:LYS:HE3	2.02	0.42
2:K:394:HIS:CD2	2:K:397:GLY:H	2.38	0.42
2:K:676:GLU:HG3	2:K:814:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:745:ASN:HB3	2:K:747:HIS:HB2	2.02	0.42
2:K:755:ILE:HA	2:K:770:ILE:HD13	2.02	0.42
2:K:2076:ILE:HG21	2:K:2081:LEU:HD22	2.01	0.42
2:B:652:VAL:HG11	2:B:715:GLY:HA2	2.01	0.42
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	2.01	0.42
2:E:3986:MET:HG2	2:E:3996:ILE:HD11	2.01	0.42
2:H:294:PRO:HD3	2:H:344:LYS:HE3	2.02	0.42
2:H:2398:ASP:OD1	2:H:2402:ARG:NH2	2.50	0.42
1:J:9:PRO:HD2	2:K:748:LEU:HD11	2.01	0.42
2:K:372:LEU:HD23	2:K:403:LEU:HD11	2.02	0.42
2:K:2716:GLU:HA	2:K:2719:GLU:HB2	2.01	0.42
2:B:3777:LYS:HB2	2:B:3777:LYS:HE3	1.87	0.42
2:B:3804:LEU:HB3	2:B:3885:SER:OG	2.20	0.42
2:E:237:LEU:HB2	2:E:404:ASN:HB3	2.02	0.42
2:E:675:TYR:CZ	2:E:790:PRO:HB3	2.55	0.42
2:E:676:GLU:HG3	2:E:814:LEU:HB3	2.01	0.42
2:E:3683:LEU:HD11	2:E:3747:ALA:HB3	2.02	0.42
2:H:675:TYR:CZ	2:H:790:PRO:HB3	2.55	0.42
2:H:940:LEU:HD23	2:H:940:LEU:HA	1.89	0.42
2:H:1714:TYR:CD1	2:H:1761:MET:HB3	2.54	0.42
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	2.01	0.42
2:K:2880:ALA:O	2:K:2884:ALA:N	2.49	0.42
2:K:3925:ILE:HD11	2:K:3936:LEU:HD13	2.02	0.42
1:A:77:THR:HB	1:A:80:VAL:HG23	2.01	0.42
2:B:1846:ILE:HG23	2:B:1894:LEU:HB3	2.02	0.42
2:E:195:SER:OG	2:E:196:TYR:N	2.53	0.42
2:E:881:ILE:O	2:E:885:LEU:HB2	2.20	0.42
2:E:1210:ALA:N	2:E:1211:GLN:OE1	2.51	0.42
2:E:1466:THR:HG22	2:E:1482:ARG:HG2	2.01	0.42
2:E:2029:ARG:O	2:E:2032:SER:OG	2.28	0.42
2:E:3605:ARG:HH12	3:F:82:SER:HB3	1.85	0.42
2:H:372:LEU:HD23	2:H:403:LEU:HD11	2.02	0.42
2:H:2213:LYS:HA	2:H:2254:LEU:HD21	2.02	0.42
2:H:2716:GLU:HA	2:H:2719:GLU:HB2	2.01	0.42
2:K:73:LEU:HB3	2:K:77:ALA:HB3	2.02	0.42
2:K:675:TYR:CZ	2:K:790:PRO:HB3	2.55	0.42
2:K:1118:SER:HB2	2:K:1122:CYS:SG	2.60	0.42
1:A:9:PRO:HD2	2:B:748:LEU:HD11	2.01	0.41
2:B:76:ARG:CZ	2:E:3806:LEU:HD21	2.50	0.41
2:B:425:LEU:HD21	2:B:452:VAL:HG13	2.01	0.41
2:B:755:ILE:HA	2:B:770:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4521:TYR:HD1	2:B:4521:TYR:HA	1.72	0.41
2:E:394:HIS:CD2	2:E:397:GLY:H	2.38	0.41
2:E:4027:LEU:HD22	2:E:4056:HIS:HB3	2.02	0.41
2:H:73:LEU:HB3	2:H:77:ALA:HB3	2.02	0.41
2:H:195:SER:OG	2:H:196:TYR:N	2.53	0.41
2:H:1446:ILE:O	2:H:1540:PHE:N	2.42	0.41
2:H:4011:VAL:HA	2:H:4014:ILE:HG12	2.00	0.41
2:K:195:SER:OG	2:K:196:TYR:N	2.53	0.41
2:K:1683:PRO:HA	2:K:1686:LEU:HD12	2.02	0.41
2:K:1846:ILE:HG23	2:K:1894:LEU:HB3	2.02	0.41
2:K:3804:LEU:HB3	2:K:3885:SER:OG	2.20	0.41
2:K:3987:LEU:HG	2:K:3990:ASN:HD21	1.85	0.41
2:B:2773:ARG:HD3	2:B:2777:LYS:HE3	2.02	0.41
2:H:1683:PRO:HA	2:H:1686:LEU:HD12	2.02	0.41
2:H:3804:LEU:HB3	2:H:3885:SER:OG	2.20	0.41
2:H:3925:ILE:HD11	2:H:3936:LEU:HD13	2.02	0.41
2:H:4780:TYR:OH	2:K:4515:ASN:HB3	2.19	0.41
2:K:2433:LEU:HD22	2:K:2488:LEU:HD22	2.01	0.41
2:B:1683:PRO:HA	2:B:1686:LEU:HD12	2.02	0.41
2:E:983:LEU:HD23	2:E:1056:THR:HA	2.02	0.41
2:E:1705:LEU:HD23	2:E:1705:LEU:HA	1.90	0.41
2:E:1836:ASN:HA	2:E:1839:LEU:HB2	2.01	0.41
2:E:2213:LYS:HA	2:E:2254:LEU:HD21	2.02	0.41
2:E:2773:ARG:HD3	2:E:2777:LYS:HE3	2.03	0.41
2:E:3683:LEU:HD23	2:E:3683:LEU:HA	1.92	0.41
2:E:3804:LEU:HB3	2:E:3885:SER:OG	2.20	0.41
2:H:394:HIS:CD2	2:H:397:GLY:H	2.38	0.41
2:H:745:ASN:HB3	2:H:747:HIS:HB2	2.02	0.41
2:H:3804:LEU:HD22	2:H:3886:ILE:HD13	2.02	0.41
2:K:1057:LEU:O	2:K:1062:TYR:N	2.51	0.41
2:K:1228:THR:HA	2:K:1232:LEU:HD12	2.01	0.41
2:K:4027:LEU:HD22	2:K:4056:HIS:HB3	2.02	0.41
2:B:195:SER:OG	2:B:196:TYR:N	2.53	0.41
2:B:881:ILE:O	2:B:885:LEU:HB2	2.20	0.41
2:B:1268:ILE:HD11	2:B:1300:MET:HG3	2.01	0.41
2:B:3831:LEU:HD13	2:B:3831:LEU:HA	1.97	0.41
2:E:1739:PHE:HA	2:E:1740:PRO:HD3	1.91	0.41
1:G:9:PRO:HD2	2:H:748:LEU:HD11	2.01	0.41
2:H:16:THR:OG1	2:H:111:ARG:O	2.29	0.41
2:H:1118:SER:HB2	2:H:1122:CYS:SG	2.60	0.41
2:K:750:ARG:N	2:K:753:ASP:OD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:LYS:H	2:B:1250:TRP:HZ3	1.67	0.41
2:B:1466:THR:HG22	2:B:1482:ARG:HG2	2.02	0.41
2:B:1689:ILE:HA	2:B:1703:TYR:CE1	2.56	0.41
2:B:1730:THR:O	2:B:1733:THR:OG1	2.28	0.41
2:E:73:LEU:HB3	2:E:77:ALA:HB3	2.02	0.41
2:E:717:GLY:H	2:E:722:LEU:HB3	1.85	0.41
2:E:4891:ILE:HD11	2:E:4916:LEU:HD13	2.03	0.41
2:H:143:LEU:HD13	2:K:2426:SER:HG	1.83	0.41
2:H:237:LEU:HB2	2:H:404:ASN:HB3	2.02	0.41
2:H:1510:VAL:HG12	2:H:1511:VAL:HG23	2.03	0.41
2:H:1689:ILE:HA	2:H:1703:TYR:CE1	2.56	0.41
2:H:2349:GLU:HA	2:H:2352:ILE:HD11	2.03	0.41
1:J:77:THR:HB	1:J:80:VAL:HG23	2.01	0.41
2:K:1091:GLU:HB3	2:K:1094:TYR:HD2	1.86	0.41
2:K:1268:ILE:HD11	2:K:1300:MET:HG3	2.02	0.41
2:K:3677:LEU:HD23	2:K:3677:LEU:HA	1.90	0.41
2:B:1118:SER:HB2	2:B:1122:CYS:SG	2.60	0.41
2:B:3683:LEU:HD11	2:B:3747:ALA:HB3	2.02	0.41
2:B:4910:THR:HG21	7:B:6003:ATP:C4	2.55	0.41
2:E:1124:PRO:HG2	2:E:1598:ARG:HG3	2.01	0.41
2:E:1640:ASP:OD1	2:E:1640:ASP:N	2.44	0.41
2:E:1683:PRO:HA	2:E:1686:LEU:HD12	2.02	0.41
2:E:1689:ILE:HA	2:E:1703:TYR:CE1	2.56	0.41
2:E:3925:ILE:HD11	2:E:3936:LEU:HD13	2.02	0.41
2:E:4052:ALA:O	2:E:4056:HIS:ND1	2.54	0.41
2:H:432:GLY:HA3	2:H:447:LEU:HG	2.03	0.41
2:H:755:ILE:HA	2:H:770:ILE:HD13	2.02	0.41
2:H:2834:LEU:HD13	2:H:2838:LEU:HB3	2.01	0.41
2:H:4020:MET:HE2	2:H:4067:LEU:HD13	2.02	0.41
2:K:123:HIS:CD2	2:K:126:SER:H	2.23	0.41
2:K:983:LEU:HD23	2:K:1056:THR:HA	2.02	0.41
2:K:4597:PRO:HA	2:K:4600:ILE:HG22	2.01	0.41
2:B:1733:THR:HA	2:B:1755:THR:HG21	2.03	0.41
2:B:1757:LEU:HD13	2:B:1757:LEU:HA	1.88	0.41
2:B:3804:LEU:HD22	2:B:3886:ILE:HD13	2.02	0.41
2:B:4891:ILE:HD11	2:B:4916:LEU:HD13	2.03	0.41
2:E:150:GLN:NE2	2:E:158:CYS:SG	2.85	0.41
2:E:1091:GLU:HB3	2:E:1094:TYR:HD2	1.86	0.41
2:K:677:LEU:HD23	2:K:802:PHE:HA	2.03	0.41
2:K:1510:VAL:HG12	2:K:1511:VAL:HG23	2.03	0.41
2:B:372:LEU:HD23	2:B:403:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1601:ASN:ND2	2:B:1643:GLU:OE2	2.36	0.41
2:B:4848:ASP:CB	2:E:4819:TYR:CE1	2.95	0.41
2:E:1092:LYS:H	2:E:1250:TRP:HZ3	1.66	0.41
2:E:1306:MET:HB2	2:E:1575:HIS:HE2	1.86	0.41
2:E:1733:THR:HA	2:E:1755:THR:HG21	2.03	0.41
2:E:4793:PHE:HD1	2:E:4833:GLU:HB2	1.86	0.41
2:H:2416:GLU:HB3	2:H:2419:ARG:HH21	1.85	0.41
2:H:3911:ILE:HD13	2:H:3911:ILE:HA	1.94	0.41
2:K:643:LEU:H	2:K:643:LEU:HG	1.60	0.41
2:K:1124:PRO:HG2	2:K:1598:ARG:HG3	2.01	0.41
2:K:2213:LYS:HA	2:K:2254:LEU:HD21	2.02	0.41
2:K:4052:ALA:O	2:K:4056:HIS:ND1	2.54	0.41
2:K:4910:THR:HG21	7:K:6003:ATP:C4	2.56	0.41
2:B:227:TYR:HE1	2:B:355:LYS:HG2	1.86	0.41
2:B:750:ARG:N	2:B:753:ASP:OD2	2.46	0.41
2:B:2213:LYS:HA	2:B:2254:LEU:HD21	2.02	0.41
2:B:3806:LEU:HD21	2:K:76:ARG:CZ	2.50	0.41
2:B:3925:ILE:HD11	2:B:3936:LEU:HD13	2.02	0.41
2:B:3966:ILE:H	2:B:3966:ILE:HG13	1.70	0.41
2:B:3987:LEU:HG	2:B:3990:ASN:HD21	1.85	0.41
2:B:4806:LYS:O	2:B:4807:CYS:SG	2.73	0.41
2:B:4953:PHE:HA	2:B:4954:PRO:HD3	1.94	0.41
2:E:372:LEU:HD23	2:E:403:LEU:HD11	2.02	0.41
2:E:432:GLY:HA3	2:E:447:LEU:HG	2.03	0.41
2:E:530:LEU:HD23	2:E:530:LEU:HA	1.91	0.41
2:E:1268:ILE:HD11	2:E:1300:MET:HG3	2.01	0.41
2:E:1846:ILE:HG23	2:E:1894:LEU:HB3	2.02	0.41
2:E:3677:LEU:HD23	2:E:3677:LEU:HA	1.91	0.41
2:E:4809:ASP:HB2	2:E:4812:THR:CG2	2.51	0.41
2:H:80:GLU:HG3	2:K:3891:TRP:CZ3	2.51	0.41
2:H:143:LEU:HD12	2:K:2427:LEU:HD11	2.01	0.41
2:H:238:HIS:N	2:H:243:GLU:O	2.43	0.41
2:H:506:HIS:CE1	2:H:564:ARG:HG2	2.56	0.41
2:H:657:PRO:HB3	2:H:834:VAL:HG22	2.03	0.41
2:H:1733:THR:HA	2:H:1755:THR:HG21	2.03	0.41
2:H:4027:LEU:HD22	2:H:4056:HIS:HB3	2.02	0.41
2:H:4100:ALA:O	2:H:4104:THR:OG1	2.33	0.41
2:H:4910:THR:HG21	7:H:6003:ATP:C4	2.55	0.41
2:K:506:HIS:CE1	2:K:564:ARG:HG2	2.56	0.41
2:K:717:GLY:H	2:K:722:LEU:HB3	1.85	0.41
2:K:881:ILE:O	2:K:885:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1689:ILE:HA	2:K:1703:TYR:CE1	2.56	0.41
2:K:1986:GLU:N	2:K:1989:CYS:SG	2.73	0.41
2:K:2349:GLU:HA	2:K:2352:ILE:HD11	2.03	0.41
2:K:3804:LEU:HD22	2:K:3886:ILE:HD13	2.02	0.41
2:K:4891:ILE:HD11	2:K:4916:LEU:HD13	2.03	0.41
2:B:618:CYS:SG	2:B:629:GLN:NE2	2.93	0.41
2:B:717:GLY:H	2:B:722:LEU:HB3	1.85	0.41
2:B:1306:MET:HB2	2:B:1575:HIS:HE2	1.85	0.41
2:B:4027:LEU:HD22	2:B:4056:HIS:HB3	2.02	0.41
2:B:4127:LEU:O	2:B:4131:GLN:N	2.54	0.41
2:E:1118:SER:HB2	2:E:1122:CYS:SG	2.60	0.41
1:G:27:THR:HG23	1:G:100:ASP:HB3	2.03	0.41
2:H:717:GLY:H	2:H:722:LEU:HB3	1.85	0.41
2:H:881:ILE:O	2:H:885:LEU:HB2	2.20	0.41
2:H:1846:ILE:HG23	2:H:1894:LEU:HB3	2.02	0.41
2:K:1057:LEU:HB3	2:K:1062:TYR:HB2	2.03	0.41
2:K:4127:LEU:O	2:K:4131:GLN:N	2.54	0.41
2:B:432:GLY:HA3	2:B:447:LEU:HG	2.03	0.40
2:E:1644:LEU:HD21	2:E:1651:LEU:HA	2.03	0.40
2:E:3804:LEU:HD22	2:E:3886:ILE:HD13	2.02	0.40
2:E:3831:LEU:HD23	2:E:3906:ASN:HD21	1.86	0.40
2:H:227:TYR:HE1	2:H:355:LYS:HG2	1.86	0.40
2:H:983:LEU:HD23	2:H:1056:THR:HA	2.02	0.40
2:H:2201:LEU:HD23	2:H:2201:LEU:HA	1.92	0.40
2:H:2773:ARG:HD3	2:H:2777:LYS:HE3	2.02	0.40
2:H:3683:LEU:HD11	2:H:3747:ALA:HB3	2.02	0.40
2:H:4809:ASP:HB2	2:H:4812:THR:CG2	2.51	0.40
2:K:150:GLN:NE2	2:K:158:CYS:SG	2.85	0.40
2:K:228:LEU:HB3	2:K:289:ILE:HB	2.04	0.40
2:K:432:GLY:HA3	2:K:447:LEU:HG	2.03	0.40
2:K:1177:LEU:N	2:K:1180:GLU:O	2.55	0.40
2:K:1644:LEU:HD21	2:K:1651:LEU:HA	2.04	0.40
2:K:1733:THR:HA	2:K:1755:THR:HG21	2.03	0.40
2:K:2416:GLU:HB3	2:K:2419:ARG:HH21	1.85	0.40
2:K:2759:LYS:HA	2:K:2760:PRO:HD3	1.92	0.40
2:K:3683:LEU:HD11	2:K:3747:ALA:HB3	2.02	0.40
2:K:3777:LYS:HE3	2:K:3777:LYS:HB2	1.87	0.40
2:B:1091:GLU:HB3	2:B:1094:TYR:HD2	1.86	0.40
2:B:1785:ASP:OD1	2:B:1788:LYS:NZ	2.50	0.40
2:B:2398:ASP:OD1	2:B:2402:ARG:NH2	2.50	0.40
2:B:4793:PHE:HD1	2:B:4833:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:145:PHE:HD1	2:E:145:PHE:HA	1.76	0.40
2:E:506:HIS:CE1	2:E:564:ARG:HG2	2.56	0.40
2:E:1057:LEU:HB3	2:E:1062:TYR:HB2	2.03	0.40
2:E:1445:TRP:N	2:E:1487:MET:HB2	2.36	0.40
2:E:4020:MET:HE2	2:E:4067:LEU:HD13	2.03	0.40
2:H:228:LEU:HB3	2:H:289:ILE:HB	2.04	0.40
2:H:608:HIS:HB2	2:H:1656:HIS:CD2	2.57	0.40
2:H:1177:LEU:N	2:H:1180:GLU:O	2.55	0.40
2:H:1268:ILE:HD11	2:H:1300:MET:HG3	2.01	0.40
2:H:4582:VAL:O	2:H:4586:PHE:HB2	2.21	0.40
2:H:4793:PHE:HD1	2:H:4833:GLU:HB2	1.86	0.40
2:K:1445:TRP:N	2:K:1487:MET:HB2	2.36	0.40
2:B:1177:LEU:N	2:B:1180:GLU:O	2.55	0.40
2:B:1510:VAL:HG12	2:B:1511:VAL:HG23	2.03	0.40
2:B:4168:GLU:HG3	2:B:4171:ARG:HH11	1.85	0.40
2:E:1162:VAL:O	2:E:1176:THR:OG1	2.33	0.40
2:H:236:LEU:HD12	2:H:236:LEU:HA	1.92	0.40
2:H:1445:TRP:N	2:H:1487:MET:HB2	2.36	0.40
2:H:1644:LEU:HD21	2:H:1651:LEU:HA	2.04	0.40
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.54	0.40
2:H:4891:ILE:HD11	2:H:4916:LEU:HD13	2.03	0.40
1:J:27:THR:HG23	1:J:100:ASP:HB3	2.03	0.40
2:K:1306:MET:HB2	2:K:1575:HIS:HE2	1.85	0.40
2:K:1446:ILE:O	2:K:1540:PHE:N	2.42	0.40
2:K:2168:MET:H	2:K:2168:MET:HG3	1.74	0.40
2:K:2773:ARG:HD3	2:K:2777:LYS:HE3	2.02	0.40
2:B:163:HIS:HA	2:B:164:PRO:HD3	1.93	0.40
2:B:227:TYR:CE1	2:B:355:LYS:HG2	2.57	0.40
2:B:1014:GLN:HA	2:B:1029:ASN:HB2	2.03	0.40
2:B:2103:LEU:HD23	2:B:2103:LEU:HA	1.92	0.40
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.54	0.40
2:E:643:LEU:H	2:E:643:LEU:HG	1.60	0.40
2:E:1014:GLN:HA	2:E:1029:ASN:HB2	2.03	0.40
2:E:4780:TYR:OH	2:H:4515:ASN:HB3	2.22	0.40
2:E:4910:THR:HG21	7:E:6003:ATP:C4	2.55	0.40
2:E:4945:TYR:OH	6:E:6002:CFF:H81	2.22	0.40
2:H:76:ARG:CZ	2:K:3806:LEU:HD21	2.51	0.40
2:H:123:HIS:CD2	2:H:126:SER:H	2.23	0.40
2:H:227:TYR:CE1	2:H:355:LYS:HG2	2.57	0.40
2:B:228:LEU:HB3	2:B:289:ILE:HB	2.04	0.40
2:B:657:PRO:HB3	2:B:834:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1809:PRO:O	2:B:1812:GLY:N	2.55	0.40
2:B:1993:ILE:HG23	3:C:112:ASN:HA	2.03	0.40
2:B:4945:TYR:OH	6:B:6002:CFF:H81	2.22	0.40
2:E:228:LEU:HB3	2:E:289:ILE:HB	2.04	0.40
2:E:608:HIS:HB2	2:E:1656:HIS:CD2	2.57	0.40
2:E:2088:LEU:HD23	2:E:2088:LEU:HA	1.89	0.40
2:E:2349:GLU:HA	2:E:2352:ILE:HD11	2.03	0.40
2:E:4668:SER:O	2:E:4672:GLY:N	2.54	0.40
2:H:1446:ILE:HB	2:H:1540:PHE:HB2	2.04	0.40
2:H:1993:ILE:HG23	3:I:112:ASN:HA	2.03	0.40
2:H:3804:LEU:HD13	2:H:3910:ALA:HB2	2.04	0.40
2:H:3831:LEU:HD23	2:H:3906:ASN:HD21	1.86	0.40
2:H:4923:LEU:HD12	2:H:4923:LEU:HA	1.93	0.40
2:K:64:ILE:H	2:K:64:ILE:HG13	1.74	0.40
2:K:439:LYS:HE3	2:K:439:LYS:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	G	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3386/4968 (68%)	2990 (88%)	383 (11%)	13 (0%)	34	72
2	E	3386/4968 (68%)	2986 (88%)	387 (11%)	13 (0%)	34	72
2	H	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	34	72
2	K	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	I	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	60
All	All	14492/20900 (69%)	12806 (88%)	1630 (11%)	56 (0%)	38	72

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1477	HIS
2	E	1477	HIS
2	H	1477	HIS
2	K	1477	HIS
2	B	1580	PRO
2	B	4916	LEU
3	C	130	ASP
2	E	1580	PRO
2	E	4916	LEU
3	F	130	ASP
2	H	1580	PRO
2	H	4916	LEU
3	I	130	ASP
2	K	1580	PRO
2	K	4916	LEU
3	L	130	ASP
2	B	730	LEU
2	B	1581	GLN
2	B	4071	ALA
2	E	730	LEU
2	E	1581	GLN
2	E	4071	ALA
2	H	730	LEU
2	H	1581	GLN
2	H	4071	ALA
2	K	730	LEU
2	K	1581	GLN
2	K	4071	ALA
2	B	3802	SER
2	E	3802	SER
2	H	3802	SER
2	K	3802	SER

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Mol	Chain	Res	Type
2	B	853	PRO
2	E	853	PRO
2	H	853	PRO
2	K	853	PRO
2	B	3801	CYS
2	B	4164	PRO
2	E	3801	CYS
2	E	4164	PRO
2	H	3801	CYS
2	H	4164	PRO
2	K	3801	CYS
2	K	4164	PRO
2	B	1535	PRO
2	E	1535	PRO
2	H	1535	PRO
2	K	1535	PRO
2	B	828	PRO
2	B	1848	PRO
2	E	828	PRO
2	E	1848	PRO
2	H	828	PRO
2	H	1848	PRO
2	K	828	PRO
2	K	1848	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	86 (98%)	2 (2%)	50	70
1	D	88/89 (99%)	86 (98%)	2 (2%)	50	70
1	G	88/89 (99%)	86 (98%)	2 (2%)	50	70
1	J	88/89 (99%)	86 (98%)	2 (2%)	50	70
2	B	2698/4355 (62%)	2670 (99%)	28 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	2698/4355 (62%)	2670 (99%)	28 (1%)	76	86
2	H	2699/4355 (62%)	2670 (99%)	29 (1%)	73	84
2	K	2699/4355 (62%)	2670 (99%)	29 (1%)	73	84
3	C	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	F	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	I	115/123 (94%)	114 (99%)	1 (1%)	78	87
3	L	115/123 (94%)	114 (99%)	1 (1%)	78	87
All	All	11606/18268 (64%)	11480 (99%)	126 (1%)	74	84

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	42	ARG
2	B	44	ASN
2	B	57	ASN
2	B	439	LYS
2	B	487	ASN
2	B	531	ASN
2	B	658	ASN
2	B	841	LYS
2	B	881	ILE
2	B	925	PRO
2	B	990	PRO
2	B	1042	THR
2	B	1054	VAL
2	B	1089	ARG
2	B	1760	ARG
2	B	1761	MET
2	B	2196	ASN
2	B	2199	ARG
2	B	2211	ASN
2	B	2328	ARG
2	B	2420	ILE
2	B	3726	LEU
2	B	3906	ASN
2	B	4136	ARG
2	B	4206	GLN
2	B	4499	ASN
2	B	4521	TYR

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Mol	Chain	Res	Type
2	B	4652	ARG
2	B	4788	ASN
3	C	116	LYS
1	D	13	ARG
1	D	42	ARG
2	E	44	ASN
2	E	57	ASN
2	E	439	LYS
2	E	487	ASN
2	E	531	ASN
2	E	658	ASN
2	E	841	LYS
2	E	881	ILE
2	E	925	PRO
2	E	990	PRO
2	E	1042	THR
2	E	1054	VAL
2	E	1089	ARG
2	E	1760	ARG
2	E	1761	MET
2	E	2196	ASN
2	E	2199	ARG
2	E	2211	ASN
2	E	2328	ARG
2	E	2420	ILE
2	E	3726	LEU
2	E	3906	ASN
2	E	4136	ARG
2	E	4206	GLN
2	E	4499	ASN
2	E	4521	TYR
2	E	4652	ARG
2	E	4788	ASN
3	F	116	LYS
1	G	13	ARG
1	G	42	ARG
2	H	44	ASN
2	H	57	ASN
2	H	439	LYS
2	H	487	ASN
2	H	531	ASN
2	H	658	ASN

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Mol	Chain	Res	Type
2	H	841	LYS
2	H	881	ILE
2	H	925	PRO
2	H	950	VAL
2	H	990	PRO
2	H	1042	THR
2	H	1054	VAL
2	H	1089	ARG
2	H	1760	ARG
2	H	1761	MET
2	H	2196	ASN
2	H	2199	ARG
2	H	2211	ASN
2	H	2328	ARG
2	H	2420	ILE
2	H	3726	LEU
2	H	3906	ASN
2	H	4136	ARG
2	H	4206	GLN
2	H	4499	ASN
2	H	4521	TYR
2	H	4652	ARG
2	H	4788	ASN
3	I	116	LYS
1	J	13	ARG
1	J	42	ARG
2	K	44	ASN
2	K	57	ASN
2	K	439	LYS
2	K	487	ASN
2	K	531	ASN
2	K	658	ASN
2	K	841	LYS
2	K	881	ILE
2	K	925	PRO
2	K	950	VAL
2	K	990	PRO
2	K	1042	THR
2	K	1054	VAL
2	K	1089	ARG
2	K	1760	ARG
2	K	1761	MET

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Mol	Chain	Res	Type
2	K	2196	ASN
2	K	2199	ARG
2	K	2211	ASN
2	K	2328	ARG
2	K	2420	ILE
2	K	3726	LEU
2	K	3906	ASN
2	K	4136	ARG
2	K	4206	GLN
2	K	4499	ASN
2	K	4521	TYR
2	K	4652	ARG
2	K	4788	ASN
3	L	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	44	ASN
2	B	57	ASN
2	B	123	HIS
2	B	252	HIS
2	B	261	HIS
2	B	293	GLN
2	B	375	GLN
2	B	394	HIS
2	B	476	GLN
2	B	486	GLN
2	B	487	ASN
2	B	531	ASN
2	B	544	ASN
2	B	621	HIS
2	B	635	ASN
2	B	776	GLN
2	B	1146	HIS
2	B	1147	GLN
2	B	1149	ASN
2	B	1242	ASN
2	B	1265	HIS
2	B	1587	HIS
2	B	1656	HIS
2	B	1669	ASN

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Mol	Chain	Res	Type
2	B	1722	ASN
2	B	1746	HIS
2	B	2090	HIS
2	B	2211	ASN
2	B	2212	GLN
2	B	2251	ASN
2	B	2310	ASN
2	B	2711	ASN
2	B	2820	HIS
2	B	3666	HIS
2	B	3902	GLN
2	B	3904	GLN
2	B	3954	HIS
2	B	3965	GLN
2	B	3976	GLN
2	B	3993	ASN
2	B	4089	HIS
2	B	4128	ASN
2	B	4494	ASN
2	B	4499	ASN
2	B	4621	GLN
2	E	44	ASN
2	E	57	ASN
2	E	123	HIS
2	E	150	GLN
2	E	252	HIS
2	E	261	HIS
2	E	293	GLN
2	E	375	GLN
2	E	394	HIS
2	E	476	GLN
2	E	486	GLN
2	E	487	ASN
2	E	531	ASN
2	E	544	ASN
2	E	621	HIS
2	E	635	ASN
2	E	776	GLN
2	E	1146	HIS
2	E	1147	GLN
2	E	1149	ASN
2	E	1242	ASN

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Mol	Chain	Res	Type
2	E	1265	HIS
2	E	1587	HIS
2	E	1656	HIS
2	E	1669	ASN
2	E	1722	ASN
2	E	1746	HIS
2	E	2090	HIS
2	E	2211	ASN
2	E	2212	GLN
2	E	2251	ASN
2	E	2310	ASN
2	E	2711	ASN
2	E	2820	HIS
2	E	3666	HIS
2	E	3902	GLN
2	E	3904	GLN
2	E	3954	HIS
2	E	3965	GLN
2	E	3976	GLN
2	E	3993	ASN
2	E	4089	HIS
2	E	4128	ASN
2	E	4494	ASN
2	E	4499	ASN
2	E	4559	HIS
2	E	4621	GLN
3	F	136	GLN
2	H	44	ASN
2	H	57	ASN
2	H	123	HIS
2	H	150	GLN
2	H	252	HIS
2	H	261	HIS
2	H	293	GLN
2	H	375	GLN
2	H	394	HIS
2	H	476	GLN
2	H	486	GLN
2	H	487	ASN
2	H	531	ASN
2	H	544	ASN
2	H	621	HIS

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Mol	Chain	Res	Type
2	H	635	ASN
2	H	1146	HIS
2	H	1147	GLN
2	H	1149	ASN
2	H	1242	ASN
2	H	1265	HIS
2	H	1587	HIS
2	H	1656	HIS
2	H	1669	ASN
2	H	1722	ASN
2	H	1746	HIS
2	H	2090	HIS
2	H	2211	ASN
2	H	2212	GLN
2	H	2251	ASN
2	H	2310	ASN
2	H	2711	ASN
2	H	2820	HIS
2	H	3666	HIS
2	H	3902	GLN
2	H	3904	GLN
2	H	3954	HIS
2	H	3965	GLN
2	H	3976	GLN
2	H	3993	ASN
2	H	4089	HIS
2	H	4128	ASN
2	H	4494	ASN
2	H	4499	ASN
2	H	4621	GLN
2	K	44	ASN
2	K	57	ASN
2	K	123	HIS
2	K	150	GLN
2	K	252	HIS
2	K	261	HIS
2	K	293	GLN
2	K	375	GLN
2	K	394	HIS
2	K	476	GLN
2	K	486	GLN
2	K	487	ASN

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Mol	Chain	Res	Type
2	K	531	ASN
2	K	544	ASN
2	K	621	HIS
2	K	635	ASN
2	K	1146	HIS
2	K	1147	GLN
2	K	1149	ASN
2	K	1242	ASN
2	K	1265	HIS
2	K	1587	HIS
2	K	1656	HIS
2	K	1669	ASN
2	K	1722	ASN
2	K	1746	HIS
2	K	2090	HIS
2	K	2211	ASN
2	K	2212	GLN
2	K	2251	ASN
2	K	2310	ASN
2	K	2711	ASN
2	K	2820	HIS
2	K	2891	GLN
2	K	3666	HIS
2	K	3902	GLN
2	K	3904	GLN
2	K	3954	HIS
2	K	3965	GLN
2	K	3976	GLN
2	K	3993	ASN
2	K	4089	HIS
2	K	4128	ASN
2	K	4494	ASN
2	K	4499	ASN
2	K	4621	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	E	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)
6	CFF	B	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)
7	ATP	K	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)
7	ATP	H	6003	-	26,33,33	0.90	1 (3%)	31,52,52	1.55	4 (12%)
6	CFF	K	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.27	1 (12%)
7	ATP	B	6003	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	4 (12%)
6	CFF	H	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)
6	CFF	E	6002	-	8,15,15	2.74	4 (50%)	8,23,23	1.28	1 (12%)

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
7	ATP	E	6003	-	-	7/18/38/38	0/3/3/3
6	CFF	B	6002	-	-	-	0/2/2/2
7	ATP	K	6003	-	-	7/18/38/38	0/3/3/3
7	ATP	H	6003	-	-	7/18/38/38	0/3/3/3
6	CFF	K	6002	-	-	-	0/2/2/2
7	ATP	B	6003	-	-	7/18/38/38	0/3/3/3
6	CFF	H	6002	-	-	-	0/2/2/2
6	CFF	E	6002	-	-	-	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6002	CFF	C5-C4	-4.92	1.32	1.39
6	E	6002	CFF	C5-C4	-4.91	1.32	1.39
6	H	6002	CFF	C5-C4	-4.91	1.32	1.39
6	K	6002	CFF	C5-C4	-4.91	1.32	1.39
6	E	6002	CFF	C6-N1	-4.82	1.31	1.38
6	B	6002	CFF	C6-N1	-4.79	1.31	1.38
6	H	6002	CFF	C6-N1	-4.79	1.31	1.38
6	K	6002	CFF	C6-N1	-4.79	1.31	1.38
6	B	6002	CFF	O13-C6	-2.33	1.18	1.24
6	E	6002	CFF	O13-C6	-2.33	1.18	1.24
6	H	6002	CFF	O13-C6	-2.33	1.18	1.24
6	K	6002	CFF	O13-C6	-2.33	1.18	1.24
6	K	6002	CFF	C5-C6	-2.19	1.37	1.41
6	B	6002	CFF	C5-C6	-2.16	1.37	1.41
6	H	6002	CFF	C5-C6	-2.16	1.37	1.41
6	E	6002	CFF	C5-C6	-2.13	1.37	1.41
7	B	6003	ATP	C5-C4	2.02	1.46	1.40
7	E	6003	ATP	C5-C4	2.02	1.46	1.40
7	H	6003	ATP	C5-C4	2.02	1.46	1.40
7	K	6003	ATP	C5-C4	2.02	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	6003	ATP	PA-O3A-PB	-3.41	121.14	132.83
7	H	6003	ATP	PA-O3A-PB	-3.41	121.14	132.83
7	E	6003	ATP	PA-O3A-PB	-3.40	121.14	132.83
7	K	6003	ATP	PA-O3A-PB	-3.40	121.16	132.83
7	B	6003	ATP	N3-C2-N1	-3.39	123.38	128.68
7	H	6003	ATP	N3-C2-N1	-3.38	123.39	128.68
7	E	6003	ATP	N3-C2-N1	-3.38	123.39	128.68
7	K	6003	ATP	N3-C2-N1	-3.38	123.40	128.68
7	B	6003	ATP	C3'-C2'-C1'	3.24	105.85	100.98
7	K	6003	ATP	C3'-C2'-C1'	3.24	105.85	100.98
7	H	6003	ATP	C3'-C2'-C1'	3.23	105.84	100.98
7	E	6003	ATP	C3'-C2'-C1'	3.22	105.82	100.98
6	B	6002	CFF	C14-N7-C8	-2.79	112.01	125.43
6	H	6002	CFF	C14-N7-C8	-2.79	112.01	125.43
6	E	6002	CFF	C14-N7-C8	-2.78	112.04	125.43
6	K	6002	CFF	C14-N7-C8	-2.78	112.04	125.43
7	K	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83
7	H	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83
7	E	6003	ATP	PB-O3B-PG	-2.51	124.20	132.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	6003	ATP	PB-O3B-PG-O2G
7	B	6003	ATP	PB-O3B-PG-O3G
7	B	6003	ATP	C5'-O5'-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O2A
7	E	6003	ATP	PB-O3B-PG-O2G
7	E	6003	ATP	PB-O3B-PG-O3G
7	E	6003	ATP	C5'-O5'-PA-O1A
7	E	6003	ATP	C5'-O5'-PA-O2A
7	H	6003	ATP	PB-O3B-PG-O2G
7	H	6003	ATP	PB-O3B-PG-O3G
7	H	6003	ATP	C5'-O5'-PA-O1A
7	H	6003	ATP	C5'-O5'-PA-O2A
7	K	6003	ATP	PB-O3B-PG-O2G
7	K	6003	ATP	PB-O3B-PG-O3G
7	K	6003	ATP	C5'-O5'-PA-O1A
7	K	6003	ATP	C5'-O5'-PA-O2A
7	B	6003	ATP	O4'-C4'-C5'-O5'
7	E	6003	ATP	O4'-C4'-C5'-O5'
7	H	6003	ATP	O4'-C4'-C5'-O5'
7	K	6003	ATP	O4'-C4'-C5'-O5'
7	B	6003	ATP	PB-O3A-PA-O1A
7	E	6003	ATP	PB-O3A-PA-O1A
7	H	6003	ATP	PB-O3A-PA-O1A
7	K	6003	ATP	PB-O3A-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O3A
7	E	6003	ATP	C5'-O5'-PA-O3A
7	H	6003	ATP	C5'-O5'-PA-O3A
7	K	6003	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

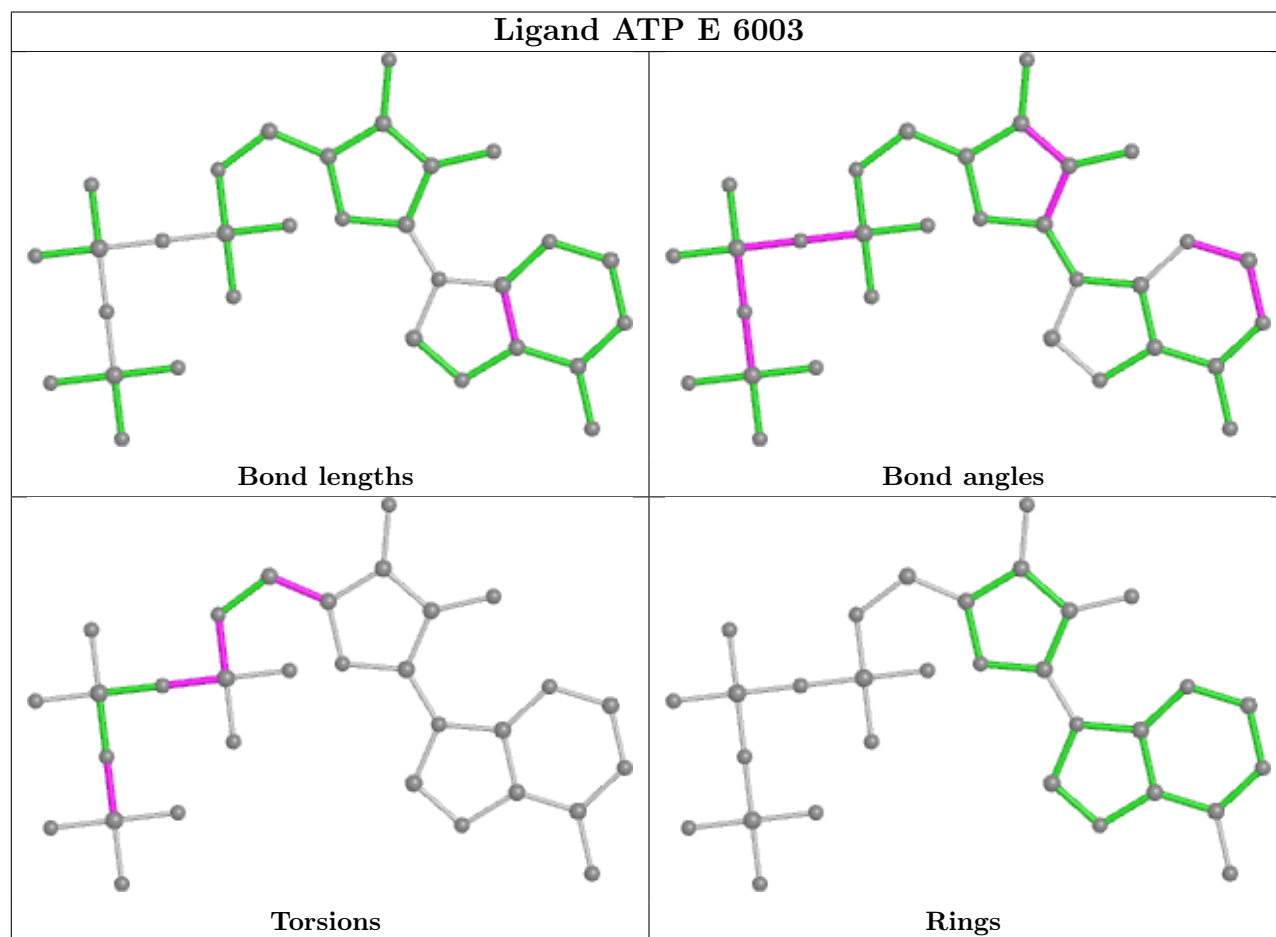
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	6003	ATP	4	0

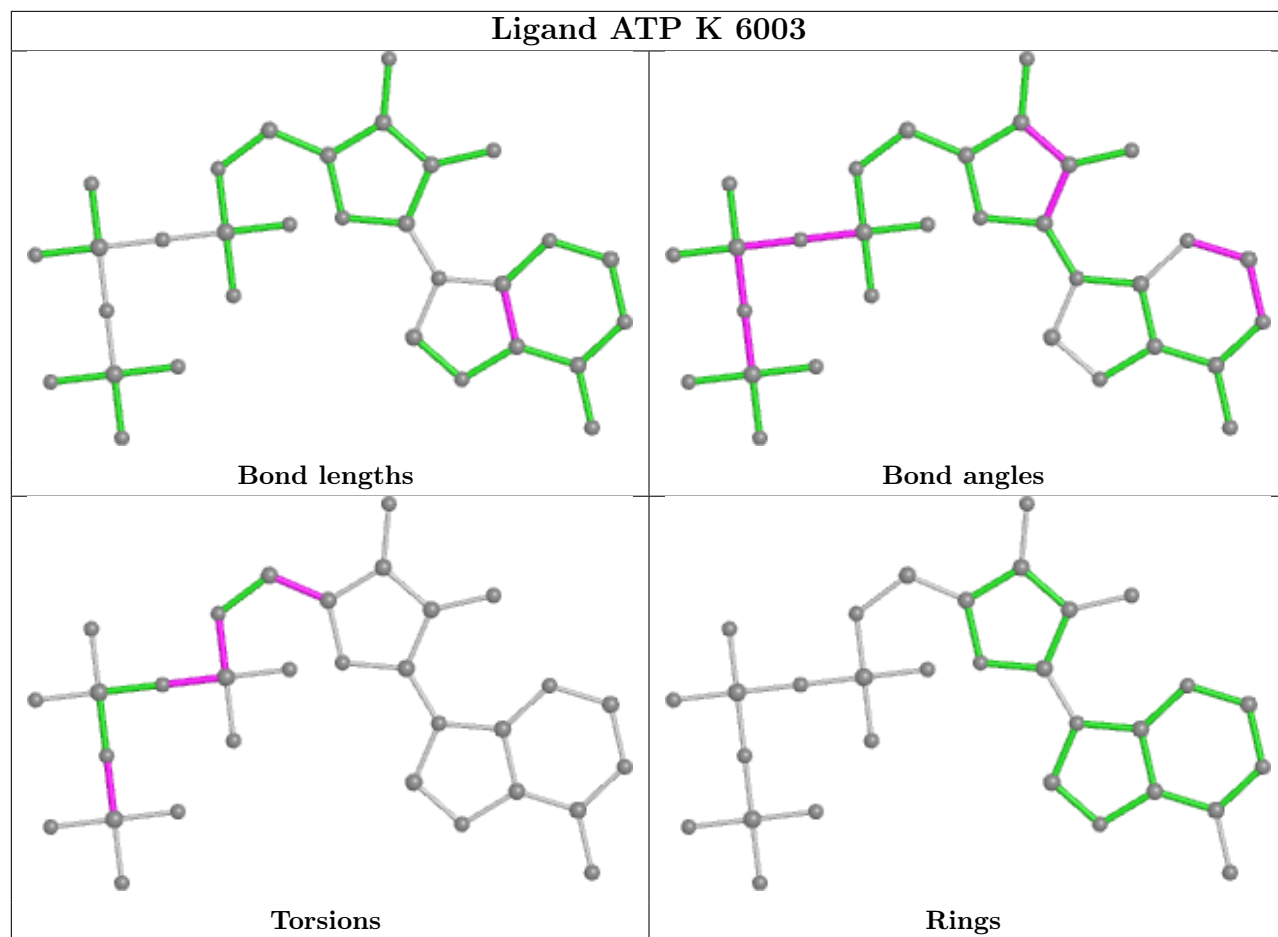
Continued on next page...

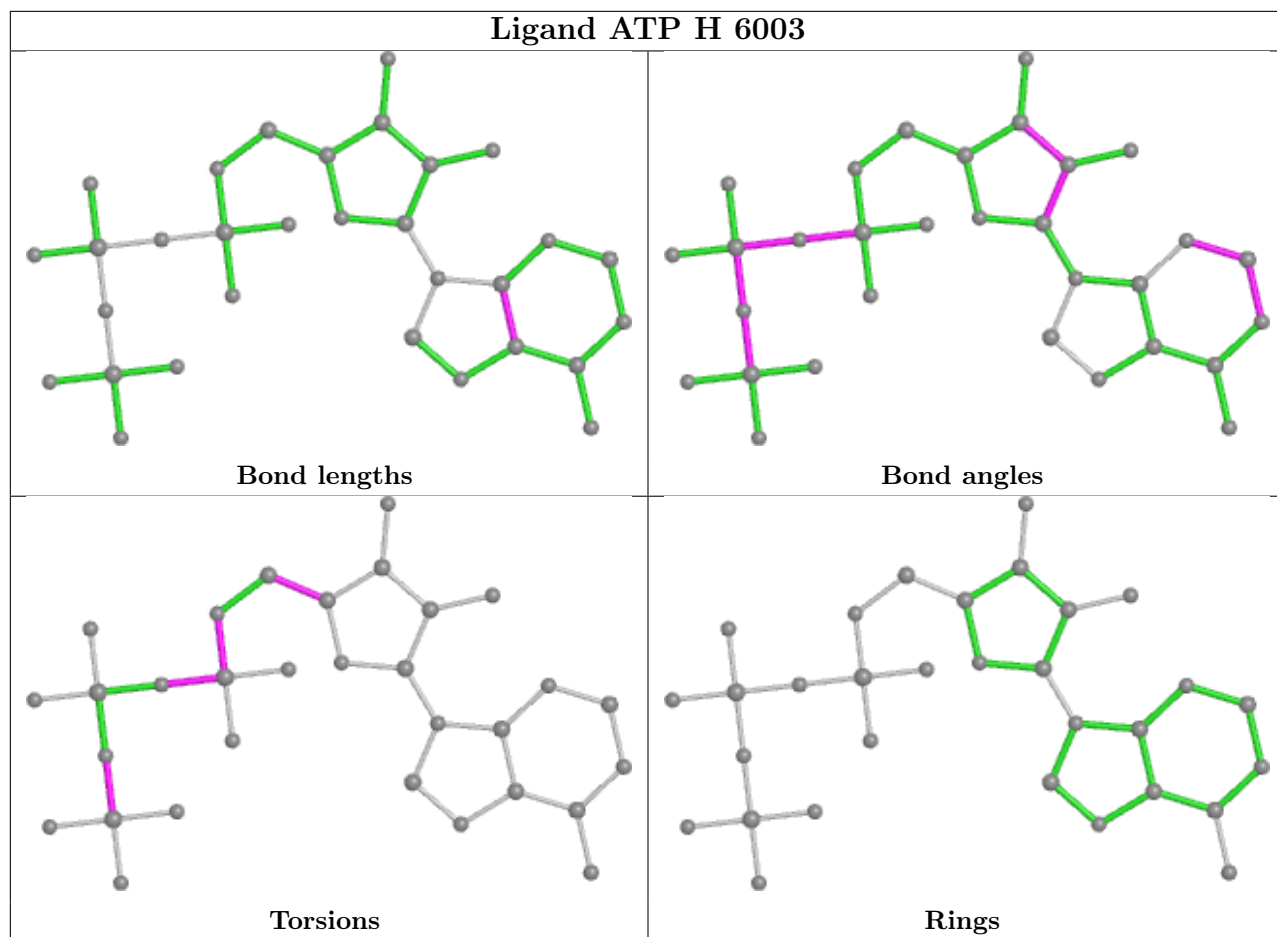
Continued from previous page...

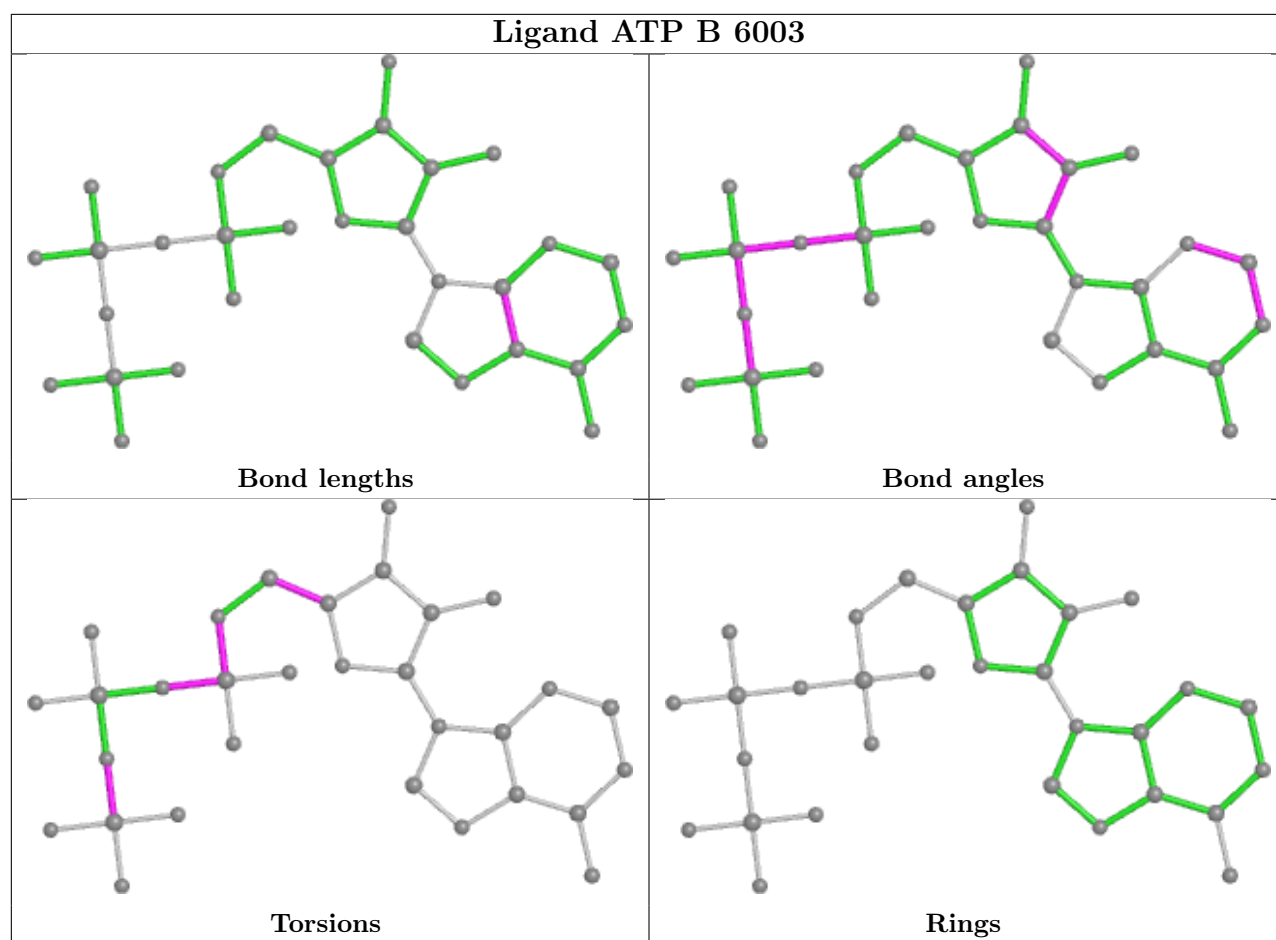
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	6002	CFF	1	0
7	K	6003	ATP	4	0
7	H	6003	ATP	5	0
7	B	6003	ATP	4	0
6	E	6002	CFF	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

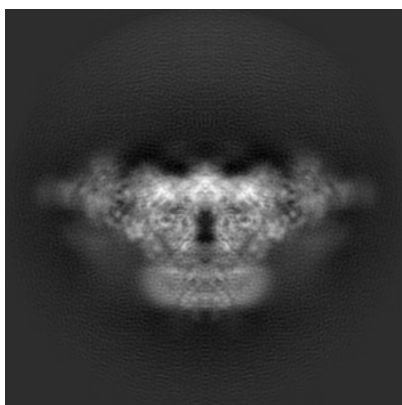
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9834. These allow visual inspection of the internal detail of the map and identification of artifacts.

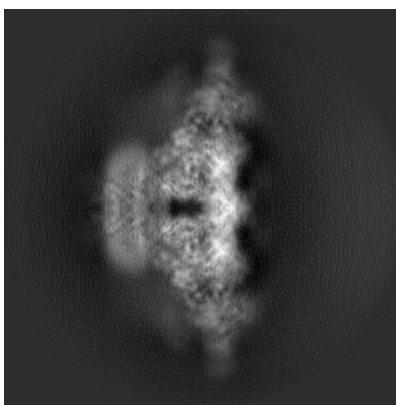
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

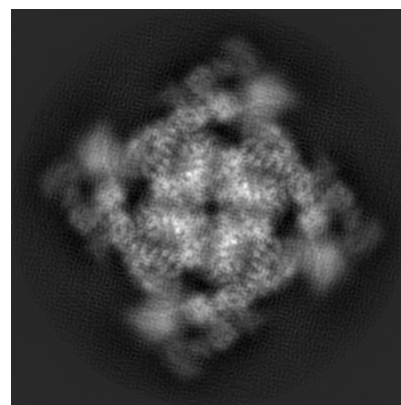
6.1.1 Primary map



X



Y

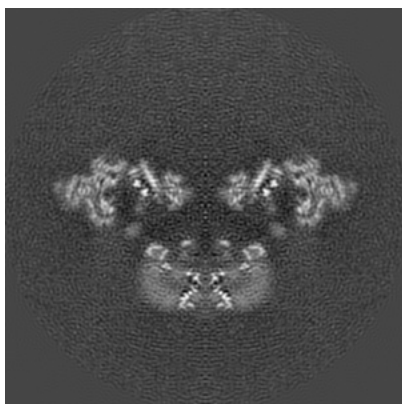


Z

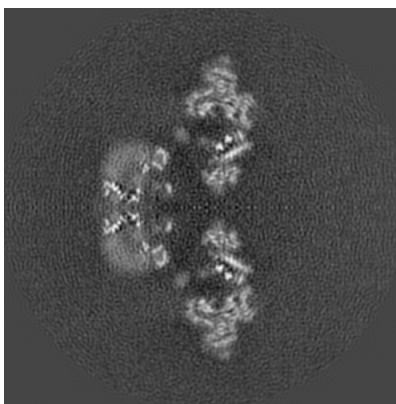
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

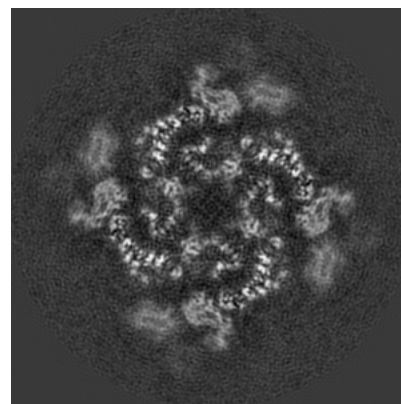
6.2.1 Primary map



X Index: 200



Y Index: 200

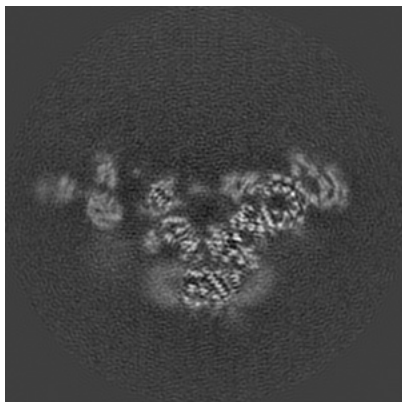


Z Index: 200

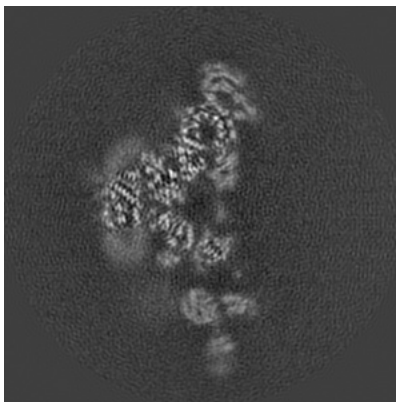
The images above show central slices of the map in three orthogonal directions.

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

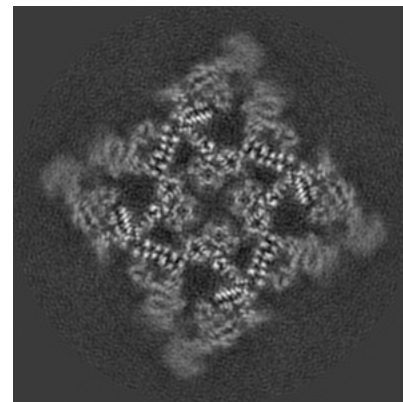
6.3.1 Primary map



X Index: 185



Y Index: 215

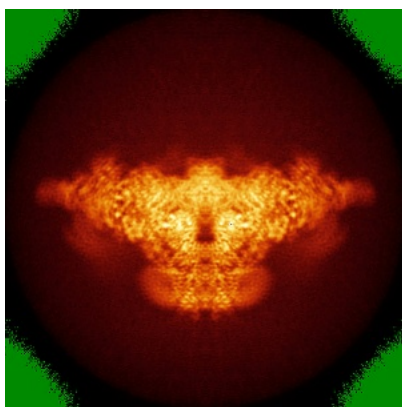


Z Index: 212

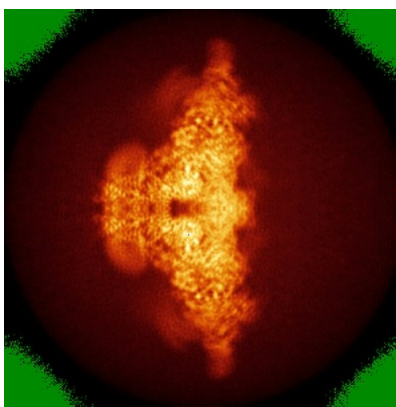
The images above show the largest variance slices of the map in three orthogonal directions.

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

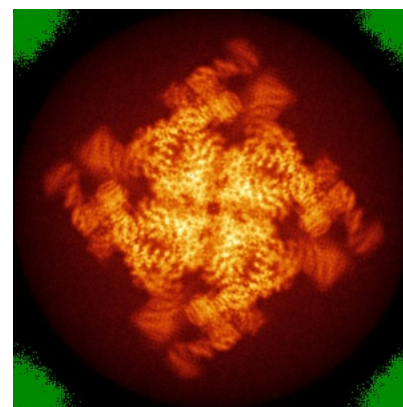
6.4.1 Primary map



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.

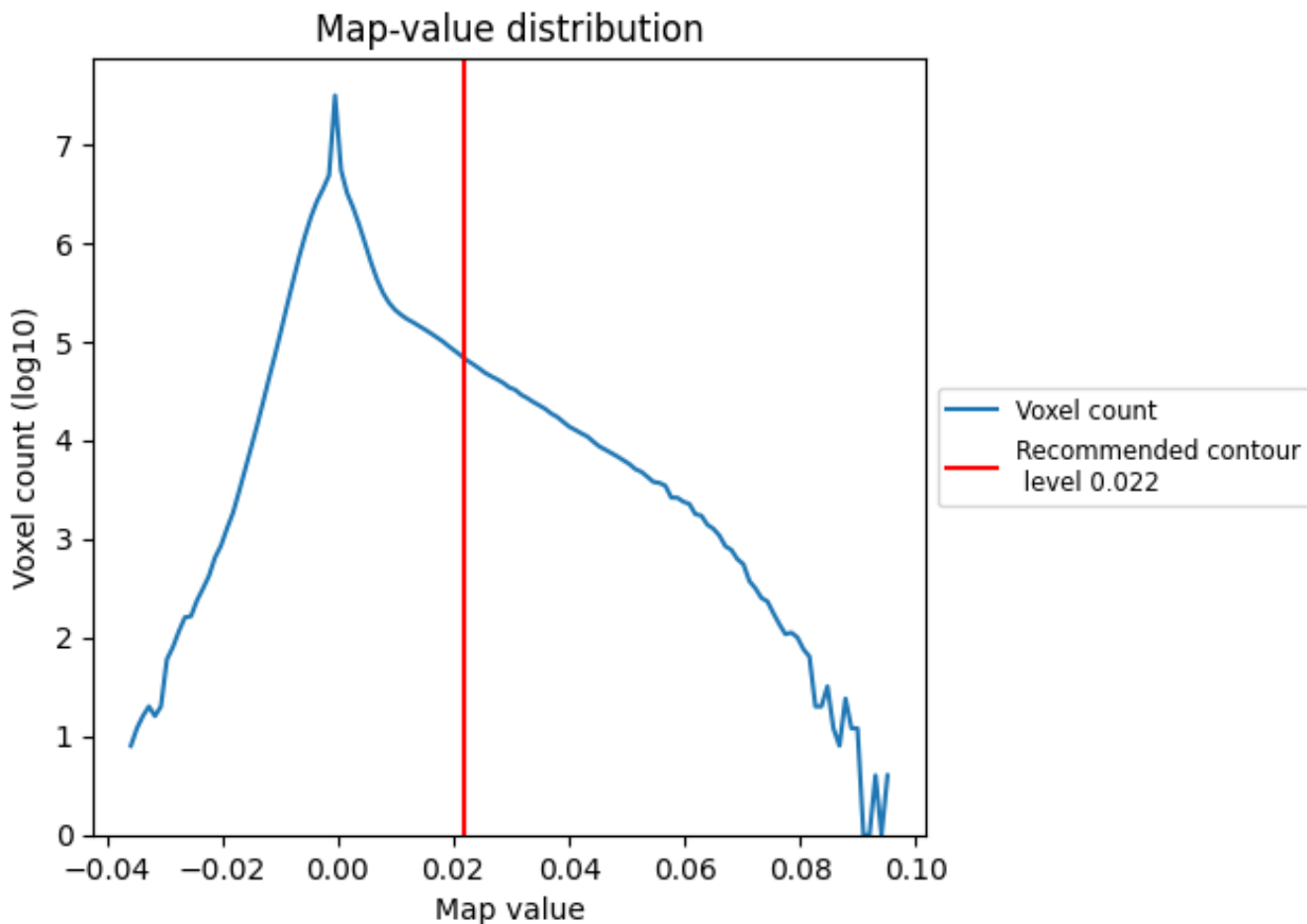
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

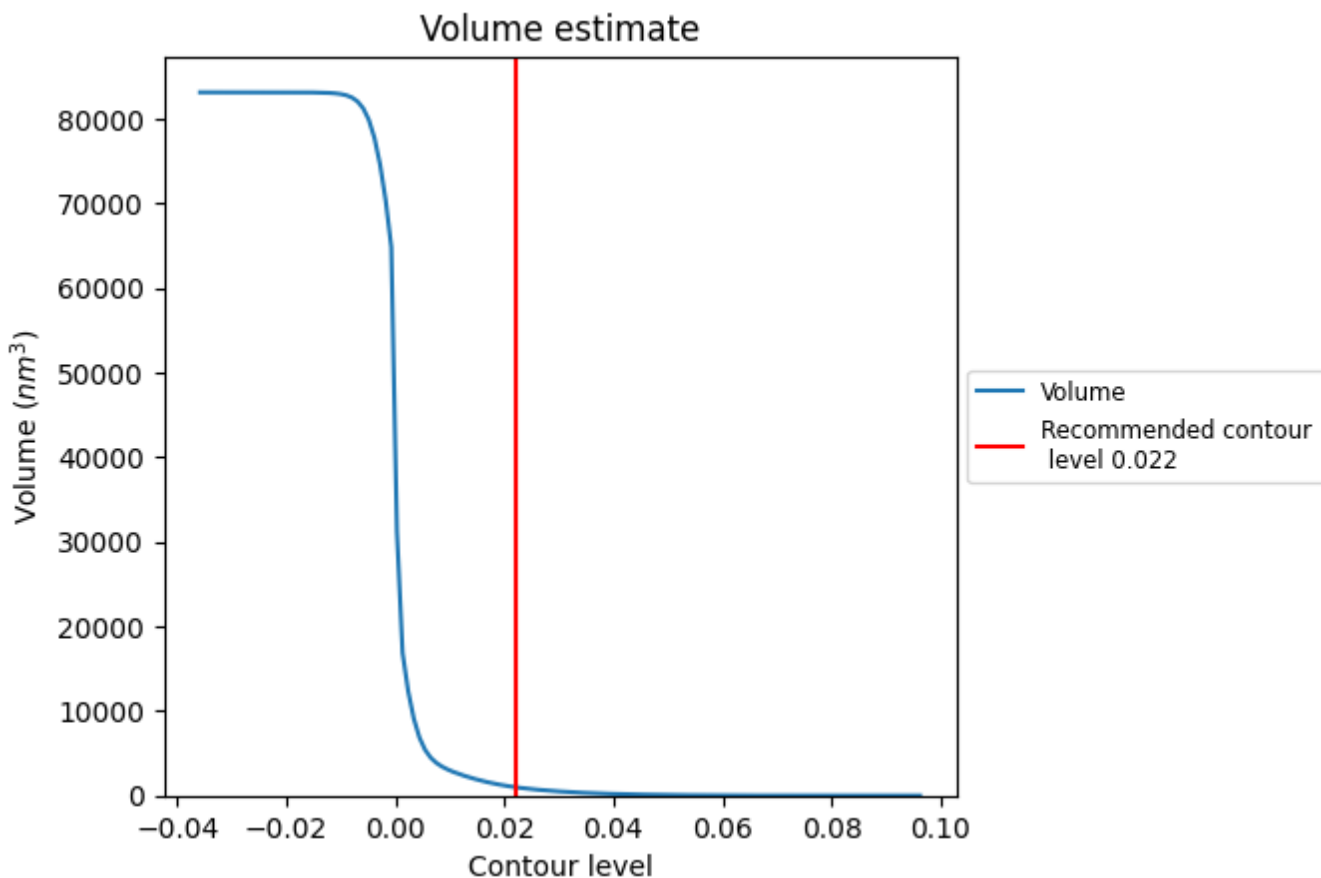
This section contains the results of statistical analysis of the map.

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.

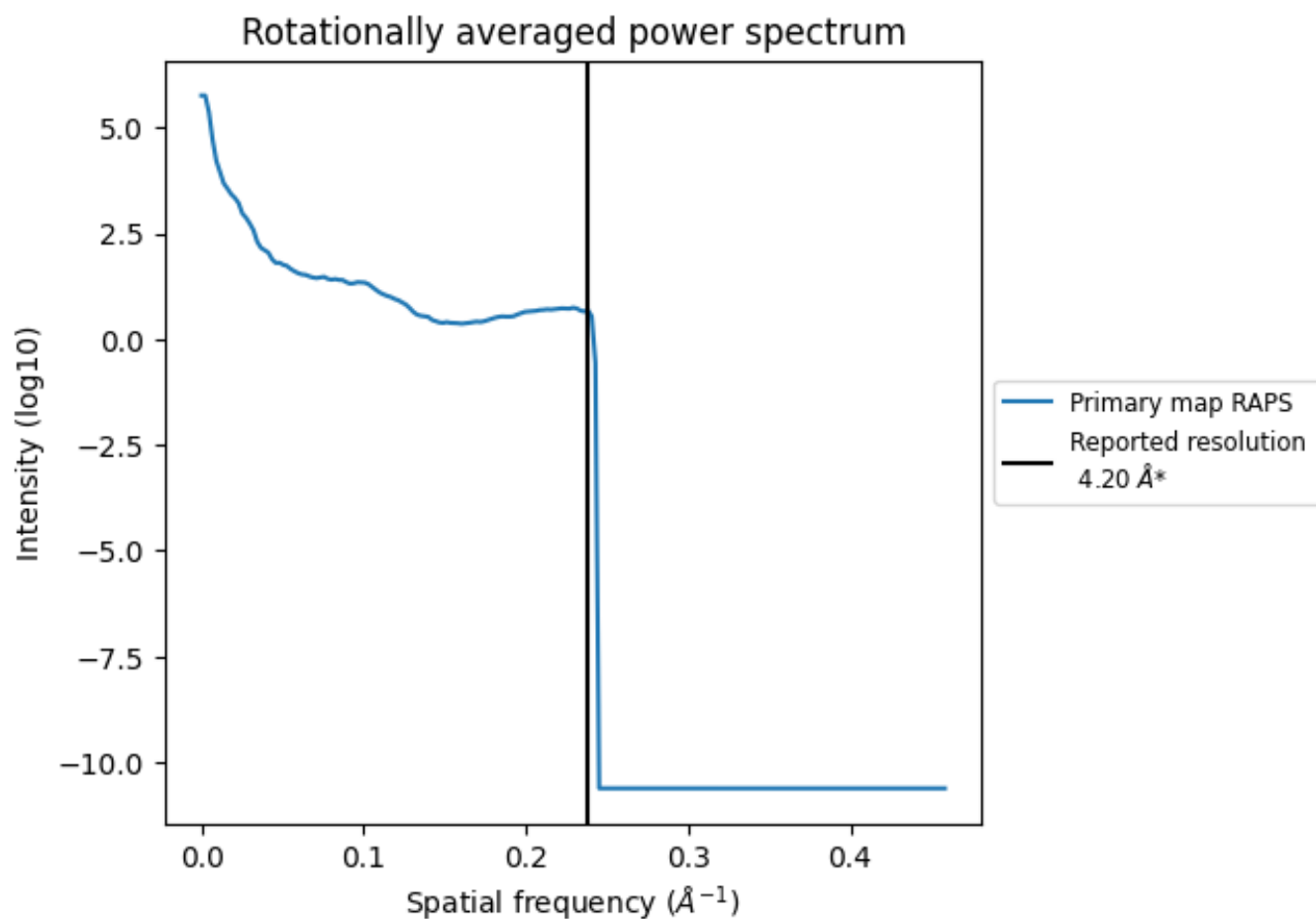
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 992 nm³; this corresponds to an approximate mass of 896 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

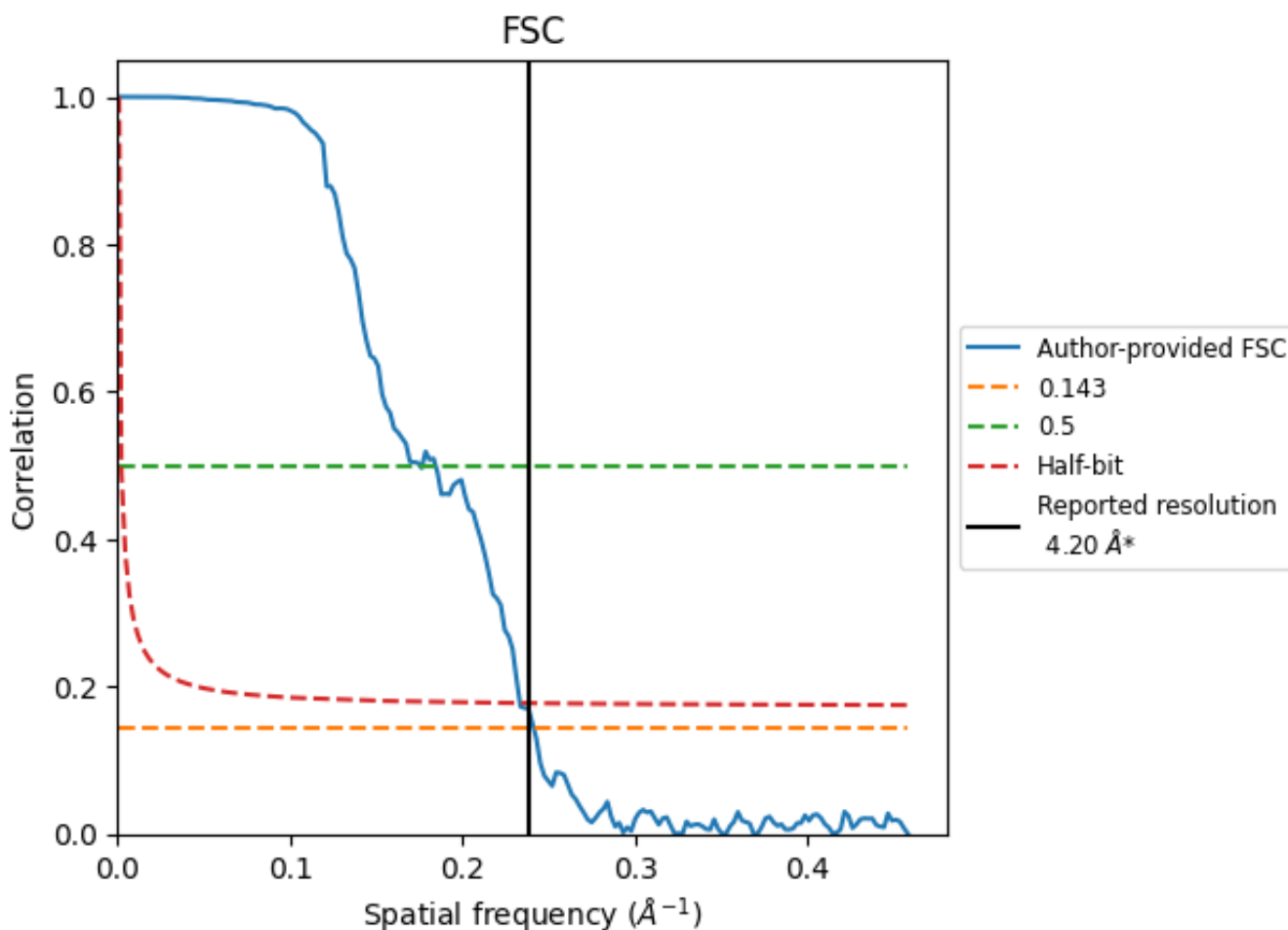


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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](#)

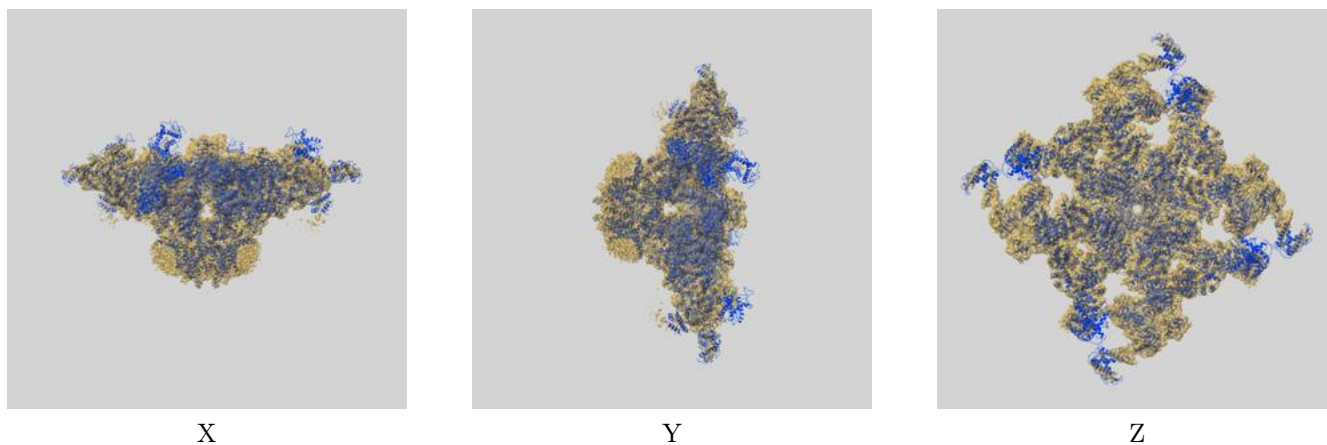
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	5.71	4.28
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

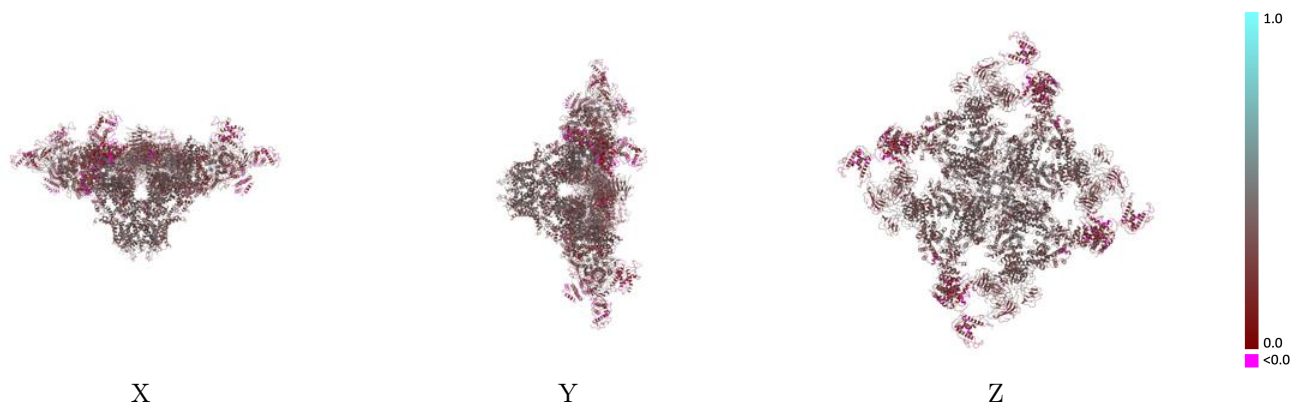
This section contains information regarding the fit between EMDB map EMD-9834 and PDB model 6JII. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



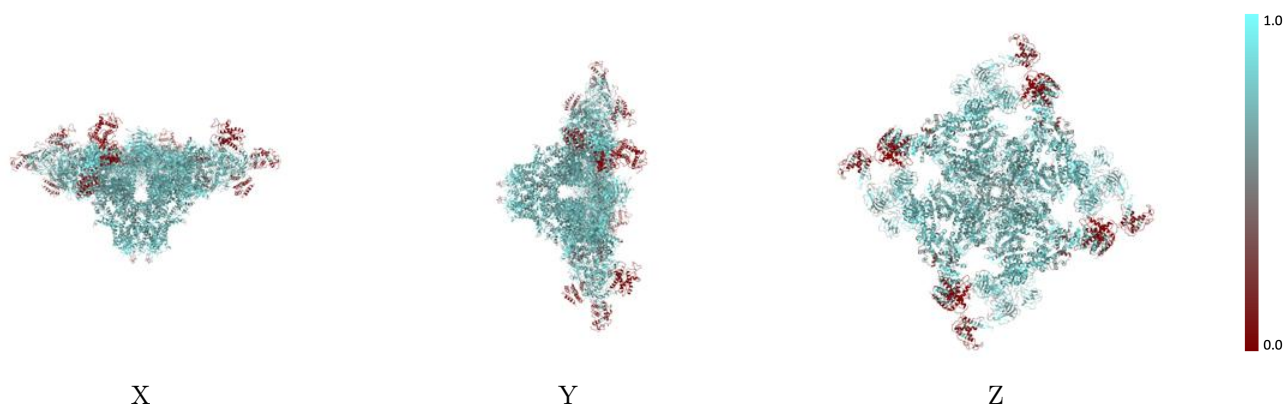
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



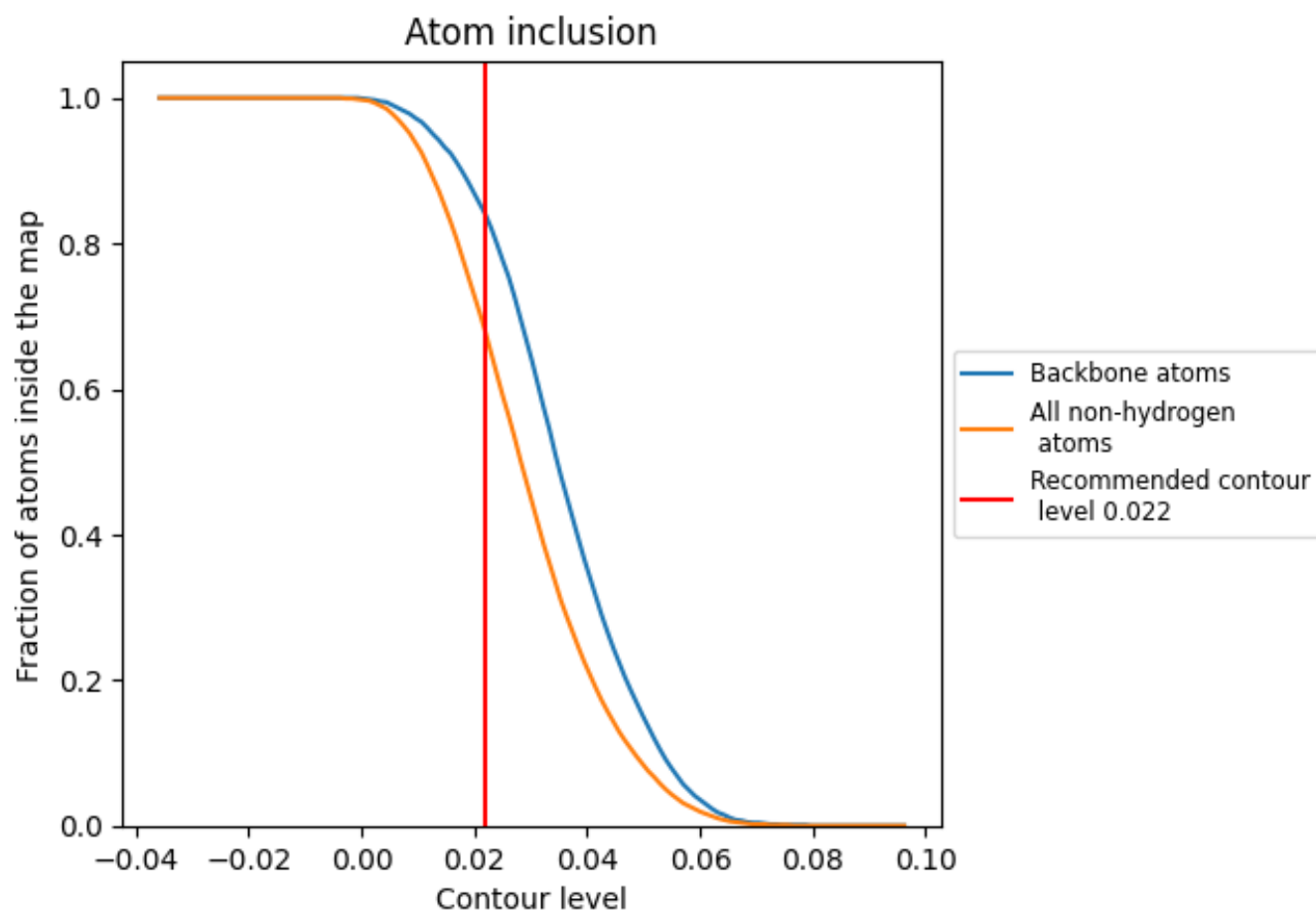
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 68% 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	 0.6770	 0.3190
A	 0.7090	 0.3340
B	 0.6840	 0.3210
C	 0.4910	 0.2490
D	 0.7100	 0.3380
E	 0.6840	 0.3220
F	 0.4910	 0.2470
G	 0.7110	 0.3370
H	 0.6840	 0.3220
I	 0.4910	 0.2480
J	 0.7100	 0.3360
K	 0.6840	 0.3210
L	 0.4910	 0.2490

